Supplementary information
(May 30, 2011)

Unique interplay between electronic states and dihedral angles
for the molecular rotor diphenyldiacetylene

Peter W. Thulstrup,*a Søren V. Hoffmann,b Bjarke K. V. Hansen,c and Jens Spanget-Larsen*c

aDepartment of Basic Science and Environment, Faculty of Life Sciences, University of Copenhagen, Thorvaldsensvej 40, DK-1871 Frederiksberg C, Denmark
bInstitute for Storage Ring Facilities, ISA, University of Aarhus, Ny Munkegade, Bldg. 1520, DK-8000 Aarhus C, Denmark
cDepartment of Science, Systems and Models, Roskilde University, P.O.Box 260, DK-4000 Roskilde, Denmark

*Corresponding authors: E-mail <pwt@life.ku.dk> (P. W. Thulstrup), <spanget@ruc.dk> (J. Spanget-Larsen)

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S 3  Calculated electronic transitions for twisted DPDA: $\Phi = 45^\circ (D_2)$
S 4  Calculated electronic transisitions for twisted DPDA: $\Phi = 90^\circ (D_{2d})$
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<table>
<thead>
<tr>
<th>Term</th>
<th>( \tilde{\nu}^a )</th>
<th>( j^b )</th>
<th>Leading configurations $^c$</th>
</tr>
</thead>
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<td>29.7 0.93</td>
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<tr>
<td>2</td>
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<td>31.2 0</td>
<td>92% (2,-1)</td>
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<tr>
<td>3</td>
<td>( 2^1A_u )</td>
<td>34.0 0</td>
<td>93% (1,-3)</td>
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<tr>
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<td>9</td>
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<td>49% (5,-1), 25% (1,-2)</td>
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<td>91% (1,-6)</td>
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<td>99% (2,-4)</td>
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<td>17</td>
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<td>50.0 0</td>
<td>88% (1,-8)</td>
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<td>99% (3,-3)</td>
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<td>99% (4,-3)</td>
</tr>
<tr>
<td>22</td>
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<td>95% (1,-9)</td>
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</tr>
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<td>89% (7,-1)</td>
</tr>
<tr>
<td>28</td>
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<td>93% (1,-11), 99% (1,-12)</td>
</tr>
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<td>32</td>
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<tr>
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</tr>
<tr>
<td>35</td>
<td>( 5^1B_{1g} )</td>
<td>55.0 0</td>
<td>54% (3,-6), 43% (4,-7)</td>
</tr>
<tr>
<td>36</td>
<td>( 5^1B_{3g} )</td>
<td>55.4 0</td>
<td>51% (5,-5), 31% (3,-2)</td>
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<td>37</td>
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<tr>
<td>38</td>
<td>( 5^1A_u )</td>
<td>55.6 0</td>
<td>87% (1,-13)</td>
</tr>
<tr>
<td>39</td>
<td>( 5^1B_{2g} )</td>
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<td>92% (1,-14)</td>
</tr>
<tr>
<td>40</td>
<td>( 7^1B_{1u} )</td>
<td>56.4 0.03</td>
<td>75% (1,-17)</td>
</tr>
</tbody>
</table>

$^a$ Wavenumber in $10^3$ cm$^{-1}$.

$^b$ Oscillator strength.

$^c$ The notation \((i,-j)\) indicates an excited singlet configuration derived from the ground configuration by promotion of an electron from the \(i\)'th highest occupied to the \(j\)'th lowest unoccupied MO.
DPDA, $\Phi = 45^\circ$ (D$_2$). TD-PBE1PBE/6-31+G*//[6-31G* (D$_{2h}$)]

<table>
<thead>
<tr>
<th>Term</th>
<th>$\tilde{\nu}^a$</th>
<th>$f^b$</th>
<th>Leading configurations$^c$</th>
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</thead>
<tbody>
<tr>
<td>1 $^1\text{B}_1$</td>
<td>30.2</td>
<td>0.60</td>
<td>76% (1,-1), 14% (2,-2)</td>
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<tr>
<td>2 $^1\text{A}$</td>
<td>30.8</td>
<td>0</td>
<td>71% (2,-1), 17% (1,-2)</td>
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<tr>
<td>3 $^1\text{A}$</td>
<td>33.3</td>
<td>0</td>
<td>63% (1,-2), 16% (2,-1)</td>
</tr>
<tr>
<td>4 $^1\text{B}_2$</td>
<td>38.5</td>
<td>2·10$^{-4}$</td>
<td>49% (1,-3), 40% (3,-1)</td>
</tr>
<tr>
<td>5 $^1\text{B}_3$</td>
<td>38.5</td>
<td>1·10$^{-4}$</td>
<td>49% (1,-4), 40% (4,-1)</td>
</tr>
<tr>
<td>6 $^1\text{B}_1$</td>
<td>40.5</td>
<td>1.40</td>
<td>72% (2,-2), 7% (1,-1)</td>
</tr>
<tr>
<td>7 $^1\text{A}$</td>
<td>42.9</td>
<td>0</td>
<td>49% (5,-1), 42% (1,-5)</td>
</tr>
<tr>
<td>8 $^2\text{B}_3$</td>
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<td>0.07</td>
<td>42% (1,-4), 40% (4,-1)</td>
</tr>
<tr>
<td>9 $^2\text{B}_2$</td>
<td>43.2</td>
<td>0.07</td>
<td>42% (1,-3), 40% (3,-1)</td>
</tr>
<tr>
<td>10 $^1\text{A}$</td>
<td>44.9</td>
<td>0</td>
<td>38% (1,-5), 32% (5,-1)</td>
</tr>
<tr>
<td>11 $^1\text{B}_3$</td>
<td>45.2</td>
<td>5·10$^{-3}$</td>
<td>66% (2,-3), 18% (3,-2)</td>
</tr>
<tr>
<td>12 $^1\text{B}_2$</td>
<td>45.2</td>
<td>0.01</td>
<td>66% (2,-4), 18% (4,-2)</td>
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<tr>
<td>13 $^4\text{B}_2$</td>
<td>46.1</td>
<td>1·10$^{-4}$</td>
<td>90% (1,-6)</td>
</tr>
<tr>
<td>14 $^1\text{B}_1$</td>
<td>46.5</td>
<td>0.05</td>
<td>58% (5,-2), 29% (2,-5)</td>
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<tr>
<td>15 $^1\text{B}_3$</td>
<td>47.5</td>
<td>0.01</td>
<td>63% (3,-2), 15% (2,-3)</td>
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<td>47.5</td>
<td>0.08</td>
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<td>17 $^5\text{B}_3$</td>
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<td>0.01</td>
<td>86% (1,-7)</td>
</tr>
<tr>
<td>18 $^4\text{B}_1$</td>
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<td>0.13</td>
<td>50% (6,-1), 33% (2,-5)</td>
</tr>
<tr>
<td>19 $^5\text{B}_1$</td>
<td>50.0</td>
<td>0.14</td>
<td>42% (1,-11), 22% (6,-1)</td>
</tr>
<tr>
<td>20 $^6\text{B}_2$</td>
<td>50.6</td>
<td>3·10$^{-3}$</td>
<td>84% (1,-8)</td>
</tr>
<tr>
<td>21 $^6\text{B}_3$</td>
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<td>6·10$^{-4}$</td>
<td>77% (2,-6), 15% (2,-8)</td>
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<td>22 $^6\text{A}$</td>
<td>51.4</td>
<td>0</td>
<td>94% (1,-9)</td>
</tr>
<tr>
<td>23 $^6\text{B}_1$</td>
<td>52.1</td>
<td>0.08</td>
<td>86% (1,-10)</td>
</tr>
<tr>
<td>24 $^7\text{A}$</td>
<td>52.2</td>
<td>0</td>
<td>58% (6,-2), 13% (3,-4)</td>
</tr>
<tr>
<td>25 $^7\text{B}_1$</td>
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<td>0.97</td>
<td>29% (4,-4), 29% (3,-3)</td>
</tr>
<tr>
<td>26 $^7\text{B}_2$</td>
<td>53.1</td>
<td>2·10$^{-4}$</td>
<td>87% (2,-7)</td>
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<tr>
<td>27 $^7\text{B}_3$</td>
<td>53.8</td>
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<td>35% (1,-12), 32% (5,-3)</td>
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<td>31 $^8\text{A}$</td>
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<td>56.5</td>
<td>4·10$^{-4}$</td>
<td>89% (1,-14)</td>
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<tr>
<td>40 $^{12}\text{B}_1$</td>
<td>56.7</td>
<td>0.03</td>
<td>55% (1,-15), 17% (2,-9)</td>
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</tbody>
</table>

$^a$ Wavenumber in 10$^3$ cm$^{-1}$.

$^b$ Oscillator strength.

$^c$ The notation ($i$,$j$) indicates an excited singlet configuration derived from the ground configuration by promotion of an electron from the $i$'th highest occupied to the $j$'th lowest unoccupied MO.
**DPDA, Φ = 90° (D_{2d}). TD-PBE1PBE/6-31+G*/[6-31G* (D_{2h})]**

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<tr>
<th>Term</th>
<th>$\tilde{\nu}^a$</th>
<th>$f^b$</th>
<th>Leading configurations $^c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$^1B_1$</td>
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<td>45% (2,-1), 45% (2,-2)</td>
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<td>$^2A_2$</td>
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<td>44% (6,-1), 44% (5,-2)</td>
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<td>15</td>
<td>$^1E$</td>
<td>47.7</td>
<td>&lt;10^{-4} 42% (1,-5), 31% (2,-5)</td>
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<tr>
<td>16</td>
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<td>42% (2,-5), 31% (1,-5)</td>
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<td>17</td>
<td>$^1A_1$</td>
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<td>37% (6,-2), 37% (5,-1)</td>
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<td>18</td>
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<td>48.5</td>
<td>34% (6,-2), 34% (5,-1), 14% (2,-8), 14% (1,-7)</td>
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<tr>
<td>19</td>
<td>$^1B_1$</td>
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<td>43% (2,-7), 43% (1,-8)</td>
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<td>21</td>
<td>$^6E$</td>
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<td>0.01 48% (1,-6), 25% (2,-6)</td>
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<tr>
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<td>23</td>
<td>$^4A_1$</td>
<td>50.0</td>
<td>41% (2,-8), 41% (2,-8)</td>
</tr>
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<td>24</td>
<td>$^2B_2$</td>
<td>52.5</td>
<td>33% (3,-3), 32% (4,-4)</td>
</tr>
<tr>
<td>25</td>
<td>$^1E$</td>
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<td>68% (2,-9), 12% (2,-5)</td>
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<td>1.36</td>
<td>68% (1,-9), 12% (1,-5)</td>
</tr>
<tr>
<td>27</td>
<td>$^4B_1$</td>
<td>53.1</td>
<td>48% (2,-10), 48% (1,-11)</td>
</tr>
<tr>
<td>28</td>
<td>$^4A_2$</td>
<td>53.1</td>
<td>48% (2,-10), 48% (1,-11)</td>
</tr>
<tr>
<td>29</td>
<td>$^5A_1$</td>
<td>54.6</td>
<td>51% (4,-3), 49% (3,-4)</td>
</tr>
<tr>
<td>30</td>
<td>$^4B_2$</td>
<td>54.6</td>
<td>50% (4,-4), 49% (3,-3)</td>
</tr>
<tr>
<td>31</td>
<td>$^6A_1$</td>
<td>54.7</td>
<td>46% (2,-11), 46% (1,-10)</td>
</tr>
<tr>
<td>32</td>
<td>$^5B_2$</td>
<td>54.7</td>
<td>44% (2,-11), 44% (1,-10)</td>
</tr>
<tr>
<td>33</td>
<td>$^6B_2$</td>
<td>55.0</td>
<td>52% (3,-5), 45% (4,-6)</td>
</tr>
<tr>
<td>34</td>
<td>$^5B_1$</td>
<td>55.0</td>
<td>52% (4,-5), 45% (3,-6)</td>
</tr>
<tr>
<td>35</td>
<td>$^8E$</td>
<td>55.7</td>
<td>2·10^{-3} 77% (1,-12)</td>
</tr>
<tr>
<td>36</td>
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<td>77% (2,-12)</td>
</tr>
<tr>
<td>37</td>
<td>$^7A_1$</td>
<td>56.3</td>
<td>28% (4,-3), 26% (3,-4)</td>
</tr>
<tr>
<td>38</td>
<td>$^9E$</td>
<td>56.3</td>
<td>0.08 16% (6,-3), 15% (6,-4), 15% (5,-3), 14% (5,-4)</td>
</tr>
<tr>
<td>39</td>
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<td></td>
<td>16% (5,-3), 15% (6,-3), 15% (5,-4), 14% (6,-4)</td>
</tr>
<tr>
<td>40</td>
<td>$^5A_2$</td>
<td>56.9</td>
<td>0     41% (8,-1), 41% (7,-2)</td>
</tr>
</tbody>
</table>

$^a$ Wavenumber in 10^3 cm^{-1}.

$^b$ Oscillator strength.

$^c$ The notation ($i,j$) indicates an excited singlet configuration derived from the ground configuration by promotion of an electron from the $i$'th highest occupied to the $j$'th lowest unoccupied MO.
Gaussian 03: x86-Linux-G03RevB.04 2-Jun-2003
7-Nov-2008

# t td(Nst=40,conver=3) pbe1pbe/6-31+G*

1,4-Diphenylbuta-1,3-diyne, D = 0.0 (pbe1pbe/6-31+G*/6-31G*)

Framework group  D2H[C2"(HCCCC.CCCCH),SG(C8H8)]

Standard orientation:

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<th>Center Number</th>
<th>Atomic Number</th>
<th>Atomic Type</th>
<th>Coordinates (Angstroms)</th>
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324 basis functions,  552 primitive gaussians,  324 cartesian basis functions
53 alpha electrons       53 beta electrons

SCF Done:  E(RPBE+HF-PBE) = -614.896831082     A.U. after 102 cycles
Convg =  0.6948D-08             -V/T =  2.0089

Excited states from <AA,BB:AA,BB> singles matrix:

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<tr>
<th>Ground to excited state Transition electric dipole moments (Au):</th>
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<tbody>
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<td>state</td>
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<tr>
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</tr>
<tr>
<td>30</td>
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<tr>
<td>31</td>
</tr>
</tbody>
</table>
Excitation energies and oscillator strengths:

→ MO parentage [in brackets] added by J. Spanget-Larsen. The notation \([i, -j]\) indicates an excited singlet configuration derived from the ground configuration by promotion of an electron from the \(i\)’th highest occupied to the \(j\)’th lowest unoccupied MO.

<table>
<thead>
<tr>
<th>Excited State</th>
<th>Singlet-B1U</th>
<th>29.72232 1000/cm</th>
<th>336.45 nm</th>
<th>f=0.9342</th>
</tr>
</thead>
<tbody>
<tr>
<td>52 -&gt; 56</td>
<td>-0.25056</td>
<td>13% [2, -3]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>53 -&gt; 54</td>
<td>0.62888</td>
<td>79% [1, -1]</td>
<td></td>
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</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Excited State</th>
<th>Singlet-AU</th>
<th>31.24026 1000/cm</th>
<th>320.10 nm</th>
<th>f=0.0000</th>
</tr>
</thead>
<tbody>
<tr>
<td>52 -&gt; 54</td>
<td>0.67975</td>
<td>92% [2, -1]</td>
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</tr>
<tr>
<td>53 -&gt; 56</td>
<td>-0.10508</td>
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<table>
<thead>
<tr>
<th>Excited State</th>
<th>Singlet-AU</th>
<th>33.98577 1000/cm</th>
<th>294.24 nm</th>
<th>f=0.0000</th>
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<tbody>
<tr>
<td>52 -&gt; 54</td>
<td>0.14079</td>
<td></td>
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</tr>
<tr>
<td>53 -&gt; 56</td>
<td>0.68361</td>
<td>93% [1, -3]</td>
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</table>

<table>
<thead>
<tr>
<th>Excited State</th>
<th>Singlet-B3G</th>
<th>38.04677 1000/cm</th>
<th>262.83 nm</th>
<th>f=0.0000</th>
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<tbody>
<tr>
<td>49 -&gt; 58</td>
<td>-0.14252</td>
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</tr>
<tr>
<td>50 -&gt; 54</td>
<td>0.45993</td>
<td>42% [4, -1]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>51 -&gt; 55</td>
<td>0.14350</td>
<td></td>
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</tr>
<tr>
<td>53 -&gt; 57</td>
<td>0.50722</td>
<td>51% [1, -4]</td>
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</table>

<table>
<thead>
<tr>
<th>Excited State</th>
<th>Singlet-B2U</th>
<th>38.05967 1000/cm</th>
<th>262.75 nm</th>
<th>f=0.0003</th>
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<tr>
<td>49 -&gt; 57</td>
<td>-0.14309</td>
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<tr>
<td>50 -&gt; 55</td>
<td>0.14334</td>
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</tr>
<tr>
<td>51 -&gt; 54</td>
<td>0.46202</td>
<td>43% [3, -1]</td>
<td></td>
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</tr>
<tr>
<td>53 -&gt; 58</td>
<td>0.50528</td>
<td>51% [1, -5]</td>
<td></td>
<td></td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Excited State</th>
<th>Singlet-AG</th>
<th>40.1051 1000/cm</th>
<th>249.34 nm</th>
<th>f=0.0000</th>
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</thead>
<tbody>
<tr>
<td>49 -&gt; 54</td>
<td>0.43191</td>
<td>37% [5, -1]</td>
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</tr>
<tr>
<td>53 -&gt; 55</td>
<td>0.56250</td>
<td>63% [1, -2]</td>
<td></td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Excited State</th>
<th>Singlet-B3G</th>
<th>42.85222 1000/cm</th>
<th>233.36 nm</th>
<th>f=0.0000</th>
</tr>
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<tbody>
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<td>49 -&gt; 58</td>
<td>-0.10146</td>
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<tr>
<td>50 -&gt; 54</td>
<td>0.48425</td>
<td>47% [4, -1]</td>
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</tr>
<tr>
<td>53 -&gt; 57</td>
<td>-0.45484</td>
<td>41% [1, -4]</td>
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</table>

<table>
<thead>
<tr>
<th>Excited State</th>
<th>Singlet-B2U</th>
<th>42.92319 1000/cm</th>
<th>232.98 nm</th>
<th>f=0.1222</th>
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<tbody>
<tr>
<td>49 -&gt; 57</td>
<td>-0.10311</td>
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<td>-0.45653</td>
<td>42% [1, -5]</td>
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<table>
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<tr>
<th>Excited State</th>
<th>Singlet-AG</th>
<th>43.6628 1000/cm</th>
<th>229.03 nm</th>
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<tbody>
<tr>
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<td>0.10832</td>
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<td>49 -&gt; 54</td>
<td>0.49331</td>
<td>49% [5, -1]</td>
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<tr>
<td>50 -&gt; 58</td>
<td>0.14551</td>
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<tr>
<td>51 -&gt; 57</td>
<td>0.14614</td>
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<tr>
<td>53 -&gt; 55</td>
<td>-0.35142</td>
<td>25% [1, -2]</td>
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<th>Excited State</th>
<th>Singlet-B1G</th>
<th>44.3516 1000/cm</th>
<th>225.47 nm</th>
<th>f=0.0000</th>
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<tr>
<td>47 -&gt; 54</td>
<td>0.14852</td>
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<tr>
<td>52 -&gt; 55</td>
<td>0.68324</td>
<td>93% [2, -2]</td>
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<table>
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<th>Excited State</th>
<th>Singlet-B2G</th>
<th>45.40012 1000/cm</th>
<th>220.27 nm</th>
<th>f=0.0000</th>
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</table>
Excited State 12: Singlet-B1U 45.82517 1000/cm 218.22 nm f=1.3046
53 -> 59  0.67529  91% [ 1,-6 ]
53 -> 61  0.17456

Excited State 13: Singlet-B2G 46.80595 1000/cm 213.65 nm f=0.0000
52 -> 57  0.70249  99% [ 2,-4 ]

Excited State 14: Singlet-B3U 46.83095 1000/cm 213.53 nm f=0.0038
52 -> 58  0.70450  99% [ 3,-3 ]

Excited State 15: Singlet-B3G 50.12572 1000/cm 199.50 nm f=0.0000
53 -> 63  0.69464  97% [ 1,-10 ]

Excited State 16: Singlet-B1G 48.14563 1000/cm 207.70 nm f=0.0000
46 -> 56  -0.12423
49 -> 56  0.68537  94% [ 5,-3 ]

Excited State 17: Singlet-B2G 50.00716 1000/cm 199.97 nm f=0.0000
53 -> 59  -0.17226
53 -> 61  0.66312  88% [ 1,-8 ]

Excited State 18: Singlet-B2U 50.11846 1000/cm 199.53 nm f=0.0011
48 -> 58  -0.13593
49 -> 57  -0.42341  36% [ 5,-4 ]
50 -> 55  0.61047  52% [ 4,-2 ]
51 -> 54  -0.15324
53 -> 58  -0.11842

Excited State 19: Singlet-B3G 50.12572 1000/cm 199.50 nm f=0.0000
48 -> 57  -0.13636
49 -> 58  -0.42109  35% [ 5,-5 ]
50 -> 54  -0.15325
51 -> 55  0.51173  52% [ 3,-2 ]
53 -> 57  -0.11783

Excited State 20: Singlet-B3U 50.58062 1000/cm 197.70 nm f=0.0000
51 -> 56  0.70450  99% [ 3,-3 ]

Excited State 21: Singlet-B2G 50.58788 1000/cm 197.68 nm f=0.0000
50 -> 56  0.70291  99% [ 4,-3 ]

Excited State 22: Singlet-AU 50.59997 1000/cm 197.63 nm f=0.0000
53 -> 62  0.69037  95% [ 1,-9 ]
53 -> 66  0.11548

Excited State 23: Singlet-B1U 50.68386 1000/cm 197.30 nm f=0.1786
48 -> 54  0.50578  51% [ 6,-1 ]
52 -> 56  0.17308
53 -> 65  0.40307  32% [ 1,-12 ]
53 -> 70  -0.12021

Excited State 24: Singlet-B1G 51.5993 1000/cm 193.80 nm f=0.0000
53 -> 63  0.69464  97% [ 1,-10 ]

Excited State 25: Singlet-B1U 51.72834 1000/cm 193.32 nm f=0.4041
49 -> 55  0.47541  45% [ 5,-2 ]
50 -> 57  0.32835  22% [ 4,-4 ]
51 -> 58  0.32366  21% [ 3,-5 ]
Excited State 26: Singlet-B3G 52.45182 1000/cm 190.65 nm f=0.0000
  52 -> 59  0.62537  78% [ 2,-6 ]
  52 -> 61  0.29422  17% [ 2,-8 ]

Excited State 27: Singlet-B1G 52.53409 1000/cm 190.35 nm f=0.0000
  44 -> 54  0.10138
  47 -> 54  0.66575  89% [ 7,-1 ]
  52 -> 55  -0.15606

Excited State 28: Singlet-B3U 53.14142 1000/cm 188.18 nm f=0.0043
  49 -> 54  0.10138
  47 -> 54  0.66575  89% [ 2,-6 ]
  52 -> 55  -0.15606

Excited State 29: Singlet-B1U 54.00121 1000/cm 185.18 nm f=1.2587
  49 -> 55  0.42605  36% [ 5,-2 ]
  50 -> 58  -0.22691  10% [ 4,-4 ]
  52 -> 56  -0.12939
  53 -> 65  0.38379  29% [ 1,-11 ]

Excited State 30: Singlet-AG 54.25205 1000/cm 184.32 nm f=0.0000
  46 -> 54  0.24696  12% [ 8,-1 ]
  47 -> 56  -0.13384
  48 -> 55  0.16269
  50 -> 58  0.35762  26% [ 4,-5 ]
  51 -> 57  0.41609  35% [ 3,-4 ]

Excited State 31: Singlet-B1U 54.60129 1000/cm 183.15 nm f=0.0006
  49 -> 57  0.49467  49% [ 4,-4 ]
  51 -> 58  0.50481  51% [ 3,-5 ]

Excited State 32: Singlet-AG 54.60210 1000/cm 183.14 nm f=0.0000
  50 -> 58  0.52126  54% [ 4,-5 ]
  51 -> 57  0.47733  46% [ 3,-4 ]

Excited State 33: Singlet-B2U 54.93924 1000/cm 182.02 nm f=0.0610
  49 -> 57  -0.23294  11% [ 5,-4 ]
  50 -> 55  -0.20193
  52 -> 60  0.60624  74% [ 2,-7 ]
  53 -> 66  -0.12866

Excited State 34: Singlet-AU 54.94569 1000/cm 182.00 nm f=0.0000
  50 -> 59  0.50977  52% [ 4,-6 ]
  51 -> 60  0.45674  42% [ 3,-7 ]
  53 -> 66  -0.12647

Excited State 35: Singlet-B1G 54.95618 1000/cm 181.96 nm f=0.0000
  50 -> 60  0.46467  43% [ 4,-7 ]
  51 -> 59  0.51876  54% [ 3,-6 ]

Excited State 36: Singlet-B3G 55.42155 1000/cm 180.43 nm f=0.0000
  49 -> 58  0.50405  51% [ 5,-5 ]
  51 -> 55  0.39648  31% [ 3,-2 ]
  52 -> 59  0.10319

Excited State 37: Singlet-B2U 55.54576 1000/cm 180.03 nm f=0.3655
  49 -> 57  0.44783  40% [ 5,-4 ]
  50 -> 55  0.35026  25% [ 4,-2 ]
  52 -> 60  0.33401  22% [ 2,-7 ]

Excited State 38: Singlet-AU 55.56592 1000/cm 179.97 nm f=0.0000
  48 -> 56  0.13545
  50 -> 59  0.10131
  53 -> 66  0.65765  87% [ 1,-13 ]
Excited State 39: Singlet-B2G    55.92162 1000/cm  178.82 nm  f=0.0000
53 -> 61    -0.10740
53 -> 67    0.67979   92% [ 1, -14 ]

Excited State 40: Singlet-B1U    56.40475 1000/cm  177.29 nm  f=0.0276
49 -> 55    -0.14255
50 -> 57    0.13521
51 -> 58    0.13624
53 -> 65    0.17406
53 -> 70    0.61238   75% [ 1, -17 ]
53 -> 74    0.11249

Orbital symmetries:
Occupied  (B1U)  (AG)  (AG)  (B1U)  (AG)  (B3G)  (B2U)  (B1U)  
            (AG)  (B1U)  (AG)  (B2U)  (B3G)  (B1U)  (AG)  (B1U)  
            (AG)  (B1U)  (AG)  (B3G)  (B2U)  (B1U)  (AG)  (B1U)  
            (B3G)  (AG)  (B1U)  (AG)  (B1U)  (AG)  (B3G)  (B3U)  
            (B3U)  (AG)  (B1U)  (B3G)  (B2U)  (B1U)  (AG)  (B1U)  
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Virtual  (B3U)  (B2G)  (B2U)  (B1G)  (AU)  (AG)  (B1U)  (AG)  (B2U)  
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        (B3G)  (B1U)  (AG)  (B2G)  (B2U)  (B1U)  (AG)  (B1U)  

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Alpha virt. eigenvalues -- 0.01017 0.01275 0.03057 0.03131 0.03358
Alpha virt. eigenvalues -- 0.04223 0.04790 0.05328 0.05516 0.06219
Alpha virt. eigenvalues -- 0.06340 0.06354 0.06977 0.07698 0.08220
Alpha virt. eigenvalues -- 0.08711 0.09300 0.09800 0.09818 0.09922
Alpha virt. eigenvalues -- 0.10391 0.11743 0.12336 0.13979 0.14442
Alpha virt. eigenvalues -- 0.14442 0.14840 0.15057 0.15267 0.15427
Alpha virt. eigenvalues -- 0.15733 0.15886 0.15901 0.16123 0.16358
Alpha virt. eigenvalues -- 0.16373 0.16936 0.17394 0.17981 0.18134
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Normal termination of Gaussian 03 at Sat Nov 8 10:04:25 2008.
# Gaussian 03: x86-Linux-G03RevB.04 2-Jun-2003 7-Nov-2008

1,4-Diphenylbuta-1,3-diyne, D=45 (based on pbe1pbe/6-31G* D2h geo.)

Framework group D2[C2(HCCCC.CCCCH),X(C8H8)]

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324 basis functions, 552 primitive gaussians, 324 cartesian basis functions
53 alpha electrons 53 beta electrons

SCF Done: E(RPBE+HF-PBE) = -614.896597490 A.U. after 26 cycles
Convg = 0.7835D-08 -V/T = 2.0089

Excited states from <AA,BB:AA,BB> singles matrix:

Ground to excited state Transition electric dipole moments (Au):

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Ground to excited state transition velocity dipole Moments (Au):

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Excitation energies and oscillator strengths:
→ MO parentage [in brackets] added by J. Spanget-Larsen. The notation [i,-j] indicates an excited singlet configuration derived from the ground configuration by promotion of an electron from the i'th highest occupied to the j'th lowest unoccupied MO.

Excited State 1: Singlet-B1 30.21513 1000/cm 330.96 nm  f=0.6032
52 -> 55  0.26193  14% [2,-2]
52 -> 58  -0.12953
53 -> 54  0.61636  76% [1,-1]

Excited State 2: Singlet-A 30.75229 1000/cm 325.18 nm  f=0.0000
49 -> 54  0.14098
52 -> 54  0.59583  71% [2,-1]
53 -> 55  0.29323  17% [1,-2]

Excited State 3: Singlet-A 33.27519 1000/cm 300.53 nm  f=0.0000
49 -> 54 -0.14826
52 -> 54 -0.28274  16% [2,-1]
53 -> 55  0.56068  63% [1,-2]
53 -> 58 -0.24551  12% [1,-5]

Excited State 4: Singlet-B2 38.5436 1000/cm 259.45 nm  f=0.0002
49 -> 57  0.10876
50 -> 55 -0.16956
51 -> 54 -0.44609  40% [3,-1]
52 -> 57 -0.14927
53 -> 56  0.49290  49% [1,-3]

Excited State 5: Singlet-B3 38.54522 1000/cm 259.44 nm  f=0.0001
49 -> 56  0.10876
50 -> 54 -0.44604  40% [4,-1]
51 -> 55 -0.16979
52 -> 56 -0.14952
53 -> 57  0.49275  49% [1,-4]

Excited State 6: Singlet-B1 40.54064 1000/cm 246.67 nm  f=1.3996
48 -> 54  0.13905
52 -> 55  0.59853  72% [2,-2]
53 -> 54 -0.18814
53 -> 64  0.10971

Excited State 7: Singlet-A 42.91835 1000/cm 233.00 nm  f=0.0000
49 -> 54  0.49284  49% [5,-1]
52 -> 54 -0.12593
53 -> 55 -0.15561
53 -> 58 -0.45582  42% [1,-5]

Excited State 8: Singlet-B3 43.16193 1000/cm 231.69 nm  f=0.0100
50 -> 54  0.44666  40% [4,-1]
52 -> 56  0.22330  10% [2,-3]
53 -> 57  0.46000  42% [1,-4]

Excited State 9: Singlet-B2 43.18613 1000/cm 231.55 nm  f=0.0714
51 -> 54  0.44540  40% [3,-1]
| Transition   | Energy (cm⁻¹) | Wavelength (nm) | Oscillator Strength | | |
|--------------|--------------|-----------------|---------------------|--------|
| 52 → 57      | 0.22743      | 10% [2,-4]      |                     |        |
| 53 → 56      | 0.45937      | 42% [1,-3]      |                     |        |
| 52 → 54      | 0.39873      | 32% [5,-1]      |                     |        |
| 51 → 57      | 0.14055      | 18% [3,-2]      |                     |        |
| 52 → 54      | -0.10477     | 12% [4,-1]      |                     |        |
| 53 → 55      | 0.29813      | 18% [3,-2]      |                     |        |
| 52 → 56      | 0.57487      | 66% [2,-3]      |                     |        |
| 53 → 55      | 0.57265      | 66% [2,-4]      |                     |        |
| 53 → 58      | 0.16470      |                |                     |        |
| 53 → 57      | 0.43415      | 38% [1,-5]      |                     |        |
| 53 → 59      | 0.66909      | 90% [1,-6]      |                     |        |
| 53 → 61      | 0.18279      |                |                     |        |
| 52 → 58      | -0.10997     | 29% [2,-5]      |                     |        |
| 53 → 57      | 0.13688      |                |                     |        |
| 53 → 60      | -0.15983     |                |                     |        |
| 53 → 64      | 0.45647      | 42% [1,-11]     |                     |        |
| 53 → 68      | -0.10841     |                |                     |        |
Excited State 20: Singlet-B2  50.59594 1000/cm  197.64 nm  f=0.0030
52 -> 60  0.17442
53 -> 59  -0.16031
53 -> 61  0.64642  84% [ 1,-8 ]
53 -> 67  0.10336

Excited State 21: Singlet-B3  50.91776 1000/cm  196.40 nm  f=0.0006
52 -> 59  0.61913  77% [ 2,-6 ]
52 -> 61  0.26976  15% [ 2,-8 ]
53 -> 60  0.15923

Excited State 22: Singlet-A  51.43153 1000/cm  194.43 nm  f=0.0000
53 -> 62  0.68428  94% [ 1,-9 ]
53 -> 66  0.11487

Excited State 23: Singlet-B1  52.1171 1000/cm  191.87 nm  f=0.0801
50 -> 57  -0.10324
51 -> 56  -0.10190
52 -> 62  -0.11040
53 -> 63  0.65431  86% [ 1,-10 ]
53 -> 64  0.12155

Excited State 24: Singlet-A  52.18405 1000/cm  191.63 nm  f=0.0000
46 -> 54  -0.16718
48 -> 55  0.53655  58% [ 6,-2 ]
50 -> 56  -0.24997  12% [ 4,-3 ]
51 -> 57  -0.25011  13% [ 3,-4 ]
52 -> 64  -0.11232

Excited State 25: Singlet-B1  52.46231 1000/cm  190.61 nm  f=0.9739
47 -> 54  0.13580
49 -> 58  0.15059
50 -> 57  0.37769  29% [ 4,-4 ]
51 -> 56  0.37917  29% [ 3,-3 ]
52 -> 58  -0.14415
53 -> 63  0.19396
53 -> 64  -0.21113

Excited State 26: Singlet-B2  53.06561 1000/cm  188.45 nm  f=0.0002
52 -> 60  0.65832  87% [ 2,-7 ]
52 -> 65  -0.11014
53 -> 59  0.12710
53 -> 61  -0.14381

Excited State 27: Singlet-B3  53.82296 1000/cm  185.79 nm  f=0.0092
49 -> 56  0.39695  32% [ 5,-3 ]
51 -> 58  -0.31642  20% [ 3,-5 ]
52 -> 61  0.13224
53 -> 65  0.41912  35% [ 1,-12 ]

Excited State 28: Singlet-B2  53.877 1000/cm  185.61 nm  f=0.0423
48 -> 56  -0.10952
49 -> 57  0.50631  51% [ 5,-4 ]
50 -> 58  -0.41779  35% [ 4,-5 ]
51 -> 54  0.10554

Excited State 29: Singlet-B3  53.91733 1000/cm  185.47 nm  f=0.0000
49 -> 56  -0.32508  21% [ 5,-3 ]
51 -> 58  0.27192  15% [ 3,-5 ]
52 -> 59  -0.11138
52 -> 61  0.17325
53 -> 65  0.48921  48% [ 1,-12 ]

Excited State 30: Singlet-B1  54.01493 1000/cm  185.13 nm  f=0.2139
Excited State 31: Singlet-A

\[ E(47 \rightarrow 54) = 0.61693 \quad 76\% \quad [7,-1] \]

\[ E(53 \rightarrow 64) = 0.23559 \quad 11\% \quad [1,-11] \]

Excited State 32: Singlet-B1

\[ E(50 \rightarrow 57) = 0.49932 \quad 50\% \quad [4,-4] \]

Excited State 33: Singlet-A

\[ E(50 \rightarrow 56) = 0.48456 \quad 47\% \quad [4,-3] \]

Excited State 34: Singlet-B1

\[ E(52 \rightarrow 60) = 0.45942 \quad 42\% \quad [4,-7] \]

Excited State 35: Singlet-A

\[ E(52 \rightarrow 62) = 0.59834 \quad 72\% \quad [2,-9] \]

Excited State 36: Singlet-B3

\[ E(52 \rightarrow 65) = -0.25598 \quad 13\% \quad [2,-6] \]

Excited State 37: Singlet-A

\[ E(52 \rightarrow 63) = -0.10236 \quad 17\% \quad [2,-9] \]

Excited State 38: Singlet-B1

\[ E(53 \rightarrow 66) = 0.63897 \quad 82\% \quad [1,-13] \]

Excited State 39: Singlet-B2

\[ E(53 \rightarrow 68) = 0.23075 \quad 11\% \quad [1,-15] \]

Excited State 40: Singlet-B1

\[ E(53 \rightarrow 70) = -0.18167 \quad 17\% \quad [2,-9] \]

Orbital symmetries:

Occupied

\[ (A) \ (B1) \ (A) \ (B1) \ (A) \ (B1) \ (B3) \ (B2) \ (B1) \ (A) \]
\[ (A) \ (B1) \ (B2) \ (B3) \ (A) \ (B1) \ (B1) \ (A) \ (B1) \ (A) \]
\[ (A) \ (B3) \ (B2) \ (A) \ (B1) \ (B2) \ (B3) \ (A) \ (B1) \ (B3) \ (B1) \]
\[ (A) \ (B1) \ (B2) \ (B3) \ (B1) \ (A) \ (B2) \ (B3) \ (A) \]
\[ (B2) \ (B1) \ (A) \ (B2) \ (B3) \ (B2) \ (B3) \ (A) \ (B1) \]
\[ (B1) \ (B3) \ (B2) \ (A) \ (B1) \ (B2) \ (B3) \ (B1) \ (A) \ (B1) \]

Virtual

\[ (B3) \ (B2) \ (A) \ (B1) \ (B2) \ (A) \ (B1) \ (A) \ (B2) \ (B3) \]
\[ (B3) \ (B1) \ (B2) \ (A) \ (B3) \ (B2) \ (B3) \ (B1) \ (B1) \ (A) \]
\[ (B3) \ (B2) \ (A) \ (B1) \ (A) \ (B2) \ (B3) \ (B1) \ (B2) \ (B3) \]
The electronic state is 1-A.

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# Gaussian 03: x86-Linux-G03RevB.04 2-Jun-2003
7-Nov-2008

#t td(Nst=40,conver=3) pbe1pbe/6-31+G*

1,4-Diphenylbuta-1,3-diyn, D=90 (based on pbe1pbe/6-31G* D2h geo.)

Framework group  D2D[C2(HCCCC.CCCCH),2SGD(C4H4)]

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324 basis functions, 552 primitive gaussians, 324 cartesian basis functions
53 alpha electrons 53 beta electrons

SCF Done: E(RPBE+HF-PBE) = -614.896422965 A.U. after 24 cycles
Convg = 0.5166D-08 -V/T = 2.0089

Excited states from <AA,BB:AA,BB> singles matrix:

Ground to excited state Transition electric dipole moments (Au):

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Ground to excited state transition velocity dipole Moments (Au):

Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics
This journal is © The Owner Societies 2011
Excitation energies and oscillator strengths:

Term symbols*) and MO parentage [in brackets] added by J. Spanget-Larsen. The notation [i,-j] indicates an excited singlet configuration derived from the ground configuration by promotion of an electron from the i'th highest occupied to the j'th lowest unoccupied MO.

*) In general, term symbols for the D2d conformation were not properly derived by the GAUSSIAN program. The symbols in brackets listed below were determined by correlation with corresponding results for slightly perturbed geometries of D2 and C2v symmetry, for which the GAUSSIAN symmetry analysis produces the correct symbols.

Excited State 1: Singlet-[B1] 30.20061 1000/cm 331.12 nm f=0.0000
52 -> 54 0.47425 45% [ 2,-1 ]
53 -> 55 0.47425 45% [ 1,-2 ]

Excited State 2: Singlet-[A2] 30.91199 1000/cm 323.50 nm f=0.0000
52 -> 54 0.48949 48% [ 2,-1 ]
53 -> 55 -0.48949 48% [ 1,-2 ]

Excited State 3: Singlet-[A1] 33.00823 1000/cm 302.96 nm f=0.0000
48 -> 55 0.12747
49 -> 54 0.12747
52 -> 55 0.45271 41% [ 2,-2 ]
52 -> 61 0.11546
53 -> 54 0.45271 41% [ 1,-1 ]
53 -> 60 0.11546

Excited State 4: Singlet-[B2] 37.92497 1000/cm 263.68 nm f=2.1837
52 -> 55 0.43420 38% [ 2,-2 ]
53 -> 55 -0.43420 38% [ 1,-2 ]

Excited State 5: Singlet-E 39.25418 1000/cm 254.75 nm f=0.0002
50 -> 54 0.10878
50 -> 55 0.32353 21% [ 4,-2 ]
51 -> 54 -0.10878
51 -> 55 0.32356 21% [ 3,-2 ]
52 -> 56 0.34692 24% [ 2,-3 ]
52 -> 57 0.34358 24% [ 2,-4 ]
53 -> 56 0.11664
53 -> 57 -0.11552

Excited State 6: Singlet-E 39.25418 1000/cm 254.75 nm f=0.0002
50 -> 54 0.32353 21% [ 4,-1 ]
50 -> 55 -0.10878
51 -> 54 -0.32356 21% [ 3,-1 ]
51 -> 55 -0.10878
52 -> 56 -0.11664
52 -> 57 -0.11552
53 -> 56 0.34692 24% [ 1,-3 ]
53 -> 57 -0.34358 24% [ 1,-4 ]

Excited State 7: Singlet-E 43.11757 1000/cm 231.93 nm f=0.0003
52 -> 56 -0.21529
52 -> 57 0.21483
53 -> 56 0.44534 40% [ 1,-3 ]
53 -> 57 0.44440 39% [ 1,-4 ]

Excited State 8: Singlet-E 43.11757 1000/cm 231.93 nm f=0.0003
Excited State 9: Singlet-E 44.26772 1000/cm 225.90 nm f=0.0000
50 -> 54 -0.18611
50 -> 55 0.45994 42% [ 4,-2 ]
51 -> 54 -0.18606
51 -> 55 -0.45983 42% [ 3,-2 ]

Excited State 10: Singlet-E 44.26772 1000/cm 225.90 nm f=0.0000
50 -> 54 0.45994 42% [ 4,-1 ]
50 -> 55 0.18611
51 -> 54 0.45983 42% [ 3,-1 ]
51 -> 55 -0.18606

Excited State 11: Singlet-E 46.07843 1000/cm 217.02 nm f=0.1203
48 -> 56 0.10458
48 -> 57 0.10553
50 -> 54 -0.16493
50 -> 55 -0.27002 15% [ 4,-2 ]
51 -> 54 0.16552
51 -> 55 -0.27100 15% [ 3,-2 ]
52 -> 56 0.26721 14% [ 2,-3 ]
52 -> 57 0.27207 15% [ 2,-4 ]
53 -> 56 0.16321
53 -> 57 -0.16618

Excited State 12: Singlet-E 46.07843 1000/cm 217.02 nm f=0.1203
49 -> 56 0.10458
49 -> 57 -0.10553
50 -> 54 -0.27002 15% [ 4,-1 ]
50 -> 55 0.16493
51 -> 54 0.27100 15% [ 3,-1 ]
51 -> 55 0.16552
52 -> 56 -0.16321
52 -> 57 -0.16618
53 -> 56 0.26721 14% [ 1,-3 ]
53 -> 57 -0.27207 15% [ 1,-4 ]

Excited State 13: Singlet-[A2] 46.35911 1000/cm 215.71 nm f=0.0000
46 -> 54 0.11383
47 -> 55 -0.11383
48 -> 54 0.46643 44% [ 6,-1 ]
49 -> 55 -0.46643 44% [ 5,-2 ]

Excited State 14: Singlet-[B1] 46.58414 1000/cm 214.66 nm f=0.0000
48 -> 54 0.47140 44% [ 6,-1 ]
49 -> 55 0.47140 44% [ 5,-2 ]
52 -> 54 -0.10399
53 -> 55 -0.10399

Excited State 15: Singlet-E 47.74639 1000/cm 209.44 nm f=0.0000
52 -> 58 0.39060 31% [ 2,-5 ]
52 -> 59 0.20061
52 -> 62 0.10059
53 -> 58 -0.46026 42% [ 1,-5 ]
53 -> 59 0.23639 11% [ 1,-6 ]
53 -> 62 -0.11854

Excited State 16: Singlet-E 47.74639 1000/cm 209.44 nm f=0.0000
52 -> 58 0.46026 42% [ 2,-5 ]
52 -> 59 0.23639 11% [ 2,-6 ]
52 -> 62 0.11854
Excited State 17: Singlet-[A1] 48.51826 1000/cm 206.11 nm f=0.0000
48 -> 55 0.42849 37% [ 6,-2 ]
49 -> 54 0.42846 37% [ 5,-1 ]
50 -> 56 0.20433
51 -> 57 0.20277

Excited State 18: Singlet-[B2] 48.52794 1000/cm 206.07 nm f=0.0000
48 -> 55 0.41003 34% [ 6,-2 ]
49 -> 54 -0.41005 34% [ 5,-1 ]
52 -> 61 -0.26805 14% [ 2,-8 ]
53 -> 60 0.26805 14% [ 1,-7 ]

Excited State 19: Singlet-[B1] 48.71506 1000/cm 205.27 nm f=0.0000
52 -> 60 0.46535 43% [ 2,-7 ]
53 -> 61 0.46535 43% [ 1,-8 ]

Excited State 20: Singlet-[A2] 49.01832 1000/cm 204.01 nm f=0.0000
52 -> 60 -0.46859 44% [ 2,-7 ]
53 -> 61 0.46859 44% [ 1,-8 ]

Excited State 21: Singlet-E 49.94264 1000/cm 200.23 nm f=0.0070
52 -> 58 -0.14350
52 -> 59 0.35340 25% [ 2,-6 ]
52 -> 62 -0.14492
53 -> 58 0.19803
53 -> 59 0.48770 48% [ 1,-6 ]
53 -> 62 0.19999

Excited State 22: Singlet-E 49.94264 1000/cm 200.23 nm f=0.0070
52 -> 58 -0.19803
52 -> 59 0.48770 48% [ 2,-6 ]
52 -> 62 -0.19999
53 -> 58 -0.14350
53 -> 59 -0.35340 25% [ 1,-6 ]
53 -> 62 -0.14492

Excited State 23: Singlet-[A1] 49.95715 1000/cm 200.17 nm f=0.0000
50 -> 56 0.14850
51 -> 57 0.14683
52 -> 61 0.45323 41% [ 2,-8 ]
53 -> 60 0.45323 41% [ 1,-7 ]

Excited State 24: Singlet-B2 52.51393 1000/cm 190.42 nm f=1.3648
50 -> 57 0.39915 32% [ 4,-4 ]
51 -> 56 0.40903 33% [ 3,-3 ]
52 -> 61 0.18997
53 -> 60 -0.18997

Excited State 25: Singlet-E 52.77606 1000/cm 189.48 nm f=0.0028
52 -> 58 -0.24328 12% [ 2,-5 ]
52 -> 59 0.14223
52 -> 62 0.58450 68% [ 2,-9 ]
52 -> 65 -0.17812
53 -> 62 -0.14082

Excited State 26: Singlet-E 52.77606 1000/cm 189.48 nm f=0.0028
52 -> 62 0.14082
53 -> 58 -0.24328 12% [ 1,-5 ]
53 -> 59 -0.14223
53 -> 62 0.58450 68% [ 1,-9 ]
53 -> 65 0.17812
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<th>Energy (1000/cm)</th>
<th>Wavelength (nm)</th>
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<td>45% [3,-6]</td>
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<td>35: E</td>
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<td>0.62223</td>
<td>77% [2,-12]</td>
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<td>-0.27508</td>
<td>15% [5,-3]</td>
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</table>

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49 -> 57 0.26846 14% [ 5,-4 ]
50 -> 60 -0.17199
50 -> 61 0.17558
51 -> 60 0.17371
51 -> 61 0.17733
52 -> 65 0.11432
53 -> 65 0.11670

Excited State 39: Singlet-E 56.29021 1000/cm 177.65 nm f=0.0445
48 -> 56 0.27508 15% [ 6,-3 ]
48 -> 57 0.26846 14% [ 6,-4 ]
49 -> 56 0.28081 16% [ 5,-3 ]
49 -> 57 -0.27407 15% [ 5,-4 ]
50 -> 60 0.17558
50 -> 61 0.17199
51 -> 60 -0.17734
51 -> 61 0.17371
52 -> 65 -0.11670
53 -> 65 0.11432

Excited State 40: Singlet-[A2] 56.91932 1000/cm 175.69 nm f=0.0000
46 -> 54 0.45203 41% [ 8,-1 ]
47 -> 55 -0.45213 41% [ 7,-2 ]
48 -> 54 -0.10242
49 -> 55 0.10243

Orbital symmetries:

Occupied
(B2) (A1) (E) (E) (E) (E) (B1) (A2) (E)
(E)

Virtual
(E) (E) (B1) (A2) (A1) (B2) (E) (E) (A1) (E)
(B2) (A1) (E) (E) (E) (B2) (B2) (A1) (E) (E)
(B1) (A2) (A1) (E) (E) (B2) (E) (E) (B1) (B2)
(E) (B2) (A1) (E) (E) (B1) (A2) (A1) (B2) (E)
(E) (A1) (E) (E) (E) (B2) (B2) (E) (E) (E)
(B2) (B2) (E) (E) (E) (E) (E) (E) (A2) (A1)
(A2) (E) (B2) (A1) (B2) (E) (E) (B1) (B2)
(A1) (B2) (A1) (E) (E) (B2) (A2) (E) (E) (E)
(A1) (A2) (E) (E) (E) (E) (E) (E) (E) (E)
(E) (E) (E) (E) (E) (E) (E) (E) (E) (E)

The electronic state is 1-A1.
| Alpha occ. eigenvalues | -0.64780 | -0.63868 | -0.63868 | -0.60725 | -0.56528 |
| Alpha occ. eigenvalues | -0.55540 | -0.50716 | -0.50324 | -0.48303 | -0.48303 |
| Alpha occ. eigenvalues | -0.45980 | -0.45835 | -0.44775 | -0.44775 | -0.40802 |
| Alpha occ. eigenvalues | -0.40802 | -0.38131 | -0.38063 | -0.37379 | -0.37379 |
| Alpha occ. eigenvalues | -0.35918 | -0.35918 | -0.30407 | -0.30407 | -0.27812 |
| Alpha virt. eigenvalues | -0.05380 | -0.05380 | -0.01558 | -0.01539 | 0.01090 |
| Alpha virt. eigenvalues | 0.01262 | 0.02753 | 0.02753 | 0.03156 | 0.03320 |
| Alpha virt. eigenvalues | 0.03320 | 0.04141 | 0.02753 | 0.03156 | 0.03320 |
| Alpha virt. eigenvalues | 0.03575 | 0.05266 | 0.05266 | 0.06689 | 0.06689 |
| Alpha virt. eigenvalues | 0.04162 | 0.04526 | 0.04526 | 0.06327 | 0.06327 |
| Alpha virt. eigenvalues | 0.05501 | 0.05732 | 0.05732 | 0.06124 | 0.06124 |
| Alpha virt. eigenvalues | 0.06436 | 0.06484 | 0.06807 | 0.07109 | 0.07109 |
| Alpha virt. eigenvalues | 0.07126 | 0.07125 | 0.07166 | 0.07166 | 0.07280 |
| Alpha virt. eigenvalues | 0.07291 | 0.07377 | 0.07400 | 0.07488 | 0.07488 |
| Alpha virt. eigenvalues | 0.07577 | 0.07586 | 0.07586 | 0.07618 | 0.07703 |
| Alpha virt. eigenvalues | 0.07735 | 0.07893 | 0.07893 | 0.08058 | 0.08058 |
| Alpha virt. eigenvalues | 0.08192 | 0.08238 | 0.08238 | 0.08423 | 0.08618 |
| Alpha virt. eigenvalues | 0.08652 | 0.08719 | 0.08719 | 0.09210 | 0.09210 |
| Alpha virt. eigenvalues | 0.09258 | 0.09330 | 0.09573 | 0.09738 | 0.09769 |
| Alpha virt. eigenvalues | 0.09766 | 0.09821 | 0.10037 | 0.10218 | 0.10217 |
| Alpha virt. eigenvalues | 1.04053 | 1.04053 | 1.06637 | 1.06637 | 1.10134 |
| Alpha virt. eigenvalues | 1.10134 | 1.12798 | 1.12964 | 1.15015 | 1.16477 |
| Alpha virt. eigenvalues | 1.19960 | 1.20351 | 1.20351 | 1.21156 | 1.23288 |
| Alpha virt. eigenvalues | 1.23846 | 1.23862 | 1.25463 | 1.28312 | 1.29149 |
| Alpha virt. eigenvalues | 1.29149 | 1.32003 | 1.34403 | 1.34652 | 1.41041 |
| Alpha virt. eigenvalues | 1.41041 | 1.43547 | 1.44254 | 1.44254 | 1.44454 |
| Alpha virt. eigenvalues | 1.44997 | 1.46091 | 1.47992 | 1.47992 | 1.49026 |
| Alpha virt. eigenvalues | 1.49026 | 1.49354 | 1.50093 | 1.50112 | 1.50281 |
| Alpha virt. eigenvalues | 1.59318 | 1.62712 | 1.65140 | 1.65140 | 1.67615 |
| Alpha virt. eigenvalues | 1.82575 | 1.84392 | 1.84751 | 1.84751 | 1.86491 |
| Alpha virt. eigenvalues | 1.90333 | 1.90333 | 1.91604 | 1.92825 | 1.93218 |
| Alpha virt. eigenvalues | 1.94642 | 1.97057 | 1.98874 | 2.00417 | 2.00417 |
| Alpha virt. eigenvalues | 2.01169 | 2.04454 | 2.07493 | 2.07493 | 2.08573 |
| Alpha virt. eigenvalues | 2.13390 | 2.15395 | 2.15524 | 2.16331 | 2.16331 |
| Alpha virt. eigenvalues | 2.18986 | 2.20462 | 2.21029 | 2.21029 | 2.21775 |
| Alpha virt. eigenvalues | 2.29712 | 2.29712 | 2.30380 | 2.30380 | 2.31492 |
| Alpha virt. eigenvalues | 2.31492 | 2.39113 | 2.51111 | 2.51111 | 2.52199 |
| Alpha virt. eigenvalues | 2.54109 | 2.59501 | 2.60780 | 2.63391 | 2.63391 |
| Alpha virt. eigenvalues | 2.65195 | 2.65232 | 2.65236 | 2.73169 | 2.75630 |
| Alpha virt. eigenvalues | 2.76615 | 2.76615 | 2.78115 | 2.81554 | 2.83065 |
| Alpha virt. eigenvalues | 2.83065 | 2.88118 | 3.02425 | 3.02425 | 3.03634 |
| Alpha virt. eigenvalues | 3.02573 | 3.02573 | 3.30611 | 3.41792 | 3.51468 |
| Alpha virt. eigenvalues | 3.77437 | 4.23486 | 4.27334 | 4.27679 | 4.27992 |
| Alpha virt. eigenvalues | 4.27992 | 4.32067 | 4.33905 | 4.39882 | 4.42266 |
| Alpha virt. eigenvalues | 4.43642 | 4.43642 | 4.59740 | 4.64075 | 4.81139 |
| Alpha virt. eigenvalues | 4.90568 | 5.64378 |
DPDA, D$_{2h}$ ($\Phi = 0^\circ$) 
PBE1PBE/6-31+G* MO energies (eV)

(-5) 2 $a_u$  \(-0.42\) 

(-4) 2 $b_{1g}$  \(-0.42\) 

(-3) 9 $b_{2u}$  \(-0.44\) 

(-2) 4 $b_{2g}$  \(-0.48\) 

(-1) 4 $b_{3u}$  \(-1.83\) [LUMO]

(1) 3 $b_{2g}$  \(-6.14\) [HOMO] 

(2) 8 $b_{3g}$  \(-7.09\) 

(3) 1 $b_{1g}$  \(-7.57\) 

(4) 1 $a_u$  \(-7.57\) 

(5) 3 $b_{3u}$  \(-7.60\)
DPDA, D₂ (Φ = 45°)
PBE1PBE/6-31+G* MO energies (eV)

(-4) 16 b₁  −0.42  (1) 11 b₂  −6.23  [HOMO]

(-3) 17 a  −0.42  (2) 11 b₃  −6.82

(-2) 12 b₂  −1.03  (3) 15 b₁  −7.57

(-1) 12 b₃  −1.74  (4) 16 a  −7.57  [LUMO]
DPDA, D$_{2d}$ ($\Phi = 90^\circ$)
PBE1PBE/6-31+G* MO energies (eV)

(-4) 2 $b_1$  $-0.42$

(1) 11 $e$  $-6.47$
[HOMO]

(-3) 2 $a_2$  $-0.42$

(2) 11 $e$  $-6.47$
[HOMO]

(-2) 12 $e$  $-1.46$
[LUMO]

(3) 1 $b_1$  $-7.57$

(-1) 12 $e$  $-1.46$
[LUMO]

(4) 1 $a_2$  $-7.57$
Frontier MO energies as a function of dihedral angle $\Phi$
#t td(Nst=40,conver=3) pbe1pbe/6-31+G*

1,4-Diphenylbuta-1,3-diyne (pbe1pbe/6-31+G*//~6-31G*)
Non-linear diyne axis, in-plane distortion

Standard orientation:

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<th>Atomic Number</th>
<th>Atomic Type</th>
<th>X (Angstroms)</th>
<th>Y (Angstroms)</th>
<th>Z (Angstroms)</th>
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324 basis functions, 552 primitive gaussians, 324 cartesian basis functions
53 alpha electrons     53 beta electrons

Excited states from <AA,BB:AA,BB> singles matrix:

Ground to excited state transition electric dipole moments (Au):
Excitation energies and oscillator strengths:
→ MO parentage [in brackets] added by J. Spanget-Larsen. The notation \([i, -j]\) indicates an excited singlet configuration derived from the ground configuration by promotion of an electron from the \(i\)’th highest occupied to the \(j\)’th lowest unoccupied MO.

Excited State 1: Singlet-B2 29.72474 1000/cm \(f=0.9253\)
52 -> 56 -0.21581
53 -> 54 0.67039 90% \([1, -1]\)

Excited State 2: Singlet-A2 31.24348 1000/cm \(f=0.0000\)
52 -> 54 0.68719 94% \([2, -1]\)
53 -> 56 -0.12558

Excited State 3: Singlet-A2 33.92286 1000/cm \(f=0.0000\)
48 -> 56 0.10105
52 -> 54 0.12914
53 -> 56 0.68596 94% \([1, -3]\)

Excited State 4: Singlet-B2 38.05402 1000/cm \(f=0.0000\)
49 -> 58 -0.13516
50 -> 54 0.45603 42% \([4, -1]\)
51 -> 55 0.13730
53 -> 57 0.50265 51% \([1, -4]\)
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Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics
This journal is © The Owner Societies 2011
Excited State 31: Singlet-B2 54.59484 1000/cm f=0.0007
50 -> 57 -0.49389 49% [ 4,-4 ]
51 -> 58 0.50529 51% [ 3,-5 ]

Excited State 32: Singlet-A1 54.59645 1000/cm f=0.0001
50 -> 58 0.52566 55% [ 4,-5 ]
51 -> 57 -0.47159 44% [ 3,-4 ]

Excited State 33: Singlet-A2 55.00537 1000/cm f=0.0000
50 -> 58 0.52566 55% [ 4,-5 ]
51 -> 57 -0.47159 44% [ 3,-4 ]

Excited State 34: Singlet-B1 55.01908 1000/cm f=0.0000
50 -> 60 0.45551 41% [ 4,-7 ]
51 -> 59 0.52732 56% [ 3,-6 ]

Excited State 35: Singlet-A1 55.05457 1000/cm f=0.1049
49 -> 57 -0.30629 19% [ 5,-4 ]
50 -> 55 -0.26325 14% [ 4,-2 ]
52 -> 60 0.55597 62% [ 2,-7 ]
52 -> 64 -0.11823

Excited State 36: Singlet-B2 55.42720 1000/cm f=0.0091
49 -> 58 0.53253 57% [ 5,-5 ]
51 -> 59 0.42609 36% [ 3,-6 ]
52 -> 59 0.10261

Excited State 37: Singlet-A2 55.52479 1000/cm f=0.0000
48 -> 56 -0.12748
50 -> 59 -0.11514
51 -> 60 -0.10493
53 -> 62 -0.10356
53 -> 66 0.64604 83% [ 1,-13 ]
53 -> 67 0.10759

Excited State 38: Singlet-A1 55.60787 1000/cm f=0.3186
49 -> 57 0.43602 38% [ 5,-4 ]
50 -> 55 0.34572 24% [ 4,-2 ]
52 -> 60 0.41114 34% [ 2,-7 ]

Excited State 39: Singlet-A2 55.95227 1000/cm f=0.0000
53 -> 67 0.66896 90% [ 1,-14 ]

Excited State 40: Singlet-B2 56.39103 1000/cm f=0.0293
49 -> 55 -0.15491
50 -> 57 0.15269
51 -> 58 0.15388
53 -> 65 0.18201
53 -> 69 0.60707 74% [ 1,-16 ]
53 -> 74 0.11150

Normal termination of Gaussian 03 at Tue Apr 12 14:02:43 2011.
**Gaussian 03: x86-Linux-G03RevB.04 2-Jun-2003**

11-Apr-2011

---

#t td(Nst=40,conver=3) sym=loose pbe1pbe/6-31+G*

---

1,4-Diphenylbuta-1,3-diyne (pbe1pbe/6-31+G*/-6-31G*)
Non-linear diyne axis, out-of-plane distortion

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Standard orientation:

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324 basis functions, 552 primitive gaussians, 324 cartesian basis functions
53 alpha electrons 53 beta electrons

Excited states from <AA,BB:AA,BB> singles matrix:

**Excited states from <AA,BB:AA,BB> singles matrix:**

**Ground to excited state transition electric dipole moments (Au):**

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Excitation energies and oscillator strengths:

→ MO parentage [in brackets] added by J. Spanget-Larsen. The notation [(i,-j)] indicates an excited singlet configuration derived from the ground configuration by promotion of an electron from the i'th highest occupied to the j'th lowest unoccupied MO.

**Excited State 1:** Singlet-B 29.70216 1000/cm  f=0.9229

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<td>52</td>
<td>-0.17316</td>
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<td>56</td>
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<tr>
<td>54</td>
<td>0.67066</td>
<td>90% [ 1,-1 ]</td>
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**Excited State 2:** Singlet-A 31.23058 1000/cm  f=0.0000

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<tbody>
<tr>
<td>52</td>
<td>0.68744</td>
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**Excited State 3:** Singlet-A 33.96561 1000/cm  f=0.0000

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<td>54</td>
<td>0.56321</td>
<td>63% [ 1,-3 ]</td>
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<tr>
<td>55</td>
<td>0.39275</td>
<td>31% [ 1,-5 ]</td>
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**Excited State 4:** Singlet-B 38.05241 1000/cm  f=0.0002

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<tbody>
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<tr>
<td>51</td>
<td>0.45698</td>
<td>42% [ 3,-1 ]</td>
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<tr>
<td>52</td>
<td>0.50157</td>
<td>50% [ 1,-4 ]</td>
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**Excited State 5:** Singlet-A 38.05322 1000/cm  f=0.0000

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<th>56</th>
<th>57</th>
<th>58</th>
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</thead>
<tbody>
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<tr>
<td>50</td>
<td>0.45488</td>
<td>41% [ 4,-1 ]</td>
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<tr>
<td>52</td>
<td>0.28150</td>
<td>16% [ 1,-3 ]</td>
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<tr>
<td>53</td>
<td>-0.41759</td>
<td>35% [ 1,-5 ]</td>
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**Excited State 6:** Singlet-A 40.0696 1000/cm  f=0.0002
| Excited State | Singlet-A | 42.84576 1000/cm | f=0.0000 |
| 49 -> 54 | 0.41878 | 35% | [ 5,-1 ] |
| 53 -> 55 | 0.56429 | 64% | [ 1,-2 ] |

| Excited State | Singlet-B | 42.9111 1000/cm | f=0.1216 |
| 51 -> 54 | 0.50678 | 51% | [ 3,-1 ] |
| 53 -> 57 | -0.47632 | 45% | [ 1,-4 ] |

| Excited State | Singlet-A | 43.63377 1000/cm | f=0.0084 |
| 47 -> 54 | 0.15010 |
| 52 -> 55 | 0.68451 | 94% | [ 2,-2 ] |

| Excited State | Singlet-B | 45.36786 1000/cm | f=0.0044 |
| 53 -> 59 | 0.67522 | 91% | [ 1,-6 ] |
| 53 -> 61 | 0.17195 |

| Excited State | Singlet-B | 45.78969 1000/cm | f=1.2769 |
| 48 -> 58 | 0.58944 | 69% | [ 2,-5 ] |
| 53 -> 54 | 0.19757 |

| Excited State | Singlet-B | 46.80917 1000/cm | f=0.0109 |
| 52 -> 56 | -0.37409 | 28% | [ 2,-3 ] |
| 52 -> 58 | 0.58944 | 69% | [ 2,-5 ] |

| Excited State | Singlet-A | 46.84062 1000/cm | f=0.0017 |
| 49 -> 56 | -0.20757 |
| 49 -> 58 | 0.36530 | 27% | [ 5,-5 ] |

| Excited State | Singlet-B | 48.12224 1000/cm | f=0.0001 |
| 53 -> 59 | -0.17039 |
| 53 -> 61 | 0.66355 | 88% | [ 1,-8 ] |

| Excited State | Singlet-A | 50.10636 1000/cm | f=0.0000 |
| 48 -> 58 | -0.10265 |
| 49 -> 57 | -0.41664 | 35% | [ 5,-4 ] |
| 50 -> 54 | 0.15741 |
| 51 -> 55 | 0.50830 | 52% | [ 3,-2 ] |

| Excited State | Singlet-B | 50.11766 1000/cm | f=0.0012 |
| 48 -> 57 | 0.13313 |
| 49 -> 56 | -0.20757 |
| 49 -> 58 | 0.36530 | 27% | [ 5,-5 ] |
| 50 -> 55 | 0.50617 | 51% | [ 4,-2 ] |
| 51 -> 54 | 0.15615 |
| 53 -> 57 | 0.12260 |
Excited State 20: Singlet-B 50.5169 1000/cm f=0.0957
48 -> 54  0.28886  17% [ 6,-1 ]
50 -> 56  0.52208  55% [ 4,-3 ]
50 -> 58  0.25918  13% [ 4,-5 ]
52 -> 58  0.10326
53 -> 65  -0.20297

Excited State 21: Singlet-A 50.58626 1000/cm f=0.0000
51 -> 56  0.57677  67% [ 3,-3 ]
51 -> 58  0.40549  33% [ 3,-5 ]

Excited State 22: Singlet-A 50.59513 1000/cm f=0.0000
53 -> 62  0.69022  95% [ 1,-9 ]
53 -> 66  0.11633

Excited State 23: Singlet-B 50.70079 1000/cm f=0.0679
48 -> 54  0.42476  36% [ 6,-1 ]
50 -> 56  -0.29224  17% [ 4,-3 ]
50 -> 58  -0.27016  15% [ 4,-5 ]
52 -> 56  0.10240
53 -> 65  -0.34333  24% [ 1,-12 ]

Excited State 24: Singlet-B 51.73721 1000/cm f=0.3813
49 -> 55  0.48072  46% [ 5,-2 ]
50 -> 56  0.13426
50 -> 58  -0.32569  21% [ 4,-5 ]
51 -> 57  0.34413  24% [ 3,-4 ]

Excited State 25: Singlet-B 51.78077 1000/cm f=0.0000
53 -> 63  0.69384  96% [ 1,-10 ]

Excited State 26: Singlet-A 52.42198 1000/cm f=0.0000
52 -> 59  0.62752  79% [ 2,-6 ]
52 -> 61  0.28941  17% [ 2,-8 ]

Excited State 27: Singlet-B 52.5357 1000/cm f=0.0002
44 -> 54  0.10255
47 -> 54  0.66840  89% [ 7,-1 ]
52 -> 55  -0.15318

Excited State 28: Singlet-A 53.40356 1000/cm f=0.0048
49 -> 61  0.11752
53 -> 64  0.68198  93% [ 1,-11 ]
53 -> 71  -0.10008

Excited State 29: Singlet-B 53.96492 1000/cm f=1.2644
49 -> 55  0.43602  38% [ 5,-2 ]
50 -> 56  -0.12630
50 -> 58  0.21383
51 -> 57  -0.24141  12% [ 3,-4 ]
52 -> 56  -0.12188
53 -> 65  -0.37762  29% [ 1,-12 ]
53 -> 68  0.10506

Excited State 30: Singlet-A 54.26254 1000/cm f=0.0143
46 -> 54  -0.24596  12% [ 8,-1 ]
47 -> 56  0.10336
48 -> 55  -0.15805
49 -> 54  0.10885
50 -> 57  0.39832  32% [ 4,-4 ]
51 -> 56  0.26104  14% [ 3,-3 ]
51 -> 58  -0.36750  27% [ 3,-5 ]

Excited State 31: Singlet-B 54.60532 1000/cm f=0.0001
Excited State 32: Singlet-A 54.60694 1000/cm f=0.0000

Excited State 33: Singlet-B 54.92311 1000/cm f=0.0265

Excited State 34: Singlet-A 55.02553 1000/cm f=0.0000

Excited State 35: Singlet-B 55.14894 1000/cm f=0.0997

Excited State 36: Singlet-A 55.40623 1000/cm f=0.0000

Excited State 37: Singlet-A 55.56028 1000/cm f=0.0000

Excited State 38: Singlet-B 55.61271 1000/cm f=0.3008

Excited State 39: Singlet-B 55.89581 1000/cm f=0.0005

Excited State 40: Singlet-B 56.3757 1000/cm f=0.0276

Normal termination of Gaussian 03 at Mon Apr 11 21:24:50 2011.
GAUSSIAN03 reference:

Gaussian 03, Revision B.04,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven,
K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Izengar, J. Tomasi,
V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega,
G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota,
R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao,
H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross,
C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev,
A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala,
K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg,
V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain,
O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford,
J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz,
I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,