Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics


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

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Planar DPDA ($D_{2h}$). TD-PBE1PBE/6-31+G*//6-31G*

| | Term | $\tilde{\nu}$ [a] | $f$ [b] | Leading configurations [c] |
|---|---|---|---|---|
| *1* | $1\,^1B_{1u}$ | 29.7 | 0.93 | 79% (1,-1), 13% (2,-3) |
| *2* | $1\,^1A_u$ | 31.2 | 0 | 92% (2,-1) |
| *3* | $2\,^1A_u$ | 34.0 | 0 | 93% (1,-3) |
| *4* | $1\,^1B_{3g}$ | 38.0 | 0 | 51% (1,-4), 42% (4,-1) |
| *5* | $1\,^1B_{2u}$ | 38.1 | $3\cdot10^{-4}$ | 51% (1,-5), 43% (3,-1) |
| *6* | $2\,^1A_g$ | 40.1 | 0 | 63% (1,-2), 37% (5,-1) |
| *7* | $2\,^1B_{3g}$ | 42.9 | 0 | 47% (4,-1), 41% (1,-4) |
| *8* | $2\,^1B_{2u}$ | 42.9 | 0.12 | 46% (3,-1), 42% (1,-5) |
| *9* | $3\,^1A_g$ | 43.7 | 0 | 49% (5,-1), 25% (1,-2) |
| *10* | $1\,^1B_{1g}$ | 44.4 | 0 | 93% (2,-2) |
| *11* | $1\,^1B_{2g}$ | 45.4 | 0 | 91% (1,-6) |
| *12* | $2\,^1B_{1u}$ | 45.8 | 1.30 | 46% (2,-3), 28% (6,-1) |
| *13* | $2\,^1B_{2g}$ | 46.8 | 0 | 99% (2,-4) |
| *14* | $1\,^1B_{3u}$ | 46.8 | $4\cdot10^{-3}$ | 59% (2,-5), 38% (1,-7) |
| *15* | $2\,^1B_{3u}$ | 46.9 | $1\cdot10^{-3}$ | 57% (1,-7), 39% (2,-5) |
| *16* | $2\,^1B_{1g}$ | 48.1 | 0 | 94% (5,-3) |
| *17* | $3\,^1B_{2g}$ | 50.0 | 0 | 88% (1,-8) |
| *18* | $3\,^1B_{2u}$ | 50.1 | $1\cdot10^{-3}$ | 52% (4,-2), 36% (5,-4) |
| *19* | $3\,^1B_{3g}$ | 50.1 | 0 | 52% (3,-2), 35% (5,-5) |
| *20* | $3\,^1B_{3u}$ | 50.6 | 0 | 99% (3,-3) |
| *21* | $4\,^1B_{2g}$ | 50.6 | 0 | 99% (4,-3) |
| *22* | $3\,^1A_u$ | 50.6 | 0 | 95% (1,-9) |
| *23* | $3\,^1B_{1u}$ | 50.7 | 0.18 | 51% (6,-1), 32% (1,-12) |
| *24* | $3\,^1B_{1g}$ | 51.6 | 0 | 97% (1,-10) |
| *25* | $4\,^1B_{1u}$ | 51.7 | 0.40 | 45% (5,-2), 22% (4,-4) |
| *26* | $4\,^1B_{3g}$ | 52.5 | 0 | 78% (2,-6), 17% (2,-8) |
| *27* | $4\,^1B_{1g}$ | 52.5 | 0 | 89% (7,-1) |
| *28* | $4\,^1B_{3u}$ | 53.1 | $4\cdot10^{-3}$ | 93% (1,-11) |
| *29* | $5\,^1B_{1u}$ | 54.0 | 1.26 | 36% (5,-2), 29% (1,-12) |
| *30* | $4\,^1A_g$ | 54.3 | 0 | 35% (3,-4), 26% (4,-5) |
| *31* | $6\,^1B_{1u}$ | 54.6 | $6\cdot10^{-4}$ | 51% (3,-5), 49% (4,-4) |
| *32* | $5\,^1A_g$ | 54.6 | 0 | 54% (4,-5), 46% (3,-4) |
| *33* | $4\,^1B_{2u}$ | 54.9 | 0.06 | 74% (2,-7), 11% (5,-4) |
| *34* | $4\,^1A_u$ | 54.9 | 0 | 52% (4,-6), 42% (3,-7) |
| *35* | $5\,^1B_{1g}$ | 55.0 | 0 | 54% (3,-6), 43% (4,-7) |
| *36* | $5\,^1B_{3g}$ | 55.4 | 0 | 51% (5,-5), 31% (3,-2) |
| *37* | $5\,^1B_{2u}$ | 55.5 | 0.37 | 40% (5,-4), 25% (4,-2) |
| *38* | $5\,^1A_u$ | 55.6 | 0 | 87% (1,-13) |
| *39* | $5\,^1B_{2g}$ | 55.9 | 0 | 92% (1,-14) |
| *40* | $7\,^1B_{1u}$ | 56.4 | 0.03 | 75% (1,-17) |

[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 = 45° ($D_2$). TD-PBE1PBE/6-31+G*//[6-31G* ($D_{2h}$)]

| | Term | $\tilde{\nu}$ [a] | $f$ [b] | Leading configurations [c] |
|---|---|---|---|---|
| *1* | $1\ ^1B_1$ | 30.2 | 0.60 | 76% (1,-1), 14% (2,-2) |
| *2* | $2\ ^1A$ | 30.8 | 0 | 71% (2,-1), 17% (1,-2) |
| *3* | $3\ ^1A$ | 33.3 | 0 | 63% (1,-2), 16% (2,-1) |
| *4* | $1\ ^1B_2$ | 38.5 | $2\cdot10^{-4}$ | 49% (1,-3), 40% (3,-1) |
| *5* | $1\ ^1B_3$ | 38.5 | $1\cdot10^{-4}$ | 49% (1,-4), 40% (4,-1) |
| *6* | $2\ ^1B_1$ | 40.5 | 1.40 | 72% (2,-2), 7% (1,-1) |
| *7* | $4\ ^1A$ | 42.9 | 0 | 49% (5,-1), 42% (1,-5) |
| *8* | $2\ ^1B_3$ | 43.2 | 0.01 | 42% (1,-4), 40% (4,-1) |
| *9* | $2\ ^1B_2$ | 43.2 | 0.07 | 42% (1,-3), 40% (3,-1) |
| *10* | $5\ ^1A$ | 44.9 | 0 | 38% (1,-5), 32% (5,-1) |
| *11* | $3\ ^1B_3$ | 45.2 | $5\cdot10^{-3}$ | 66% (2,-3), 18% (3,-2) |
| *12* | $3\ ^1B_2$ | 45.2 | 0.01 | 66% (2,-4), 18% (4,-2) |
| *13* | $4\ ^1B_2$ | 46.1 | $1\cdot10^{-4}$ | 90% (1,-6) |
| *14* | $3\ ^1B_1$ | 46.5 | 0.05 | 58% (5,-2), 29% (2,-5) |
| *15* | $4\ ^1B_3$ | 47.5 | 0.01 | 63% (3,-2), 15% (2,-3) |
| *16* | $5\ ^1B_2$ | 47.5 | 0.08 | 66% (4,-2), 15% (2,-4) |
| *17* | $5\ ^1B_3$ | 47.6 | 0.01 | 86% (1,-7) |
| *18* | $4\ ^1B_1$ | 47.8 | 0.13 | 50% (6,-1), 33% (2,-5) |
| *19* | $5\ ^1B_1$ | 50.0 | 0.14 | 42% (1,-11), 22% (6,-1) |
| *20* | $6\ ^1B_2$ | 50.6 | $3\cdot10^{-3}$ | 84% (1,-8) |
| *21* | $6\ ^1B_3$ | 50.9 | $6\cdot10^{-4}$ | 77% (2,-6), 15% (2,-8) |
| *22* | $6\ ^1A$ | 51.4 | 0 | 94% (1,-9) |
| *23* | $6\ ^1B_1$ | 52.1 | 0.08 | 86% (1,-10) |
| *24* | $7\ ^1A$ | 52.2 | 0 | 58% (6,-2), 13% (3,-4) |
| *25* | $7\ ^1B_1$ | 52.5 | 0.97 | 29% (4,-4), 29% (3,-3) |
| *26* | $7\ ^1B_2$ | 53.1 | $2\cdot10^{-4}$ | 87% (2,-7) |
| *27* | $7\ ^1B_3$ | 53.8 | 0.01 | 35% (1,-12), 32% (5,-3) |
| *28* | $8\ ^1B_2$ | 53.9 | 0.04 | 51% (5,-4), 15% (4,-5) |
| *29* | $8\ ^1B_3$ | 53.9 | $< 10^{-4}$ | 48% (1,-12), 15% (3,-5) |
| *30* | $8\ ^1B_1$ | 54.0 | 0.21 | 76% (7,-1), 11% (1,-11) |
| *31* | $8\ ^1A$ | 54.6 | 0 | 53% (2,-11), 17% (6,-2) |
| *32* | $9\ ^1A$ | 54.6 | 0 | 52% (3,-4), 47% (4,-3) |
| *33* | $9\ ^1B_1$ | 54.6 | $< 10^{-4}$ | 50% (4,-4), 50% (3,-3) |
| *34* | $10\ ^1B_1$ | 55.1 | $1\cdot10^{-4}$ | 55% (3,-6), 42% (4,-7) |
| *35* | $10\ ^1A$ | 55.1 | 0 | 54% (4,-6), 42% (3,-7) |
| *36* | $9\ ^1B_3$ | 55.8 | $9\cdot10^{-4}$ | 65% (2,-8), 13% (2,-6) |
| *37* | $11\ ^1A$ | 56.2 | 0 | 82% (2,-13), 12% (2,-10) |
| *38* | $11\ ^1B_1$ | 56.3 | $3\cdot10^{-4}$ | 72% (2,-9), 11% (1,-15) |
| *39* | $9\ ^1B_2$ | 56.5 | $4\cdot10^{-4}$ | 89% (1,-14) |
| *40* | $12\ ^1B_1$ | 56.7 | 0.03 | 55% (1,-15), 17% (2,-9) |

[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* ($D_{2h}$)]

| | Term | $\tilde{\nu}$ [a] | $f$ [b] | Leading configurations [c] |
|---|---|---|---|---|
| *1* | $1\ ^1B_1$ | 30.2 | 0 | 45% (2,-1), 45% (2,-2) |
| *2* | $1\ ^1A_2$ | 30.9 | 0 | 48% (2,-1), 48% (1,-2) |
| *3* | $2\ ^1A_1$ | 33.0 | 0 | 41% (2,-2), 41% (1,-1) |
| *4* | $1\ ^1B_2$ | 37.9 | 2.18 | 38% (2,-2), 38% (1,-1) |
| *5* | $1\ ^1E$ | 39.3 | $4\cdot10^{-4}$ | 24% (2,-3), 24% (2,-4), 21% (3,-2), 21% (4,-2) |
| *6* | | | | 24% (1,-3), 24% (1,-4), 21% (3,-1), 21% (4,-1) |
| *7* | $2\ ^1E$ | 43.1 | $6\cdot10^{-4}$ | 40% (1,-3), 39% (1,-4) |
| *8* | | | | 40% (2,-3), 39% (2,-4) |
| *9* | $3\ ^1E$ | 44.3 | $< 10^{-4}$ | 42% (4,-2), 42% (3,-2) |
| *10* | | | | 42% (4,-1), 42% (3,-1) |
| *11* | $4\ ^1E$ | 46.1 | 0.24 | 15% (4,-2), 15% (3,-2), 15% (2,-4), 14% (2,-3) |
| *12* | | | | 15% (4,-1), 15% (3,-1), 15% (1,-4), 14% (1,-3) |
| *13* | $2\ ^1A_2$ | 46.4 | 0 | 44% (6,-1), 44% (5,-2) |
| *14* | $2\ ^1B_1$ | 46.6 | 0 | 44% (6,-1), 44% (5,-2) |
| *15* | $5\ ^1E$ | 47.7 | $< 10^{-4}$ | 42% (1,-5), 31% (2,-5) |
| *16* | | | | 42% (2,-5), 31% (1,-5) |
| *17* | $3\ ^1A_1$ | 48.5 | 0 | 37% (6,-2), 37% (5,-1) |
| *18* | $2\ ^1B_2$ | 48.5 | 0 | 34% (6,-2), 34% (5,-1), 14% (2,-8), 14% (1,-7) |
| *19* | $3\ ^1B_1$ | 48.7 | 0 | 43% (2,-7), 43% (1,-8) |
| *20* | $3\ ^1A_2$ | 49.0 | 0 | 44% (2,-7), 44% (1,-8) |
| *21* | $6\ ^1E$ | 49.9 | 0.01 | 48% (1,-6), 25% (2,-6) |
| *22* | | | | 48% (2,-6), 25% (1,-6) |
| *23* | $4\ ^1A_1$ | 50.0 | 0 | 41% (2,-8), 41% (2,-8) |
| *24* | $3\ ^1B_2$ | 52.5 | 1.36 | 33% (3,-3), 32% (4,-4) |
| *25* | $7\ ^1E$ | 52.8 | $6\cdot10^{-4}$ | 68% (2,-9), 12% (2,-5) |
| *26* | | | | 68% (1,-9), 12% (1,-5) |
| *27* | $4\ ^1B_1$ | 53.1 | 0 | 48% (2,-10), 48% (1,-11) |
| *28* | $4\ ^1A_2$ | 53.1 | 0 | 48% (2,-10), 48% (1,-11) |
| *29* | $5\ ^1A_1$ | 54.6 | 0 | 51% (4,-3), 49% (3,-4) |
| *30* | $4\ ^1B_2$ | 54.6 | $1\cdot10^{-4}$ | 50% (4,-4), 49% (3,-3) |
| *31* | $6\ ^1A_1$ | 54.7 | 0 | 46% (2,-11), 46% (1,-10) |
| *32* | $5\ ^1B_2$ | 54.7 | $4\cdot10^{-3}$ | 44% (2,-11), 44% (1,-10) |
| *33* | $6\ ^1B_2$ | 55.0 | 0 | 52% (3,-5), 45% (4,-6) |
| *34* | $5\ ^1B_1$ | 55.0 | 0 | 52% (4,-5), 45% (3,-6) |
| *35* | $8\ ^1E$ | 55.7 | $2\cdot10^{-3}$ | 77% (1,-12) |
| *36* | | | | 77% (2,-12) |
| *37* | $7\ ^1A_1$ | 56.3 | 0 | 28% (4,-3), 26% (3,-4) |
| *38* | $9\ ^1E$ | 56.3 | 0.08 | 16% (6,-3), 15% (6,-4), 15% (5,-3), 14% (5,-4) |
| *39* | | | | 16% (5,-3), 15% (6,-3), 15% (5,-4), 14% (6,-4) |
| *40* | $5\ ^1A_2$ | 56.9 | 0 | 41% (8,-1), 41% (7,-2) |

[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:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6             0        0.000000    0.000000    0.679461
   2          6             0        0.000000    0.000000   -0.679461
   3          6             0        0.000000    0.000000    1.899660
   4          6             0        0.000000    0.000000   -1.899660
   5          6             0        0.000000    0.000000    3.318498
   6          6             0        0.000000    0.000000   -3.318498
   7          6             0        0.000000    1.211722    4.030916
   8          6             0        0.000000    1.211722   -4.030916
   9          6             0        0.000000   -1.211722    4.030916
  10          6             0        0.000000   -1.211722   -4.030916
  11          6             0        0.000000    1.206087    5.419091
  12          6             0        0.000000    1.206087   -5.419091
  13          6             0        0.000000   -1.206087    5.419091
  14          6             0        0.000000   -1.206087   -5.419091
  15          6             0        0.000000    0.000000    6.117221
  16          6             0        0.000000    0.000000   -6.117221
  17          1             0        0.000000    2.148075    3.481442
  18          1             0        0.000000    2.148075   -3.481442
  19          1             0        0.000000   -2.148075    3.481442
  20          1             0        0.000000   -2.148075   -3.481442
  21          1             0        0.000000    2.148474    5.959837
  22          1             0        0.000000    2.148474   -5.959837
  23          1             0        0.000000   -2.148474    5.959837
  24          1             0        0.000000   -2.148474   -5.959837
  25          1             0        0.000000    0.000000    7.203732
  26          1             0        0.000000    0.000000   -7.203732
---------------------------------------------------------------------
  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:
*****************************************************************

Ground to excited state Transition electric dipole moments (Au):
      state          X           Y           Z          Osc.
        1         0.0000      0.0000     -3.2167      0.9342
        2         0.0000      0.0000      0.0000      0.0000
        3         0.0000      0.0000      0.0000      0.0000
        4         0.0000      0.0000      0.0000      0.0000
        5         0.0000      0.0467      0.0000      0.0003
        6         0.0000      0.0000      0.0000      0.0000
        7         0.0000      0.0000      0.0000      0.0000
        8         0.0000      0.9681      0.0000      0.1222
```

| | | | | |
|---|---|---|---|---|
| 9 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 10 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 11 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 12 | 0.0000 | 0.0000 | -3.0614 | 1.3046 |
| 13 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 14 | 0.1630 | 0.0000 | 0.0000 | 0.0038 |
| 15 | 0.0835 | 0.0000 | 0.0000 | 0.0010 |
| 16 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 17 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 18 | 0.0000 | 0.0841 | 0.0000 | 0.0011 |
| 19 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 20 | -0.0034 | 0.0000 | 0.0000 | 0.0000 |
| 21 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 22 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 23 | 0.0000 | 0.0000 | -1.0771 | 0.1786 |
| 24 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 25 | 0.0000 | 0.0000 | -1.6037 | 0.4041 |
| 26 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 27 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 28 | 0.1633 | 0.0000 | 0.0000 | 0.0043 |
| 29 | 0.0000 | 0.0000 | 2.7701 | 1.2587 |
| 30 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 31 | 0.0000 | 0.0000 | -0.0583 | 0.0006 |
| 32 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 33 | 0.0000 | -0.6044 | 0.0000 | 0.0610 |
| 34 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 35 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 36 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 37 | 0.0000 | 1.4718 | 0.0000 | 0.3655 |
| 38 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 39 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 40 | 0.0000 | 0.0000 | -0.4017 | 0.0276 |

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

| state | X | Y | Z | Osc. |
|---|---|---|---|---|
| 1 | 0.0000 | 0.0000 | 0.4286 | 0.9041 |
| 2 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 3 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 4 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 5 | 0.0000 | -0.0053 | 0.0000 | 0.0001 |
| 6 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 7 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 8 | 0.0000 | -0.1961 | 0.0000 | 0.1311 |
| 9 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 10 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 11 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 12 | 0.0000 | 0.0000 | 0.6306 | 1.2695 |
| 13 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 14 | -0.0164 | 0.0000 | 0.0000 | 0.0008 |
| 15 | -0.0245 | 0.0000 | 0.0000 | 0.0019 |
| 16 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 17 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 18 | 0.0000 | -0.0180 | 0.0000 | 0.0009 |
| 19 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 20 | 0.0044 | 0.0000 | 0.0000 | 0.0001 |
| 21 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 22 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 23 | 0.0000 | 0.0000 | 0.2561 | 0.1894 |
| 24 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 25 | 0.0000 | 0.0000 | 0.3718 | 0.3910 |
| 26 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 27 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 28 | -0.0391 | 0.0000 | 0.0000 | 0.0042 |
| 29 | 0.0000 | 0.0000 | -0.6703 | 1.2175 |
| 30 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 31 | 0.0000 | 0.0000 | 0.0142 | 0.0005 |

| | | | | |
|---|---|---|---|---|
| 32 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 33 | 0.0000 | 0.1446 | 0.0000 | 0.0557 |
| 34 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 35 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 36 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 37 | 0.0000 | -0.3726 | 0.0000 | 0.3658 |
| 38 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 39 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 40 | 0.0000 | 0.0000 | 0.1097 | 0.0312 |

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.

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 Excited State   1:   Singlet-B1U     29.72232 1000/cm  336.45 nm  f=0.9342
      52 -> 56        -0.25056   13% [ 2,-3 ]
      53 -> 54         0.62888   79% [ 1,-1 ]

 Excited State   2:   Singlet-AU      31.24026 1000/cm  320.10 nm  f=0.0000
      52 -> 54         0.67975   92% [ 2,-1 ]
      53 -> 56        -0.10508

 Excited State   3:   Singlet-AU      33.98577 1000/cm  294.24 nm  f=0.0000
      52 -> 54         0.14079
      53 -> 56         0.68361   93% [ 1,-3 ]

 Excited State   4:   Singlet-B3G     38.04677 1000/cm  262.83 nm  f=0.0000
      49 -> 58        -0.14252
      50 -> 54         0.45993   42% [ 4,-1 ]
      51 -> 55         0.14350
      53 -> 57         0.50722   51% [ 1,-4 ]

 Excited State   5:   Singlet-B2U     38.05967 1000/cm  262.75 nm  f=0.0003
      49 -> 57        -0.14309
      50 -> 55         0.14334
      51 -> 54         0.46202   43% [ 3,-1 ]
      53 -> 58         0.50528   51% [ 1,-5 ]

 Excited State   6:   Singlet-AG      40.1051 1000/cm  249.34 nm  f=0.0000
      49 -> 54         0.43191   37% [ 5,-1 ]
      53 -> 55         0.56250   63% [ 1,-2 ]

 Excited State   7:   Singlet-B3G     42.85222 1000/cm  233.36 nm  f=0.0000
      49 -> 58        -0.10146
      50 -> 54         0.48425   47% [ 4,-1 ]
      53 -> 57        -0.45484   41% [ 1,-4 ]

 Excited State   8:   Singlet-B2U     42.92319 1000/cm  232.98 nm  f=0.1222
      49 -> 57        -0.10311
      51 -> 54         0.48206   46% [ 3,-1 ]
      53 -> 58        -0.45653   42% [ 1,-5 ]

 Excited State   9:   Singlet-AG      43.6628 1000/cm  229.03 nm  f=0.0000
      47 -> 56         0.10832
      49 -> 54         0.49331   49% [ 5,-1 ]
      50 -> 58         0.14551
      51 -> 57         0.14614
      53 -> 55        -0.35142   25% [ 1,-2 ]

 Excited State  10:   Singlet-B1G     44.3516 1000/cm  225.47 nm  f=0.0000
      47 -> 54         0.14852
      52 -> 55         0.68324   93% [ 2,-2 ]

 Excited State  11:   Singlet-B2G     45.40012 1000/cm  220.27 nm  f=0.0000
```

```
     53 -> 59         0.67529   91% [ 1,-6 ]
     53 -> 61         0.17456

Excited State  12:   Singlet-B1U     45.82517 1000/cm  218.22 nm  f=1.3046
     48 -> 54        -0.37574   28% [ 6,-1 ]
     52 -> 56         0.47884   46% [ 2,-3 ]
     53 -> 54         0.15190
     53 -> 65         0.20911

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         0.54441   59% [ 2,-5 ]
     53 -> 60         0.43602   38% [ 1,-7 ]

Excited State  15:   Singlet-B3U     46.87208 1000/cm  213.35 nm  f=0.0010
     52 -> 58        -0.44402   39% [ 2,-5 ]
     53 -> 60         0.53581   57% [ 1,-7 ]

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         0.51047   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 -> 61         0.11244
     53 -> 64         0.68220   93% [ 1,-11 ]

Excited State  29:   Singlet-B1U     54.00121 1000/cm  185.18 nm  f=1.2587
     49 -> 55         0.42605   36% [ 5,-2 ]
     50 -> 57        -0.22691   10% [ 4,-4 ]
     51 -> 58        -0.20851
     52 -> 56        -0.12939
     53 -> 65         0.38379   29% [ 1,-12 ]

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
     50 -> 57        -0.49467   49% [ 4,-4 ]
     51 -> 58         0.50481   51% [ 3,-5 ]

Excited State  32:   Singlet-AG      54.6021 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 ]
     52 -> 64        -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) (B1U) (B3G) (B2U) (B1U)
                (AG) (B1U) (AG) (B2U) (B3G) (B1U) (AG) (AG) (B1U)
                (AG) (B1U) (AG) (B3G) (B2U) (B1U) (AG) (B1U) (B2U)
                (B3G) (AG) (B1U) (AG) (B1U) (AG) (B2U) (B3G) (B1U)
                (AG) (B2U) (B3G) (B3U) (B2G) (B1U) (AG) (B2U)
                (B3G) (B3U) (B2U) (B2G) (B3U) (AU) (B1G) (B3G)
                (B2G)
      Virtual   (B3U) (B2G) (B2U) (B1G) (AU) (AG) (B1U) (AG) (B2U)
                (B3G) (B1U) (B3U) (B2U) (AG) (B3G) (B2G) (B3U)
                (B1U) (AG) (B1U) (B3U) (B2U) (B1G) (AG) (AU) (B2G)
                (B3G) (B1U) (B2G) (B3U) (B1G) (AG) (B3U) (AU)
                (B2U) (B1U) (B2G) (B3G) (AG) (B2U) (B3G) (B3U)
                (B3G) (B1U) (AG) (B2G) (B2U) (AG) (B1U) (B3U)
                (B2U) (B3G) (AG) (B2G) (B1U) (B1U) (AG) (B3G)
                (B2U) (B1U) (B1U) (B3G) (B2G) (AG) (B2U) (B1U)
                (AG) (B3G) (B2U) (B3U) (B2U) (AG) (B3G) (B1U)
                (B1U) (AG) (AG) (B1U) (B3G) (B2U) (B2G) (B1U)
                (B3G) (AG) (B2U) (B3G) (B2U) (B1U) (B3G) (AG)
                (B1U) (B3G) (B2U) (AG) (B1U) (AG) (B1U) (B3U)
                (B2G) (B3U) (AG) (B2U) (B3G) (B1G) (B2G) (AU)
                (AG) (B1U) (B2U) (B3U) (B3G) (B1G) (AU) (B2G)
                (B1U) (AG) (B2U) (B3U) (B3G) (B2U) (B1U) (AG)
                (B2G) (B3U) (B2G) (AG) (B1U) (B3U) (B3G) (B1U)
                (AG) (B2U) (B3G) (B2U) (B3G) (AG) (B2G) (B2U)
                (B1U) (AG) (B1U) (B2U) (B3G) (B2U) (B3G) (AG)
                (B1U) (AG) (B1U) (B2U) (AG) (AG) (B3G) (B3G) (B1U)
                (B1G) (AU) (B3U) (B1U) (B1U) (B2U) (AG) (AG) (B1U)
                (B3G) (B3U) (B1U) (B2G) (B1G) (AG) (B2U) (AU)
                (B2G) (B3U) (B3G) (B1G) (B2G) (AU) (AG) (B1G)
                (AU) (B2U) (B1U) (B3U) (B1U) (AG) (B3G) (B1G)
                (B2U) (AG) (B1U) (B2G) (B3G) (AG) (B1U) (AG) (B1U)
                (B2U) (AG) (B3G) (AU) (B1U) (B2U) (B3U) (B1U)
                (AG) (B3G) (B1G) (AU) (B2U) (AG) (B2G) (B1U) (B1U)
                (B3G) (B3U) (B1G) (AU) (B3U) (B2G) (B2G) (AG)
                (B2U) (AG) (B1U) (B1U) (AG) (B2U) (B3G) (B1G)
                (AU) (B1U) (B3U) (B3G) (AG) (B2U) (AG) (B3G) (B1U)
                (B1U) (B2U) (AG) (B3G) (B1U) (B2U) (B2G) (AG)
                (B3G) (B1U) (AG) (B1U) (AG) (B1U) (AG) (B2U) (B3G)
                (AG) (B1U) (B1U) (AG) (B2U) (B3G) (B1U) (AG) (B1U)
                (AG) (B1U)
The electronic state is 1-AG.
Alpha  occ. eigenvalues --  -10.27807 -10.27807 -10.26222 -10.26165 -10.25925
Alpha  occ. eigenvalues --  -10.25910 -10.25749 -10.25749 -10.25748 -10.25748
Alpha  occ. eigenvalues --  -10.25560 -10.25560 -10.25443 -10.25443 -10.25428
Alpha  occ. eigenvalues --  -10.25428  -0.90258  -0.90218  -0.83491  -0.81684
Alpha  occ. eigenvalues --   -0.78882  -0.78490  -0.78490  -0.74627  -0.67347
Alpha  occ. eigenvalues --   -0.64788  -0.63877  -0.63873  -0.60745  -0.56537
Alpha  occ. eigenvalues --   -0.55554  -0.50721  -0.50331  -0.48341  -0.48273
Alpha  occ. eigenvalues --   -0.45987  -0.45843  -0.44782  -0.44779  -0.41078
Alpha  occ. eigenvalues --   -0.40515  -0.38133  -0.38065  -0.37601  -0.37105
Alpha  occ. eigenvalues --   -0.36448  -0.35310  -0.32120  -0.27919  -0.27816
```

```
Alpha  occ. eigenvalues --   -0.27815  -0.26039  -0.22581
Alpha virt. eigenvalues --   -0.06728  -0.01782  -0.01629  -0.01559  -0.01541
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   0.11899   0.12336   0.13979
Alpha virt. eigenvalues --    0.14442   0.14480   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   0.17436   0.17981
Alpha virt. eigenvalues --    0.18134   0.19859   0.19871   0.19997   0.21421
Alpha virt. eigenvalues --    0.21484   0.21639   0.21920   0.21940   0.22205
Alpha virt. eigenvalues --    0.22865   0.23341   0.23689   0.24018   0.24229
Alpha virt. eigenvalues --    0.24918   0.25115   0.25663   0.26098   0.26574
Alpha virt. eigenvalues --    0.27311   0.27607   0.28326   0.28701   0.28797
Alpha virt. eigenvalues --    0.29540   0.29776   0.30807   0.31028   0.32151
Alpha virt. eigenvalues --    0.32505   0.33934   0.34361   0.34589   0.35331
Alpha virt. eigenvalues --    0.35681   0.35906   0.36072   0.36445   0.39082
Alpha virt. eigenvalues --    0.44022   0.45498   0.47299   0.49594   0.50766
Alpha virt. eigenvalues --    0.55036   0.57676   0.57872   0.61239   0.61293
Alpha virt. eigenvalues --    0.64257   0.65561   0.67116   0.68282   0.69673
Alpha virt. eigenvalues --    0.69875   0.71330   0.71349   0.72800   0.72887
Alpha virt. eigenvalues --    0.72913   0.73282   0.74029   0.74122   0.74885
Alpha virt. eigenvalues --    0.75754   0.75768   0.76186   0.76747   0.76977
Alpha virt. eigenvalues --    0.77365   0.78154   0.79087   0.80184   0.81430
Alpha virt. eigenvalues --    0.82034   0.82085   0.83502   0.84407   0.85878
Alpha virt. eigenvalues --    0.86852   0.87049   0.88642   0.89889   0.93082
Alpha virt. eigenvalues --    0.93333   0.93737   0.95617   0.96014   0.97760
Alpha virt. eigenvalues --    0.98167   0.98378   0.99180   1.01065   1.02158
Alpha virt. eigenvalues --    1.02369   1.03964   1.04403   1.09329   1.10159
Alpha virt. eigenvalues --    1.12654   1.12901   1.15025   1.16483   1.19629
Alpha virt. eigenvalues --    1.19911   1.21131   1.23354   1.23636   1.23675
Alpha virt. eigenvalues --    1.23842   1.23859   1.24919   1.25817   1.28371
Alpha virt. eigenvalues --    1.31059   1.31885   1.34108   1.34719   1.35217
Alpha virt. eigenvalues --    1.42947   1.43751   1.43992   1.44434   1.44740
Alpha virt. eigenvalues --    1.45677   1.46084   1.47499   1.48443   1.48751
Alpha virt. eigenvalues --    1.49337   1.49845   1.50110   1.50217   1.50276
Alpha virt. eigenvalues --    1.59285   1.61751   1.62479   1.67810   1.67876
Alpha virt. eigenvalues --    1.82279   1.82510   1.84360   1.86694   1.87304
Alpha virt. eigenvalues --    1.89813   1.90192   1.90524   1.92921   1.93215
Alpha virt. eigenvalues --    1.95315   1.97088   2.00162   2.00335   2.01021
Alpha virt. eigenvalues --    2.01136   2.02792   2.06618   2.08452   2.09171
Alpha virt. eigenvalues --    2.13380   2.14635   2.15392   2.15522   2.18295
Alpha virt. eigenvalues --    2.18565   2.20235   2.20650   2.21984   2.22213
Alpha virt. eigenvalues --    2.27845   2.30377   2.30626   2.31263   2.31323
Alpha virt. eigenvalues --    2.35118   2.38614   2.39796   2.51293   2.54569
Alpha virt. eigenvalues --    2.59565   2.60735   2.63059   2.63949   2.65193
Alpha virt. eigenvalues --    2.65230   2.65290   2.66768   2.70337   2.73058
Alpha virt. eigenvalues --    2.76190   2.76300   2.77849   2.78187   2.81790
Alpha virt. eigenvalues --    2.87049   2.88032   2.98042   3.04050   3.15154
Alpha virt. eigenvalues --    3.18177   3.33028   3.35591   3.41856   3.51340
Alpha virt. eigenvalues --    3.77405   4.22614   4.27414   4.27679   4.27731
Alpha virt. eigenvalues --    4.29924   4.31868   4.33865   4.40114   4.42230
Alpha virt. eigenvalues --    4.44037   4.45499   4.60097   4.64011   4.81350
Alpha virt. eigenvalues --    4.90386   5.64359

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
*****************************************
---------------------------------------
#t td(Nst=40,conver=3) pbe1pbe/6-31+G*
---------------------------------------
---------------------------------------------------------------------
1,4-Diphenylbuta-1,3-diyne, D=45 (based on pbe1pbe/6-31G* D2h geo.)
---------------------------------------------------------------------

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

                      Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6             0        0.000000    0.000000    0.679461
   2          6             0        0.000000    0.000000   -0.679461
   3          6             0        0.000000    0.000000    1.899660
   4          6             0        0.000000    0.000000   -1.899660
   5          6             0        0.000000    0.000000    3.318498
   6          6             0        0.000000    0.000000   -3.318498
   7          6             0       -0.463706    1.119485    4.030916
   8          6             0        0.463706    1.119485   -4.030916
   9          6             0        0.463706   -1.119485    4.030916
  10          6             0       -0.463706   -1.119485   -4.030916
  11          6             0       -0.461549    1.114279    5.419091
  12          6             0        0.461549    1.114279   -5.419091
  13          6             0        0.461549   -1.114279    5.419091
  14          6             0       -0.461549   -1.114279   -5.419091
  15          6             0        0.000000    0.000000    6.117221
  16          6             0        0.000000    0.000000   -6.117221
  17          1             0       -0.822033    1.984562    3.481442
  18          1             0        0.822033    1.984562   -3.481442
  19          1             0        0.822033   -1.984562    3.481442
  20          1             0       -0.822033   -1.984562   -3.481442
  21          1             0       -0.822185    1.984931    5.959837
  22          1             0        0.822185    1.984931   -5.959837
  23          1             0        0.822185   -1.984931    5.959837
  24          1             0       -0.822185   -1.984931   -5.959837
  25          1             0        0.000000    0.000000    7.203732
  26          1             0        0.000000    0.000000   -7.203732
---------------------------------------------------------------------
  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):
      state          X           Y           Z          Osc.
        1         0.0000      0.0000      2.5635      0.6032
        2         0.0000      0.0000      0.0000      0.0000
        3         0.0000      0.0000      0.0000      0.0000
        4         0.0000     -0.0436      0.0000      0.0002
        5         0.0245      0.0000      0.0000      0.0001
        6         0.0000      0.0000     -3.3713      1.3996
```

| | | | | |
|---|---|---|---|---|
| 7 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 8 | -0.2764 | 0.0000 | 0.0000 | 0.0100 |
| 9 | 0.0000 | 0.7378 | 0.0000 | 0.0714 |
| 10 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 11 | 0.1861 | 0.0000 | 0.0000 | 0.0048 |
| 12 | 0.0000 | -0.3177 | 0.0000 | 0.0139 |
| 13 | 0.0000 | -0.0247 | 0.0000 | 0.0001 |
| 14 | 0.0000 | 0.0000 | 0.5966 | 0.0503 |
| 15 | -0.2979 | 0.0000 | 0.0000 | 0.0128 |
| 16 | 0.0000 | 0.7568 | 0.0000 | 0.0826 |
| 17 | -0.2315 | 0.0000 | 0.0000 | 0.0077 |
| 18 | 0.0000 | 0.0000 | -0.9303 | 0.1256 |
| 19 | 0.0000 | 0.0000 | -0.9507 | 0.1374 |
| 20 | 0.0000 | 0.1401 | 0.0000 | 0.0030 |
| 21 | -0.0617 | 0.0000 | 0.0000 | 0.0006 |
| 22 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 23 | 0.0000 | 0.0000 | 0.7115 | 0.0801 |
| 24 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 25 | 0.0000 | 0.0000 | -2.4722 | 0.9739 |
| 26 | 0.0000 | 0.0393 | 0.0000 | 0.0002 |
| 27 | -0.2368 | 0.0000 | 0.0000 | 0.0092 |
| 28 | 0.0000 | 0.5084 | 0.0000 | 0.0423 |
| 29 | -0.0147 | 0.0000 | 0.0000 | 0.0000 |
| 30 | 0.0000 | 0.0000 | 1.1417 | 0.2139 |
| 31 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 32 | 0.0000 | 0.0000 | -0.0019 | 0.0000 |
| 33 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 34 | 0.0000 | 0.0000 | 0.0277 | 0.0001 |
| 35 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 36 | -0.0748 | 0.0000 | 0.0000 | 0.0009 |
| 37 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 38 | 0.0000 | 0.0000 | 0.0385 | 0.0003 |
| 39 | 0.0000 | -0.0455 | 0.0000 | 0.0004 |
| 40 | 0.0000 | 0.0000 | 0.4421 | 0.0336 |

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

| state | X | Y | Z | Osc. |
|---|---|---|---|---|
| 1 | 0.0000 | 0.0000 | -0.3475 | 0.5848 |
| 2 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 3 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 4 | 0.0000 | 0.0055 | 0.0000 | 0.0001 |
| 5 | -0.0013 | 0.0000 | 0.0000 | 0.0000 |
| 6 | 0.0000 | 0.0000 | 0.6150 | 1.3650 |
| 7 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 8 | 0.0625 | 0.0000 | 0.0000 | 0.0133 |
| 9 | 0.0000 | -0.1471 | 0.0000 | 0.0733 |
| 10 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 11 | -0.0259 | 0.0000 | 0.0000 | 0.0022 |
| 12 | 0.0000 | 0.0734 | 0.0000 | 0.0174 |
| 13 | 0.0000 | -0.0005 | 0.0000 | 0.0000 |
| 14 | 0.0000 | 0.0000 | -0.1239 | 0.0483 |
| 15 | 0.0637 | 0.0000 | 0.0000 | 0.0125 |
| 16 | 0.0000 | -0.1679 | 0.0000 | 0.0868 |
| 17 | 0.0420 | 0.0000 | 0.0000 | 0.0054 |
| 18 | 0.0000 | 0.0000 | 0.1966 | 0.1184 |
| 19 | 0.0000 | 0.0000 | 0.2215 | 0.1435 |
| 20 | 0.0000 | -0.0333 | 0.0000 | 0.0032 |
| 21 | 0.0181 | 0.0000 | 0.0000 | 0.0009 |
| 22 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 23 | 0.0000 | 0.0000 | -0.1679 | 0.0792 |
| 24 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 25 | 0.0000 | 0.0000 | 0.5817 | 0.9439 |
| 26 | 0.0000 | -0.0142 | 0.0000 | 0.0006 |
| 27 | 0.0612 | 0.0000 | 0.0000 | 0.0102 |
| 28 | 0.0000 | -0.1222 | 0.0000 | 0.0406 |
| 29 | -0.0043 | 0.0000 | 0.0000 | 0.0001 |

| | | | | |
|---|---|---|---|---|
| 30 | 0.0000 | 0.0000 | -0.2736 | 0.2028 |
| 31 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 32 | 0.0000 | 0.0000 | 0.0005 | 0.0000 |
| 33 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 34 | 0.0000 | 0.0000 | -0.0070 | 0.0001 |
| 35 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 36 | 0.0209 | 0.0000 | 0.0000 | 0.0011 |
| 37 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 38 | 0.0000 | 0.0000 | -0.0093 | 0.0002 |
| 39 | 0.0000 | 0.0091 | 0.0000 | 0.0002 |
| 40 | 0.0000 | 0.0000 | -0.1098 | 0.0311 |

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 ]
```

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     52 -> 57         0.22743   10% [ 2,-4 ]
     53 -> 56         0.45937   42% [ 1,-3 ]

Excited State  10:   Singlet-A       44.90732 1000/cm  222.68 nm  f=0.0000
     49 -> 54         0.39873   32% [ 5,-1 ]
     50 -> 56         0.14055
     51 -> 57         0.14052
     52 -> 54        -0.10477
     53 -> 55         0.16470
     53 -> 58         0.43415   38% [ 1,-5 ]

Excited State  11:   Singlet-B3      45.22429 1000/cm  221.12 nm  f=0.0048
     50 -> 54        -0.24927   12% [ 4,-1 ]
     51 -> 55         0.29813   18% [ 3,-2 ]
     52 -> 56         0.57487   66% [ 2,-3 ]

Excited State  12:   Singlet-B2      45.22994 1000/cm  221.09 nm  f=0.0139
     50 -> 55         0.30148   18% [ 4,-2 ]
     51 -> 54        -0.25111   13% [ 3,-1 ]
     52 -> 57         0.57265   66% [ 2,-4 ]

Excited State  13:   Singlet-B2      46.10021 1000/cm  216.92 nm  f=0.0001
     53 -> 59         0.66909   90% [ 1,-6 ]
     53 -> 61         0.18279

Excited State  14:   Singlet-B1      46.53494 1000/cm  214.89 nm  f=0.0503
     47 -> 54         0.12828
     48 -> 54         0.11914
     49 -> 55         0.53849   58% [ 5,-2 ]
     52 -> 58         0.37895   29% [ 2,-5 ]

Excited State  15:   Singlet-B3      47.46651 1000/cm  210.68 nm  f=0.0128
     49 -> 56        -0.17727
     51 -> 55         0.56091   63% [ 3,-2 ]
     52 -> 56        -0.26981   15% [ 2,-3 ]
     53 -> 57         0.13688
     53 -> 60        -0.15983

Excited State  16:   Singlet-B2      47.49797 1000/cm  210.54 nm  f=0.0826
     49 -> 57        -0.18611
     50 -> 55         0.57392   66% [ 4,-2 ]
     52 -> 57        -0.27711   15% [ 2,-4 ]
     53 -> 56         0.14375

Excited State  17:   Singlet-B3      47.59637 1000/cm  210.10 nm  f=0.0077
     51 -> 55         0.13388
     52 -> 59        -0.17331
     53 -> 60         0.65462   86% [ 1,-7 ]

Excited State  18:   Singlet-B1      47.78107 1000/cm  209.29 nm  f=0.1256
     48 -> 54         0.50238   50% [ 6,-1 ]
     49 -> 55         0.16228
     49 -> 58        -0.11015
     52 -> 55        -0.10997
     52 -> 58        -0.40873   33% [ 2,-5 ]

Excited State  19:   Singlet-B1      50.02651 1000/cm  199.89 nm  f=0.1374
     47 -> 54        -0.13169
     48 -> 54        -0.33228   22% [ 6,-1 ]
     49 -> 55         0.28448   16% [ 5,-2 ]
     50 -> 57         0.10001
     51 -> 56         0.10016
     52 -> 58        -0.15474
     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
```

```
     47 -> 54         0.61693   76% [ 7,-1 ]
     53 -> 64         0.23559   11% [ 1,-11 ]

Excited State  31:   Singlet-A       54.58758 1000/cm  183.19 nm  f=0.0000
     46 -> 54         0.10478
     48 -> 55         0.29114   17% [ 6,-2 ]
     48 -> 58        -0.12239
     50 -> 56         0.19630
     51 -> 57         0.11201
     52 -> 64         0.51562   53% [ 2,-11 ]

Excited State  32:   Singlet-B1      54.59725 1000/cm  183.16 nm  f=0.0000
     50 -> 57         0.49932   50% [ 4,-4 ]
     51 -> 56        -0.49854   50% [ 3,-3 ]

Excited State  33:   Singlet-A       54.59725 1000/cm  183.16 nm  f=0.0000
     50 -> 56         0.48456   47% [ 4,-3 ]
     51 -> 57        -0.51039   52% [ 3,-4 ]

Excited State  34:   Singlet-B1      55.05054 1000/cm  181.65 nm  f=0.0001
     50 -> 60         0.45942   42% [ 4,-7 ]
     51 -> 59         0.52248   55% [ 3,-6 ]

Excited State  35:   Singlet-A       55.05295 1000/cm  181.64 nm  f=0.0000
     50 -> 59         0.52168   54% [ 4,-6 ]
     51 -> 60         0.45919   42% [ 3,-7 ]

Excited State  36:   Singlet-B3      55.83048 1000/cm  179.11 nm  f=0.0009
     52 -> 59        -0.25598   13% [ 2,-6 ]
     52 -> 61         0.56901   65% [ 2,-8 ]
     52 -> 67         0.15191
     53 -> 65        -0.22940   11% [ 1,-12 ]

Excited State  37:   Singlet-A       56.22811 1000/cm  177.85 nm  f=0.0000
     52 -> 63         0.24188   12% [ 2,-10 ]
     53 -> 66         0.63897   82% [ 1,-13 ]

Excited State  38:   Singlet-B1      56.26521 1000/cm  177.73 nm  f=0.0003
     52 -> 62         0.59834   72% [ 2,-9 ]
     52 -> 66         0.15030
     53 -> 68         0.23075   11% [ 1,-15 ]

Excited State  39:   Singlet-B2      56.51201 1000/cm  176.95 nm  f=0.0004
     52 -> 65        -0.15392
     53 -> 61        -0.10236
     53 -> 67         0.66618   89% [ 1,-14 ]

Excited State  40:   Singlet-B1      56.65639 1000/cm  176.50 nm  f=0.0336
     49 -> 58         0.13342
     52 -> 62        -0.28738   17% [ 2,-9 ]
     53 -> 63        -0.10718
     53 -> 64         0.15669
     53 -> 68         0.52265   55% [ 1,-15 ]
     53 -> 70        -0.18167

Orbital symmetries:
      Occupied  (A) (B1) (A) (B1) (A) (B1) (B3) (B2) (B1) (A)
                (A) (B1) (B2) (B3) (A) (B1) (A) (B1) (A) (B1)
                (A) (B3) (B2) (B1) (A) (B1) (B2) (B3) (A) (B1)
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                (B1) (B3) (B2)
      Virtual   (B3) (B2) (A) (B1) (B2) (A) (B1) (A) (B2) (B3)
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                (B3) (B1) (A) (B1) (A) (B1)
 The electronic state is 1-A.
 Alpha  occ. eigenvalues --  -10.27800 -10.27800 -10.26203 -10.26146 -10.25906
 Alpha  occ. eigenvalues --  -10.25891 -10.25752 -10.25752 -10.25751 -10.25751
 Alpha  occ. eigenvalues --  -10.25567 -10.25567 -10.25443 -10.25443 -10.25429
 Alpha  occ. eigenvalues --  -10.25429  -0.90256  -0.90216  -0.83478  -0.81678
 Alpha  occ. eigenvalues --   -0.78875  -0.78490  -0.78490  -0.74613  -0.67343
 Alpha  occ. eigenvalues --   -0.64785  -0.63874  -0.63871  -0.60736  -0.56533
 Alpha  occ. eigenvalues --   -0.55548  -0.50719  -0.50328  -0.48330  -0.48282
 Alpha  occ. eigenvalues --   -0.45984  -0.45840  -0.44780  -0.44778  -0.40998
 Alpha  occ. eigenvalues --   -0.40603  -0.38133  -0.38065  -0.37536  -0.37204
 Alpha  occ. eigenvalues --   -0.36281  -0.35518  -0.31614  -0.28935  -0.27815
 Alpha  occ. eigenvalues --   -0.27814  -0.25065  -0.22887
 Alpha virt. eigenvalues --   -0.06388  -0.03777  -0.01551  -0.01550   0.00600
 Alpha virt. eigenvalues --    0.01053   0.01404   0.03103   0.03197   0.03366
 Alpha virt. eigenvalues --    0.04256   0.04307   0.05426   0.05512   0.05984
 Alpha virt. eigenvalues --    0.06352   0.06449   0.07098   0.07806   0.08026
 Alpha virt. eigenvalues --    0.08635   0.09108   0.09805   0.09859   0.09968
 Alpha virt. eigenvalues --    0.10605   0.11579   0.12049   0.12473   0.13923
 Alpha virt. eigenvalues --    0.14357   0.14398   0.14470   0.15209   0.15590
 Alpha virt. eigenvalues --    0.15743   0.15818   0.15998   0.16116   0.16439
 Alpha virt. eigenvalues --    0.16678   0.16880   0.17757   0.17788   0.18051
 Alpha virt. eigenvalues --    0.18165   0.19759   0.19930   0.21163   0.21568
 Alpha virt. eigenvalues --    0.21617   0.21712   0.21919   0.22210   0.22283
 Alpha virt. eigenvalues --    0.22808   0.23555   0.23579   0.24168   0.24560
 Alpha virt. eigenvalues --    0.24959   0.24969   0.25520   0.26158   0.26430
 Alpha virt. eigenvalues --    0.27063   0.27628   0.27714   0.28437   0.29447
 Alpha virt. eigenvalues --    0.29509   0.29793   0.30177   0.30993   0.32684
 Alpha virt. eigenvalues --    0.33511   0.33925   0.33986   0.34929   0.35416
 Alpha virt. eigenvalues --    0.35914   0.36187   0.36527   0.36952   0.39889
 Alpha virt. eigenvalues --    0.43511   0.45506   0.46477   0.48243   0.50856
 Alpha virt. eigenvalues --    0.57401   0.57804   0.61220   0.61265   0.64296
 Alpha virt. eigenvalues --    0.65495   0.67509   0.68232   0.70218   0.70365
 Alpha virt. eigenvalues --    0.71263   0.71365   0.72547   0.72855   0.72862
 Alpha virt. eigenvalues --    0.73450   0.73484   0.74835   0.75043   0.75292
 Alpha virt. eigenvalues --    0.76034   0.76055   0.76418   0.77002   0.77360
 Alpha virt. eigenvalues --    0.79061   0.79068   0.80221   0.81160   0.81959
 Alpha virt. eigenvalues --    0.82196   0.84051   0.84638   0.86035   0.86835
 Alpha virt. eigenvalues --    0.86903   0.88211   0.90341   0.92972   0.93350
 Alpha virt. eigenvalues --    0.93481   0.95623   0.95913   0.97679   0.97819
 Alpha virt. eigenvalues --    0.98856   0.99006   1.01688   1.01979   1.02164
 Alpha virt. eigenvalues --    1.04045   1.04121   1.09417   1.09445   1.11090
```

```
Alpha virt. eigenvalues --    1.12762   1.13142   1.15018   1.15726   1.16627
Alpha virt. eigenvalues --    1.19808   1.19931   1.21162   1.21597   1.23852
Alpha virt. eigenvalues --    1.23852   1.25259   1.27704   1.27908   1.30433
Alpha virt. eigenvalues --    1.31949   1.33969   1.34261   1.36631   1.43325
Alpha virt. eigenvalues --    1.43760   1.43881   1.44738   1.44745   1.45335
Alpha virt. eigenvalues --    1.45450   1.47727   1.48268   1.48686   1.49541
Alpha virt. eigenvalues --    1.49585   1.49640   1.50263   1.50281   1.60910
Alpha virt. eigenvalues --    1.61007   1.62793   1.64021   1.67283   1.82364
Alpha virt. eigenvalues --    1.83212   1.85493   1.85976   1.86128   1.90236
Alpha virt. eigenvalues --    1.90344   1.90433   1.92671   1.92865   1.94901
Alpha virt. eigenvalues --    1.96781   1.99156   2.00235   2.00699   2.01842
Alpha virt. eigenvalues --    2.03295   2.06860   2.08174   2.08838   2.13388
Alpha virt. eigenvalues --    2.15121   2.15459   2.15463   2.17505   2.17644
Alpha virt. eigenvalues --    2.18770   2.20548   2.21308   2.21567   2.28318
Alpha virt. eigenvalues --    2.30505   2.30505   2.31227   2.31382   2.32594
Alpha virt. eigenvalues --    2.38814   2.43986   2.51639   2.54275   2.59165
Alpha virt. eigenvalues --    2.59457   2.60753   2.63138   2.63977   2.65206
Alpha virt. eigenvalues --    2.65212   2.65260   2.73103   2.76302   2.76323
Alpha virt. eigenvalues --    2.76385   2.77573   2.77742   2.81583   2.86200
Alpha virt. eigenvalues --    2.88081   2.98958   3.03653   3.08749   3.24271
Alpha virt. eigenvalues --    3.33041   3.34172   3.41812   3.51391   3.75089
Alpha virt. eigenvalues --    4.22958   4.27193   4.27677   4.27774   4.28725
Alpha virt. eigenvalues --    4.29495   4.31940   4.39618   4.42254   4.43865
Alpha virt. eigenvalues --    4.44029   4.58599   4.64041   4.81183   4.90466
Alpha virt. eigenvalues --    5.62494

Normal termination of Gaussian 03 at Sat Nov  8 13:25:11 2008.
```

```
*****************************************
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=90 (based on pbe1pbe/6-31G* D2h geo.)
---------------------------------------------------------------------

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

                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6             0        0.000000    0.000000    0.679461
   2          6             0        0.000000    0.000000   -0.679461
   3          6             0        0.000000    0.000000    1.899660
   4          6             0        0.000000    0.000000   -1.899660
   5          6             0        0.000000    0.000000    3.318498
   6          6             0        0.000000    0.000000   -3.318498
   7          6             0        0.000000    1.211722    4.030916
   8          6             0        1.211722    0.000000   -4.030916
   9          6             0        0.000000   -1.211722    4.030916
  10          6             0       -1.211722    0.000000   -4.030916
  11          6             0        0.000000    1.206087    5.419091
  12          6             0        1.206087    0.000000   -5.419091
  13          6             0        0.000000   -1.206087    5.419091
  14          6             0       -1.206087    0.000000   -5.419091
  15          6             0        0.000000    0.000000    6.117221
  16          6             0        0.000000    0.000000   -6.117221
  17          1             0        0.000000    2.148075    3.481442
  18          1             0        2.148075    0.000000   -3.481442
  19          1             0        0.000000   -2.148075    3.481442
  20          1             0       -2.148075    0.000000   -3.481442
  21          1             0        0.000000    2.148474    5.959837
  22          1             0        2.148474    0.000000   -5.959837
  23          1             0        0.000000   -2.148474    5.959837
  24          1             0       -2.148474    0.000000   -5.959837
  25          1             0        0.000000    0.000000    7.203732
  26          1             0        0.000000    0.000000   -7.203732
---------------------------------------------------------------------
  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):
      state          X           Y           Z          Osc.
        1         0.0000      0.0000      0.0000      0.0000
        2         0.0000      0.0000      0.0000      0.0000
        3         0.0000      0.0000      0.0000      0.0000
        4         0.0000      0.0000     -4.3538      2.1837
        5        -0.0144     -0.0427      0.0000      0.0002
        6        -0.0427      0.0144      0.0000      0.0002
        7         0.0417     -0.0201      0.0000      0.0003
        8         0.0201      0.0417      0.0000      0.0003
```

| | | | | |
|---|---|---|---|---|
| 9 | -0.0011 | 0.0028 | 0.0000 | 0.0000 |
| 10 | 0.0028 | 0.0011 | 0.0000 | 0.0000 |
| 11 | 0.4832 | 0.7912 | 0.0000 | 0.1203 |
| 12 | 0.7912 | -0.4832 | 0.0000 | 0.1203 |
| 13 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 14 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 15 | 0.0033 | -0.0039 | 0.0000 | 0.0000 |
| 16 | 0.0039 | 0.0033 | 0.0000 | 0.0000 |
| 17 | 0.0000 | 0.0000 | -0.0001 | 0.0000 |
| 18 | 0.0000 | 0.0000 | 0.0031 | 0.0000 |
| 19 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 20 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 21 | -0.1261 | 0.1740 | 0.0000 | 0.0070 |
| 22 | -0.1740 | -0.1261 | 0.0000 | 0.0070 |
| 23 | 0.0000 | 0.0000 | -0.0001 | 0.0000 |
| 24 | 0.0000 | 0.0000 | -2.9250 | 1.3648 |
| 25 | 0.1291 | -0.0311 | 0.0000 | 0.0028 |
| 26 | 0.0311 | 0.1291 | 0.0000 | 0.0028 |
| 27 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 28 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 29 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 30 | 0.0000 | 0.0000 | -0.0277 | 0.0001 |
| 31 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 32 | 0.0000 | 0.0000 | -0.1508 | 0.0038 |
| 33 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 34 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 35 | 0.0096 | 0.0851 | 0.0000 | 0.0012 |
| 36 | -0.0851 | 0.0096 | 0.0000 | 0.0012 |
| 37 | 0.0000 | 0.0000 | 0.0014 | 0.0000 |
| 38 | 0.3569 | -0.3644 | 0.0000 | 0.0445 |
| 39 | -0.3644 | -0.3569 | 0.0000 | 0.0445 |
| 40 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |

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

| state | X | Y | Z | Osc. |
|---|---|---|---|---|
| 1 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 2 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 3 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 4 | 0.0000 | 0.0000 | 0.7425 | 2.1270 |
| 5 | 0.0019 | 0.0056 | 0.0000 | 0.0001 |
| 6 | 0.0056 | -0.0019 | 0.0000 | 0.0001 |
| 7 | 0.0013 | -0.0006 | 0.0000 | 0.0000 |
| 8 | 0.0006 | 0.0013 | 0.0000 | 0.0000 |
| 9 | 0.0009 | -0.0023 | 0.0000 | 0.0000 |
| 10 | -0.0023 | -0.0009 | 0.0000 | 0.0000 |
| 11 | -0.1036 | -0.1696 | 0.0000 | 0.1254 |
| 12 | -0.1696 | 0.1036 | 0.0000 | 0.1254 |
| 13 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 14 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 15 | -0.0060 | 0.0070 | 0.0000 | 0.0003 |
| 16 | -0.0070 | -0.0060 | 0.0000 | 0.0003 |
| 17 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 18 | 0.0000 | 0.0000 | 0.0068 | 0.0001 |
| 19 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 20 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 21 | 0.0308 | -0.0425 | 0.0000 | 0.0081 |
| 22 | 0.0425 | 0.0308 | 0.0000 | 0.0081 |
| 23 | 0.0000 | 0.0000 | -0.0001 | 0.0000 |
| 24 | 0.0000 | 0.0000 | 0.6907 | 1.3290 |
| 25 | -0.0301 | 0.0073 | 0.0000 | 0.0027 |
| 26 | -0.0073 | -0.0301 | 0.0000 | 0.0027 |
| 27 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 28 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 29 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 30 | 0.0000 | 0.0000 | 0.0067 | 0.0001 |
| 31 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |

| | | | | |
|---|---|---|---|---|
| 32 | 0.0000 | 0.0000 | 0.0361 | 0.0035 |
| 33 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 34 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 35 | -0.0020 | -0.0177 | 0.0000 | 0.0008 |
| 36 | 0.0177 | -0.0020 | 0.0000 | 0.0008 |
| 37 | 0.0000 | 0.0000 | -0.0004 | 0.0000 |
| 38 | -0.0917 | 0.0936 | 0.0000 | 0.0446 |
| 39 | 0.0936 | 0.0917 | 0.0000 | 0.0446 |
| 40 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |

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 -> 54        -0.43420   38% [ 1,-1 ]

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
```

```
     52 -> 56         0.44534   40% [ 2,-3 ]
     52 -> 57        -0.44440   39% [ 2,-4 ]
     53 -> 56         0.21529
     53 -> 57         0.21483

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
```

```
     53 -> 58         0.39060   31% [ 1,-5 ]
     53 -> 59        -0.20061
     53 -> 62         0.10059

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
```

```
Excited State  27:   Singlet-[B1]     53.06561 1000/cm  188.45 nm  f=0.0000
     52 -> 63         0.48748   48% [ 2,-10 ]
     53 -> 64        -0.48748   48% [ 1,-11 ]

Excited State  28:   Singlet-[A2]     53.08739 1000/cm  188.37 nm  f=0.0000
     52 -> 63         0.48833   48% [ 2,-10 ]
     53 -> 64         0.48833   48% [ 1,-11 ]

Excited State  29:   Singlet-A1      54.59967 1000/cm  183.15 nm  f=0.0000
     50 -> 56         0.50408   51% [ 4,-3 ]
     51 -> 57        -0.49596   49% [ 3,-4 ]

Excited State  30:   Singlet-B2      54.59967 1000/cm  183.15 nm  f=0.0001
     50 -> 57         0.50244   50% [ 4,-4 ]
     51 -> 56        -0.49709   49% [ 3,-3 ]

Excited State  31:   Singlet-[A1]     54.68517 1000/cm  182.87 nm  f=0.0000
     52 -> 64         0.47705   46% [ 2,-11 ]
     52 -> 68         0.12847
     53 -> 63         0.47706   46% [ 1,-10 ]
     53 -> 67         0.12843

Excited State  32:   Singlet-[B2]     54.72146 1000/cm  182.74 nm  f=0.0038
     52 -> 64        -0.47114   44% [ 2,-11 ]
     52 -> 68        -0.12217
     53 -> 63         0.47113   44% [ 1,-10 ]
     53 -> 67         0.12220

Excited State  33:   Singlet-[B2]    55.00376 1000/cm  181.80 nm  f=0.0000
     50 -> 59         0.47221   45% [ 4,-6 ]
     51 -> 58         0.51096   52% [ 3,-5 ]

Excited State  34:   Singlet-B1      55.00618 1000/cm  181.80 nm  f=0.0000
     50 -> 58         0.51088   52% [ 4,-5 ]
     51 -> 59         0.47221   45% [ 3,-6 ]

Excited State  35:   Singlet-E       55.72885 1000/cm  179.44 nm  f=0.0012
     48 -> 56        -0.11275
     48 -> 57        -0.11142
     53 -> 59         0.10372
     53 -> 62        -0.12010
     53 -> 65         0.62223   77% [ 1,-12 ]
     53 -> 66        -0.17062

Excited State  36:   Singlet-E       55.72885 1000/cm  179.44 nm  f=0.0012
     49 -> 56         0.11275
     49 -> 57        -0.11142
     52 -> 59         0.10372
     52 -> 62         0.12010
     52 -> 65         0.62223   77% [ 2,-12 ]
     52 -> 66         0.17061

Excited State  37:   Singlet-A1      56.2886 1000/cm  177.65 nm  f=0.0000
     48 -> 55        -0.14239
     49 -> 54        -0.14229
     50 -> 56         0.36149   26% [ 4,-3 ]
     51 -> 57         0.37446   28% [ 3,-4 ]
     52 -> 61        -0.13518
     53 -> 60        -0.13490

Excited State  38:   Singlet-E       56.29021 1000/cm  177.65 nm  f=0.0445
     48 -> 56         0.28082   16% [ 6,-3 ]
     48 -> 57         0.27406   15% [ 6,-4 ]
     49 -> 56        -0.27508   15% [ 5,-3 ]
```

```
     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

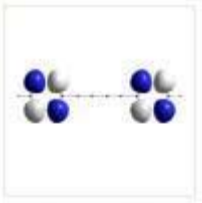
Excited State  40:   Singlet-[A2]     56.91932 1000/cm  175.69 nm  f=0.0000
     46 -> 54         0.45203   41% [ 8,-1 ]
     47 -> 55        -0.45213   41% [ 7,-2 ]
     48 -> 54        -0.10242
     49 -> 55         0.10243

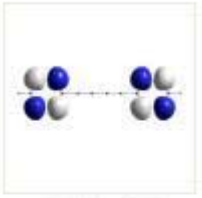
Orbital symmetries:
      Occupied  (B2) (A1) (A1) (B2) (A1) (B2) (E) (E) (B2) (A1)
                (B2) (A1) (E) (E) (B2) (A1) (A1) (B2) (A1) (B2)
                (A1) (E) (E) (B2) (A1) (B2) (E) (E) (A1) (B2)
                (A1) (B2) (A1) (E) (E) (B2) (A1) (E) (E) (E) (E)
                (B2) (A1) (E) (E) (E) (E) (E) (E) (B1) (A2) (E)
                (E)
      Virtual   (E) (E) (B1) (A2) (A1) (B2) (E) (E) (A1) (E) (E)
                (B2) (A1) (E) (E) (E) (E) (B2) (B2) (A1) (E) (E)
                (B1) (A2) (A1) (E) (E) (B2) (E) (E) (B1) (B2)
                (E) (E) (A2) (A1) (E) (E) (A1) (E) (E) (B2) (E)
                (E) (A1) (E) (E) (B2) (B2) (E) (E) (A1) (B2) (A1)
                (B2) (E) (E) (E) (E) (A1) (E) (E) (B2) (A1) (E)
                (E) (B2) (A1) (E) (E) (A1) (E) (E) (B2) (B2) (A1)
                (A1) (B2) (E) (E) (B2) (E) (E) (A1) (E) (E) (E)
                (E) (B2) (A1) (B2) (E) (E) (B2) (A1) (A1) (B2)
                (E) (E) (A1) (E) (E) (E) (E) (B1) (A2) (A1) (B2)
                (E) (E) (B1) (E) (E) (A2) (B2) (A1) (E) (E) (E)
                (E) (B2) (A1) (E) (E) (B2) (A1) (E) (E) (E) (E)
                (B2) (A1) (E) (E) (E) (E) (B2) (A1) (B2) (A1)
                (E) (E) (E) (E) (E) (E) (B2) (A1) (A1) (B2) (A1)
                (E) (E) (A1) (B2) (B1) (A2) (B2) (B2) (E) (E)
                (A1) (A1) (B2) (E) (E) (B2) (E) (E) (B1) (A1)
                (A2) (E) (E) (E) (E) (B1) (B2) (A2) (B1) (A2)
                (A1) (E) (E) (B2) (A1) (B1) (E) (E) (B2) (E) (E)
                (B2) (A1) (B2) (A1) (B2) (A1) (E) (E) (A2) (A1)
                (E) (E) (B2) (A1) (B1) (A2) (E) (E) (A1) (B2)
                (E) (E) (B2) (E) (E) (B1) (A2) (E) (E) (A1) (E)
                (E) (A1) (B2) (B2) (A1) (E) (E) (B1) (A2) (B2)
                (A1) (A1) (E) (E) (B2) (B2) (E) (E) (A1) (E) (E)
                (B2) (E) (E) (A1) (B2) (A1) (B2) (A1) (B2) (A1)
                (E) (E) (A1) (B2) (B2) (A1) (E) (E) (B2) (A1)
                (B2) (A1) (B2)
The electronic state is 1-A1.
Alpha  occ. eigenvalues --  -10.27787 -10.27787 -10.26179 -10.26122 -10.25883
Alpha  occ. eigenvalues --  -10.25868 -10.25750 -10.25750 -10.25749 -10.25749
Alpha  occ. eigenvalues --  -10.25570 -10.25569 -10.25440 -10.25440 -10.25426
Alpha  occ. eigenvalues --  -10.25426  -0.90251  -0.90212  -0.83464  -0.81671
Alpha  occ. eigenvalues --   -0.78866  -0.78488  -0.78488  -0.74597  -0.67337
```

```
 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  occ. eigenvalues --   -0.27812  -0.23768  -0.23768
 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   0.05510   0.05671   0.05671
 Alpha virt. eigenvalues --    0.06411   0.06411   0.06970   0.07853   0.07916
 Alpha virt. eigenvalues --    0.08814   0.08814   0.09802   0.09923   0.10006
 Alpha virt. eigenvalues --    0.11082   0.11082   0.11841   0.12958   0.12958
 Alpha virt. eigenvalues --    0.14448   0.14537   0.14790   0.14790   0.15268
 Alpha virt. eigenvalues --    0.15788   0.16042   0.16042   0.16097   0.16481
 Alpha virt. eigenvalues --    0.16481   0.17213   0.17358   0.17358   0.18099
 Alpha virt. eigenvalues --    0.19245   0.19245   0.19339   0.20687   0.21577
 Alpha virt. eigenvalues --    0.21577   0.21915   0.22387   0.22768   0.22817
 Alpha virt. eigenvalues --    0.23183   0.23183   0.23863   0.23863   0.23868
 Alpha virt. eigenvalues --    0.24699   0.24699   0.24750   0.26219   0.26730
 Alpha virt. eigenvalues --    0.26730   0.27216   0.27701   0.28583   0.28583
 Alpha virt. eigenvalues --    0.29810   0.29860   0.29860   0.30406   0.31453
 Alpha virt. eigenvalues --    0.33016   0.33925   0.34059   0.34620   0.34620
 Alpha virt. eigenvalues --    0.35759   0.36256   0.36256   0.36689   0.41622
 Alpha virt. eigenvalues --    0.41622   0.45426   0.45426   0.46327   0.51019
 Alpha virt. eigenvalues --    0.55017   0.57532   0.57532   0.61242   0.61262
 Alpha virt. eigenvalues --    0.64356   0.65484   0.68076   0.68076   0.71090
 Alpha virt. eigenvalues --    0.71259   0.71259   0.71566   0.71566   0.72801
 Alpha virt. eigenvalues --    0.72913   0.73771   0.74007   0.74887   0.74887
 Alpha virt. eigenvalues --    0.75770   0.75866   0.75866   0.76187   0.77038
 Alpha virt. eigenvalues --    0.77354   0.78993   0.78993   0.80586   0.80586
 Alpha virt. eigenvalues --    0.81924   0.82385   0.84283   0.84283   0.86818
 Alpha virt. eigenvalues --    0.86952   0.87198   0.87198   0.92180   0.92180
 Alpha virt. eigenvalues --    0.92958   0.93370   0.95738   0.95738   0.97669
 Alpha virt. eigenvalues --    0.97669   0.98921   1.00379   1.02181   1.02197
 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   2.30629   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   2.76530
 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 --    3.30257   3.30257   3.33061   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

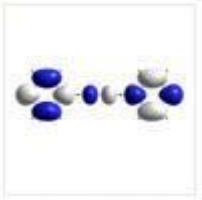
 Normal termination of Gaussian 03 at Sat Nov  8 16:35:02 2008.
```

DPDA, $D_{2h}$ ($\Phi = 0°$)
PBE1PBE/6-31+G* MO energies (eV)

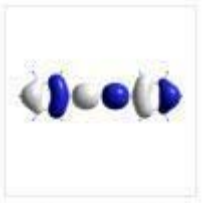
(-5) 2 $a_u$ –0.42 

(-4) 2 $b_{1g}$ –0.42 

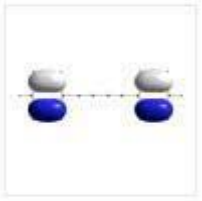
(-3) 9 $b_{2u}$ –0.44 

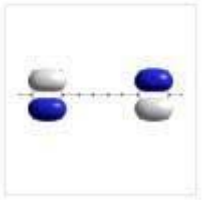
(-2) 4 $b_{2g}$ –0.48 

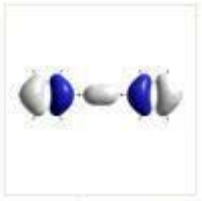
(-1) 4 $b_{3u}$ –1.83 [LUMO] 

(1) 3 $b_{2g}$ –6.14 [HOMO] 

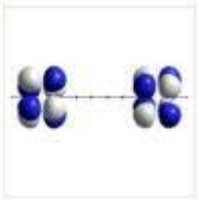
(2) 8 $b_{3g}$ –7.09 

(3) 1 $b_{1g}$ –7.57 

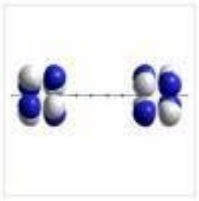
(4) 1 $a_u$ –7.57 

(5) 3 $b_{3u}$ –7.60 

DPDA, $D_2$ ($\Phi = 45°$)
PBE1PBE/6-31+G* MO energies (eV)

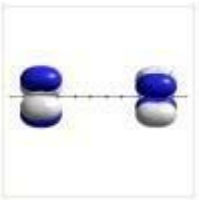
(-4) 16 $b_1$ –0.42 

(1) 11 $b_2$ –6.23 [HOMO] 

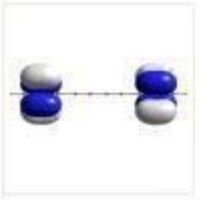
(-3) 17 $a$ –0.42 

(2) 11 $b_3$ –6.82 

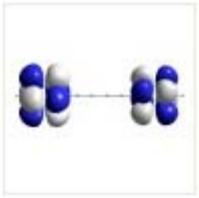
(-2) 12 $b_2$ –1.03 

(3) 15 $b_1$ –7.57 

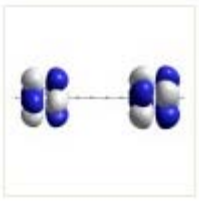
(-1) 12 $b_3$ –1.74 [LUMO] 

(4) 16 $a$ –7.57 

DPDA, $D_{2d}$ ($\Phi = 90°$)
PBE1PBE/6-31+G* MO energies (eV)

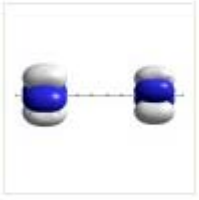
(-4) 2 $b_1$ –0.42 

(1) 11 $e$ –6.47 [HOMO] 

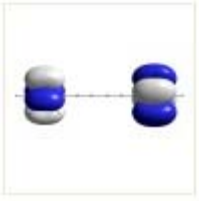
(-3) 2 $a_2$ –0.42 

(2) 11 $e$ –6.47 [HOMO] 

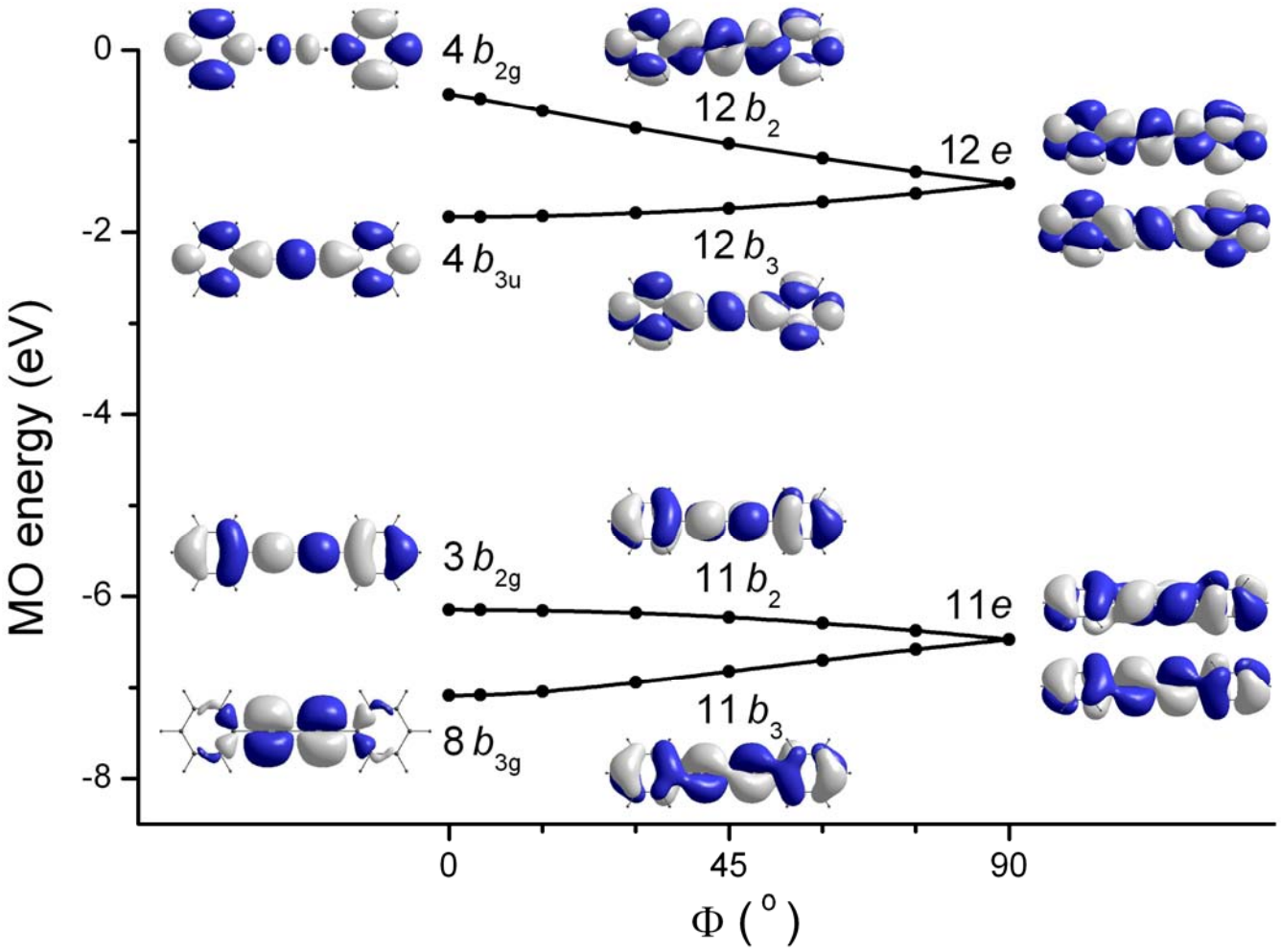
(-2) 12 $e$ –1.46 [LUMO] 

(3) 1 $b_1$ –7.57 

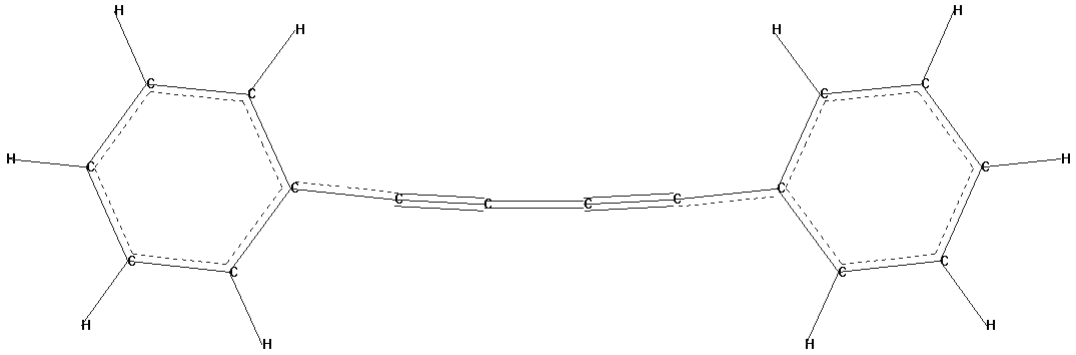
(-1) 12 $e$ –1.46 [LUMO] 

(4) 1 $a_2$ –7.57 

Frontier MO energies as a function of dihedral angle Φ



```
*****************************************
 Gaussian 03:  x86-Linux-G03RevB.04 2-Jun-2003
               11-Apr-2011
 *****************************************
 ----------------------------
 #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:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        0.000000   -0.679401   -0.289764
      2          6           0        0.000000    0.679401   -0.289764
      3          6           0        0.000000   -1.897728   -0.225917
      4          6           0        0.000000    1.897728   -0.225917
      5          6           0        0.000000   -3.308756   -0.077610
      6          6           0        0.000000    3.308756   -0.077610
      7          6           0        0.000000   -3.890554    1.201820
      8          6           0        0.000000    4.143853   -1.208097
      9          6           0        0.000000   -4.143853   -1.208097
     10          6           0        0.000000    3.890554    1.201820
     11          6           0        0.000000   -5.271627    1.341309
     12          6           0        0.000000    5.523747   -1.057391
     13          6           0        0.000000   -5.523747   -1.057391
     14          6           0        0.000000    5.271627    1.341309
     15          6           0        0.000000   -6.091906    0.214940
     16          6           0        0.000000    6.091906    0.214940
     17          1           0        0.000000   -3.246255    2.075551
     18          1           0        0.000000    3.695338   -2.196604
     19          1           0        0.000000   -3.695338   -2.196604
     20          1           0        0.000000    3.246255    2.075551
     21          1           0        0.000000   -5.710899    2.335052
     22          1           0        0.000000    6.160035   -1.938084
     23          1           0        0.000000   -6.160035   -1.938084
     24          1           0        0.000000    5.710899    2.335052
     25          1           0        0.000000   -7.172453    0.328512
     26          1           0        0.000000    7.172453    0.328512
 ---------------------------------------------------------------------
   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):
```

| state | X | Y | Z | Dip. S. | Osc. |
|---|---|---|---|---|---|
| 1 | 0.0000 | 3.2012 | 0.0000 | 10.2477 | 0.9253 |
| 2 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 3 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 4 | 0.0000 | -0.0001 | 0.0000 | 0.0000 | 0.0000 |
| 5 | 0.0000 | 0.0000 | 0.0452 | 0.0020 | 0.0002 |
| 6 | 0.0000 | 0.0000 | -0.0255 | 0.0007 | 0.0001 |
| 7 | 0.0000 | 0.0975 | 0.0000 | 0.0095 | 0.0012 |
| 8 | 0.0000 | 0.0000 | 0.9657 | 0.9325 | 0.1216 |
| 9 | 0.0000 | 0.0000 | 0.1602 | 0.0257 | 0.0034 |
| 10 | -0.0070 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 11 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 12 | 0.0000 | 3.0672 | 0.0000 | 9.4075 | 1.3085 |
| 13 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 14 | 0.0979 | 0.0000 | 0.0000 | 0.0096 | 0.0014 |
| 15 | 0.1548 | 0.0000 | 0.0000 | 0.0240 | 0.0034 |
| 16 | 0.0232 | 0.0000 | 0.0000 | 0.0005 | 0.0001 |
| 17 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 18 | 0.0000 | 0.0000 | 0.0833 | 0.0069 | 0.0011 |
| 19 | 0.0000 | -0.0042 | 0.0000 | 0.0000 | 0.0000 |
| 20 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 21 | -0.0036 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 22 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 23 | 0.0000 | 1.0687 | 0.0000 | 1.1421 | 0.1758 |
| 24 | 0.0183 | 0.0000 | 0.0000 | 0.0003 | 0.0001 |
| 25 | 0.0000 | 1.5935 | 0.0000 | 2.5392 | 0.3990 |
| 26 | 0.0000 | 0.0045 | 0.0000 | 0.0000 | 0.0000 |
| 27 | -0.0006 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 28 | 0.1716 | 0.0000 | 0.0000 | 0.0295 | 0.0048 |
| 29 | 0.0000 | -2.7458 | 0.0000 | 7.5395 | 1.2366 |
| 30 | 0.0000 | 0.0000 | -0.2090 | 0.0437 | 0.0072 |
| 31 | 0.0000 | 0.0656 | 0.0000 | 0.0043 | 0.0007 |
| 32 | 0.0000 | 0.0000 | -0.0225 | 0.0005 | 0.0001 |
| 33 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 34 | 0.0028 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 35 | 0.0000 | 0.0000 | -0.7921 | 0.6273 | 0.1049 |
| 36 | 0.0000 | 0.2321 | 0.0000 | 0.0539 | 0.0091 |
| 37 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 38 | 0.0000 | 0.0000 | 1.3735 | 1.8864 | 0.3186 |
| 39 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 40 | 0.0000 | 0.4135 | 0.0000 | 0.1709 | 0.0293 |

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 ]
```

```
Excited State   5:      Singlet-A1   38.06774 1000/cm   f=0.0002
     49 -> 57        -0.13591
     50 -> 55         0.13764
     51 -> 54         0.45780   42% [ 3,-1 ]
     53 -> 58         0.50015   50% [ 1,-5 ]

Excited State   6:      Singlet-A1   40.11316 1000/cm   f=0.0001
     49 -> 54         0.42050   35% [ 5,-1 ]
     53 -> 55         0.56252   63% [ 1,-2 ]

Excited State   7:      Singlet-B2   42.85544 1000/cm   f=0.0012
     50 -> 54         0.50801   52% [ 4,-1 ]
     53 -> 57        -0.47562   45% [ 1,-4 ]

Excited State   8:      Singlet-A1   42.92884 1000/cm   f=0.1216
     51 -> 54         0.50569   51% [ 3,-1 ]
     53 -> 58        -0.47695   45% [ 1,-5 ]

Excited State   9:      Singlet-A1   43.67168 1000/cm   f=0.0034
     49 -> 54         0.53712   58% [ 5,-1 ]
     50 -> 58         0.13758
     51 -> 57         0.13830
     53 -> 55        -0.39481   31% [ 1,-2 ]

Excited State  10:      Singlet-B1   44.35483 1000/cm   f=0.0000
     47 -> 54        -0.15058
     52 -> 55         0.68459   94% [ 2,-2 ]

Excited State  11:      Singlet-A2   45.35899 1000/cm   f=0.0000
     53 -> 59         0.67556   91% [ 1,-6 ]
     53 -> 61         0.15264

Excited State  12:      Singlet-B2   45.7905 1000/cm    f=1.3085
     48 -> 54        -0.36935   27% [ 6,-1 ]
     52 -> 56         0.50763   52% [ 2,-3 ]
     53 -> 54         0.20020
     53 -> 65         0.20044

Excited State  13:      Singlet-A2   46.80514 1000/cm   f=0.0000
     52 -> 57         0.70337   99% [ 2,-4 ]

Excited State  14:      Singlet-B1   46.84788 1000/cm   f=0.0014
     52 -> 58         0.69949   98% [ 2,-5 ]

Excited State  15:      Singlet-B1   47.03178 1000/cm   f=0.0034
     49 -> 59        -0.11541
     53 -> 60         0.68504   94% [ 1,-7 ]

Excited State  16:      Singlet-B1   48.07949 1000/cm   f=0.0001
     46 -> 56        -0.12653
     49 -> 56         0.68526   94% [ 5,-3 ]

Excited State  17:      Singlet-A2   49.97893 1000/cm   f=0.0000
     53 -> 59        -0.16899
     53 -> 61         0.63252   80% [ 1,-8 ]
     53 -> 62         0.20634

Excited State  18:      Singlet-A1   50.12169 1000/cm   f=0.0011
     48 -> 58        -0.13347
     49 -> 57        -0.41884   35% [ 5,-4 ]
     50 -> 55         0.50664   51% [ 4,-2 ]
     51 -> 54        -0.15717
     53 -> 58        -0.12316

Excited State  19:      Singlet-B2   50.12975 1000/cm   f=0.0000
```

```
     48 -> 57        -0.13388
     49 -> 58        -0.41567   35% [ 5,-5 ]
     50 -> 54        -0.15752
     51 -> 55         0.50685   51% [ 3,-2 ]
     53 -> 57        -0.12269

Excited State  20:      Singlet-A2   50.49754 1000/cm   f=0.0000
     50 -> 56         0.67938   92% [ 4,-3 ]
     53 -> 61        -0.10003
     53 -> 62         0.15538

Excited State  21:      Singlet-B1   50.49916 1000/cm   f=0.0000
     51 -> 56         0.70409   99% [ 3,-3 ]

Excited State  22:      Singlet-A2   50.61772 1000/cm   f=0.0000
     50 -> 56        -0.18411
     53 -> 61        -0.20663
     53 -> 62         0.63192   80% [ 1,-9 ]
     53 -> 66         0.11469

Excited State  23:      Singlet-B2   50.68466 1000/cm   f=0.1758
     48 -> 54         0.51435   53% [ 6,-1 ]
     50 -> 57         0.10348
     51 -> 58         0.10290
     52 -> 56         0.19144
     53 -> 65         0.38954   30% [ 1,-12 ]
     53 -> 69        -0.11319

Excited State  24:      Singlet-B1   51.67914 1000/cm   f=0.0001
     53 -> 63         0.69322   96% [ 1,-10 ]

Excited State  25:      Singlet-B2   51.73318 1000/cm   f=0.3990
     49 -> 55         0.47784   46% [ 5,-2 ]
     50 -> 57         0.34923   24% [ 4,-4 ]
     51 -> 58         0.34309   24% [ 3,-5 ]

Excited State  26:      Singlet-B2   52.39859 1000/cm   f=0.0000
     52 -> 59         0.62675   79% [ 2,-6 ]
     52 -> 61         0.25273   13% [ 2,-8 ]
     52 -> 62         0.14434

Excited State  27:      Singlet-B1   52.55586 1000/cm   f=0.0000
     44 -> 54         0.10275
     47 -> 54         0.66862   89% [ 7,-1 ]
     52 -> 55         0.15379

Excited State  28:      Singlet-B1   53.38743 1000/cm   f=0.0048
     49 -> 61         0.10640
     53 -> 64         0.68139   93% [ 1,-11 ]

Excited State  29:      Singlet-B2   53.99718 1000/cm   f=1.2366
     49 -> 55         0.43981   39% [ 5,-2 ]
     50 -> 57        -0.24881   12% [ 4,-4 ]
     51 -> 58        -0.22885   10% [ 3,-5 ]
     52 -> 56        -0.14827
     53 -> 65         0.38321   29% [ 1,-12 ]
     53 -> 69         0.10123

Excited State  30:      Singlet-A1   54.26092 1000/cm   f=0.0072
     46 -> 54         0.24592   12% [ 8,-1 ]
     47 -> 56         0.12750
     48 -> 55         0.15735
     49 -> 54        -0.10885
     50 -> 58         0.39084   31% [ 4,-5 ]
     51 -> 57         0.45549   41% [ 3,-4 ]
```

```
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 -> 59         0.51534   53% [ 4,-6 ]
     51 -> 60         0.44431   39% [ 3,-7 ]
     53 -> 66         0.14498

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   55.4272 1000/cm    f=0.0091
     49 -> 58         0.53253   57% [ 5,-5 ]
     51 -> 55         0.42609   36% [ 3,-2 ]
     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

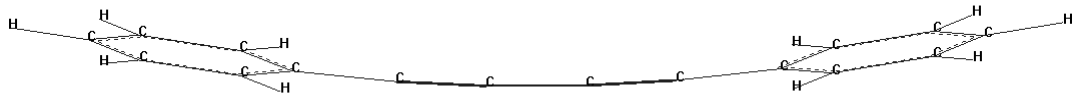
Excited State  38:      Singlet-A1   55.60787 1000/cm   f=0.3186
     49 -> 57         0.43602   38% [ 5,-4 ]
     50 -> 55         0.34572   24% [ 4,-2 ]
     52 -> 60         0.41114   34% [ 2,-7 ]

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
 ------------------------------------------------------
```



Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | -0.679450 | 0.348572 |
| 2 | 6 | 0 | 0.000000 | 0.679450 | 0.348572 |
| 3 | 6 | 0 | 0.000000 | -1.897877 | 0.284716 |
| 4 | 6 | 0 | 0.000000 | 1.897877 | 0.284716 |
| 5 | 6 | 0 | 0.000000 | -3.308904 | 0.136408 |
| 6 | 6 | 0 | 0.000000 | 3.308904 | 0.136408 |
| 7 | 6 | 0 | 1.211691 | -4.012549 | 0.024997 |
| 8 | 6 | 0 | -1.211691 | 4.012549 | 0.024997 |
| 9 | 6 | 0 | -1.211692 | -4.012518 | 0.024927 |
| 10 | 6 | 0 | 1.211692 | 4.012518 | 0.024927 |
| 11 | 6 | 0 | 1.206042 | -5.383548 | -0.192152 |
| 12 | 6 | 0 | -1.206042 | 5.383548 | -0.192152 |
| 13 | 6 | 0 | -1.206066 | -5.383515 | -0.192222 |
| 14 | 6 | 0 | 1.206066 | 5.383515 | -0.192222 |
| 15 | 6 | 0 | 0.000000 | -6.073033 | -0.301395 |
| 16 | 6 | 0 | 0.000000 | 6.073033 | -0.301395 |
| 17 | 1 | 0 | 2.147989 | -3.469889 | 0.110975 |
| 18 | 1 | 0 | -2.147989 | 3.469889 | 0.110975 |
| 19 | 1 | 0 | -2.147980 | -3.469832 | 0.110854 |
| 20 | 1 | 0 | 2.147980 | 3.469832 | 0.110854 |
| 21 | 1 | 0 | 2.148417 | -5.917645 | -0.276719 |
| 22 | 1 | 0 | -2.148417 | 5.917645 | -0.276719 |
| 23 | 1 | 0 | -2.148451 | -5.917588 | -0.276841 |
| 24 | 1 | 0 | 2.148451 | 5.917588 | -0.276841 |
| 25 | 1 | 0 | 0.000000 | -7.146156 | -0.471367 |
| 26 | 1 | 0 | 0.000000 | 7.146156 | -0.471367 |

```
  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):

| state | X | Y | Z | Dip. S. | Osc. |
|---|---|---|---|---|---|
| 1 | 0.0000 | 3.1983 | 0.0000 | 10.2293 | 0.9229 |
| 2 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 3 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 4 | -0.0437 | 0.0000 | 0.0000 | 0.0019 | 0.0002 |
| 5 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 6 | 0.0000 | 0.0000 | 0.0360 | 0.0013 | 0.0002 |
| 7 | 0.0000 | 0.0000 | -0.0001 | 0.0000 | 0.0000 |

| | | | | | |
|---|---|---|---|---|---|
| 8 | -0.9659 | 0.0002 | 0.0000 | 0.9330 | 0.1216 |
| 9 | 0.0000 | 0.0000 | -0.2522 | 0.0636 | 0.0084 |
| 10 | 0.0203 | -0.0006 | 0.0000 | 0.0004 | 0.0001 |
| 11 | 0.0000 | 0.1778 | 0.0000 | 0.0316 | 0.0044 |
| 12 | 0.0001 | 3.0300 | 0.0000 | 9.1806 | 1.2769 |
| 13 | 0.0000 | 0.2766 | 0.0000 | 0.0765 | 0.0109 |
| 14 | 0.0000 | 0.0000 | -0.1093 | 0.0120 | 0.0017 |
| 15 | 0.0000 | 0.0000 | 0.1479 | 0.0219 | 0.0031 |
| 16 | 0.0288 | -0.0001 | 0.0000 | 0.0008 | 0.0001 |
| 17 | 0.0000 | 0.0617 | 0.0000 | 0.0038 | 0.0006 |
| 18 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 19 | 0.0877 | -0.0005 | 0.0000 | 0.0077 | 0.0012 |
| 20 | 0.0000 | 0.7899 | 0.0000 | 0.6240 | 0.0957 |
| 21 | 0.0000 | 0.0000 | -0.0154 | 0.0002 | 0.0000 |
| 22 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 23 | 0.0000 | 0.6639 | 0.0000 | 0.4408 | 0.0679 |
| 24 | 0.0003 | 1.5576 | 0.0000 | 2.4261 | 0.3813 |
| 25 | -0.0131 | -0.0006 | 0.0000 | 0.0002 | 0.0000 |
| 26 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 27 | -0.0324 | 0.0002 | 0.0000 | 0.0010 | 0.0002 |
| 28 | 0.0000 | 0.0000 | 0.1717 | 0.0295 | 0.0048 |
| 29 | 0.0002 | -2.7773 | 0.0000 | 7.7135 | 1.2644 |
| 30 | 0.0000 | 0.0000 | -0.2948 | 0.0869 | 0.0143 |
| 31 | -0.0009 | 0.0195 | 0.0000 | 0.0004 | 0.0001 |
| 32 | 0.0000 | 0.0000 | -0.0162 | 0.0003 | 0.0000 |
| 33 | -0.3983 | -0.0001 | 0.0000 | 0.1586 | 0.0265 |
| 34 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 35 | -0.7716 | -0.0001 | 0.0000 | 0.5954 | 0.0997 |
| 36 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 37 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 38 | 1.3343 | 0.0001 | 0.0000 | 1.7804 | 0.3008 |
| 39 | 0.0000 | -0.0530 | 0.0000 | 0.0028 | 0.0005 |
| 40 | 0.0001 | 0.4012 | 0.0000 | 0.1610 | 0.0276 |

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
      52 -> 56        -0.17316
      52 -> 58        -0.12752
      53 -> 54         0.67066   90% [ 1,-1 ]

 Excited State   2:      Singlet-A    31.23058 1000/cm    f=0.0000
      52 -> 54         0.68744   95% [ 2,-1 ]

 Excited State   3:      Singlet-A    33.96561 1000/cm    f=0.0000
      52 -> 54         0.12585
      53 -> 56         0.56321   63% [ 1,-3 ]
      53 -> 58         0.39275   31% [ 1,-5 ]

 Excited State   4:      Singlet-B    38.05241 1000/cm    f=0.0002
      49 -> 58        -0.10478
      50 -> 55        -0.13736
      51 -> 54         0.45698   42% [ 3,-1 ]
      53 -> 57         0.50157   50% [ 1,-4 ]

 Excited State   5:      Singlet-A    38.05322 1000/cm    f=0.0000
      49 -> 57         0.13534
      50 -> 54         0.45488   41% [ 4,-1 ]
      51 -> 55        -0.13767
      53 -> 56         0.28150   16% [ 1,-3 ]
      53 -> 58        -0.41759   35% [ 1,-5 ]

 Excited State   6:      Singlet-A    40.0696 1000/cm   f=0.0002
```

```
     49 -> 54         0.41878   35% [ 5,-1 ]
     53 -> 55         0.56429   64% [ 1,-2 ]

Excited State   7:      Singlet-A    42.84576 1000/cm   f=0.0000
     50 -> 54         0.50847   52% [ 4,-1 ]
     53 -> 56        -0.27993   16% [ 1,-3 ]
     53 -> 58         0.38342   29% [ 1,-5 ]

Excited State   8:      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   9:      Singlet-A    43.63377 1000/cm   f=0.0084
     49 -> 54         0.53853   58% [ 5,-1 ]
     50 -> 57        -0.13544
     53 -> 55        -0.39284   31% [ 1,-2 ]

Excited State  10:      Singlet-B    44.31531 1000/cm   f=0.0001
     47 -> 54         0.15010
     52 -> 55         0.68451   94% [ 2,-2 ]

Excited State  11:      Singlet-B    45.36786 1000/cm   f=0.0044
     53 -> 59         0.67522   91% [ 1,-6 ]
     53 -> 61         0.17195

Excited State  12:      Singlet-B    45.78969 1000/cm   f=1.2769
     48 -> 54        -0.36367   26% [ 6,-1 ]
     52 -> 56         0.45979   42% [ 2,-3 ]
     52 -> 58         0.22493   10% [ 2,-5 ]
     53 -> 54         0.19757
     53 -> 65        -0.20124

Excited State  13:      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  14:      Singlet-A    46.84062 1000/cm   f=0.0017
     52 -> 57         0.69791   97% [ 2,-4 ]

Excited State  15:      Singlet-A    47.03904 1000/cm   f=0.0031
     49 -> 59        -0.11694
     53 -> 60         0.68692   94% [ 1,-7 ]

Excited State  16:      Singlet-B    48.12224 1000/cm   f=0.0001
     49 -> 56         0.57281   66% [ 5,-3 ]
     49 -> 58         0.38005   29% [ 5,-5 ]

Excited State  17:      Singlet-B    50.02893 1000/cm   f=0.0006
     53 -> 59        -0.17039
     53 -> 61         0.66355   88% [ 1,-8 ]
     53 -> 67         0.10085

Excited State  18:      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  19:      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
```

```
     50 -> 56        -0.27983   16% [ 4,-3 ]
     50 -> 58         0.41285   34% [ 4,-5 ]
     51 -> 57         0.50094   50% [ 3,-4 ]

 Excited State  32:      Singlet-A    54.60694 1000/cm   f=0.0000
     50 -> 57         0.52033   54% [ 4,-4 ]
     51 -> 56        -0.26698   14% [ 3,-3 ]
     51 -> 58         0.39656   31% [ 3,-5 ]

 Excited State  33:      Singlet-B    54.92311 1000/cm   f=0.0265
     49 -> 58         0.13806
     50 -> 55        -0.15299
     50 -> 60         0.31953   20% [ 4,-7 ]
     51 -> 59        -0.38139   29% [ 3,-6 ]
     52 -> 60         0.42808   37% [ 2,-7 ]

 Excited State  34:      Singlet-A    55.02553 1000/cm   f=0.0000
     50 -> 59         0.51229   52% [ 4,-6 ]
     51 -> 60        -0.44306   39% [ 3,-7 ]
     53 -> 66         0.15300

 Excited State  35:      Singlet-B    55.14894 1000/cm   f=0.0997
     49 -> 56        -0.17031
     49 -> 58         0.23211   11% [ 5,-5 ]
     50 -> 55        -0.23750   11% [ 4,-2 ]
     50 -> 60        -0.31405   20% [ 4,-7 ]
     51 -> 59         0.35417   25% [ 3,-6 ]
     52 -> 60         0.33804   23% [ 2,-7 ]

 Excited State  36:      Singlet-A    55.40623 1000/cm   f=0.0000
     49 -> 57         0.53147   56% [ 5,-4 ]
     51 -> 55         0.42567   36% [ 3,-2 ]
     52 -> 59        -0.10379

 Excited State  37:      Singlet-A    55.56028 1000/cm   f=0.0000
     48 -> 56        -0.11134
     50 -> 59        -0.12541
     51 -> 60         0.11327
     53 -> 66         0.65104   85% [ 1,-13 ]

 Excited State  38:      Singlet-B    55.61271 1000/cm   f=0.3008
     49 -> 56         0.24326   12% [ 5,-3 ]
     49 -> 58        -0.33915   23% [ 5,-5 ]
     50 -> 55         0.32948   22% [ 4,-2 ]
     52 -> 60         0.42700   36% [ 2,-7 ]

 Excited State  39:      Singlet-B    55.89581 1000/cm   f=0.0005
     53 -> 61        -0.10940
     53 -> 67         0.67974   92% [ 1,-14 ]

 Excited State  40:      Singlet-B    56.3757 1000/cm   f=0.0276
     49 -> 55        -0.15236
     50 -> 58        -0.12300
     51 -> 57         0.15299
     53 -> 65        -0.17692
     53 -> 68         0.60851   74% [ 1,-15 ]
     53 -> 74         0.11052

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