Supplementary information

Excited states of diphenylacetylene (Tolan): Near and vacuum UV polarization spectroscopy

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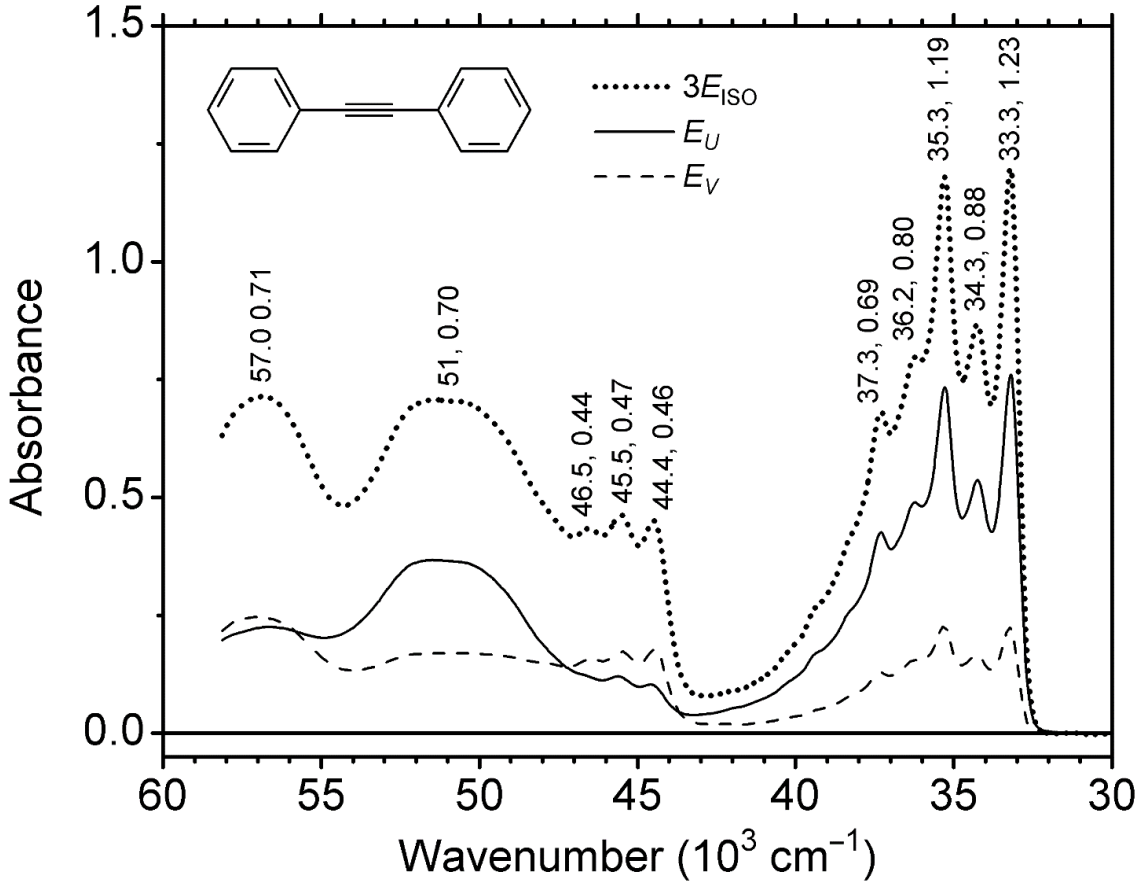
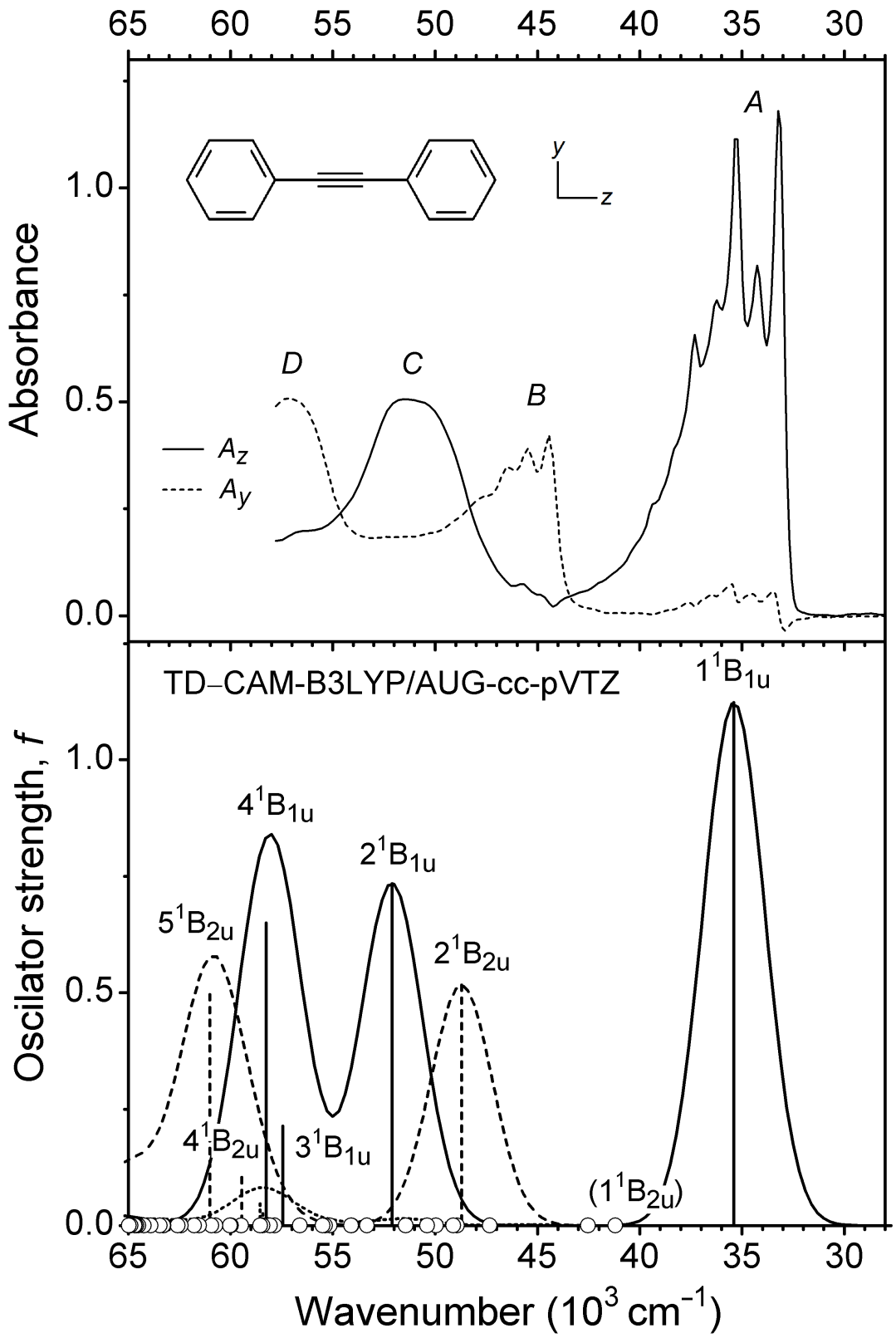
S1. Peak wavenumbers and absorbances for diphenylacetylene (tolan) in stretched polyethylene at room temperature. The curve $3E_{\mathrm{ISO}}(\tilde{\nu}) = E_U(\tilde{\nu}) + 2E_V(\tilde{\nu})$ is three times the absorbance that would have been measured in an isotropic experiment on the same sample.



S2. Computational results obtained with CAM-B3LYP/AUG-cc-pVTZ.



Observed				TD–CAM-B3LYP/AUG-cc-pVTZ [a]				
	$\tilde{\nu}$ [b]	Abs [c]	Pol [d]		Term	$\tilde{\nu}$ [b]	f [e]	Leading configurations
A	33.2 [f]	1.18 [f]	*z*	*1*	$1\,^1B_{1u}$	35.4	1.12	94%[$3b_{3u}(\pi)\rightarrow 3b_{2g}(\pi^*)$]
				2	$1\,^1B_{2u}$	40.9	$2\cdot10^{-4}$	49%[$3b_{3u}(\pi)\rightarrow 2b_{1g}(\pi^*)$], 32%[$1a_u(\pi)\rightarrow 3b_{2g}(\pi^*)$]
				3	$1\,^1B_{3g}$	41.2	0	44%[$3b_{3u}(\pi)\rightarrow 2a_u(\pi^*)$], 35%[$1b_{1g}(\sigma)\rightarrow 3b_{2g}(\pi^*)$]
				4	$1\,^1A_u$	42.5	0	94%[$8b_{2u}(\pi_{C\equiv C})\rightarrow 3b_{2g}(\pi^*)$]
				5	$1\,^1B_{3u}$	45.3	$2\cdot10^{-3}$	76%[$3b_{3u}(\pi)\rightarrow 14a_g(\sigma^*)$], 11%[$3b_{3u}(\pi)\rightarrow 15a_g(\sigma^*)$]
				6	$2\,^1A_g$	47.3	0	59%[$3b_{3u}(\pi)\rightarrow 4b_{3u}(\pi^*)$], 18%[$2b_{2g}(\pi)\rightarrow 3b_{2g}(\pi^*)$]
B	44.4 [f]	0.42 [f]	*y*	*7*	$2\,^1B_{2u}$	48.7	0.52	48%[$1a_u(\pi)\rightarrow 3b_{2g}(\pi^*)$], 43%[$3b_{3u}(\pi)\rightarrow 2b_{1g}(\pi^*)$]
				8	$1\,^1B_{2g}$	48.9	0	81%[$3b_{3u}(\pi)\rightarrow 13b_{1u}(\sigma^*)$]
				9	$2\,^1B_{3g}$	49.1	0	47%[$1b_{1g}(\pi)\rightarrow 3b_{2g}(\pi^*)$], 46%[$3b_{3u}(\pi)\rightarrow 2a_u(\pi^*)$]
				10	$1\,^1B_{1g}$	50.0	0	86%[$3b_{3u}(\pi)\rightarrow 9b_{2u}(\sigma^*)$]
				11	$2\,^1A_u$	50.4	0	53%[$3b_{3u}(\pi)\rightarrow 11b_{3g}(\sigma^*)$], 26%[$3b_{3u}(\pi)\rightarrow 10b_{3g}(\sigma^*)$]
				12	$3\,^1A_g$	51.4	0	52%[$2b_{2g}(\pi)\rightarrow 3b_{2g}(\pi^*)$], 33%[$3b_{3u}(\pi)\rightarrow 4b_{3u}(\pi^*)$]
				13	$2\,^1B_{3u}$	51.5	0.01	66%[$3b_{3u}(\pi)\rightarrow 15a_g(\sigma^*)$], 13%[$3b_{3u}(\pi)\rightarrow 14a_g(\sigma^*)$]
C	51	0.50	*z*	*14*	$2\,^1B_{1u}$	52.1	0.73	46%[$1a_u(\pi)\rightarrow 2b_{1g}(\pi^*)$], 41%[$1b_{1g}(\pi)\rightarrow 2a_u(\pi^*)$]
				15	$3\,^1A_u$	53.2	0	79%[$3b_{3u}(\pi)\rightarrow 8b_{3g}(\pi_{C\equiv C}^*)$]
				16	$2\,^1B_{1g}$	54.1	0	54%[$1b_{1g}(\pi)\rightarrow 14a_g\,(\sigma^*)$], 30%[$1a_u(\pi)\rightarrow 13b_{1u}(\sigma^*)$]
				17	$4\,^1A_u$	54.1	0	53%[$1a_u(\pi)\rightarrow 14a_g\,(\sigma^*)$], 28%[$1b_{1g}(\pi)\rightarrow 13b_{1u}(\sigma^*)$]
				18	$4\,^1A_g$	55.2	0	89%[$3b_{3u}(\pi)\rightarrow 5b_{3u}(\pi^*)$]
				19	$5\,^1A_g$	55.4	0	36%[$1b_{1g}(\pi)\rightarrow 2b_{1g}(\pi^*)$], 32%[$1a_u(\pi)\rightarrow 2a_u(\pi^*)$]
				20	$3\,^1B_{3u}$	55.4	$5\cdot10^{-3}$	54%[$3b_{3u}(\pi)\rightarrow 17a_g(\sigma^*)$], 33%[$3b_{3u}(\pi)\rightarrow 16a_g(\sigma^*)$]
				21	$2\,^1B_{2g}$	55.5	0	64%[$3b_{3u}(\pi)\rightarrow 14b_{1u}(\sigma^*)$], 14%[$3b_{3u}(\pi)\rightarrow 15b_{1u}(\sigma^*)$]
				22	$3\,^1B_{1g}$	56.6	0	82%[$3b_{3u}(\pi)\rightarrow 10b_{2u}(\sigma^*)$]
				23	$3\,^1B_{1u}$	57.4	0.21	68%[$3b_{3u}(\pi)\rightarrow 4b_{2g}(\pi^*)$], 14%[$2b_{3u}(\pi)\rightarrow 3b_{2g}(\pi^*)$]
				24	$4\,^1B_{3u}$	57.7	$8\cdot10^{-3}$	93%[$8b_{2u}(\pi_{C\equiv C})\rightarrow 2b_{1g}(\pi^*)$]
				25	$3\,^1B_{2g}$	57.9	0	48%[$3b_{3u}(\pi)\rightarrow 15b_{1u}(\sigma^*)$], 12%[$3b_{3u}(\pi)\rightarrow 14b_{1u}(\sigma^*)$]
				26	$4\,^1B_{1g}$	58.1	0	72%[$8b_{2u}(\pi_{C\equiv C})\rightarrow 4b_{3u}(\pi^*)$], 18%[$7b_{3g}(\sigma)\rightarrow 3b_{2g}(\pi^*)$]
				27	$3\,^1B_{2u}$	58.2	0.02	56%[$8b_{2u}(\pi_{C\equiv C})\rightarrow 14a_g\,(\sigma^*)$], 20%[$8b_{2u}(\pi_{C\equiv C})\rightarrow 15a_g\,(\sigma^*)$]
				28	$4\,^1B_{1u}$	58.3	0.65	30% $2b_{3u}(\pi)\rightarrow 3b_{2g}(\pi^*)$], 18%[$3b_{3u}(\pi)\rightarrow 4b_{2g}(\pi^*)$]
				29	$5\,^1B_{3u}$	58.4	0.03	32%[$1b_{1g}(\pi)\rightarrow 9b_{2u}(\sigma^*)$], 17%[$3b_{3u}(\pi)\rightarrow 16a_g(\sigma^*)$]
				30	$4\,^1B_{2g}$	58.4	0	46%[$8b_{2u}(\pi_{C\equiv C})\rightarrow 2a_u(\pi^*)$], 25%[$1a_u(\pi)\rightarrow 9b_{2u}(\sigma^*)$]
				31	$5\,^1B_{2g}$	58.6	0	45%[$8b_{2u}(\pi_{C\equiv C})\rightarrow 2a_u(\pi^*)$], 24%[$1a_u(\pi)\rightarrow 9b_{2u}(\sigma^*)$]
				32	$6\,^1B_{3u}$	58.7	0.05	24%[$1b_{1g}(\pi)\rightarrow 9b_{2u}(\sigma^*)$], 19%[$3b_{3u}(\pi)\rightarrow 17a_g\,(\sigma^*)$]
				33	$4\,^1B_{2u}$	59.5	0.10	37%[$2b_{2g}(\pi)\rightarrow 2a_u(\pi^*)$], 20%[$1b_{1g}(\pi)\rightarrow 4b_{3u}(\pi^*)$]
				34	$3\,^1B_{3g}$	59.5	0	57%[$2b_{2g}(\pi)\rightarrow 2b_{1g}(\pi^*)$], 11% $2b_{3u}(\pi)\rightarrow 2a_u(\pi^*)$]
				35	$5\,^1A_u$	60.0	0	55%[$1a_u(\pi)\rightarrow 15a_g(\sigma^*)$], 22%[$1b_{1g}(\pi)\rightarrow 13b_{1u}(\sigma^*)$]
				36	$5\,^1B_{1g}$	60.0	0	54%[$1b_{1g}(\pi)\rightarrow 15a_g(\sigma^*)$], 22%[$1a_u(\pi)\rightarrow 13b_{1u}(\sigma^*)$]
				37	$4\,^1B_{3g}$	60.7	0	59%[$1a_u(\pi)\rightarrow 4b_{3u}(\pi^*)$], 13%[$1b_{1g}(\pi)\rightarrow 4b_{2g}(\pi^*)$]
				38	$6\,^1B_{2g}$	60.9	0	65%[$2b_{2g}(\pi)\rightarrow 14a_g(\sigma^*)$]
E	57.1	0.51	*y*	*39*	$5\,^1B_{2u}$	61.0	0.50	43%[$1b_{1g}(\pi)\rightarrow 4b_{3u}(\pi^*)$], 21%[$2b_{2g}(\pi)\rightarrow 2a_u(\pi^*)$]
				40	$6\,^1A_u$	61.5	0	80%[$3b_{3u}(\pi)\rightarrow 9b_{3g}(\sigma^*)$]
				41	$6\,^1B_{2u}$	61.7	0.02	84%[$3b_{3u}(\pi)\rightarrow 3b_{1g}(\pi^*)$]

[a] Complete list of calculated transitions provided below.
[b] Peak wavenumber in 1000 cm^{-1}.
[c] Peak absorbance estimated from the partial absorbance curves in Fig. 1.
[d] Polarization direction.
[e] Oscillator strength.
[f] Onset.

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****************************************
Gaussian 16:  AS64L-G16RevA.03 25-Dec-2016
              28-Dec-2022
****************************************
--------------------------------------------------------------------------
#t cam-b3lyp/aug-cc-pvtz opt=tight freq scrf(pcm,solvent=n-hexadecane)
 empiricaldispersion=gd3bj
--------------------------------------------------------------------------
------------------------------
Tolan (diphenylacetylene), D2h
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         Item               Value     Threshold  Converged?
Maximum Force            0.000008     0.000015     YES
RMS     Force            0.000002     0.000010     YES
Maximum Displacement     0.000055     0.000060     YES
RMS     Displacement     0.000017     0.000040     YES
Optimization completed.
   -- Stationary point found.

                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.000000    0.000000    2.024916
     2          6           0        0.000000    0.000000    0.599842
     3          6           0        0.000000    0.000000   -0.599842
     4          6           0        0.000000    0.000000   -2.024916
     5          6           0        0.000000    1.202396   -2.732113
     6          6           0        0.000000    1.198704   -4.113842
     7          6           0       -0.000000    0.000000   -4.808888
     8          6           0       -0.000000   -1.198704   -4.113842
     9          6           0       -0.000000   -1.202396   -2.732113
    10          6           0       -0.000000   -1.202396    2.732113
    11          6           0       -0.000000   -1.198704    4.113842
    12          6           0       -0.000000   -0.000000    4.808888
    13          6           0       -0.000000    1.198704    4.113842
    14          6           0       -0.000000    1.202396    2.732113
    15          1           0        0.000000    2.135299   -2.187639
    16          1           0        0.000000    2.136285   -4.651346
    17          1           0       -0.000000    0.000000   -5.889538
    18          1           0       -0.000000   -2.136285   -4.651346
    19          1           0       -0.000000   -2.135299   -2.187639
    20          1           0       -0.000000   -2.135299    2.187639
    21          1           0       -0.000000   -2.136285    4.651346
    22          1           0       -0.000000   -0.000000    5.889538
    23          1           0       -0.000000    2.136285    4.651346
    24          1           0       -0.000000    2.135299    2.187639
---------------------------------------------------------------------
  874 basis functions,  1278 primitive gaussians,  1020 cartesian basis functions
   47 alpha electrons       47 beta electrons

SCF Done:  E(RCAM-B3LYP) =  -539.355136208     A.U. after    5 cycles
           NFock=  5  Conv=0.87D-08     -V/T= 2.0053

Full mass-weighted force constant matrix:
Low frequencies ---  -18.1333   -6.4422   -4.4846   -2.9751   -0.0012   -0.0008
Low frequencies ---   -0.0008   44.7917   49.0494
******    1 imaginary frequencies (negative Signs) ******

                     1                      2                      3
                    AU                    B2U                    B3U
Frequencies --     -2.9751                44.7917                49.0494
Red. masses --      3.6386                 4.7518                 5.4972
Frc consts  --      0.0000                 0.0056                 0.0078
IR Inten    --      0.0000                 0.7040                 1.5022
 Atom  AN      X      Y      Z        X      Y      Z        X      Y      Z
    1   6    -0.00  -0.00   0.00     0.00   0.11   0.00     0.16  -0.00  -0.00
    2   6    -0.00  -0.00  -0.00     0.00   0.22  -0.00     0.27  -0.00  -0.00
    3   6     0.00  -0.00   0.00    -0.00   0.22   0.00     0.27   0.00  -0.00
    4   6     0.00  -0.00  -0.00    -0.00   0.11  -0.00     0.16   0.00  -0.00
    5   6     0.17   0.00   0.00     0.00   0.04  -0.12     0.06   0.00  -0.00
```

6	6	0.17	0.00	0.00	0.00	-0.10	-0.12	-0.14	-0.00	-0.00
7	6	-0.00	0.00	0.00	0.00	-0.17	-0.00	-0.24	-0.00	0.00
8	6	-0.17	0.00	-0.00	-0.00	-0.10	0.12	-0.14	-0.00	0.00
9	6	-0.17	-0.00	-0.00	-0.00	0.04	0.12	0.06	0.00	0.00
10	6	0.17	-0.00	0.00	0.00	0.04	-0.12	0.06	-0.00	0.00
11	6	0.17	0.00	0.00	0.00	-0.10	-0.12	-0.14	0.00	0.00
12	6	0.00	0.00	-0.00	-0.00	-0.17	0.00	-0.24	0.00	0.00
13	6	-0.17	0.00	-0.00	-0.00	-0.10	0.12	-0.14	0.00	-0.00
14	6	-0.17	0.00	-0.00	-0.00	0.04	0.12	0.06	-0.00	-0.00
15	1	0.31	-0.00	0.00	-0.00	0.10	-0.21	0.14	0.00	-0.00
16	1	0.31	0.00	0.00	0.00	-0.16	-0.22	-0.21	-0.00	-0.00
17	1	-0.00	0.00	0.00	0.00	-0.28	-0.00	-0.41	-0.00	-0.00
18	1	-0.31	0.00	-0.00	-0.00	-0.16	0.22	-0.21	-0.00	0.00
19	1	-0.31	-0.00	-0.00	-0.00	0.10	0.21	0.14	0.00	0.00
20	1	0.31	-0.00	0.00	0.00	0.10	-0.21	0.14	-0.00	0.00
21	1	0.31	0.00	0.00	0.00	-0.16	-0.22	-0.21	0.00	0.00
22	1	0.00	0.00	-0.00	-0.00	-0.28	0.00	-0.41	0.00	-0.00
23	1	-0.31	0.00	-0.00	-0.00	-0.16	0.22	-0.21	0.00	-0.00
24	1	-0.31	-0.00	-0.00	0.00	0.10	0.21	0.14	-0.00	-0.00

Normal termination of Gaussian 16

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****************************************
Gaussian 16:  AS64L-G16RevA.03 25-Dec-2016
               29-Dec-2022
****************************************
```

```
---------------------------------------------------------------------
#t td(nst=70) cam-b3lyp/aug-cc-pvtz scrf(pcm,solvent=n-hexadecane) gue
ss=read geom=check
---------------------------------------------------------------------
```

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------------------------------
Tolan (diphenylacetylene), D2h
------------------------------
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-0.000000	2.024916
2	6	0	0.000000	0.000000	0.599842
3	6	0	0.000000	0.000000	-0.599842
4	6	0	0.000000	-0.000000	-2.024916
5	6	0	0.000000	1.202396	-2.732113
6	6	0	0.000000	1.198704	-4.113842
7	6	0	0.000000	0.000000	-4.808888
8	6	0	-0.000000	-1.198704	-4.113842
9	6	0	-0.000000	-1.202396	-2.732113
10	6	0	-0.000000	-1.202396	2.732113
11	6	0	-0.000000	-1.198704	4.113842
12	6	0	-0.000000	0.000000	4.808888
13	6	0	-0.000000	1.198704	4.113842
14	6	0	-0.000000	1.202396	2.732113
15	1	0	0.000000	2.135299	-2.187639
16	1	0	0.000000	2.136285	-4.651346
17	1	0	0.000000	0.000000	-5.889538
18	1	0	-0.000000	-2.136285	-4.651346
19	1	0	-0.000000	-2.135299	-2.187639
20	1	0	-0.000000	-2.135299	2.187639
21	1	0	-0.000000	-2.136285	4.651346
22	1	0	-0.000000	-0.000000	5.889538
23	1	0	-0.000000	2.136285	4.651346
24	1	0	-0.000000	2.135299	2.187639

```
---------------------------------------------------------------------
  874 basis functions,  1278 primitive gaussians,  1020 cartesian basis functions
   47 alpha electrons       47 beta electrons
```

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

state	X	Y	Z	Dip. S.	Osc.
1	-0.0000	-0.0000	-3.2330	10.4522	1.1237
2	-0.0000	0.0388	-0.0000	0.0015	0.0002
3	-0.0000	0.0000	0.0000	0.0000	0.0000
4	0.0000	-0.0000	-0.0000	0.0000	0.0000

5	0.1321	-0.0000	0.0000	0.0175	0.0024
6	-0.0000	0.0000	0.0000	0.0000	0.0000
7	-0.0000	-1.8691	-0.0000	3.4936	0.5169
8	0.0000	0.0000	-0.0000	0.0000	0.0000
9	-0.0000	-0.0000	-0.0000	0.0000	0.0000
10	-0.0000	-0.0000	-0.0000	0.0000	0.0000
11	-0.0000	0.0000	0.0000	0.0000	0.0000
12	0.0000	-0.0000	0.0000	0.0000	0.0000
13	0.3058	-0.0000	-0.0000	0.0935	0.0146
14	0.0000	0.0000	-2.1544	4.6413	0.7348
15	-0.0000	0.0000	0.0000	0.0000	0.0000
16	0.0000	0.0000	-0.0000	0.0000	0.0000
17	-0.0000	0.0000	0.0000	0.0000	0.0000
18	0.0000	0.0000	0.0000	0.0000	0.0000
19	0.0000	0.0000	-0.0000	0.0000	0.0000
20	0.1648	-0.0000	-0.0000	0.0271	0.0046
21	0.0000	0.0000	-0.0000	0.0000	0.0000
22	-0.0000	-0.0000	0.0000	0.0000	0.0000
23	-0.0000	0.0000	-1.1065	1.2243	0.2136
24	-0.2195	0.0000	0.0000	0.0482	0.0084
25	0.0000	-0.0000	0.0000	0.0000	0.0000
26	0.0000	0.0000	-0.0000	0.0000	0.0000
27	0.0000	0.2954	0.0000	0.0872	0.0154
28	0.0000	-0.0000	1.9173	3.6762	0.6506
29	-0.3823	0.0000	-0.0000	0.1462	0.0259
30	-0.0000	0.0000	0.0000	0.0000	0.0000
31	0.0000	0.0000	0.0000	0.0000	0.0000
32	-0.5159	0.0000	0.0000	0.2662	0.0474
33	-0.0000	-0.7571	-0.0000	0.5732	0.1035
34	-0.0000	0.0000	-0.0000	0.0000	0.0000
35	0.0000	-0.0000	0.0000	0.0000	0.0000
36	0.0000	0.0000	-0.0000	0.0000	0.0000
37	-0.0000	0.0000	0.0000	0.0000	0.0000
38	0.0000	0.0000	0.0000	0.0000	0.0000
39	0.0000	1.6368	0.0000	2.6790	0.4965
40	0.0000	0.0000	0.0000	0.0000	0.0000
41	0.0000	-0.2908	0.0000	0.0846	0.0158
42	0.0000	-0.0000	-0.0000	0.0000	0.0000
43	0.0000	0.0000	-0.0000	0.0000	0.0000
44	0.0000	0.0000	-0.0000	0.0000	0.0000
45	-0.1875	-0.0000	0.0000	0.0352	0.0067
46	0.0000	-0.0000	0.0000	0.0000	0.0000
47	0.0000	0.0000	0.0000	0.0000	0.0000
48	-0.0000	-0.0000	0.0000	0.0000	0.0000
49	-0.0135	-0.0000	-0.0000	0.0002	0.0000
50	0.0000	0.0000	-0.0000	0.0000	0.0000
51	-0.1936	-0.0000	0.0000	0.0375	0.0073
52	-0.0000	0.0000	-0.0000	0.0000	0.0000
53	0.0144	0.0000	0.0000	0.0002	0.0000
54	0.0000	-0.0000	0.0000	0.0000	0.0000
55	0.0000	-0.0000	-0.0000	0.0000	0.0000
56	-0.0000	0.0000	-0.0000	0.0000	0.0000
57	-0.0000	-0.0000	-0.0000	0.0000	0.0000
58	-0.0000	0.0000	0.1161	0.0135	0.0027
59	0.0000	-0.0000	-0.0000	0.0000	0.0000
60	0.0000	-0.0000	0.0000	0.0000	0.0000
61	0.0000	0.0000	-0.0000	0.0000	0.0000
62	0.0000	-0.7961	0.0000	0.6337	0.1253
63	0.0000	-0.0000	0.0000	0.0000	0.0000
64	0.0000	-0.0000	0.0000	0.0000	0.0000
65	-0.0000	-0.0000	0.0000	0.0000	0.0000
66	0.0000	0.0000	0.2100	0.0441	0.0088
67	0.0000	-0.0000	-0.2517	0.0634	0.0127
68	-0.1403	-0.0000	-0.0000	0.0197	0.0040
69	-0.0000	-0.0000	-0.0000	0.0000	0.0000
70	-0.0699	0.0000	-0.0000	0.0049	0.0010

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kK (kiloKaiser) = 1000/cm
p = pi, s = sigma
ip indicates an in-plane pi-type component of the triple bond

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Excited State   1:      1 Singlet-B1U  35.39482 kK  282.53 nm  f=1.1237
     47 -> 48         0.68578   94% [3b3u(p)->3b2g(p*)]

Excited State   2:      1 Singlet-B2U  40.91245 kK  244.43 nm  f=0.0002
     44 -> 54        -0.21216
     45 -> 56        -0.19345
     46 -> 48         0.40217   32% [1au(p)->3b2g(p*)]
     47 -> 52         0.49325   49% [3b3u(p)->2b1g(p*)]

Excited State   3:      1 Singlet-B3G  41.19071 kK  242.77 nm  f=0.0000
     44 -> 52        -0.21755
     45 -> 48        -0.42042   35% [1b1g(p)->3b2g(p*)]
     46 -> 56         0.20327
     47 -> 54         0.47024   44% [3b3u(p)->2au(p*)]

Excited State   4:      1 Singlet-AU   42.52798 kK  235.14 nm  f=0.0000
     43 -> 48         0.68417   94% [8b2u(ip)->3b2g(p*)]

Excited State   5:      1 Singlet-B3U  45.29849 kK  220.76 nm  f=0.0024
     47 -> 49         0.61476   76% [3b3u(p)->14ag(s*)]
     47 -> 53        -0.23315   11% [3b3u(p)->15ag(s*)]
     47 -> 59        -0.15741
     47 -> 67        -0.10943

Excited State   6:      2 Singlet-AG   47.31972 kK  211.33 nm  f=0.0000
     44 -> 48        -0.29790   18% [2b2g(p)->3b2g(p*)]
     45 -> 52         0.22694   10% [1b1g(p)->2b1g(p*)]
     46 -> 54        -0.21828   10% [1au(p)->2au(p*)]
     47 -> 56         0.54526   59% [3b3u(p)->4b3u(p*)]

Excited State   7:      2 Singlet-B2U  48.71103 kK  205.29 nm  f=0.5169
     45 -> 56        -0.16326
     46 -> 48         0.49242   48% [1au(p)->3b2g(p*)]
     47 -> 52        -0.46628   43% [3b3u(p)->2b1g(p*)]

Excited State   8:      1 Singlet-B2G  48.9296 kK  204.37 nm  f=0.0000
     44 -> 49        -0.19052
     47 -> 50         0.63683   81% [3b3u(p)->13b1u(s*)]
     47 -> 57        -0.10033
     47 -> 63        -0.15405

Excited State   9:      2 Singlet-B3G  49.10382 kK  203.65 nm  f=0.0000
     45 -> 48         0.48370   47% [1b1g(p)->3b2g(p*)]
     46 -> 56        -0.15448
     47 -> 54         0.48084   46% [3b3u(p)->2au(p*)]

Excited State  10:      1 Singlet-B1G  49.96683 kK  200.13 nm  f=0.0000
     47 -> 51         0.65460   86% [3b3u(p)->9b2u(s*)]
     47 -> 58        -0.17375
     47 -> 71        -0.13942

Excited State  11:      2 Singlet-AU   50.39591 kK  198.43 nm  f=0.0000
     42 -> 74         0.15786
     47 -> 55         0.13393
     47 -> 64        -0.12315
     47 -> 72        -0.35859   26% [3b3u(p)->10b3g(s*)]
     47 -> 74         0.51487   53% [3b3u(p)->11b3g(s*)]
     47 -> 83        -0.11459

Excited State  12:      3 Singlet-AG   51.4396 kK  194.40 nm  f=0.0000
     42 -> 56         0.12489
     44 -> 48         0.51048   52% [2b2g(p)->3b2g(p*)]
     45 -> 52        -0.15095
     46 -> 54         0.14823
     47 -> 56         0.40419   33% [3b3u(p)->4b3u(p*)]

Excited State  13:      2 Singlet-B3U  51.54767 kK  193.99 nm  f=0.0146
     44 -> 50        -0.18225
     47 -> 49         0.25609   13% [3b3u(p)->14ag(s*)]
     47 -> 53         0.57477   66% [3b3u(p)->15ag(s*)]
     47 -> 59         0.14569
     47 -> 67         0.15979
```

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Excited State  14:      2-Singlet-B1U  52.12113 kK  191.86 nm  f=0.7348
     42 -> 48         0.14968
     44 -> 56         0.14210
     45 -> 54        -0.45300   41% [1b1g(p)->2au(p*)]
     46 -> 52         0.47751   46% [1au(p)->2b1g(p*)]

Excited State  15:      3 Singlet-AU   53.335 kK  187.49 nm  f=0.0000
     44 -> 51         0.13297
     46 -> 49         0.14129
     47 -> 55         0.63013   79% [3b3u(p)->8b3g(ip*)]
     47 -> 64         0.13248
     47 -> 74        -0.14499

Excited State  16:      2 Singlet-B1G  54.0988 kK  184.85 nm  f=0.0000
     45 -> 49         0.52200   54% [1b1g(p)->14ag(s*)]
     45 -> 73        -0.11388
     46 -> 50        -0.38808   30% [1au(p)->13b1u(s*)]
     46 -> 63         0.12280

Excited State  17:      4 Singlet-AU   54.10042 kK  184.84 nm  f=0.0000
     45 -> 50        -0.37611   28% [1b1g(p)->13b1u(s*)]
     45 -> 63         0.11924
     46 -> 49         0.51245   53% [1au(p)->14ag(s*)]
     46 -> 73        -0.11141
     47 -> 55        -0.16961

Excited State  18:      4 Singlet-AG   55.15781 kK  181.30 nm  f=0.0000
     44 -> 61         0.10701
     47 -> 60         0.66732   89% [3b3u(p)->5b3u(p*)]
     47 -> 68        -0.13694

Excited State  19:      5 Singlet-AG   55.37638 kK  180.58 nm  f=0.0000
     44 -> 48         0.34151   23% [2b2g(p)->3b2g(p*)]
     45 -> 52         0.42623   36% [1b1g(p)->2b1g(p*)]
     46 -> 54        -0.39853   32% [1au(p)->2au(p*)]
     47 -> 56        -0.14073

Excited State  20:      3 Singlet-B3U  55.44817 kK  180.35 nm  f=0.0046
     44 -> 63         0.10135
     47 -> 53         0.13689
     47 -> 59        -0.40614   33% [3b3u(p)->16ag(s*)]
     47 -> 62         0.51902   54% [3b3u(p)->17ag(s*)]

Excited State  21:      2 Singlet-B2G  55.50866 kK  180.15 nm  f=0.0000
     44 -> 53        -0.17782
     47 -> 50         0.15057
     47 -> 57         0.56719   64% [3b3u(p)->14b1u(s*)]
     47 -> 63         0.26807   14% [3b3u(p)->15b1u(s*)]
     47 -> 78        -0.12921

Excited State  22:      3 Singlet-B1G  56.608 kK  176.65 nm  f=0.0000
     44 -> 55         0.13284
     47 -> 51         0.16605
     47 -> 58         0.63974   82% [3b3u(p)->10b2u(s*)]
     47 -> 77        -0.15088

Excited State  23:      3 Singlet-B1U  57.44117 kK  174.09 nm  f=0.2136
     42 -> 48        -0.26793   14% 2b3u(p)->3b2g(p*)]
     43 -> 74         0.10609
     44 -> 60         0.20614
     47 -> 61         0.58416   68% [3b3u(p)->4b2g(p*)]

Excited State  24:      4 Singlet-B3U  57.71217 kK  173.27 nm  f=0.0084
     41 -> 54        -0.13622
     43 -> 52         0.68319   93% [8b2u(ip)->2b1g(p*)]

Excited State  25:      3 Singlet-B2G  57.85493 kK  172.85 nm  f=0.0000
     44 -> 49         0.11162
     44 -> 59        -0.11557
     44 -> 62         0.11600
     45 -> 55        -0.14795
     46 -> 51        -0.19708
     47 -> 50         0.10884
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     47 -> 57        -0.24820   12% [3b3u(p)->14b1u(s*)]
     47 -> 63         0.49030   48% [3b3u(p)->15b1u(s*)]
     47 -> 66        -0.23220   11% [3b3u(p)->16b1u(s*)]

Excited State  26:      4 Singlet-B1G  58.07511 kK  172.19 nm  f=0.0000
     40 -> 56         0.10671
     41 -> 48        -0.30102   18% [7b3g(s)->3b2g(p*)]
     43 -> 56         0.59952   72% [8b2u(ip)->4b3u(p*)]
     43 -> 60        -0.12761

Excited State  27:      3 Singlet-B2U  58.19691 kK  171.83 nm  f=0.0154
     43 -> 49         0.52952   56% [8b2u(ip)->14ag(s*)]
     43 -> 53        -0.31279   20% [8b2u(ip)->15ag(s*)]
     43 -> 59        -0.20474
     43 -> 67        -0.18924
     44 -> 54         0.12222

Excited State  28:      4 Singlet-B1U  58.26465 kK  171.63 nm  f=0.6506
     42 -> 48         0.38998   30% 2b3u(p)->3b2g(p*)]
     43 -> 72         0.16977
     43 -> 74        -0.26479   14% [8b2u(ip)->11b3g(s*)]
     44 -> 56         0.22551   10% [2b2g(p)->4b3u(p*)]
     45 -> 54         0.14121
     46 -> 52        -0.15736
     47 -> 61         0.30207   18% [3b3u(p)->4b2g(p*)]
     47 -> 76         0.12439

Excited State  29:      5 Singlet-B3U  58.42597 kK  171.16 nm  f=0.0259
     44 -> 57        -0.10196
     45 -> 51         0.39782   32% [1b1g(p)->9b2u(s*)]
     45 -> 71        -0.10396
     46 -> 55         0.28051   16% [1au(p)->8b3g(ip*)]
     47 -> 53         0.18469
     47 -> 59        -0.28795   17% [3b3u(p)->16ag(s*)]
     47 -> 62        -0.19963
     47 -> 67        -0.17938

Excited State  30:      4 Singlet-B2G  58.44774 kK  171.09 nm  f=0.0000
     41 -> 52        -0.11573
     43 -> 54         0.48129   46% [8b2u(ip)->2au(p*)]
     45 -> 55        -0.25009   13% [1b1g(p)->8b3g(ip*)]
     46 -> 51        -0.35035   25% [1au(p)->9b2u(s*)]
     47 -> 57         0.12641
     47 -> 63        -0.11315

Excited State  31:      5 Singlet-B2G  58.56228 kK  170.76 nm  f=0.0000
     41 -> 52        -0.10475
     43 -> 54         0.47458   45% [8b2u(ip)->2au(p*)]
     45 -> 55         0.24442   12% [1b1g(p)->8b3g(ip*)]
     46 -> 51         0.34852   24% [1au(p)->9b2u(s*)]
     47 -> 57        -0.14264
     47 -> 63         0.14938

Excited State  32:      6 Singlet-B3U  58.56792 kK  170.74 nm  f=0.0474
     45 -> 51         0.34961   24% [1b1g(p)->9b2u(s*)]
     46 -> 55         0.26585   14% [1au(p)->8b3g(ip*)]
     47 -> 53        -0.10405
     47 -> 59         0.27577   15% [3b3u(p)->16ag(s*)]
     47 -> 62         0.30832   19% [3b3u(p)->17ag(s*)]
     47 -> 67         0.22703   10% [3b3u(p)->18ag(s*)]
     47 -> 80        -0.10219

Excited State  33:      4 Singlet-B2U  59.46481 kK  168.17 nm  f=0.1035
     42 -> 52         0.21185
     43 -> 49        -0.10142
     44 -> 54         0.43208   37% [2b2g(p)->2au(p*)]
     45 -> 56         0.31603   20% [1b1g(p)->4b3u(p*)]
     46 -> 48         0.27037   15% [1au(p)->3b2g(p*)]
     47 -> 52         0.12497
     47 -> 65         0.21339

Excited State  34:      3 Singlet-B3G  59.48175 kK  168.12 nm  f=0.0000
     42 -> 54         0.23969   11% 2b3u(p)->2au(p*)]
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     44 -> 52         0.53478   57% [2b2g(p)->2b1g(p*)]
     45 -> 48        -0.22673   10% [1b1g(p)->3b2g(p*)]
     46 -> 56        -0.23075   11% [1au(p)->4b3u(p*)]
     47 -> 54         0.18893

Excited State  35:      5 Singlet-AU   59.98423 kK  166.71 nm  f=0.0000
     45 -> 50        -0.33113   22% [1b1g(p)->13b1u(s*)]
     45 -> 57        -0.16570
     46 -> 49        -0.16059
     46 -> 53         0.52225   55% [1au(p)->15ag(s*)]
     46 -> 59         0.12879
     46 -> 67         0.10445

Excited State  36:      5 Singlet-B1G  60.02778 kK  166.59 nm  f=0.0000
     45 -> 49        -0.16767
     45 -> 53         0.51957   54% [1b1g(p)->15ag(s*)]
     45 -> 59         0.13072
     45 -> 67         0.10350
     46 -> 50        -0.32811   22% [1au(p)->13b1u(s*)]
     46 -> 57        -0.16798

Excited State  37:      4 Singlet-B3G  60.73997 kK  164.64 nm  f=0.0000
     44 -> 52         0.22670   10% [2b2g(p)->2b1g(p*)]
     45 -> 48         0.16747
     45 -> 61         0.25515   13% [1b1g(p)->4b2g(p*)]
     46 -> 56         0.54266   59% [1au(p)->4b3u(p*)]
     46 -> 60         0.17562

Excited State  38:      6 Singlet-B2G  60.9279 kK  164.13 nm  f=0.0000
     44 -> 49         0.57149   65% [2b2g(p)->14ag(s*)]
     44 -> 53        -0.15806
     47 -> 50         0.17397
     47 -> 63        -0.10187
     47 -> 66         0.16035
     47 -> 69         0.12447

Excited State  39:      5 Singlet-B2U  61.01823 kK  163.89 nm  f=0.4965
     42 -> 52        -0.14030
     44 -> 54        -0.32288   21% [2b2g(p)->2au(p*)]
     45 -> 56         0.46538   43% [1b1g(p)->4b3u(p*)]
     45 -> 60         0.21083
     46 -> 48         0.10092
     46 -> 61         0.26925   14% [1au(p)->4b2g(p*)]

Excited State  40:      6 Singlet-AU   61.54249 kK  162.49 nm  f=0.0000
     44 -> 58        -0.15800
     47 -> 55        -0.11271
     47 -> 64         0.63224   80% [3b3u(p)->9b3g(s*)]
     47 -> 87        -0.12236

Excited State  41:      6 Singlet-B2U  61.65299 kK  162.20 nm  f=0.0158
     44 -> 54        -0.11552
     44 -> 70         0.10985
     45 -> 56        -0.16524
     47 -> 65         0.64904   84% [3b3u(p)->3b1g(p*)]

Excited State  42:      7 Singlet-AU   61.7893 kK  161.84 nm  f=0.0000
     40 -> 48         0.60999   74% [7b2u(s)->3b2g(p*)]
     41 -> 56        -0.30461   19% [7b3g(s)->4b3u(p*)]
     41 -> 60         0.11179

Excited State  43:      6 Singlet-B1G  62.42325 kK  160.20 nm  f=0.0000
     40 -> 56        -0.26906   14% [7b2u(s)->4b3u(p*)]
     41 -> 48         0.54540   59% [7b3g(s)->3b2g(p*)]
     43 -> 56         0.32495   21% [8b2u(ip)->4b3u(p*)]

Excited State  44:      6 Singlet-AG   62.58617 kK  159.78 nm  f=0.0000
     43 -> 51        -0.10910
     44 -> 61         0.19318
     47 -> 60         0.10723
     47 -> 68         0.63671   81% [3b3u(p)->6b3u(p*)]

Excited State  45:      7 Singlet-B3U  62.83862 kK  159.14 nm  f=0.0067
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     42 -> 49         0.16163
     44 -> 50         0.46379   43% [2b2g(p)->13b1u(s*)]
     44 -> 63        -0.17187
     45 -> 51        -0.10801
     45 -> 58         0.11094
     47 -> 49         0.16457
     47 -> 53         0.15664
     47 -> 59         0.13642
     47 -> 62         0.12006
     47 -> 67        -0.23477   11% [3b3u(p)->18ag(s*)]
     47 -> 73         0.14099

Excited State  46:      7 Singlet-B1G  63.28465 kK  158.02 nm  f=0.0000
     45 -> 59        -0.29837   18% [1b1g(p)->16ag(s*)]
     45 -> 62         0.39964   32% [1b1g(p)->17ag(s*)]
     45 -> 67         0.10353
     46 -> 63         0.36160   26% [1au(p)->15b1u(s*)]
     46 -> 66        -0.21175

Excited State  47:      8 Singlet-AU   63.29836 kK  157.98 nm  f=0.0000
     45 -> 63         0.35703   25% [1b1g(p)->15b1u(s*)]
     45 -> 66        -0.20721
     46 -> 53         0.10010
     46 -> 59        -0.29661   18% [1au(p)->16ag(s*)]
     46 -> 62         0.39490   31% [1au(p)->17ag(s*)]
     46 -> 67         0.10251

Excited State  48:      7 Singlet-B2G  63.4508 kK  157.60 nm  f=0.0000
     38 -> 56         0.28839   17% [12b1u(s)->4b3u(p*)]
     38 -> 60        -0.10933
     39 -> 48         0.62105   77% [13ag(s)->3b2g(p*)]

Excited State  49:      8 Singlet-B3U  63.65969 kK  157.08 nm  f=0.0000
     44 -> 50         0.21221
     47 -> 49         0.10605
     47 -> 59        -0.26211   14% [3b3u(p)->16ag(s*)]
     47 -> 62        -0.18225
     47 -> 67         0.47300   45% [3b3u(p)->18ag(s*)]
     47 -> 73         0.25099   13% [3b3u(p)->19ag(s*)]

Excited State  50:      7 Singlet-AG   63.90166 kK  156.49 nm  f=0.0000
     43 -> 51         0.61643   76% [8b2u(ip)->9b2u(s*)]
     43 -> 58        -0.24444   12% [8b2u(ip)->10b2u(s*)]
     43 -> 71        -0.14591
     47 -> 68         0.11784

Excited State  51:      9 Singlet-B3U  64.24283 kK  155.66 nm  f=0.0073
     38 -> 48         0.59575   71% [12b1u(s)->3b2g(p*)]
     39 -> 56         0.31492   20% [13ag(s)->4b3u(p*)]
     39 -> 60        -0.11747

Excited State  52:      8 Singlet-B2G  64.24526 kK  155.65 nm  f=0.0000
     44 -> 49         0.10658
     44 -> 53        -0.12181
     45 -> 55         0.35691   25% [1b1g(p)->8b3g(ip*)]
     45 -> 64        -0.14530
     46 -> 51        -0.23021   11% [1au(p)->9b2u(s*)]
     46 -> 58         0.44553   40% [1au(p)->10b2u(s*)]
     46 -> 77        -0.12023
     47 -> 66        -0.13385

Excited State  53:      10 Singlet-B3U  64.41382 kK  155.25 nm  f=0.0000
     44 -> 50        -0.12275
     45 -> 51        -0.25151   13% [1b1g(p)->9b2u(s*)]
     45 -> 58         0.44995   40% [1b1g(p)->10b2u(s*)]
     45 -> 77        -0.11655
     46 -> 55         0.37850   29% [1au(p)->8b3g(ip*)]
     46 -> 64        -0.13479

Excited State  54:      9 Singlet-AU   64.51948 kK  154.99 nm  f=0.0000
     44 -> 51        -0.32343   21% [2b2g(p)->9b2u(s*)]
     45 -> 50        -0.23272   11% [1b1g(p)->13b1u(s*)]
     45 -> 57         0.36726   27% [1b1g(p)->14b1u(s*)]
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     45 -> 63         0.11339
     46 -> 49        -0.29544   17% [1au(p)->14ag(s*)]
     46 -> 53        -0.15000
     46 -> 59         0.14427
     46 -> 62         0.11177

Excited State  55:      8 Singlet-B1G  64.60982 kK  154.77 nm  f=0.0000
     45 -> 49        -0.33724   23% [1b1g(p)->14ag(s*)]
     45 -> 53        -0.17139
     45 -> 59         0.17998
     46 -> 50        -0.29147   17% [1au(p)->13b1u(s*)]
     46 -> 57         0.42105   35% [1au(p)->14b1u(s*)]
     46 -> 63         0.10927

Excited State  56:      9 Singlet-B2G  64.67514 kK  154.62 nm  f=0.0000
     44 -> 49        -0.16047
     44 -> 62        -0.13649
     46 -> 51        -0.13864
     46 -> 58         0.12839
     47 -> 57        -0.12063
     47 -> 63         0.23529   11% [3b3u(p)->15b1u(s*)]
     47 -> 66         0.53083   56% [3b3u(p)->16b1u(s*)]
     47 -> 69         0.12692
     47 -> 92         0.12312

Excited State  57:      5 Singlet-B3G  64.70096 kK  154.56 nm  f=0.0000
     44 -> 65         0.15453
     45 -> 61         0.16223
     46 -> 56        -0.12126
     46 -> 60         0.22984   11% [1au(p)->5b3u(p*)]
     47 -> 70         0.59645   71% [3b3u(p)->3au(p*)]

Excited State  58:      5 Singlet-B1U  64.85823 kK  154.18 nm  f=0.0027
     45 -> 54         0.49491   49% [1b1g(p)->2au(p*)]
     46 -> 52         0.48962   48% [1au(p)->2b1g(p*)]

Excited State  59:      8 Singlet-AG   64.88404 kK  154.12 nm  f=0.0000
     45 -> 52         0.48082   46% [1b1g(p)->2b1g(p*)]
     46 -> 54         0.51074   52% [1au(p)->2au(p*)]

Excited State  60:      10 Singlet-AU   64.98567 kK  153.88 nm  f=0.0000
     44 -> 51         0.52392   55% [2b2g(p)->9b2u(s*)]
     44 -> 71        -0.11436
     45 -> 50        -0.20908
     45 -> 57         0.19710
     46 -> 49        -0.17659
     46 -> 59         0.10117
     47 -> 55        -0.13854
     47 -> 64        -0.12220
     47 -> 72        -0.12466

Excited State  61:      6 Singlet-B3G  65.03245 kK  153.77 nm  f=0.0000
     43 -> 50        -0.15725
     44 -> 52        -0.17280
     45 -> 61         0.33099   22% [1b1g(p)->4b2g(p*)]
     46 -> 56        -0.18081
     46 -> 60         0.41885   35% [1au(p)->5b3u(p*)]
     47 -> 70        -0.29970   18% [3b3u(p)->3au(p*)]

Excited State  62:      7 Singlet-B2U  65.11714 kK  153.57 nm  f=0.1253
     44 -> 54         0.23150   11% [2b2g(p)->2au(p*)]
     45 -> 56        -0.23131   11% [1b1g(p)->4b3u(p*)]
     45 -> 60         0.47657   45% [1b1g(p)->5b3u(p*)]
     46 -> 61         0.36992   27% [1au(p)->4b2g(p*)]

Excited State  63:      9 Singlet-B1G  65.17037 kK  153.44 nm  f=0.0000
     44 -> 55        -0.16935
     47 -> 51         0.15776
     47 -> 71         0.59694   71% [3b3u(p)->11b2u(s*)]
     47 -> 77        -0.14423
     47 -> 79        -0.10514

Excited State  64:      7 Singlet-B3G  65.41637 kK  152.87 nm  f=0.0000
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     43 -> 50         0.62065   77% [8b2u(ip)->13b1u(s*)]
     43 -> 57        -0.19521
     43 -> 63        -0.16471
     46 -> 60         0.10562

Excited State  65:      10 Singlet-B2G  65.4196 kK  152.86 nm  f=0.0000
     42 -> 50         0.11570
     44 -> 53         0.44915   40% [2b2g(p)->15ag(s*)]
     44 -> 59         0.13891
     44 -> 67         0.13779
     44 -> 73        -0.11386
     45 -> 55         0.10959
     47 -> 50         0.16007
     47 -> 57         0.16251
     47 -> 69         0.35298   25% [3b3u(p)->17b1u(s*)]

Excited State  66:      6 Singlet-B1U  65.60994 kK  152.42 nm  f=0.0088
     42 -> 48        -0.37487   28% 2b3u(p)->3b2g(p*)]
     44 -> 56         0.46260   43% [2b2g(p)->4b3u(p*)]
     47 -> 76         0.26860   14% [3b3u(p)->5b2g(p*)]
     47 -> 86         0.10749
     47 -> 93         0.11422
     47 -> 95        -0.10127

Excited State  67:      7 Singlet-B1U  66.16324 kK  151.14 nm  f=0.0127
     42 -> 48         0.13703
     43 -> 72        -0.13620
     43 -> 74         0.20287
     44 -> 56         0.40394   33% [2b2g(p)->4b3u(p*)]
     45 -> 54         0.10743
     47 -> 48         0.10007
     47 -> 76        -0.37787   29% [3b3u(p)->5b2g(p*)]
     47 -> 93        -0.13303
     47 -> 95         0.13184

Excited State  68:      11 Singlet-B3U  66.22616 kK  151.00 nm  f=0.0040
     40 -> 52         0.47585   45% [7b2u(s)->2b1g(p*)]
     41 -> 54        -0.47140   44% [7b3g(s)->2au(p*)]
     43 -> 52        -0.15159

Excited State  69:      11 Singlet-B2G  66.35923 kK  150.69 nm  f=0.0000
     40 -> 54        -0.46673   44% [7b2u(s)->2au(p*)]
     41 -> 52         0.47700   46% [7b3g(s)->2b1g(p*)]
     43 -> 54         0.17996

Excited State  70:      12 Singlet-B3U  66.51006 kK  150.35 nm  f=0.0010
     44 -> 50        -0.25685   13% [2b2g(p)->13b1u(s*)]
     44 -> 57        -0.13051
     44 -> 63        -0.16445
     47 -> 73         0.28509   16% [3b3u(p)->19ag(s*)]
     47 -> 75         0.46687   44% [3b3u(p)->20ag(s*)]
     47 -> 80        -0.19416

Orbital symmetries:

      Occupied  ( 1B1U) ( 1AG) ( 2B1U) ( 1B3G) ( 1B2U) ( 2AG)   ( 3B1U) ( 3AG) ( 2B3G)
                ( 2B2U) ( 4B1U) ( 4AG) ( 5AG)  ( 5B1U) ( 6AG)   ( 6B1U) ( 7AG) ( 7B1U)
                ( 3B2U) ( 3B3G) ( 8AG) ( 8B1U) ( 4B2U) ( 4B3G)  ( 9AG)  ( 9B1U)
                ( 10AG) (10B1U) (11AG) ( 5B2U) ( 5B3G) (11B1U)  (12AG)  ( 6B2U) ( 6B3G)

                   36      37      38      39      40      41      42      43
                ( 1B3U) ( 1B2G) (12B1U) (13AG) ( 7B2U) ( 7B3G)  ( 2B3U) ( 8B2U)
                   12      11      10       9       8       7       6       5

                   44      45      46      47
                ( 2B2G) ( 1B1G) ( 1AU)  ( 3B3U)
                   4       3       2       1

                   48      49      50      51      52      53      54      55      56
       Virtual  ( 3B2G) (14AG)  (13B1U) ( 9B2U) ( 2B1G) (15AG)  ( 2AU)  ( 8B3G) ( 4B3U)
                  -1      -2      -3      -4      -5      -6      -7      -8      -9

                   57      58      59      60      61      62      63      64
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(14B1U) (10B2U) (16AG)  ( 5B3U) ( 4B2G) (17AG)  (15B1U) ( 9B3G)
  -10     -11     -12     -13     -14     -15     -16     -17

   65      66      67      68      69      70      71      72
( 3B1G) (16B1U) (18AG)  ( 6B3U) (17B1U) ( 3AU)  (11B2U) (10B3G)
  -18     -19     -20     -21     -22     -23     -24     -25

   73      74      75      76      77      78      79      80      81
(19AG)  (11B3G) (20AG)  ( 5B2G) (12B2U) (18B1U) (13B2U) (21AG)  (14B2U)
  -26     -27     -28     -29     -30     -31     -32     -33     -34

( 4B1G) (12B3G) ( 7B3U) (19B1U) ( 6B2G) (13B3G) ( 8B3U) (22AG)
(14B3G) ( 4AU)  (20B1U) ( 7B2G) (15B2U) ( 8B2G) (21B1U) (23AG)
(AG) (B3U) (B1U) (B3G) (AG) (B3U) (B2U) (B1U)
(AG) (B2U) (B2G) (B3G) (B2U) (B1U) (AG) (B1U)
(B3U) (B3G) (B1G) (B3G) (B2G) (B2U) (AG) (B1U)
(B2G) (AG) (B2U) (AU) (B3G) (B1U) (B3U) (B1U)
(B2U) (B3G) (B1G) (AG) (AG) (B2U) (AG) (B1U) (B2U)
(B2G) (B3G) (AG) (B1G) (B1U) (B1U) (B3U) (AU)
(B2G) (AG) (B1G) (B3G) (AU) (B3U) (B1G) (B2U)
(AU) (AG) (B3U) (B2G) (B2U) (B3U) (B1U) (AG) (AG)
(B2G) (B1U) (AU) (B1U) (B3G) (B2U) (B3G) (AG)
(B1U) (B2G) (B2U) (B1U) (AG) (B3U) (B3G) (AG)
(B2U) (B3G) (B1U) (AG) (B2U) (AG) (B3G) (B1U)
(B2U) (B2G) (B3G) (AG) (B1U) (B3U) (B1G) (B2U)
(B3G) (B1U) (B2U) (B1U) (B2G) (B3G) (AG) (B3U)
(AU) (B1G) (B3U) (B2G) (AG) (B1U) (AG) (B2U) (AU)
(AG) (B3G) (B1U) (B2U) (B3G) (B2G) (B1G) (B3U)
(B2U) (AG) (B3G) (B1U) (B1G) (B2U) (AG) (AU) (B3G)
(B1U) (B1U) (AG) (B2U) (B2G) (B3G) (B1U) (B3G)
(B3U) (B1G) (AU) (AG) (B2U) (B1U) (AG) (AU) (B2U)
(B1G) (B3U) (B3G) (B1U) (AG) (B2G) (AG) (B2G)
(B3G) (B1U) (B3U) (AG) (AU) (B2U) (B2G) (B1U)
(AG) (B1G) (B1U) (B3U) (B2G) (B3G) (AU) (B2U)
(B1U) (B2U) (B3U) (B3G) (AG) (B1G) (AG) (B2U)
(B1U) (B2G) (B3U) (B3G) (B2U) (AG) (AU) (AG) (B3U)
(B3G) (B2G) (B1G) (B3U) (B2G) (B1U) (B1G) (AU)
(B3U) (AU) (B1U) (B1G) (AG) (B1U) (B2U) (B3G)
(B1U) (B2G) (AG) (AU) (B3G) (B2U) (B3U) (AG) (B1U)
(B3G) (B2U) (B2G) (B1G) (AG) (B2G) (B1U) (B2U)
(B3G) (AU) (B1G) (B2U) (B3U) (B1U) (B2G) (AG)
(B1U) (AG) (B3G) (B2U) (B1U) (B3G) (B2U) (AG)
(B2U) (AG) (B3G) (B3U) (AG) (B1G) (B2U) (B1U)
(AU) (B3U) (AG) (B1U) (B3G) (B1U) (B2G) (AG) (B1G)
(B1U) (B3G) (B2U) (B3U) (B1U) (B3G) (AG) (B3G)
(B3G) (AU) (B2U) (B1U) (AG) (B2G) (B1G) (B3U)
(AU) (B2G) (B1U) (AG) (B2U) (AU) (B1U) (B3G) (B3U)
(B1G) (B2G) (AG) (B3U) (B2U) (AG) (B1U) (AG) (B2G)
(B2U) (B1U) (AU) (B2G) (B3G) (B2U) (AG) (B1U)
(B1U) (B3G) (AG) (B3U) (B2U) (B2G) (B1G) (B3U)
(B3G) (B1U) (AU) (B1G) (AG) (B3G) (AU) (B2U) (B1G)
(B3U) (AG) (B2U) (AU) (B1U) (B3G) (B2G) (B2U)
(B1U) (AG) (B3G) (B2U) (B2G) (B1U) (B3G) (AG)
(B3U) (B1G) (B3G) (B2U) (B2G) (B3U) (AU) (B1G)
(B2U) (B1U) (B2G) (B2U) (AG) (AG) (B3G) (B1U)
(B3U) (B2G) (AU) (B1U) (B3G) (B3U) (AG) (B1G)
(AG) (AU) (B3U) (B1U) (B2U) (B3G) (B1U) (B2U)
(B3G) (B2G) (AG) (AG) (B2U) (B1U) (B1G) (B1U)
(AG) (B3G) (B2U) (AG) (AU) (B1U) (B3U) (B3G) (B2G)
(B2U) (B3U) (B2G) (B3G) (B1U) (B1G) (B2U) (AG)
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(B1U) (AG) (B2U) (B1U) (B2U) (AG) (B2G) (B3U)
(B1G) (B1U) (B3G) (B3U) (AU) (B1U) (B3G) (AU)
(AG) (B3U) (AG) (B2G) (B1U) (B3G) (B1G) (AG) (B2U)
(B1U) (AU) (B1U) (AG) (B2U) (B3G) (B2U) (B3G)
(B2U) (B1U) (B2G) (AG) (B1G) (B1U) (AU) (B2U)
(B1U) (B3G) (AG) (B3U) (B3G) (B2U) (B2G) (B3G)
(B2U) (AG) (B3G) (B2U) (B3U) (B1U) (AG) (B1U)
(B1G) (B3U) (AG) (AU) (B2G) (B2U) (B1G) (B3G)
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(B2G) (B3U) (AG) (B3G) (B1G) (B3U) (AU) (AG) (B1U)
(B2U) (B2G) (B1U) (B3G) (AG) (B3U) (B3G) (AU)
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                (B2U) (AG) (B1G) (B3U) (B2G) (B3U) (B2G) (B1U)
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                (B2U) (B1U) (B3G) (AU) (B1G) (AG) (B2U) (B3G)
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                (B1U) (B3U) (B3G) (AG) (B1U) (B1G) (B2U) (B2G)
                (B3G) (B1U) (B2U) (B3G) (AG) (B1U) (B2G) (B1G)
                (AU) (B3G) (AU) (AG) (B2U) (B1G) (B3U) (B1U) (AU)
                (B2U) (B2G) (AG) (B1G) (B3U) (B3G) (B1U) (B2G)
                (AG) (B2U) (AU) (B1U) (B3U) (B1U) (AG) (B3G) (B2G)
                (B1U) (AG) (B3G) (B3U) (B2U) (B2G) (B3G) (AG)
                (B1G) (AU) (B3U) (B2U) (B3G) (B2U) (B1U) (B2G)
                (B3U) (B1U) (B1G) (B3U) (B2G) (AU) (B3G) (B1G)
                (AG) (B2U) (AU) (B1U) (B3G) (B2U) (AG) (AG) (B1G)
                (B2G) (B3G) (B3U) (B1U) (B2G) (B2U) (AU) (AG)
                (B3U) (B1G) (AU) (B1U) (AG) (B1U) (B3G) (B2U)
                (B1U) (AG) (B3G) (B2U) (B1U) (B2G) (AG) (B3G)
                (B2U) (B2U) (B3U) (B3G) (B1U) (AG) (B3G) (B1U)
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                (B2G) (B3G) (AG) (B2U) (B1U) (AG) (B1U) (B3G)
                (B2U) (AG) (B3G) (B1U) (B2U) (B2U) (B3G) (AG)
                (B1U) (B3G) (AG) (B1U) (B2U) (B3G) (AG) (B2U)
                (B3G) (B1U) (AG) (AG) (B1U) (AG) (B1U) (B2U) (B1U)
                (AG) (B3G) (B1U)
 The electronic state is 1-AG.
 Alpha  occ. eigenvalues --  -10.27991 -10.27990 -10.25855 -10.25855 -10.25855
 Alpha  occ. eigenvalues --  -10.25854 -10.25668 -10.25667 -10.25607 -10.25606
 Alpha  occ. eigenvalues --  -10.25573 -10.25573 -10.25114 -10.24850  -0.96054
 Alpha  occ. eigenvalues --   -0.95762  -0.88154  -0.85666  -0.83976  -0.83957
 Alpha  occ. eigenvalues --   -0.80324  -0.71720  -0.69307  -0.69140  -0.68953
 Alpha  occ. eigenvalues --   -0.62735  -0.61177  -0.56141  -0.54872  -0.53956
 Alpha  occ. eigenvalues --   -0.53413  -0.51263  -0.50658  -0.49864  -0.49826
 Alpha  occ. eigenvalues --   -0.46983  -0.45730  -0.43099  -0.42665  -0.42131

 Alpha  occ. eigenvalues --   -0.41724  -0.39279  -0.34117  -0.33608  -0.32178
                               41        42        43        44        45
 Alpha  occ. eigenvalues --   -0.32156  -0.27289
                               46        47


 Alpha virt. eigenvalues --   -0.01754   0.00876   0.01306   0.01919   0.02227
                               48        49        50        51        52
 Alpha virt. eigenvalues --    0.02470   0.02556   0.02637   0.03404   0.03896
                               53        54        55        56        57

 Alpha virt. eigenvalues --    0.04188   0.04951   0.05709   0.06051   0.06292
 Alpha virt. eigenvalues --    0.06302   0.06322   0.07942   0.08250   0.08408
 Alpha virt. eigenvalues --    0.08420   0.08766   0.09095   0.09150   0.09336
 Alpha virt. eigenvalues --    0.09420   0.10140   0.10533   0.10553   0.10688
 Alpha virt. eigenvalues --    0.10998   0.11013   0.11257   0.11387   0.12128
 Alpha virt. eigenvalues --    0.12327   0.12637   0.13019   0.13123   0.13269
 Alpha virt. eigenvalues --    0.13770   0.14787   0.14915   0.15371   0.15620
 Alpha virt. eigenvalues --    0.15692   0.15854   0.16862   0.17183   0.17557
 Alpha virt. eigenvalues --    0.17941   0.18005   0.19134   0.19358   0.19773
 Alpha virt. eigenvalues --    0.20654   0.20916   0.21308   0.21546   0.21932
 Alpha virt. eigenvalues --    0.22335   0.22550   0.23316   0.23333   0.23542
 Alpha virt. eigenvalues --    0.23714   0.24702   0.24869   0.25094   0.25119
 Alpha virt. eigenvalues --    0.25217   0.25433   0.25451   0.25935   0.25954
 Alpha virt. eigenvalues --    0.26442   0.26503   0.26615   0.26869   0.27117
 Alpha virt. eigenvalues --    0.27513   0.27701   0.27760   0.27889   0.28388
 Alpha virt. eigenvalues --    0.28395   0.29427   0.30145   0.30695   0.31073
 Alpha virt. eigenvalues --    0.31483   0.31919   0.32042   0.32553   0.32677
 Alpha virt. eigenvalues --    0.32740   0.34053   0.34178   0.34216   0.34911
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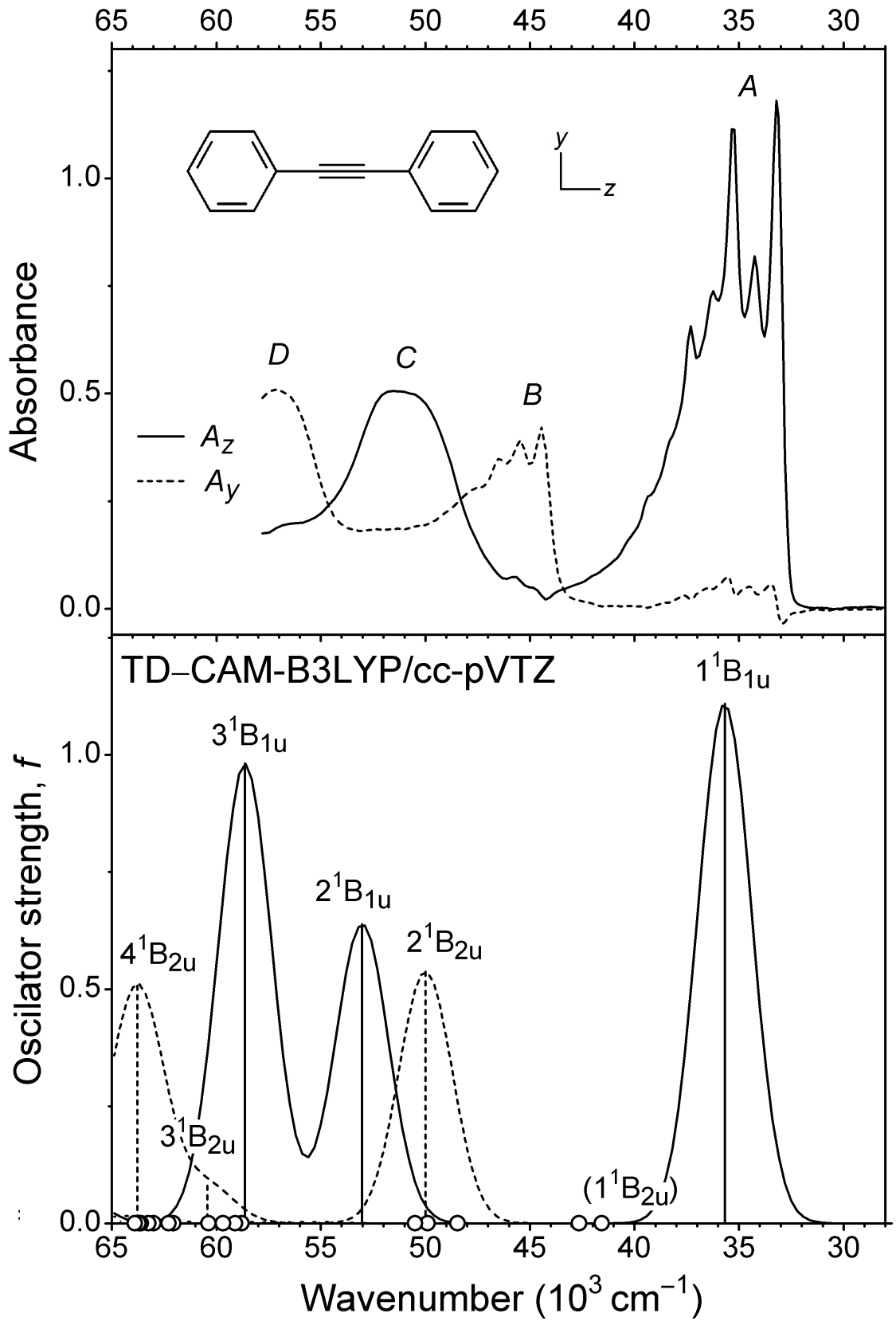
Alpha virt. eigenvalues --    0.35254   0.35563   0.36163   0.36244   0.36677
Alpha virt. eigenvalues --    0.37688   0.38038   0.38376   0.38395   0.38470
Alpha virt. eigenvalues --    0.38967   0.39025   0.39361   0.39749   0.39808
Alpha virt. eigenvalues --    0.40055   0.40123   0.40856   0.41014   0.41515
Alpha virt. eigenvalues --    0.41752   0.42096   0.42255   0.42587   0.43367
Alpha virt. eigenvalues --    0.43477   0.43603   0.43692   0.43757   0.44245
Alpha virt. eigenvalues --    0.44800   0.45428   0.45435   0.45564   0.46180
Alpha virt. eigenvalues --    0.46194   0.46865   0.46886   0.47284   0.47791
Alpha virt. eigenvalues --    0.48111   0.48319   0.48593   0.48679   0.49445
Alpha virt. eigenvalues --    0.49612   0.49806   0.49917   0.50365   0.50469
Alpha virt. eigenvalues --    0.51316   0.51423   0.51750   0.52599   0.52637
Alpha virt. eigenvalues --    0.54665   0.55041   0.55265   0.55338   0.55354
Alpha virt. eigenvalues --    0.55444   0.56063   0.57274   0.57617   0.59416
Alpha virt. eigenvalues --    0.59608   0.59700   0.61296   0.61503   0.61504
Alpha virt. eigenvalues --    0.61537   0.61629   0.62187   0.63103   0.63473
Alpha virt. eigenvalues --    0.63486   0.63492   0.63534   0.64774   0.64949
Alpha virt. eigenvalues --    0.66309   0.66572   0.66609   0.66934   0.67508
Alpha virt. eigenvalues --    0.67888   0.68114   0.69021   0.69403   0.70922
Alpha virt. eigenvalues --    0.70954   0.71135   0.71739   0.72035   0.72950
Alpha virt. eigenvalues --    0.73451   0.75143   0.75831   0.76304   0.76673
Alpha virt. eigenvalues --    0.76834   0.77019   0.77247   0.77777   0.77860
Alpha virt. eigenvalues --    0.78628   0.79095   0.79430   0.79448   0.79871
Alpha virt. eigenvalues --    0.80492   0.80617   0.80773   0.81144   0.81472
Alpha virt. eigenvalues --    0.82001   0.82147   0.82183   0.82603   0.83999
Alpha virt. eigenvalues --    0.84142   0.84322   0.84720   0.84799   0.85174
Alpha virt. eigenvalues --    0.85367   0.85391   0.86347   0.87662   0.87673
Alpha virt. eigenvalues --    0.87799   0.88322   0.88717   0.88933   0.89301
Alpha virt. eigenvalues --    0.89858   0.90677   0.91222   0.91461   0.91669
Alpha virt. eigenvalues --    0.91993   0.92422   0.93629   0.94122   0.94626
Alpha virt. eigenvalues --    0.94829   0.94901   0.95132   0.95884   0.96808
Alpha virt. eigenvalues --    0.96839   0.96936   0.97002   0.97090   0.97212
Alpha virt. eigenvalues --    0.97317   0.98486   0.98790   0.99066   0.99304
Alpha virt. eigenvalues --    0.99454   0.99747   1.00571   1.00952   1.01094
Alpha virt. eigenvalues --    1.02068   1.02243   1.02729   1.03623   1.03782
Alpha virt. eigenvalues --    1.04216   1.04307   1.04358   1.04418   1.05071
Alpha virt. eigenvalues --    1.05622   1.05966   1.06381   1.06888   1.06958
Alpha virt. eigenvalues --    1.07168   1.07342   1.07410   1.08007   1.08939
Alpha virt. eigenvalues --    1.09505   1.09866   1.10016   1.10628   1.10705
Alpha virt. eigenvalues --    1.10930   1.11047   1.11312   1.12208   1.12458
Alpha virt. eigenvalues --    1.12855   1.13168   1.15135   1.15268   1.15400
Alpha virt. eigenvalues --    1.15797   1.16894   1.17171   1.18110   1.18849
Alpha virt. eigenvalues --    1.19626   1.21059   1.21406   1.21970   1.22263
Alpha virt. eigenvalues --    1.24043   1.24200   1.24326   1.25144   1.25676
Alpha virt. eigenvalues --    1.25752   1.26638   1.26897   1.26941   1.27306
Alpha virt. eigenvalues --    1.27429   1.27776   1.28797   1.29917   1.30017
Alpha virt. eigenvalues --    1.31106   1.31291   1.32352   1.32451   1.33654
Alpha virt. eigenvalues --    1.34130   1.34220   1.34729   1.35613   1.35968
Alpha virt. eigenvalues --    1.37300   1.37519   1.37648   1.39232   1.39835
Alpha virt. eigenvalues --    1.40077   1.41052   1.41189   1.41896   1.42145
Alpha virt. eigenvalues --    1.43478   1.43774   1.43881   1.47418   1.47495
Alpha virt. eigenvalues --    1.48132   1.48595   1.48692   1.51021   1.51053
Alpha virt. eigenvalues --    1.52776   1.53589   1.53955   1.54303   1.54606
Alpha virt. eigenvalues --    1.54810   1.55693   1.55916   1.56293   1.57655
Alpha virt. eigenvalues --    1.58542   1.59954   1.61681   1.61774   1.62538
Alpha virt. eigenvalues --    1.62674   1.64350   1.64870   1.65212   1.66077
Alpha virt. eigenvalues --    1.66329   1.67493   1.67699   1.67999   1.68515
Alpha virt. eigenvalues --    1.68712   1.69062   1.69805   1.70599   1.71293
Alpha virt. eigenvalues --    1.71373   1.72139   1.73795   1.73967   1.74187
Alpha virt. eigenvalues --    1.75396   1.76024   1.76507   1.76543   1.76767
Alpha virt. eigenvalues --    1.76900   1.77116   1.78594   1.78655   1.79892
Alpha virt. eigenvalues --    1.80137   1.81405   1.83405   1.83527   1.83900
Alpha virt. eigenvalues --    1.84229   1.85641   1.85772   1.86247   1.86393
Alpha virt. eigenvalues --    1.87800   1.88090   1.89046   1.91262   1.91457
Alpha virt. eigenvalues --    1.91514   1.92000   1.92133   1.92562   1.93215
Alpha virt. eigenvalues --    1.93421   1.94527   1.95989   1.96479   1.96481
Alpha virt. eigenvalues --    1.97506   1.98328   1.98640   1.99344   1.99521
Alpha virt. eigenvalues --    1.99536   2.01816   2.01959   2.02085   2.03398
Alpha virt. eigenvalues --    2.03561   2.06235   2.06240   2.07957   2.07962
Alpha virt. eigenvalues --    2.08062   2.08287   2.09990   2.11643   2.13928
Alpha virt. eigenvalues --    2.15003   2.16804   2.17676   2.18011   2.18405
Alpha virt. eigenvalues --    2.19411   2.20817   2.21129   2.21640   2.21674
Alpha virt. eigenvalues --    2.22512   2.23671   2.23889   2.23903   2.24978
Alpha virt. eigenvalues --    2.25301   2.25764   2.25998   2.30682   2.31227
```

```
Alpha virt. eigenvalues --    2.31339   2.32312   2.33793   2.33968   2.34748
Alpha virt. eigenvalues --    2.35614   2.39216   2.39303   2.41437   2.42263
Alpha virt. eigenvalues --    2.42938   2.44725   2.45783   2.47001   2.48978
Alpha virt. eigenvalues --    2.50654   2.53090   2.54360   2.55271   2.56452
Alpha virt. eigenvalues --    2.57968   2.58142   2.58800   2.59708   2.59838
Alpha virt. eigenvalues --    2.60889   2.62522   2.63331   2.64764   2.66149
Alpha virt. eigenvalues --    2.67700   2.74278   2.75125   2.76855   2.81200
Alpha virt. eigenvalues --    2.83216   2.87225   2.89020   2.92272   2.93545
Alpha virt. eigenvalues --    2.93864   2.94620   2.94974   2.95413   2.95758
Alpha virt. eigenvalues --    2.95804   2.99702   2.99841   3.01753   3.04581
Alpha virt. eigenvalues --    3.04780   3.06062   3.06982   3.07223   3.07268
Alpha virt. eigenvalues --    3.07766   3.07829   3.09042   3.10938   3.11337
Alpha virt. eigenvalues --    3.12675   3.12942   3.13382   3.13906   3.15918
Alpha virt. eigenvalues --    3.16390   3.16733   3.16741   3.17317   3.19150
Alpha virt. eigenvalues --    3.19343   3.19611   3.21082   3.21370   3.22295
Alpha virt. eigenvalues --    3.22803   3.23178   3.25322   3.26856   3.26857
Alpha virt. eigenvalues --    3.27506   3.28104   3.28134   3.29913   3.30482
Alpha virt. eigenvalues --    3.30534   3.30597   3.30877   3.31055   3.32479
Alpha virt. eigenvalues --    3.33755   3.34532   3.34989   3.35459   3.36598
Alpha virt. eigenvalues --    3.37162   3.37190   3.38802   3.39673   3.40451
Alpha virt. eigenvalues --    3.40916   3.41448   3.41861   3.42039   3.44644
Alpha virt. eigenvalues --    3.45099   3.45449   3.45951   3.45978   3.46058
Alpha virt. eigenvalues --    3.47294   3.47624   3.48717   3.52269   3.54401
Alpha virt. eigenvalues --    3.54710   3.55277   3.55575   3.55577   3.57059
Alpha virt. eigenvalues --    3.57455   3.57927   3.58148   3.59975   3.60224
Alpha virt. eigenvalues --    3.60593   3.62188   3.62456   3.63478   3.63858
Alpha virt. eigenvalues --    3.64356   3.65241   3.66158   3.66286   3.66332
Alpha virt. eigenvalues --    3.66909   3.67264   3.67762   3.67863   3.69881
Alpha virt. eigenvalues --    3.71202   3.71304   3.72897   3.72900   3.73741
Alpha virt. eigenvalues --    3.74537   3.74815   3.75720   3.75926   3.76510
Alpha virt. eigenvalues --    3.76989   3.77507   3.77523   3.77745   3.79132
Alpha virt. eigenvalues --    3.80124   3.81471   3.82633   3.83127   3.84792
Alpha virt. eigenvalues --    3.84988   3.85036   3.88830   3.89111   3.89490
Alpha virt. eigenvalues --    3.89493   3.89853   3.90140   3.90647   3.90934
Alpha virt. eigenvalues --    3.93875   3.95772   3.95967   3.96464   3.98348
Alpha virt. eigenvalues --    4.00453   4.00838   4.01117   4.01812   4.02939
Alpha virt. eigenvalues --    4.03513   4.03667   4.04900   4.05697   4.06652
Alpha virt. eigenvalues --    4.07293   4.07588   4.08416   4.08666   4.09963
Alpha virt. eigenvalues --    4.10370   4.10549   4.12177   4.12696   4.13192
Alpha virt. eigenvalues --    4.14005   4.14644   4.14665   4.15511   4.16982
Alpha virt. eigenvalues --    4.17538   4.18484   4.19975   4.20301   4.20419
Alpha virt. eigenvalues --    4.20574   4.20701   4.22280   4.22427   4.23130
Alpha virt. eigenvalues --    4.25454   4.26794   4.30460   4.30631   4.31124
Alpha virt. eigenvalues --    4.32103   4.34056   4.34539   4.35948   4.38832
Alpha virt. eigenvalues --    4.40462   4.42450   4.43175   4.45604   4.45615
Alpha virt. eigenvalues --    4.46206   4.46730   4.47169   4.48618   4.49668
Alpha virt. eigenvalues --    4.50288   4.53937   4.54710   4.55716   4.56432
Alpha virt. eigenvalues --    4.59691   4.61421   4.62990   4.63163   4.65647
Alpha virt. eigenvalues --    4.65749   4.66111   4.66925   4.68119   4.70062
Alpha virt. eigenvalues --    4.70239   4.71691   4.72642   4.77799   4.78799
Alpha virt. eigenvalues --    4.78932   4.79644   4.80002   4.80547   4.80630
Alpha virt. eigenvalues --    4.82395   4.83813   4.85708   4.86060   4.86104
Alpha virt. eigenvalues --    4.87356   4.87563   4.89717   4.91321   4.91467
Alpha virt. eigenvalues --    4.91674   4.91811   4.91832   4.92494   4.93317
Alpha virt. eigenvalues --    4.94285   4.95438   4.97506   5.02388   5.02926
Alpha virt. eigenvalues --    5.03160   5.04979   5.05828   5.06750   5.07480
Alpha virt. eigenvalues --    5.09732   5.10057   5.11013   5.11070   5.12510
Alpha virt. eigenvalues --    5.12878   5.18229   5.18365   5.19755   5.23120
Alpha virt. eigenvalues --    5.24548   5.25417   5.27716   5.31729   5.32079
Alpha virt. eigenvalues --    5.36361   5.42651   5.46191   5.49594   5.50635
Alpha virt. eigenvalues --    5.50964   5.51109   5.57435   5.57665   5.59992
Alpha virt. eigenvalues --    5.60961   5.62144   5.69547   5.78810   5.80479
Alpha virt. eigenvalues --    5.88613   5.89990   5.90069   5.92084   5.94110
Alpha virt. eigenvalues --    5.94785   5.97052   5.99308   6.02110   6.03399
Alpha virt. eigenvalues --    6.07062   6.07399   6.10591   6.16185   6.22070
Alpha virt. eigenvalues --    6.25968   6.30323   6.39243   6.43479   6.44621
Alpha virt. eigenvalues --    6.55146   6.56847   6.58951   6.64836   6.68828
Alpha virt. eigenvalues --    6.68940   6.89310   6.95596   7.06382   7.18776
Alpha virt. eigenvalues --   15.17761  15.56621  15.62196  15.94307  16.87575
Alpha virt. eigenvalues --   18.12969  18.46438  18.78353  18.93642  19.26674
Alpha virt. eigenvalues --   19.40683  19.64492  19.67850  21.62667

Normal termination of Gaussian 16
```

S3. Computational results obtained with CAM-B3LYP/cc-pVTZ.



```
****************************************
Gaussian 16:  AS64L-G16RevA.03 25-Dec-2016
              29-Dec-2022
****************************************
------------------------------------------------------------------------
#t cam-b3lyp/cc-pvtz opt=tight freq scrf(pcm,solvent=n-hexadecane) emp
iricaldispersion=gd3bj
------------------------------------------------------------------------
------------------------------
Tolan (diphenylacetylene), D2h
------------------------------

         Item               Value     Threshold  Converged?
Maximum Force            0.000007     0.000015     YES
RMS     Force            0.000002     0.000010     YES
Maximum Displacement     0.000051     0.000060     YES
RMS     Displacement     0.000016     0.000040     YES
Optimization completed.
   -- Stationary point found.

                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.000000    0.000000    2.024922
     2          6           0        0.000000    0.000000    0.599962
     3          6           0        0.000000    0.000000   -0.599962
     4          6           0        0.000000    0.000000   -2.024922
     5          6           0        0.000000    1.202325   -2.732151
     6          6           0        0.000000    1.198599   -4.113667
     7          6           0       -0.000000    0.000000   -4.808568
     8          6           0       -0.000000   -1.198599   -4.113667
     9          6           0       -0.000000   -1.202325   -2.732151
    10          6           0       -0.000000   -1.202325    2.732151
    11          6           0       -0.000000   -1.198599    4.113667
    12          6           0       -0.000000   -0.000000    4.808568
    13          6           0       -0.000000    1.198599    4.113667
    14          6           0       -0.000000    1.202325    2.732151
    15          1           0        0.000000    2.135168   -2.187363
    16          1           0        0.000000    2.136318   -4.651200
    17          1           0       -0.000000    0.000000   -5.889347
    18          1           0       -0.000000   -2.136318   -4.651200
    19          1           0       -0.000000   -2.135168   -2.187363
    20          1           0       -0.000000   -2.135168    2.187363
    21          1           0       -0.000000   -2.136318    4.651200
    22          1           0       -0.000000   -0.000000    5.889347
    23          1           0       -0.000000    2.136318    4.651200
    24          1           0       -0.000000    2.135168    2.187363
---------------------------------------------------------------------
  560 basis functions,   898 primitive gaussians,   640 cartesian basis functions
   47 alpha electrons       47 beta electrons

SCF Done:  E(RCAM-B3LYP) =  -539.350614410     A.U. after    1 cycles
           NFock=  1  Conv=0.19D-08     -V/T= 2.0059

Full mass-weighted force constant matrix:
Low frequencies ---  -19.2666   -6.7730   -4.5650   -0.0010   -0.0008   -0.0007
Low frequencies ---    2.4015   45.2168   49.0252

                     1                      2                      3
                    AU                    B2U                    B3U
Frequencies --      2.4015                45.2168                49.0252
Red. masses --      3.6408                 4.7513                 5.4970
Frc consts  --      0.0000                 0.0057                 0.0078
IR Inten    --      0.0000                 0.7131                 1.4810
 Atom  AN      X      Y      Z        X      Y      Z        X      Y      Z
    1   6    -0.00  -0.00  -0.00    -0.00   0.11   0.00     0.16   0.00   0.00
    2   6    -0.00  -0.00  -0.00    -0.00   0.22  -0.00     0.27   0.00   0.00
    3   6     0.00  -0.00   0.00     0.00   0.22   0.00     0.27  -0.00   0.00
    4   6     0.00  -0.00   0.00     0.00   0.11  -0.00     0.16  -0.00   0.00
    5   6     0.17  -0.00   0.00     0.00   0.04  -0.12     0.06  -0.00   0.00
    6   6     0.17   0.00   0.00     0.00  -0.10  -0.12    -0.14   0.00   0.00
```

7	6	-0.00	0.00	-0.00	-0.00	-0.17	-0.00	-0.24	0.00	-0.00
8	6	-0.17	0.00	-0.00	-0.00	-0.10	0.12	-0.14	0.00	-0.00
9	6	-0.17	-0.00	-0.00	-0.00	0.04	0.12	0.06	-0.00	-0.00
10	6	0.17	-0.00	0.00	0.00	0.04	-0.12	0.06	0.00	-0.00
11	6	0.17	0.00	0.00	0.00	-0.10	-0.12	-0.14	-0.00	-0.00
12	6	0.00	0.00	0.00	0.00	-0.17	0.00	-0.24	-0.00	-0.00
13	6	-0.17	0.00	-0.00	-0.00	-0.10	0.12	-0.14	-0.00	0.00
14	6	-0.17	-0.00	-0.00	-0.00	0.04	0.12	0.06	0.00	0.00
15	1	0.31	-0.00	0.00	0.00	0.10	-0.21	0.14	-0.00	0.00
16	1	0.31	0.00	0.00	0.00	-0.16	-0.22	-0.21	0.00	0.00
17	1	-0.00	0.00	-0.00	-0.00	-0.28	-0.00	-0.41	0.00	-0.00
18	1	-0.31	0.00	-0.00	-0.00	-0.16	0.22	-0.21	0.00	-0.00
19	1	-0.31	-0.00	-0.00	-0.00	0.10	0.21	0.14	-0.00	-0.00
20	1	0.31	-0.00	0.00	0.00	0.10	-0.21	0.14	0.00	-0.00
21	1	0.31	0.00	0.00	0.00	-0.16	-0.22	-0.21	-0.00	-0.00
22	1	0.00	0.00	0.00	0.00	-0.28	0.00	-0.41	-0.00	-0.00
23	1	-0.31	0.00	-0.00	-0.00	-0.16	0.22	-0.21	-0.00	0.00
24	1	-0.31	-0.00	-0.00	-0.00	0.10	0.21	0.14	0.00	0.00

Normal termination of Gaussian 16

```
****************************************
Gaussian 16:  AS64L-G16RevA.03 25-Dec-2016
               29-Dec-2022
****************************************
```

```
--------------------------------------------------------------------------
#T td(nst=70) cam-b3lyp/cc-pvtz scrf(pcm,solvent=n-hexadecane) guess=r
ead geom=check
--------------------------------------------------------------------------
```

```
------------------------------
Tolan (diphenylacetylene), D2h
------------------------------
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	2.024922
2	6	0	0.000000	0.000000	0.599962
3	6	0	0.000000	0.000000	-0.599962
4	6	0	0.000000	0.000000	-2.024922
5	6	0	0.000000	1.202325	-2.732151
6	6	0	0.000000	1.198599	-4.113667
7	6	0	0.000000	0.000000	-4.808568
8	6	0	-0.000000	-1.198599	-4.113667
9	6	0	-0.000000	-1.202325	-2.732151
10	6	0	-0.000000	-1.202325	2.732151
11	6	0	-0.000000	-1.198599	4.113667
12	6	0	-0.000000	-0.000000	4.808568
13	6	0	-0.000000	1.198599	4.113667
14	6	0	-0.000000	1.202325	2.732151
15	1	0	0.000000	2.135168	-2.187363
16	1	0	0.000000	2.136318	-4.651200
17	1	0	0.000000	0.000000	-5.889347
18	1	0	-0.000000	-2.136318	-4.651200
19	1	0	-0.000000	-2.135168	-2.187363
20	1	0	-0.000000	-2.135168	2.187363
21	1	0	-0.000000	-2.136318	4.651200
22	1	0	-0.000000	-0.000000	5.889347
23	1	0	-0.000000	2.136318	4.651200
24	1	0	-0.000000	2.135168	2.187363

```
--------------------------------------------------------------------
  560 basis functions,   898 primitive gaussians,   640 cartesian basis functions
   47 alpha electrons       47 beta electrons
```

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

state	X	Y	Z	Dip. S.	Osc.
1	-0.0000	0.0000	3.1997	10.2380	1.1097
2	-0.0000	0.0079	-0.0000	0.0001	0.0000
3	0.0000	0.0000	-0.0000	0.0000	0.0000
4	0.0000	0.0000	0.0000	0.0000	0.0000
5	-0.0000	0.0000	-0.0000	0.0000	0.0000

6	-0.0000	-0.0000	0.0000	0.0000	0.0000
7	-0.0000	-1.8818	0.0000	3.5412	0.5378
8	0.0000	0.0000	-0.0000	0.0000	0.0000
9	-0.0000	-0.0000	0.0000	0.0000	0.0000
10	0.0000	0.0000	1.9916	3.9666	0.6389
11	0.1260	-0.0000	-0.0000	0.0159	0.0027
12	-0.0000	-0.0000	0.0000	0.0000	0.0000
13	0.0000	0.0000	-2.3474	5.5102	0.9814
14	0.0000	0.0000	0.0000	0.0000	0.0000
15	0.1234	-0.0000	0.0000	0.0152	0.0027
16	-0.0000	-0.0000	0.0000	0.0000	0.0000
17	0.0000	0.0000	-0.0000	0.0000	0.0000
18	0.0000	-0.0000	-0.0000	0.0000	0.0000
19	-0.0000	-0.6631	-0.0000	0.4397	0.0807
20	-0.0000	0.0000	0.0000	0.0000	0.0000
21	0.0000	-0.0000	-0.0000	0.0000	0.0000
22	-0.0000	-0.0000	0.0000	0.0000	0.0000
23	-0.0000	0.0000	-0.0000	0.0000	0.0000
24	0.2438	-0.0000	0.0000	0.0594	0.0115
25	-0.0000	0.0000	0.0000	0.0000	0.0000
26	0.0000	0.0000	-0.0000	0.0000	0.0000
27	0.0000	1.6194	0.0000	2.6225	0.5080
28	0.0000	0.0000	-0.0000	0.0000	0.0000
29	0.1609	-0.0000	-0.0000	0.0259	0.0051
30	-0.0000	-0.0000	0.0000	0.0000	0.0000
31	-0.0000	-0.0000	0.0202	0.0004	0.0001
32	0.0000	0.0000	0.0000	0.0000	0.0000
33	-0.0000	-0.0000	0.5268	0.2776	0.0564
34	0.2214	0.0000	0.0000	0.0490	0.0100
35	-0.0000	0.0000	0.0000	0.0000	0.0000
36	-0.0000	0.0000	0.0000	0.0000	0.0000
37	0.0000	-0.0000	-0.0000	0.0000	0.0000
38	0.0000	0.0000	-0.5670	0.3215	0.0662
39	-0.0000	0.9990	0.0000	0.9981	0.2058
40	0.0000	0.0000	-0.0000	0.0000	0.0000
41	0.3591	-0.0000	0.0000	0.1290	0.0272
42	0.0000	0.0000	0.0000	0.0000	0.0000
43	0.0000	-0.0000	-0.0000	0.0000	0.0000
44	-0.2326	0.0000	-0.0000	0.0541	0.0117
45	0.0000	0.0000	-0.0000	0.0000	0.0000
46	-0.0000	-0.0000	-0.0000	0.0000	0.0000
47	0.0000	-0.0000	-0.0000	0.0000	0.0000
48	0.0000	-0.0000	-0.0000	0.0000	0.0000
49	0.0000	-0.0000	-0.0000	0.0000	0.0000
50	0.0000	0.0000	-0.0000	0.0000	0.0000
51	0.2391	-0.0000	0.0000	0.0572	0.0128
52	0.0000	0.3198	0.0000	0.1023	0.0231
53	0.0000	0.0000	-0.0000	0.0000	0.0000
54	0.0000	0.0000	-0.6269	0.3930	0.0897
55	0.0324	-0.0000	-0.0000	0.0011	0.0002
56	0.0000	0.0000	-0.0000	0.0000	0.0000
57	0.0000	-0.0000	0.0000	0.0000	0.0000
58	0.0000	0.0000	-0.0000	0.0000	0.0000
59	0.0000	-0.0000	0.0000	0.0000	0.0000
60	0.0000	0.0000	0.0000	0.0000	0.0000
61	0.0000	-0.0000	-0.0000	0.0000	0.0000
62	-0.0000	-0.0000	-0.0000	0.0000	0.0000
63	0.0000	0.0000	0.0000	0.0000	0.0000
64	0.0000	0.0000	-0.0000	0.0000	0.0000
65	-0.0000	0.0000	1.1724	1.3744	0.3295
66	-0.0000	-0.0000	0.0000	0.0000	0.0000
67	0.0000	-0.0000	-0.0000	0.0000	0.0000
68	-0.1085	0.0000	-0.0000	0.0118	0.0028
69	-0.0000	0.0000	-0.0000	0.0000	0.0000
70	-0.0000	-0.0000	-0.0000	0.0000	0.0000

---

kK = 1000/cm. The notation [i,-j] indicates the singlet configuration derived by promotion of an electron from the i'th highest occupied to the j'th lowest unoccupied molecular orbital.

Excited State 1: 1 Singlet-B1U 35.68437 kK 280.23 nm f=1.1097

```
     47 -> 48         0.68626   94% [ 1,-1 ]

Excited State   2:      1 Singlet-B2U  41.45849 kK  241.20 nm  f=0.0000
     44 -> 50         0.21651
     45 -> 51         0.21891   10% [ 3,-4 ]
     46 -> 48         0.42690   36% [ 2,-1 ]
     47 -> 49         0.46889   44% [ 1,-2 ]

Excited State   3:      1 Singlet-B3G  41.55205 kK  240.66 nm  f=0.0000
     44 -> 49         0.21909   10% [ 4,-2 ]
     45 -> 48         0.42998   37% [ 3,-1 ]
     46 -> 51         0.22145   10% [ 2,-4 ]
     47 -> 50         0.46349   43% [ 1,-3 ]

Excited State   4:      1 Singlet-AU   42.64493 kK  234.49 nm  f=0.0000
     43 -> 48         0.68627   94% [ 5,-1 ]
     43 -> 61        -0.14598

Excited State   5:      2 Singlet-AG   48.46583 kK  206.33 nm  f=0.0000
     44 -> 48         0.36684   27% [ 4,-1 ]
     45 -> 49        -0.24948   12% [ 3,-2 ]
     46 -> 50        -0.24702   12% [ 2,-3 ]
     47 -> 51         0.48274   47% [ 1,-4 ]

Excited State   6:      2 Singlet-B3G  49.88618 kK  200.46 nm  f=0.0000
     45 -> 48        -0.48545   47% [ 3,-1 ]
     46 -> 51        -0.12536
     47 -> 50         0.49148   48% [ 1,-3 ]

Excited State   7:      2 Singlet-B2U  49.99345 kK  200.03 nm  f=0.5378
     45 -> 51        -0.12357
     46 -> 48        -0.48802   48% [ 2,-1 ]
     47 -> 49         0.48943   48% [ 1,-2 ]

Excited State   8:      2 Singlet-AU   50.49754 kK  198.03 nm  f=0.0000
     42 -> 54         0.18545
     47 -> 54         0.64356   83% [ 1,-7 ]
     47 -> 57        -0.17894

Excited State   9:      3 Singlet-AG   52.35987 kK  190.98 nm  f=0.0000
     42 -> 51        -0.12724
     44 -> 48         0.49886   50% [ 4,-1 ]
     47 -> 51        -0.46312   43% [ 1,-4 ]

Excited State  10:      2 Singlet-B1U  53.02931 kK  188.58 nm  f=0.6389
     42 -> 48         0.17799
     44 -> 51        -0.15134
     45 -> 50         0.46036   42% [ 3,-3 ]
     46 -> 49         0.46903   44% [ 2,-2 ]

Excited State  11:      1 Singlet-B3U  55.07958 kK  181.56 nm  f=0.0027
     44 -> 53        -0.12105
     47 -> 52         0.67049   90% [ 1,-5 ]
     47 -> 56        -0.14358

Excited State  12:      4 Singlet-AG   56.55718 kK  176.81 nm  f=0.0000
     44 -> 48         0.31115   19% [ 4,-1 ]
     45 -> 49         0.42606   36% [ 3,-2 ]
     46 -> 50         0.41955   35% [ 2,-3 ]
     47 -> 51         0.19643

Excited State  13:      3 Singlet-B1U  58.63164 kK  170.56 nm  f=0.9814
     42 -> 48         0.47975   46% [ 6,-1 ]
     43 -> 54        -0.34156   23% [ 5,-7 ]
     43 -> 57         0.10345
     44 -> 51        -0.22752   10% [ 4,-4 ]
     45 -> 50        -0.15165
     46 -> 49        -0.15509
     47 -> 61        -0.11591

Excited State  14:      1 Singlet-B1G  58.7873 kK  170.11 nm  f=0.0000
     40 -> 51         0.13852
     41 -> 48         0.34504   24% [ 7,-1 ]
```

```
     43 -> 51         0.58985   70% [ 5,-4 ]

Excited State  15:      2 Singlet-B3U  58.93329 kK  169.68 nm  f=0.0027
     41 -> 50         0.15808
     43 -> 49         0.67849   92% [ 5,-2 ]

Excited State  16:      1 Singlet-B2G  59.09783 kK  169.21 nm  f=0.0000
     41 -> 49         0.16159
     43 -> 50         0.67345   91% [ 5,-3 ]

Excited State  17:      2 Singlet-B2G  59.68177 kK  167.56 nm  f=0.0000
     44 -> 52        -0.25474   13% [ 4,-5 ]
     44 -> 56        -0.10251
     47 -> 53         0.63325   80% [ 1,-6 ]

Excited State  18:      3 Singlet-B3G  60.37218 kK  165.64 nm  f=0.0000
     42 -> 50        -0.24691   12% [ 6,-3 ]
     44 -> 49         0.51583   53% [ 4,-2 ]
     45 -> 48        -0.23278   11% [ 3,-1 ]
     46 -> 51         0.27345   15% [ 2,-4 ]
     47 -> 50        -0.18930

Excited State  19:      3 Singlet-B2U  60.42945 kK  165.48 nm  f=0.0807
     42 -> 49        -0.24705   12% [ 6,-2 ]
     44 -> 50         0.50432   51% [ 4,-3 ]
     45 -> 51         0.29059   17% [ 3,-4 ]
     46 -> 48        -0.23984   12% [ 2,-1 ]
     47 -> 49        -0.18048

Excited State  20:      3 Singlet-AU   62.06514 kK  161.12 nm  f=0.0000
     40 -> 48         0.61385   75% [ 8,-1 ]
     41 -> 51         0.32725   21% [ 7,-4 ]

Excited State  21:      2 Singlet-B1G  62.28129 kK  160.56 nm  f=0.0000
     45 -> 52         0.34089   23% [ 3,-5 ]
     46 -> 53        -0.23648   11% [ 2,-6 ]
     47 -> 55         0.53120   56% [ 1,-8 ]
     47 -> 59        -0.12537

Excited State  22:      3 Singlet-B1G  63.00881 kK  158.71 nm  f=0.0000
     40 -> 51         0.27701   15% [ 8,-4 ]
     41 -> 48         0.51804   54% [ 7,-1 ]
     43 -> 51        -0.36432   27% [ 5,-4 ]

Excited State  23:      4 Singlet-AU   63.24513 kK  158.11 nm  f=0.0000
     45 -> 53        -0.42147   36% [ 3,-6 ]
     46 -> 52         0.53996   58% [ 2,-5 ]

Excited State  24:      3 Singlet-B3U  63.56049 kK  157.33 nm  f=0.0115
     38 -> 48         0.10457
     42 -> 52        -0.13199
     44 -> 53        -0.27187   15% [ 4,-6 ]
     47 -> 56         0.59844   72% [ 1,-9 ]

Excited State  25:      4 Singlet-B3G  63.61292 kK  157.20 nm  f=0.0000
     42 -> 50         0.11430
     44 -> 49        -0.32822   22% [ 4,-2 ]
     45 -> 48        -0.15121
     45 -> 61         0.11264
     46 -> 51         0.58144   68% [ 2,-4 ]

Excited State  26:      3 Singlet-B2G  63.71615 kK  156.95 nm  f=0.0000
     38 -> 51         0.31120   19% [ 10,-4 ]
     39 -> 48         0.62302   78% [ 9,-1 ]

Excited State  27:      4 Singlet-B2U  63.77503 kK  156.80 nm  f=0.5080
     42 -> 49         0.12117
     44 -> 50        -0.33732   23% [ 4,-3 ]
     45 -> 51         0.57109   65% [ 3,-4 ]
     46 -> 48        -0.14022
     46 -> 61         0.10901

Excited State  28:      4 Singlet-B1G  63.90085 kK  156.49 nm  f=0.0000
```

```
     45 -> 52        -0.40851   33% [ 3,-5 ]
     46 -> 53         0.35200   25% [ 2,-6 ]
     47 -> 55         0.41234   34% [ 1,-8 ]

Excited State  29:      4 Singlet-B3U  64.57191 kK  154.87 nm  f=0.0051
     38 -> 48         0.59537   71% [ 10,-1 ]
     39 -> 51         0.33646   23% [ 9,-4 ]
     47 -> 56        -0.11159

Excited State  30:      5 Singlet-AG   66.16163 kK  151.15 nm  f=0.0000
     45 -> 49        -0.49667   49% [ 3,-2 ]
     46 -> 50         0.50323   51% [ 2,-3 ]

Excited State  31:      4 Singlet-B1U  66.16243 kK  151.14 nm  f=0.0001
     45 -> 50         0.50385   51% [ 3,-3 ]
     46 -> 49        -0.49600   49% [ 2,-2 ]

Excited State  32:      4 Singlet-B2G  66.86896 kK  149.55 nm  f=0.0000
     40 -> 50         0.46879   44% [ 8,-3 ]
     41 -> 49         0.47228   45% [ 7,-2 ]
     43 -> 50        -0.18667

Excited State  33:      5 Singlet-B1U  66.8714 kK  149.54 nm  f=0.0564
     42 -> 48         0.37204   28% [ 6,-1 ]
     44 -> 51         0.51774   54% [ 4,-4 ]
     47 -> 61         0.25562   13% [ 1,-14 ]

Excited State  34:      5 Singlet-B3U  66.88188 kK  149.52 nm  f=0.0100
     40 -> 49         0.47488   45% [ 8,-2 ]
     41 -> 50         0.47161   44% [ 7,-3 ]
     43 -> 49        -0.18095

Excited State  35:      5 Singlet-AU   67.06255 kK  149.12 nm  f=0.0000
     38 -> 49        -0.14134
     39 -> 50        -0.14681
     44 -> 55        -0.22737   10% [ 4,-8 ]
     47 -> 54         0.16717
     47 -> 57         0.59095   70% [ 1,-10 ]

Excited State  36:      5 Singlet-B1G  67.4989 kK  148.15 nm  f=0.0000
     38 -> 50         0.47983   46% [ 10,-3 ]
     39 -> 49         0.50597   51% [ 9,-2 ]

Excited State  37:      6 Singlet-AU   67.54003 kK  148.06 nm  f=0.0000
     38 -> 49         0.46263   43% [ 10,-2 ]
     39 -> 50         0.48113   46% [ 9,-3 ]
     47 -> 57         0.18636

Excited State  38:      6 Singlet-B1U  67.83361 kK  147.42 nm  f=0.0662
     36 -> 48         0.11238
     42 -> 48        -0.21042
     42 -> 61        -0.10636
     43 -> 54        -0.35016   25% [ 5,-7 ]
     43 -> 57         0.10070
     44 -> 51         0.36074   26% [ 4,-4 ]
     47 -> 48        -0.11173
     47 -> 61        -0.34860   24% [ 1,-14 ]
     47 -> 67        -0.10634

Excited State  39:      5 Singlet-B2U  67.87474 kK  147.33 nm  f=0.2058
     43 -> 52         0.63286   80% [ 5,-5 ]
     43 -> 56        -0.26439   14% [ 5,-9 ]

Excited State  40:      5 Singlet-B2G  68.51837 kK  145.95 nm  f=0.0000
     42 -> 53         0.12063
     44 -> 56         0.20702
     45 -> 54         0.19543
     45 -> 57         0.24956   12% [ 3,-10 ]
     46 -> 55        -0.35536   25% [ 2,-8 ]
     47 -> 58         0.41248   34% [ 1,-11 ]
     47 -> 62         0.10549

Excited State  41:      6 Singlet-B3U  69.4322 kK  144.03 nm  f=0.0272
```

```
     45 -> 55        -0.43360   38% [ 3,-8 ]
     46 -> 54         0.44339   39% [ 2,-7 ]
     46 -> 57         0.26137   14% [ 2,-10 ]
     47 -> 56        -0.10500

Excited State  42:      6 Singlet-B2G  70.00485 kK  142.85 nm  f=0.0000
     44 -> 52         0.17120
     44 -> 56        -0.17444
     45 -> 54         0.45863   42% [ 3,-7 ]
     46 -> 55        -0.22491   10% [ 2,-8 ]
     47 -> 58        -0.36876   27% [ 1,-11 ]

Excited State  43:      6 Singlet-B1G  70.23311 kK  142.38 nm  f=0.0000
     37 -> 54         0.10475
     44 -> 54         0.61313   75% [ 4,-7 ]
     47 -> 59        -0.30988   19% [ 1,-12 ]

Excited State  44:      7 Singlet-B3U  71.23566 kK  140.38 nm  f=0.0117
     45 -> 55         0.29783   18% [ 3,-8 ]
     46 -> 54         0.52421   55% [ 2,-7 ]
     46 -> 57        -0.34658   24% [ 2,-10 ]

Excited State  45:      7 Singlet-B2G  71.33325 kK  140.19 nm  f=0.0000
     44 -> 52        -0.20344
     45 -> 54         0.47267   45% [ 3,-7 ]
     45 -> 57        -0.32066   21% [ 3,-10 ]
     46 -> 55         0.27421   15% [ 2,-8 ]
     47 -> 58         0.17878

Excited State  46:      7 Singlet-AU   71.83654 kK  139.21 nm  f=0.0000
     45 -> 53        -0.31261   20% [ 3,-6 ]
     45 -> 58         0.19517
     46 -> 52        -0.28633   16% [ 2,-5 ]
     46 -> 56         0.50636   51% [ 2,-9 ]

Excited State  47:      7 Singlet-B1G  71.8809 kK  139.12 nm  f=0.0000
     45 -> 52        -0.28398   16% [ 3,-5 ]
     45 -> 56         0.49845   50% [ 3,-9 ]
     46 -> 53        -0.30670   19% [ 2,-6 ]
     46 -> 58         0.19480

Excited State  48:      8 Singlet-B2G  72.24546 kK  138.42 nm  f=0.0000
     42 -> 53         0.11652
     44 -> 52         0.56246   63% [ 4,-5 ]
     45 -> 57        -0.11263
     46 -> 55         0.18743
     47 -> 53         0.22226   10% [ 1,-6 ]
     47 -> 58         0.21913   10% [ 1,-11 ]

Excited State  49:      8 Singlet-B1G  72.6439 kK  137.66 nm  f=0.0000
     44 -> 54         0.24717   12% [ 4,-7 ]
     44 -> 57        -0.26578   14% [ 4,-10 ]
     44 -> 63         0.10853
     47 -> 59         0.56216   63% [ 1,-12 ]

Excited State  50:      6 Singlet-AG   73.10525 kK  136.79 nm  f=0.0000
     36 -> 51        -0.13092
     37 -> 48         0.50132   50% [ 11,-1 ]
     42 -> 51         0.43087   37% [ 6,-4 ]
     43 -> 55        -0.11614
     44 -> 61        -0.10844

Excited State  51:      8 Singlet-B3U  73.92875 kK  135.27 nm  f=0.0128
     44 -> 58         0.25390   13% [ 4,-11 ]
     47 -> 60         0.61291   75% [ 1,-13 ]
     47 -> 65         0.14158

Excited State  52:      6 Singlet-B2U  74.38444 kK  134.44 nm  f=0.0231
     37 -> 50         0.20878
     42 -> 49         0.60959   74% [ 6,-2 ]
     44 -> 50         0.26440   14% [ 4,-3 ]

Excited State  53:      5 Singlet-B3G  74.47559 kK  134.27 nm  f=0.0000
```

```
     37 -> 49         0.21701
     42 -> 50         0.60932   74% [ 6,-3 ]
     44 -> 49         0.25582   13% [ 4,-2 ]

Excited State  54:      7 Singlet-B1U  75.14422 kK  133.08 nm  f=0.0897
     36 -> 48         0.47696   45% [ 12,-1 ]
     37 -> 51        -0.20885
     42 -> 48        -0.12643
     43 -> 54        -0.17536
     47 -> 61         0.38806   30% [ 1,-14 ]

Excited State  55:      9 Singlet-B3U  75.99513 kK  131.59 nm  f=0.0002
     42 -> 52         0.23940   11% [ 6,-5 ]
     44 -> 53         0.53346   57% [ 4,-6 ]
     45 -> 55        -0.13336
     47 -> 52         0.16826
     47 -> 56         0.24759   12% [ 1,-9 ]
     47 -> 60        -0.11478

Excited State  56:      7 Singlet-AG   76.41938 kK  130.86 nm  f=0.0000
     36 -> 51        -0.11094
     37 -> 48         0.25901   13% [ 11,-1 ]
     42 -> 51        -0.11340
     43 -> 55         0.57861   67% [ 5,-8 ]
     43 -> 59        -0.19855
     47 -> 64         0.12087

Excited State  57:      6 Singlet-B3G  76.78475 kK  130.23 nm  f=0.0000
     41 -> 52        -0.10129
     43 -> 53         0.64254   83% [ 5,-6 ]
     43 -> 58         0.21481
     43 -> 62         0.12361

Excited State  58:      8 Singlet-AU   76.90411 kK  130.03 nm  f=0.0000
     36 -> 54         0.15226
     42 -> 54         0.43951   39% [ 6,-7 ]
     44 -> 59         0.20233
     46 -> 52         0.10112
     47 -> 54        -0.18891
     47 -> 63         0.38998   30% [ 1,-16 ]

Excited State  59:      8 Singlet-AG   77.41628 kK  129.17 nm  f=0.0000
     36 -> 51         0.15951
     37 -> 48        -0.32253   21% [ 11,-1 ]
     42 -> 51         0.44178   39% [ 6,-4 ]
     43 -> 55         0.29373   17% [ 5,-8 ]
     44 -> 61        -0.13404
     47 -> 64        -0.21580

Excited State  60:      9 Singlet-B2G  77.88005 kK  128.40 nm  f=0.0000
     42 -> 53         0.10000
     44 -> 56         0.16066
     44 -> 60        -0.23626   11% [ 4,-13 ]
     47 -> 58        -0.15881
     47 -> 62         0.56847   65% [ 1,-15 ]
     47 -> 66         0.14272

Excited State  61:      9 Singlet-AU   77.96796 kK  128.26 nm  f=0.0000
     44 -> 55         0.18235
     45 -> 53         0.25047   13% [ 3,-6 ]
     45 -> 58         0.42200   36% [ 3,-11 ]
     46 -> 52         0.26170   14% [ 2,-5 ]
     46 -> 56         0.17079
     46 -> 60         0.29276   17% [ 2,-13 ]

Excited State  62:      9 Singlet-B1G  78.02281 kK  128.17 nm  f=0.0000
     45 -> 52         0.28529   16% [ 3,-5 ]
     45 -> 56         0.17703
     45 -> 60         0.29983   18% [ 3,-13 ]
     46 -> 53         0.27695   15% [ 2,-6 ]
     46 -> 58         0.44179   39% [ 2,-11 ]

Excited State  63:      10 Singlet-AU   78.58094 kK  127.26 nm  f=0.0000
```

```
     34 -> 48         0.51580   53% [ 14,-1 ]
     35 -> 51         0.26136   14% [ 13,-4 ]
     40 -> 48         0.12198
     40 -> 61        -0.12011
     41 -> 51        -0.20841
     43 -> 61        -0.22387   10% [ 5,-14 ]

Excited State  64:      10 Singlet-B1G  78.735 kK  127.01 nm  f=0.0000
     31 -> 48         0.12450
     34 -> 51         0.27361   15% [ 14,-4 ]
     35 -> 48         0.53276   57% [ 13,-1 ]
     40 -> 51        -0.22089   10% [ 8,-4 ]
     41 -> 61        -0.15210

Excited State  65:      8 Singlet-B1U  78.92696 kK  126.70 nm  f=0.3295
     36 -> 48         0.40250   32% [ 12,-1 ]
     37 -> 51        -0.14566
     42 -> 48         0.12078
     43 -> 54         0.32685   21% [ 5,-7 ]
     44 -> 64        -0.13952
     47 -> 61        -0.32624   21% [ 1,-14 ]
     47 -> 67         0.20861

Excited State  66:      11 Singlet-AU   78.9939 kK  126.59 nm  f=0.0000
     36 -> 54         0.11499
     42 -> 54         0.28321   16% [ 6,-7 ]
     44 -> 55         0.48551   47% [ 4,-8 ]
     44 -> 59        -0.18104
     47 -> 57         0.21946   10% [ 1,-10 ]
     47 -> 63        -0.20762

Excited State  67:      10 Singlet-B2G  79.01245 kK  126.56 nm  f=0.0000
     44 -> 56        -0.18554
     45 -> 57        -0.28133   16% [ 3,-10 ]
     45 -> 63         0.22895   10% [ 3,-16 ]
     46 -> 55        -0.25378   13% [ 2,-8 ]
     46 -> 59         0.47090   44% [ 2,-12 ]

Excited State  68:      10 Singlet-B3U  79.34798 kK  126.03 nm  f=0.0028
     44 -> 53        -0.10804
     45 -> 55        -0.25305   13% [ 3,-8 ]
     45 -> 59         0.48919   48% [ 3,-12 ]
     46 -> 57        -0.31928   20% [ 2,-10 ]
     46 -> 63         0.22510   10% [ 2,-16 ]

Excited State  69:      11 Singlet-B2G  79.88192 kK  125.19 nm  f=0.0000
     29 -> 48        -0.12590
     32 -> 51         0.23905   11% [ 16,-4 ]
     33 -> 48         0.56519   64% [ 15,-1 ]
     38 -> 51        -0.22269   10% [ 10,-4 ]
     39 -> 61        -0.11741

Excited State  70:      12 Singlet-AU   80.26503 kK  124.59 nm  f=0.0000
     30 -> 48        -0.13273
     42 -> 57        -0.13448
     43 -> 61         0.39255   31% [ 5,-14 ]
     43 -> 67         0.16098
     44 -> 55        -0.28246   16% [ 4,-8 ]
     45 -> 53         0.14965
     47 -> 63        -0.30235   18% [ 1,-16 ]

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

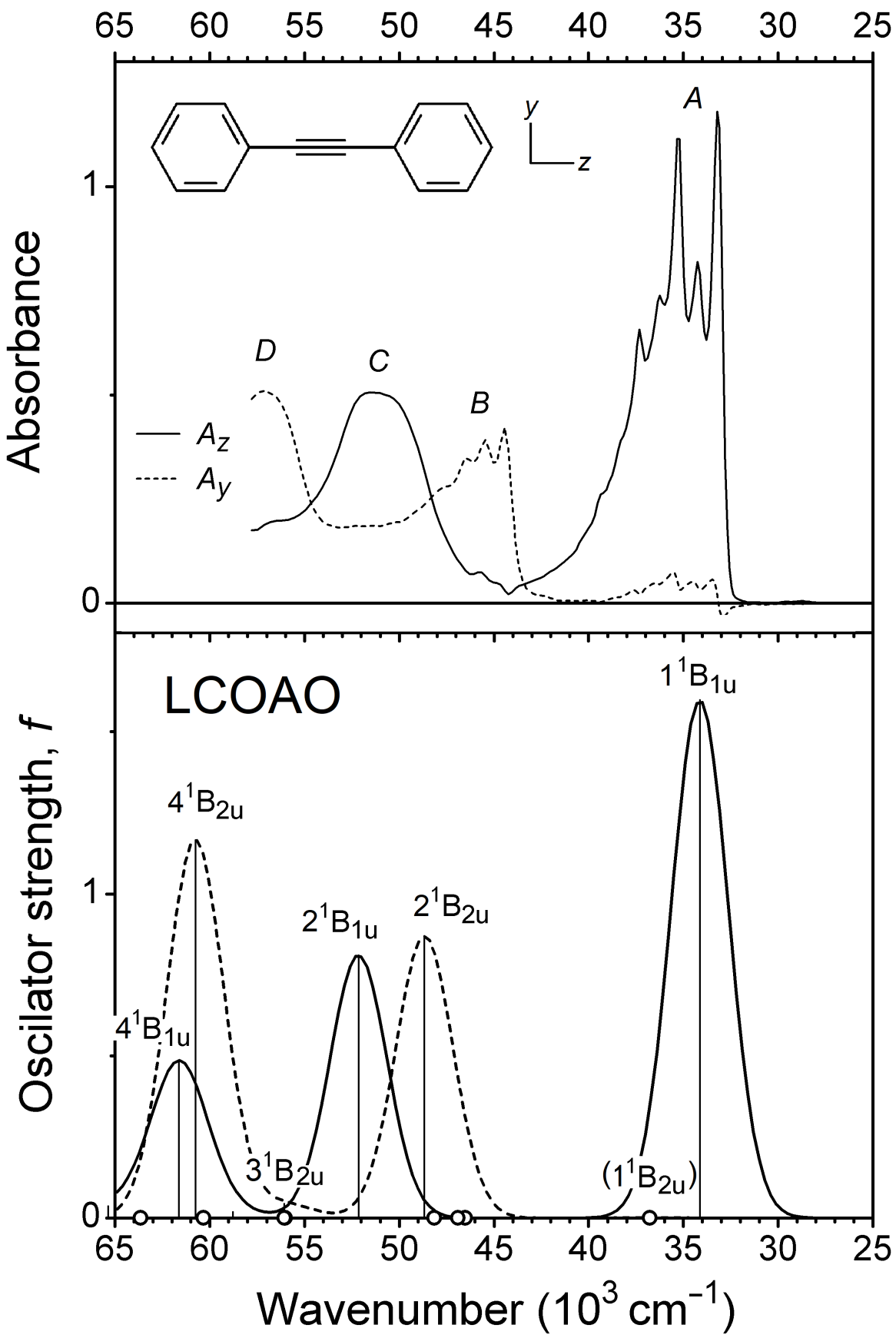
```
                 (B1U) (B2U) (B3U) (B2U) (AG) (B1G) (B1U) (B1U)
                 (AU) (B3G) (B2G) (AG) (B3U) (B3G) (B2U) (B2G)
                 (AG) (B3G) (B1U) (B2U) (B3U) (AG) (B1U) (B2U)
                 (B3G) (AG) (B2G) (AG) (B1U) (B2U) (B1U) (B3G)
                 (B3U) (B1G) (B3G) (AG) (B2U) (B1U) (AU) (AG) (B2G)
                 (B1G) (AU) (B3G) (B2U) (B1G) (B3U) (AG) (B2U)
                 (B3G) (B1U) (B2U) (B1U) (B3G) (AU) (AG) (B1U)
                 (AG) (B2G) (B1U) (B1G) (B3U) (AG) (B1U) (B2U)
                 (B3G) (B2G) (B1U) (B3G) (AG) (B3G) (AU) (B2U)
                 (AG) (B3U) (AG) (B1U) (B2G) (B1G) (B3U) (B2G)
                 (B2U) (B3U) (AG) (B1U) (B3G) (AU) (B2G) (B1U)
                 (B1G) (B1U) (B2U) (AG) (AU) (B1U) (B3U) (B2U)
                 (B3G) (B3G) (AG) (B1U) (B2U) (B2G) (AG) (B2U)
                 (B1U) (B3G) (B3U) (B1G) (B2U) (B3G) (AG) (AU)
                 (B2G) (B1U) (AG) (B3G) (B2U) (B1G) (B1U) (B3G)
                 (AG) (AU) (B2U) (B1U) (B3G) (B3U) (B1U) (AG) (B2U)
                 (AG) (B2G) (B3G) (AG) (B1U) (B2U) (B1U) (B1G)
                 (B3U) (AU) (AG) (B2G) (B1U) (B3G) (AG) (B2U) (B3G)
                 (B2U) (B1U) (AG) (B3G) (B3U) (B1U) (AG) (B2G)
                 (B2U) (B3U) (B1U) (AG) (B1G) (AU) (B3G) (B2U)
                 (B1U) (B3U) (B2G) (AG) (B1G) (AU) (B1U) (B3G)
                 (B2U) (B3U) (B1G) (B2G) (B2U) (B3G) (AG) (AU)
                 (AG) (B1U) (B1U) (B2U) (B1U) (B3G) (B2G) (B2U)
                 (B3G) (AG) (AG) (B3U) (B2G) (B3U) (AG) (B1U) (B3U)
                 (B2U) (B3G) (B2G) (B1G) (B2U) (AG) (B2G) (B3G)
                 (B3U) (B1U) (AU) (B1G) (B3U) (B2U) (B2G) (B3U)
                 (AG) (B2G) (B3G) (B1U) (AU) (B1G) (AU) (B2U) (AG)
                 (B3G) (B1U) (B1G) (AG) (B3U) (B2U) (B3U) (B1U)
                 (B2G) (AG) (B1U) (AU) (B2U) (B3G) (B2G) (B3U)
                 (B1G) (AG) (B2G) (AG) (B3G) (B3G) (AU) (B2G) (B1U)
                 (B2U) (B3U) (AG) (B1G) (B1U) (AG) (B3G) (B1U)
                 (B3G) (B2U) (B1G) (AU) (B2U) (B2G) (AG) (B3G)
                 (B1U) (B1U) (B3U) (AG) (B1G) (B2U) (AU) (B2U)
                 (AG) (B1G) (B3U) (AU) (B3G) (B2G) (B1U) (B1U)
                 (B2U) (B2G) (B3G) (B3U) (AG) (B1G) (AG) (AU) (B2U)
                 (B3G) (B1U) (B3U) (B1U) (B1G) (AU) (B2U) (B3G)
                 (B2G) (B1U) (AG) (B3U) (B2U) (B2G) (AG) (AU) (B1U)
                 (B3G) (B3G) (B1G) (AG) (B1U) (B2G) (AG) (B2U)
                 (B3U) (B1U) (AU) (AG) (B1G) (B3G) (AG) (B2U) (B2G)
                 (B1G) (B3U) (AU) (B1U) (B3G) (B2U) (B3G) (B1U)
                 (AU) (B2G) (AG) (B3U) (B1G) (B2U) (B2G) (B3U)
                 (B1U) (B1G) (AU) (B3G) (AG) (B2U) (AG) (B2G) (B1U)
                 (AU) (AG) (B2U) (B3U) (B3G) (B1U) (B2U) (B3G)
                 (B1G) (B1U) (AG) (B2G) (B1U) (AU) (B2U) (AG) (B3G)
                 (B3U) (B1U) (B2G) (AG) (B3G) (B2U) (B2U) (B1U)
                 (AG) (B1U) (B3G) (B1G) (B3U) (B2G) (B1G) (AU)
                 (B1U) (B3U) (B2U) (B3G) (AG) (B2G) (B1U) (AU)
                 (AG) (B3G) (AG) (B2U) (B3G) (B1U) (B3U) (B1U)
                 (AG) (B2U) (B2G) (AG) (B1U) (B3U) (B3U) (B2G)
                 (B1G) (B3G) (AU) (B2U) (B1G) (AU) (B2U) (B3G)
                 (AG) (B2G) (B1U) (B3U) (B3G) (B2U) (AG) (B1U)
                 (B1G) (AU) (B1U) (B2U) (B3G) (AG) (B1U) (AG) (B2U)
                 (B3G) (B3G) (B1U) (B2G) (B2U) (AG) (B3U) (B3G)
                 (B1U) (AG) (B2U) (B1U) (AG) (B1U) (B2G) (B3G)
                 (B2U) (AG) (B3G) (B1U) (B2U) (B3G) (B2U) (B1U)
                 (AG) (B3G) (B1U) (AG) (B2U) (B3G) (AG) (B1U) (AG)
                 (AG) (B2U) (B1U) (B3G) (AG) (B1U) (B2U) (B3G)
                 (B1U) (AG) (B1U)
 The electronic state is 1-AG.
 Alpha  occ. eigenvalues --  -10.27896 -10.27895 -10.25741 -10.25740 -10.25738
 Alpha  occ. eigenvalues --  -10.25738 -10.25553 -10.25553 -10.25492 -10.25492
 Alpha  occ. eigenvalues --  -10.25463 -10.25463 -10.25026 -10.24767  -0.95922
 Alpha  occ. eigenvalues --   -0.95630  -0.88027  -0.85540  -0.83851  -0.83832
 Alpha  occ. eigenvalues --   -0.80190  -0.71600  -0.69189  -0.69023  -0.68831
 Alpha  occ. eigenvalues --   -0.62619  -0.61061  -0.56033  -0.54764  -0.53831
 Alpha  occ. eigenvalues --   -0.53289  -0.51150  -0.50541  -0.49751  -0.49713
 Alpha  occ. eigenvalues --   -0.46862  -0.45609  -0.42986  -0.42552  -0.42018
 Alpha  occ. eigenvalues --   -0.41611  -0.39161  -0.33994  -0.33487  -0.32057
 Alpha  occ. eigenvalues --   -0.32038  -0.27160
 Alpha virt. eigenvalues --   -0.01453   0.03009   0.03094   0.04431   0.07243
 Alpha virt. eigenvalues --    0.08593   0.09923   0.10256   0.10617   0.11694
 Alpha virt. eigenvalues --    0.13309   0.13855   0.14818   0.15262   0.16874
 Alpha virt. eigenvalues --    0.17774   0.20369   0.22039   0.22383   0.24001
```

```
Alpha virt. eigenvalues --    0.24824   0.26228   0.27820   0.29147   0.29685
Alpha virt. eigenvalues --    0.29870   0.30380   0.31104   0.31109   0.32698
Alpha virt. eigenvalues --    0.33122   0.34753   0.35622   0.36263   0.36574
Alpha virt. eigenvalues --    0.36756   0.37028   0.38414   0.38889   0.39556
Alpha virt. eigenvalues --    0.40519   0.40775   0.41095   0.43249   0.43721
Alpha virt. eigenvalues --    0.43825   0.44183   0.45314   0.45398   0.45413
Alpha virt. eigenvalues --    0.45524   0.45858   0.46124   0.46834   0.47448
Alpha virt. eigenvalues --    0.47996   0.49053   0.49366   0.50185   0.51080
Alpha virt. eigenvalues --    0.51997   0.52252   0.53058   0.53415   0.54400
Alpha virt. eigenvalues --    0.55794   0.55853   0.56420   0.58087   0.59691
Alpha virt. eigenvalues --    0.60116   0.60154   0.60911   0.61772   0.61903
Alpha virt. eigenvalues --    0.62135   0.62385   0.63779   0.65655   0.67756
Alpha virt. eigenvalues --    0.70101   0.71832   0.73147   0.73150   0.74203
Alpha virt. eigenvalues --    0.74746   0.75548   0.76021   0.76348   0.76553
Alpha virt. eigenvalues --    0.78099   0.78160   0.80092   0.80161   0.80225
Alpha virt. eigenvalues --    0.80641   0.82751   0.83071   0.84212   0.84379
Alpha virt. eigenvalues --    0.84839   0.85766   0.86251   0.87817   0.90187
Alpha virt. eigenvalues --    0.91195   0.91503   0.92104   0.92651   0.95208
Alpha virt. eigenvalues --    0.96413   0.97945   0.98816   0.99123   0.99228
Alpha virt. eigenvalues --    1.01851   1.02434   1.03932   1.04211   1.06473
Alpha virt. eigenvalues --    1.06475   1.06990   1.07608   1.08752   1.09294
Alpha virt. eigenvalues --    1.09706   1.10645   1.12224   1.13643   1.13739
Alpha virt. eigenvalues --    1.15776   1.16466   1.18024   1.19028   1.21172
Alpha virt. eigenvalues --    1.21742   1.22672   1.23420   1.24015   1.25498
Alpha virt. eigenvalues --    1.25546   1.29716   1.30499   1.31124   1.31527
Alpha virt. eigenvalues --    1.31861   1.31883   1.32634   1.33492   1.34394
Alpha virt. eigenvalues --    1.35239   1.36659   1.37803   1.38614   1.39103
Alpha virt. eigenvalues --    1.40781   1.41075   1.41780   1.42081   1.43726
Alpha virt. eigenvalues --    1.43957   1.44665   1.45047   1.45083   1.46202
Alpha virt. eigenvalues --    1.46286   1.50354   1.50626   1.50858   1.51792
Alpha virt. eigenvalues --    1.53648   1.56156   1.56344   1.57621   1.58195
Alpha virt. eigenvalues --    1.61684   1.62068   1.64580   1.66214   1.67362
Alpha virt. eigenvalues --    1.69093   1.71168   1.74671   1.78467   1.87198
Alpha virt. eigenvalues --    1.87498   1.89270   1.94391   1.97386   1.98297
Alpha virt. eigenvalues --    1.99314   2.00661   2.01200   2.03872   2.05350
Alpha virt. eigenvalues --    2.05901   2.06542   2.07999   2.08850   2.12625
Alpha virt. eigenvalues --    2.15739   2.16809   2.17834   2.18454   2.20218
Alpha virt. eigenvalues --    2.21609   2.21841   2.22350   2.24361   2.27333
Alpha virt. eigenvalues --    2.29941   2.30527   2.31004   2.33796   2.34727
Alpha virt. eigenvalues --    2.34985   2.38547   2.39696   2.40784   2.41286
Alpha virt. eigenvalues --    2.42912   2.45391   2.48607   2.49100   2.50098
Alpha virt. eigenvalues --    2.51660   2.52787   2.52900   2.53184   2.53494
Alpha virt. eigenvalues --    2.54215   2.54467   2.55873   2.57244   2.58355
Alpha virt. eigenvalues --    2.59206   2.61562   2.62681   2.64210   2.65497
Alpha virt. eigenvalues --    2.65571   2.68302   2.68762   2.69970   2.70860
Alpha virt. eigenvalues --    2.71148   2.71557   2.71676   2.73447   2.75398
Alpha virt. eigenvalues --    2.75412   2.76210   2.76835   2.77153   2.78678
Alpha virt. eigenvalues --    2.79634   2.80274   2.81212   2.81293   2.81379
Alpha virt. eigenvalues --    2.82642   2.83404   2.86469   2.86497   2.88258
Alpha virt. eigenvalues --    2.88966   2.89009   2.90439   2.92143   2.92320
Alpha virt. eigenvalues --    2.92676   2.93458   2.96671   2.97170   2.97226
Alpha virt. eigenvalues --    2.97573   2.97827   2.97861   2.98575   3.00179
Alpha virt. eigenvalues --    3.03791   3.04262   3.04451   3.04995   3.05188
Alpha virt. eigenvalues --    3.05636   3.05767   3.05886   3.05930   3.07685
Alpha virt. eigenvalues --    3.10495   3.10899   3.11812   3.11883   3.12466
Alpha virt. eigenvalues --    3.12550   3.12563   3.13151   3.13575   3.13603
Alpha virt. eigenvalues --    3.14439   3.14613   3.14941   3.16225   3.16629
Alpha virt. eigenvalues --    3.17466   3.18859   3.19066   3.19100   3.19895
Alpha virt. eigenvalues --    3.23358   3.23578   3.24947   3.26486   3.28324
Alpha virt. eigenvalues --    3.30402   3.32235   3.32324   3.33243   3.34535
Alpha virt. eigenvalues --    3.35235   3.37083   3.37277   3.37548   3.38982
Alpha virt. eigenvalues --    3.39828   3.39889   3.41335   3.41431   3.41884
Alpha virt. eigenvalues --    3.43992   3.44181   3.44299   3.44409   3.44989
Alpha virt. eigenvalues --    3.45311   3.46916   3.48591   3.48934   3.49848
Alpha virt. eigenvalues --    3.50140   3.50299   3.52788   3.53045   3.53553
Alpha virt. eigenvalues --    3.53865   3.59158   3.59763   3.60441   3.63403
Alpha virt. eigenvalues --    3.65013   3.68822   3.69553   3.70581   3.72554
Alpha virt. eigenvalues --    3.72838   3.74115   3.76439   3.77571   3.80810
Alpha virt. eigenvalues --    3.83656   3.84433   3.84698   3.84705   3.84757
Alpha virt. eigenvalues --    3.85308   3.86004   3.86396   3.86701   3.87845
Alpha virt. eigenvalues --    3.87901   3.88650   3.89170   3.89965   3.90741
Alpha virt. eigenvalues --    3.92097   3.92510   3.94256   3.94702   3.95642
Alpha virt. eigenvalues --    3.95658   3.95715   3.95959   3.96244   3.99808
```

```
Alpha virt. eigenvalues --    4.00384   4.01393   4.02057   4.08307   4.08423
Alpha virt. eigenvalues --    4.10139   4.10167   4.12416   4.15378   4.16413
Alpha virt. eigenvalues --    4.16967   4.17827   4.18431   4.19096   4.20299
Alpha virt. eigenvalues --    4.20411   4.20935   4.24421   4.24531   4.24601
Alpha virt. eigenvalues --    4.28540   4.28947   4.29211   4.31577   4.31864
Alpha virt. eigenvalues --    4.34188   4.34217   4.34842   4.35622   4.35676
Alpha virt. eigenvalues --    4.36886   4.39274   4.40114   4.40496   4.40822
Alpha virt. eigenvalues --    4.41365   4.41410   4.41830   4.42641   4.42915
Alpha virt. eigenvalues --    4.44616   4.47586   4.49520   4.53374   4.57146
Alpha virt. eigenvalues --    4.59872   4.60887   4.63284   4.70423   4.70653
Alpha virt. eigenvalues --    4.71922   4.73424   4.75397   4.76630   4.78091
Alpha virt. eigenvalues --    4.80026   4.80068   4.80459   4.80685   4.84824
Alpha virt. eigenvalues --    4.85213   4.85281   4.85360   4.88264   4.95798
Alpha virt. eigenvalues --    4.96362   4.96601   4.97486   4.98429   4.99780
Alpha virt. eigenvalues --    5.06421   5.06914   5.07026   5.07501   5.09246
Alpha virt. eigenvalues --    5.10829   5.11188   5.13831   5.14648   5.15555
Alpha virt. eigenvalues --    5.16212   5.20323   5.22945   5.24830   5.25648
Alpha virt. eigenvalues --    5.31237   5.39224   5.42421   5.42832   5.50944
Alpha virt. eigenvalues --    5.51802   5.57420   5.63272   5.66054   5.71088
Alpha virt. eigenvalues --    5.74555   5.78746   5.79700   5.81094   5.95457
Alpha virt. eigenvalues --    5.99774   6.00913   6.05379   6.07239   6.07310
Alpha virt. eigenvalues --    6.11424   6.16660   6.20511   6.22836   6.41635
Alpha virt. eigenvalues --    6.53055   6.55045   6.97306   7.03438   8.70400
Alpha virt. eigenvalues --    9.60001  10.57121  12.48892  12.81811  12.85643
Alpha virt. eigenvalues --   12.86381  12.96750  13.14181  13.47152  13.95635
Alpha virt. eigenvalues --   15.64571  15.66281  18.25559

Normal termination of Gaussian 16.
```

S4. Computational results obtained with LCOAO.



```
                  >-----------<
                    L C O A O
                  >-----------<

"Linear Combination of Orthogonalized Atomic Orbitals"
 J. Spanget-Larsen: Theor. Chem. Acc. 59, 137 (1997)

        100 atoms - 300 orbitals development-vs.
                      Dec. 2005
-------------------------------------------------BKVH-

---------------------------
Tolan, CAM-B3LYP/aVTZ geom.
---------------------------

    I           X             Y             Z         N(Z)
 ------------------------------------------------------------
    1      -2.187639      2.135299      0.000000       1
    2      -4.651346      2.136285      0.000000       1
    3      -5.889538      0.000000      0.000000       1
    4      -4.651346     -2.136285      0.000000       1
    5      -2.187639     -2.135299      0.000000       1
    6       2.187639     -2.135299      0.000000       1
    7       4.651346     -2.136285      0.000000       1
    8       5.889538      0.000000      0.000000       1
    9       4.651346      2.136285      0.000000       1
   10       2.187639      2.135299      0.000000       1
   11       2.024916      0.000000      0.000000       6
   12       0.599842      0.000000      0.000000       6
   13      -0.599842      0.000000      0.000000       6
   14      -2.024916      0.000000      0.000000       6
   15      -2.732113      1.202396      0.000000       6
   16      -4.113842      1.198704      0.000000       6
   17      -4.808888      0.000000      0.000000       6
   18      -4.113842     -1.198704      0.000000       6
   19      -2.732113     -1.202396      0.000000       6
   20       2.732113     -1.202396      0.000000       6
   21       4.113842     -1.198704      0.000000       6
   22       4.808888      0.000000      0.000000       6
   23       4.113842      1.198704      0.000000       6
   24       2.732113      1.202396      0.000000       6

 MO ENERGIES (EV) AND HALF OCCUPATION NUMBERS

           66:   182.921903    0.000000
           65:   130.788941    0.000000
           64:   129.484529    0.000000
           63:   113.845753    0.000000
           62:   111.540678    0.000000
           61:   111.432375    0.000000
           60:   111.407148    0.000000
           59:    90.175416    0.000000
           58:    88.252741    0.000000
           57:    82.612414    0.000000
           56:    82.514107    0.000000
           55:    64.346072    0.000000
           54:    54.162478    0.000000
           53:    35.546574    0.000000
           52:    35.503811    0.000000
           51:    31.636586    0.000000
           50:    30.304206    0.000000
           49:    24.252464    0.000000
           48:    24.207335    0.000000
           47:    23.368571    0.000000
           46:    23.099441    0.000000
           45:    22.474184    0.000000
           44:    22.421186    0.000000
           43:    22.023434    0.000000
           42:    21.977593    0.000000
           41:     3.746887    0.000000 5b2g(pi*)
           40:     3.163959    0.000000 5b3u(pi*)
           39:     1.590819    0.000000 4b2g(pi*)
           38:     0.813383    0.000000   8b3g(ip ethyne pi*)
           37:    -0.340126    0.000000 4b3u(pi*)
           36:    -0.487988    0.000000 2au(pi*)
           35:    -0.496037    0.000000 2b1g(pi*)
           34:    -1.904261    0.000000 3b2g(pi*)

           33:    -8.855200    1.000000 3b3u(pi)
           32:   -10.093568    1.000000   8b2u(ip ethyne pi)
           31:   -10.122620    1.000000 1au(pi)
           30:   -10.129598    1.000000 1b1g(pi)
           29:   -10.418839    1.000000 2b2g(pi)
           28:   -11.920619    1.000000
           27:   -11.942228    1.000000
           26:   -11.944963    1.000000
           25:   -12.118907    1.000000
           24:   -12.336642    1.000000 2b3u(pi)
           23:   -13.131524    1.000000
           22:   -13.346247    1.000000
           21:   -13.503083    1.000000
           20:   -13.655421    1.000000
           19:   -14.160787    1.000000 1b2g(pi)
           18:   -14.566575    1.000000
           17:   -14.650628    1.000000 1b3u(pi)
           16:   -14.918337    1.000000
           15:   -15.135888    1.000000
           14:   -15.388485    1.000000
           13:   -17.227139    1.000000
           12:   -18.406761    1.000000
           11:   -19.434167    1.000000
           10:   -20.235477    1.000000
            9:   -20.719806    1.000000
            8:   -21.361394    1.000000
            7:   -25.363092    1.000000
            6:   -29.413478    1.000000
            5:   -29.539952    1.000000
            4:   -30.980489    1.000000
```

```
          3:   -35.888275    1.000000
          2:   -44.103520    1.000000
          1:   -45.667114    1.000000

MO COEFFICIENTS STORED COLUMNWISE (LOWDIN BASIS)
```

	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33
1	-0.1960	0.0000	-0.1402	0.1716	-0.1872	0.1032	0.0000	0.1139	0.1876	0.0970	-0.1826	0.0000	0.0000	0.0000	-0.0726	0.0000
2	0.2125	0.0000	0.1889	0.1869	-0.1889	-0.0819	0.0000	0.0990	-0.1799	0.1070	0.1824	0.0000	0.0000	0.0000	-0.0390	0.0000
3	-0.1535	0.0000	0.1179	0.0000	0.0000	-0.2226	0.0000	-0.2550	0.0000	-0.2063	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4	0.2125	0.0000	0.1889	-0.1869	0.1889	-0.0819	0.0000	0.0990	0.1799	0.1070	-0.1824	0.0000	0.0000	0.0000	0.0390	0.0000
5	-0.1960	0.0000	-0.1402	-0.1716	0.1872	0.1032	0.0000	0.1139	-0.1876	0.0970	0.1826	0.0000	0.0000	0.0000	0.0726	0.0000
6	-0.1960	0.0000	0.1402	-0.1716	-0.1872	0.1032	0.0000	-0.1139	-0.1876	0.0970	-0.1826	0.0000	0.0000	0.0000	0.0726	0.0000
7	0.2125	0.0000	-0.1889	-0.1869	-0.1889	-0.0819	0.0000	-0.0990	0.1799	0.1070	0.1824	0.0000	0.0000	0.0000	0.0390	0.0000
8	-0.1535	0.0000	-0.1179	0.0000	0.0000	-0.2226	0.0000	0.2550	0.0000	-0.2063	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9	0.2125	0.0000	-0.1889	0.1869	0.1889	-0.0819	0.0000	-0.0990	-0.1799	0.1070	-0.1824	0.0000	0.0000	0.0000	-0.0390	0.0000
10	-0.1960	0.0000	0.1402	0.1716	0.1872	0.1032	0.0000	-0.1139	0.1876	0.0970	0.1826	0.0000	0.0000	0.0000	-0.0726	0.0000
11	0.0980	0.0000	-0.0950	0.0000	0.0000	-0.0316	0.0000	-0.0119	0.0000	0.0008	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12	0.0050	0.0000	0.0701	0.0000	0.0000	-0.0035	0.0000	0.0560	0.0000	-0.0361	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13	0.0050	0.0000	-0.0701	0.0000	0.0000	-0.0035	0.0000	-0.0560	0.0000	-0.0361	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
14	0.0980	0.0000	0.0950	0.0000	0.0000	-0.0316	0.0000	0.0119	0.0000	0.0008	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15	-0.0822	0.0000	-0.0062	-0.0496	0.0383	-0.0246	0.0000	-0.0069	0.0083	0.0007	-0.0063	0.0000	0.0000	0.0000	-0.0466	0.0000
16	0.0821	0.0000	0.0056	-0.0307	0.0365	0.0236	0.0000	0.0109	-0.0052	0.0024	0.0036	0.0000	0.0000	0.0000	0.0249	0.0000
17	-0.0887	0.0000	-0.0644	0.0000	0.0000	0.0389	0.0000	0.0013	0.0000	-0.0058	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18	0.0821	0.0000	0.0056	0.0307	-0.0365	0.0236	0.0000	0.0109	0.0052	0.0024	-0.0036	0.0000	0.0000	0.0000	-0.0249	0.0000
19	-0.0822	0.0000	-0.0062	0.0496	-0.0383	-0.0246	0.0000	-0.0069	-0.0083	0.0007	0.0063	0.0000	0.0000	0.0000	0.0466	0.0000
20	-0.0822	0.0000	0.0062	0.0496	0.0383	-0.0246	0.0000	0.0069	-0.0083	0.0007	-0.0063	0.0000	0.0000	0.0000	0.0466	0.0000
21	0.0821	0.0000	-0.0056	0.0307	0.0365	0.0236	0.0000	-0.0109	0.0052	0.0024	0.0036	0.0000	0.0000	0.0000	-0.0249	0.0000
22	-0.0887	0.0000	0.0644	0.0000	0.0000	0.0389	0.0000	-0.0013	0.0000	-0.0058	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23	0.0821	0.0000	-0.0056	-0.0307	-0.0365	0.0236	0.0000	-0.0109	-0.0052	0.0024	-0.0036	0.0000	0.0000	0.0000	0.0249	0.0000
24	-0.0822	0.0000	0.0062	-0.0496	-0.0383	-0.0246	0.0000	0.0069	0.0083	0.0007	0.0063	0.0000	0.0000	0.0000	-0.0466	0.0000
25	-0.1524	0.0000	-0.2547	0.0000	0.0000	-0.3090	0.0000	-0.1562	0.0000	0.2637	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26	0.2412	0.0000	0.0921	0.0000	0.0000	0.2934	0.0000	0.0837	0.0000	-0.2170	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27	-0.2412	0.0000	0.0921	0.0000	0.0000	-0.2934	0.0000	0.0837	0.0000	0.2170	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28	0.1524	0.0000	-0.2547	0.0000	0.0000	0.3090	0.0000	-0.1562	0.0000	-0.2637	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29	-0.0708	0.0000	0.0497	0.1258	-0.1872	0.0035	0.0000	0.2445	0.0181	0.2432	-0.0066	0.0000	0.0000	0.0000	-0.1582	0.0000
30	-0.1027	0.0000	-0.0674	-0.1443	0.1876	-0.0484	0.0000	-0.2621	-0.0134	-0.2464	0.0053	0.0000	0.0000	0.0000	0.0913	0.0000
31	0.1319	0.0000	-0.2080	0.0000	0.0000	0.3161	0.0000	0.3084	0.0000	0.2406	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32	-0.1027	0.0000	-0.0674	0.1443	-0.1876	-0.0484	0.0000	-0.2621	0.0134	-0.2464	-0.0053	0.0000	0.0000	0.0000	-0.0913	0.0000
33	-0.0708	0.0000	0.0497	-0.1258	0.1872	0.0035	0.0000	0.2445	-0.0181	0.2432	0.0066	0.0000	0.0000	0.0000	0.1582	0.0000
34	0.0708	0.0000	0.0497	0.1258	0.1872	-0.0035	0.0000	0.2445	0.0181	-0.2432	0.0066	0.0000	0.0000	0.0000	-0.1582	0.0000
35	0.1027	0.0000	-0.0674	-0.1443	-0.1876	0.0484	0.0000	-0.2621	-0.0134	0.2464	-0.0053	0.0000	0.0000	0.0000	0.0913	0.0000
36	-0.1319	0.0000	-0.2080	0.0000	0.0000	-0.3161	0.0000	0.3084	0.0000	-0.2406	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37	0.1027	0.0000	-0.0674	0.1443	0.1876	0.0484	0.0000	-0.2621	0.0134	0.2464	0.0053	0.0000	0.0000	0.0000	-0.0913	0.0000
38	0.0708	0.0000	0.0497	-0.1258	-0.1872	-0.0035	0.0000	0.2445	-0.0181	-0.2432	-0.0066	0.0000	0.0000	0.0000	0.1582	0.0000
39	0.0000	0.0000	0.0000	-0.2177	-0.1451	0.0000	0.0000	0.0000	-0.2261	0.0000	-0.2385	0.0000	0.0000	0.0000	-0.1894	0.0000
40	0.0000	0.0000	0.0000	0.1091	0.0318	0.0000	0.0000	0.0000	-0.0641	0.0000	-0.0315	0.0000	0.0000	0.0000	0.6139	0.0000
41	0.0000	0.0000	0.0000	0.1091	-0.0318	0.0000	0.0000	0.0000	-0.0641	0.0000	0.0315	0.0000	0.0000	0.0000	0.6139	0.0000
42	0.0000	0.0000	0.0000	-0.2177	0.1451	0.0000	0.0000	0.0000	-0.2261	0.0000	0.2385	0.0000	0.0000	0.0000	-0.1894	0.0000
43	-0.1759	0.0000	-0.2363	0.2260	-0.2083	0.1815	0.0000	0.0259	0.2413	-0.0091	-0.2426	0.0000	0.0000	0.0000	0.0123	0.0000
44	0.1909	0.0000	0.2396	0.2241	-0.2063	-0.1715	0.0000	-0.0236	-0.2508	0.0043	0.2510	0.0000	0.0000	0.0000	-0.0223	0.0000
45	0.0000	0.0000	0.0000	-0.1711	0.1363	0.0000	0.0000	0.0000	0.2572	0.0000	-0.2551	0.0000	0.0000	0.0000	0.0071	0.0000
46	-0.1909	0.0000	-0.2396	0.2241	-0.2063	0.1715	0.0000	0.0236	-0.2508	-0.0043	0.2510	0.0000	0.0000	0.0000	-0.0223	0.0000
47	0.1759	0.0000	0.2363	0.2260	-0.2083	-0.1815	0.0000	-0.0259	0.2413	0.0091	-0.2426	0.0000	0.0000	0.0000	0.0123	0.0000
48	0.1759	0.0000	-0.2363	0.2260	0.2083	-0.1815	0.0000	0.0259	0.2413	0.0091	0.2426	0.0000	0.0000	0.0000	0.0123	0.0000
49	-0.1909	0.0000	0.2396	0.2241	0.2063	0.1715	0.0000	-0.0236	-0.2508	-0.0043	-0.2510	0.0000	0.0000	0.0000	-0.0223	0.0000
50	0.0000	0.0000	0.0000	-0.1711	-0.1363	0.0000	0.0000	0.0000	0.2572	0.0000	0.2551	0.0000	0.0000	0.0000	0.0071	0.0000
51	0.1909	0.0000	-0.2396	0.2241	0.2063	-0.1715	0.0000	0.0236	-0.2508	0.0043	-0.2510	0.0000	0.0000	0.0000	-0.0223	0.0000
52	-0.1759	0.0000	0.2363	0.2260	0.2083	0.1815	0.0000	-0.0259	0.2413	-0.0091	0.2426	0.0000	0.0000	0.0000	0.0123	0.0000
53	0.0000	0.3055	0.0000	0.0000	0.0000	0.0000	0.1357	0.0000	0.0000	0.0000	0.0000	0.4049	0.0000	0.0000	0.0000	-0.3160
54	0.0000	0.0907	0.0000	0.0000	0.0000	0.0000	0.4936	0.0000	0.0000	0.0000	0.0000	0.1698	0.0000	0.0000	0.0000	0.3557
55	0.0000	-0.0907	0.0000	0.0000	0.0000	0.0000	0.4936	0.0000	0.0000	0.0000	0.0000	-0.1698	0.0000	0.0000	0.0000	0.3557
56	0.0000	-0.3055	0.0000	0.0000	0.0000	0.0000	0.1357	0.0000	0.0000	0.0000	0.0000	-0.4049	0.0000	0.0000	0.0000	-0.3160
57	0.0000	-0.2881	0.0000	0.0000	0.0000	0.0000	-0.0730	0.0000	0.0000	0.0000	0.0000	-0.1615	0.3548	-0.3545	0.0000	-0.2522
58	0.0000	-0.2799	0.0000	0.0000	0.0000	0.0000	-0.2514	0.0000	0.0000	0.0000	0.0000	0.2179	0.3523	-0.3526	0.0000	0.1209
59	0.0000	-0.2753	0.0000	0.0000	0.0000	0.0000	-0.3175	0.0000	0.0000	0.0000	0.0000	0.4002	0.0000	0.0000	0.0000	0.3424
60	0.0000	-0.2799	0.0000	0.0000	0.0000	0.0000	-0.2514	0.0000	0.0000	0.0000	0.0000	0.2179	-0.3523	0.3526	0.0000	0.1209
61	0.0000	-0.2881	0.0000	0.0000	0.0000	0.0000	-0.0730	0.0000	0.0000	0.0000	0.0000	-0.1615	-0.3548	0.3545	0.0000	-0.2522
62	0.0000	0.2881	0.0000	0.0000	0.0000	0.0000	-0.0730	0.0000	0.0000	0.0000	0.0000	0.1615	-0.3548	-0.3545	0.0000	-0.2522
63	0.0000	0.2799	0.0000	0.0000	0.0000	0.0000	-0.2514	0.0000	0.0000	0.0000	0.0000	-0.2179	-0.3523	-0.3526	0.0000	0.1209
64	0.0000	0.2753	0.0000	0.0000	0.0000	0.0000	-0.3175	0.0000	0.0000	0.0000	0.0000	-0.4002	0.0000	0.0000	0.0000	0.3424
65	0.0000	0.2799	0.0000	0.0000	0.0000	0.0000	-0.2514	0.0000	0.0000	0.0000	0.0000	-0.2179	0.3523	0.3526	0.0000	0.1209
66	0.0000	0.2881	0.0000	0.0000	0.0000	0.0000	-0.0730	0.0000	0.0000	0.0000	0.0000	0.1615	0.3548	0.3545	0.0000	-0.2522

	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49
1	0.0000	0.0000	0.0000	0.0000	0.0374	0.0000	0.0000	0.0000	-0.1604	0.1315	-0.2542	0.2474	0.2634	0.2641	0.2460	-0.2532
2	0.0000	0.0000	0.0000	0.0000	0.0054	0.0000	0.0000	0.0000	0.2590	-0.2620	0.2463	-0.2535	-0.0125	-0.0528	0.2554	-0.2483
3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.2636	0.2876	0.0000	0.0000	-0.3383	-0.3310	0.0000	0.0000
4	0.0000	0.0000	0.0000	0.0000	-0.0054	0.0000	0.0000	0.0000	0.2590	-0.2620	-0.2463	0.2535	-0.0125	-0.0528	-0.2554	0.2483
5	0.0000	0.0000	0.0000	0.0000	-0.0374	0.0000	0.0000	0.0000	-0.1604	0.1315	0.2542	-0.2474	0.2634	0.2641	-0.2460	0.2532
6	0.0000	0.0000	0.0000	0.0000	0.0374	0.0000	0.0000	0.0000	0.1604	0.1315	0.2542	0.2474	-0.2634	0.2641	-0.2460	-0.2532
7	0.0000	0.0000	0.0000	0.0000	0.0054	0.0000	0.0000	0.0000	-0.2590	-0.2620	-0.2463	-0.2535	0.0125	-0.0528	-0.2554	-0.2483
8	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2636	0.2876	0.0000	0.0000	0.3383	-0.3310	0.0000	0.0000
9	0.0000	0.0000	0.0000	0.0000	-0.0054	0.0000	0.0000	0.0000	-0.2590	-0.2620	0.2463	0.2535	0.0125	-0.0528	0.2554	0.2483
10	0.0000	0.0000	0.0000	0.0000	-0.0374	0.0000	0.0000	0.0000	0.1604	0.1315	-0.2542	-0.2474	-0.2634	0.2641	0.2460	0.2532
11	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0087	0.0087	0.0000	0.0000	0.0084	-0.0088	0.0000	0.0000
12	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0075	-0.0045	0.0000	0.0000	0.0152	-0.0136	0.0000	0.0000
13	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0075	-0.0045	0.0000	0.0000	-0.0152	-0.0136	0.0000	0.0000
14	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0087	0.0087	0.0000	0.0000	-0.0084	-0.0088	0.0000	0.0000
15	0.0000	0.0000	0.0000	0.0000	0.0378	0.0000	0.0000	0.0000	0.0248	-0.0219	0.0248	-0.0239	-0.0337	-0.0355	-0.0371	0.0380
16	0.0000	0.0000	0.0000	0.0000	-0.0100	0.0000	0.0000	0.0000	-0.0341	0.0344	-0.0248	0.0260	0.0036	0.0098	-0.0384	0.0376
17	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0351	-0.0368	0.0000	0.0000	0.0367	0.0385	0.0000	0.0000
18	0.0000	0.0000	0.0000	0.0000	0.0100	0.0000	0.0000	0.0000	-0.0341	0.0344	0.0248	-0.0260	0.0036	0.0098	0.0384	-0.0376
19	0.0000	0.0000	0.0000	0.0000	-0.0378	0.0000	0.0000	0.0000	0.0248	-0.0219	-0.0248	0.0239	-0.0337	-0.0355	0.0371	-0.0380
20	0.0000	0.0000	0.0000	0.0000	0.0378	0.0000	0.0000	0.0000	-0.0248	-0.0219	-0.0248	-0.0239	0.0337	-0.0355	0.0371	0.0380
21	0.0000	0.0000	0.0000	0.0000	-0.0100	0.0000	0.0000	0.0000	0.0341	0.0344	0.0248	0.0260	-0.0036	0.0098	0.0384	0.0376
22	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0351	-0.0368	0.0000	0.0000	-0.0367	0.0385	0.0000	0.0000
23	0.0000	0.0000	0.0000	0.0000	0.0100	0.0000	0.0000	0.0000	0.0341	0.0344	-0.0248	-0.0260	-0.0036	0.0098	-0.0384	-0.0376
24	0.0000	0.0000	0.0000	0.0000	-0.0378	0.0000	0.0000	0.0000	-0.0248	-0.0219	0.0248	0.0239	0.0337	-0.0355	-0.0371	-0.0380
25	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0313	-0.0114	0.0000	0.0000	0.0785	-0.0457	0.0000	0.0000

26	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0157	-0.0016	0.0000	0.0000	0.0352	-0.0042	0.0000	0.0000
27	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0157	0.0016	0.0000	0.0000	0.0352	0.0042	0.0000	0.0000
28	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0313	0.0114	0.0000	0.0000	0.0785	0.0457	0.0000	0.0000
29	0.0000	0.0000	0.0000	0.0000	0.0557	0.0000	0.0000	0.0000	0.0936	-0.0826	0.1370	-0.1355	-0.1449	-0.1600	-0.0479	0.0515
30	0.0000	0.0000	0.0000	0.0000	-0.0250	0.0000	0.0000	0.0000	0.1266	-0.1231	0.1360	-0.1376	-0.0798	-0.1042	0.0695	-0.0663
31	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.2586	0.2822	0.0000	0.0000	-0.3195	-0.3085	0.0000	0.0000
32	0.0000	0.0000	0.0000	0.0000	0.0250	0.0000	0.0000	0.0000	0.1266	-0.1231	-0.1360	0.1376	-0.0798	-0.1042	-0.0695	0.0663
33	0.0000	0.0000	0.0000	0.0000	-0.0557	0.0000	0.0000	0.0000	0.0936	-0.0826	-0.1370	0.1355	-0.1449	-0.1600	0.0479	-0.0515
34	0.0000	0.0000	0.0000	0.0000	-0.0557	0.0000	0.0000	0.0000	0.0936	0.0826	0.1370	0.1355	-0.1449	0.1600	-0.0479	-0.0515
35	0.0000	0.0000	0.0000	0.0000	0.0250	0.0000	0.0000	0.0000	0.1266	0.1231	0.1360	0.1376	-0.0798	0.1042	0.0695	0.0663
36	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.2586	-0.2822	0.0000	0.0000	-0.3195	0.3085	0.0000	0.0000
37	0.0000	0.0000	0.0000	0.0000	-0.0250	0.0000	0.0000	0.0000	0.1266	0.1231	-0.1360	-0.1376	-0.0798	0.1042	-0.0695	-0.0663
38	0.0000	0.0000	0.0000	0.0000	0.0557	0.0000	0.0000	0.0000	0.0936	0.0826	-0.1370	-0.1355	-0.1449	0.1600	0.0479	0.0515
39	0.0000	0.0000	0.0000	0.0000	-0.0959	0.0000	0.0000	0.0000	0.0000	0.0000	0.0455	0.0429	0.0000	0.0000	-0.1299	-0.1327
40	0.0000	0.0000	0.0000	0.0000	0.6903	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0016	-0.0140	0.0000	0.0000	-0.0031	0.0121
41	0.0000	0.0000	0.0000	0.0000	-0.6903	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0016	0.0140	0.0000	0.0000	-0.0031	-0.0121
42	0.0000	0.0000	0.0000	0.0000	0.0959	0.0000	0.0000	0.0000	0.0000	0.0000	0.0455	-0.0429	0.0000	0.0000	-0.1299	0.1327
43	0.0000	0.0000	0.0000	0.0000	-0.0218	0.0000	0.0000	0.0000	0.1182	-0.0946	0.2095	-0.2025	-0.1943	-0.1878	-0.2248	0.2301
44	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.2173	0.2224	-0.2014	0.2076	-0.0371	-0.0086	-0.2215	0.2155
45	0.0000	0.0000	0.0000	0.0000	-0.0061	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0384	0.0418	0.0000	0.0000	-0.1118	0.1101
46	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2173	-0.2224	-0.2014	0.2076	0.0371	0.0086	-0.2215	0.2155
47	0.0000	0.0000	0.0000	0.0000	-0.0218	0.0000	0.0000	0.0000	-0.1182	0.0946	0.2095	-0.2025	0.1943	0.1878	-0.2248	0.2301
48	0.0000	0.0000	0.0000	0.0000	0.0218	0.0000	0.0000	0.0000	0.1182	0.0946	0.2095	0.2025	-0.1943	0.1878	-0.2248	-0.2301
49	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.2173	-0.2224	-0.2014	-0.2076	-0.0371	0.0086	-0.2215	-0.2155
50	0.0000	0.0000	0.0000	0.0000	0.0061	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0384	-0.0418	0.0000	0.0000	-0.1118	-0.1101
51	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2173	0.2224	-0.2014	-0.2076	0.0371	-0.0086	-0.2215	-0.2155
52	0.0000	0.0000	0.0000	0.0000	0.0218	0.0000	0.0000	0.0000	-0.1182	-0.0946	0.2095	0.2025	0.1943	-0.1878	-0.2248	-0.2301
53	0.2717	0.0000	0.0000	-0.4216	0.0000	-0.1770	-0.2945	-0.3710	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
54	0.3867	0.0000	0.0000	0.1233	0.0000	0.4553	0.0573	0.3259	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
55	-0.3867	0.0000	0.0000	0.1233	0.0000	-0.4553	0.0573	-0.3259	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
56	-0.2717	0.0000	0.0000	-0.4216	0.0000	0.1770	-0.2945	0.3710	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
57	0.2653	-0.3523	0.3526	0.1802	0.0000	0.0747	0.2832	-0.2549	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
58	0.1041	0.3548	-0.3545	0.2056	0.0000	-0.2637	-0.2881	0.2093	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
59	-0.3381	0.0000	0.0000	-0.3969	0.0000	0.3334	0.2892	-0.1965	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
60	0.1041	-0.3548	0.3545	0.2056	0.0000	-0.2637	-0.2881	0.2093	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
61	0.2653	0.3523	-0.3526	0.1802	0.0000	0.0747	0.2832	-0.2549	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
62	-0.2653	0.3523	0.3526	0.1802	0.0000	-0.0747	0.2832	0.2549	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
63	-0.1041	-0.3548	-0.3545	0.2056	0.0000	0.2637	-0.2881	-0.2093	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
64	0.3381	0.0000	0.0000	-0.3969	0.0000	-0.3334	0.2892	0.1965	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
65	-0.1041	0.3548	0.3545	0.2056	0.0000	0.2637	-0.2881	-0.2093	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
66	-0.2653	-0.3523	-0.3526	0.1802	0.0000	-0.0747	0.2832	0.2549	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

CONFIGURATION INTERACTION:

OCC.ORB. NO.		VIRT.ORB. NO.	CONFIGURATION ENERGY IN EV SINGLET	TRIPLET	CONF. NO.	TRANSITION MOMENT SX	SY	SZ	OSC
3b3u	---->	3b2g	4.3186	3.0114	2	9.88229	0.00000	0.00000	1.59962
1au	---->	3b2g	5.5611	4.8698	3	0.00000	-4.26757	0.00000	0.38413
1b1g	---->	3b2g	5.5370	4.8762	4	0.00000	0.00000	0.00000	0.00000
2b2g	---->	3b2g	6.0360	4.8332	5	0.00000	0.00000	0.00000	0.00000
2b3u	---->	3b2g	7.6826	6.4299	6	-0.08095	0.00000	0.00000	0.00019
1b2g	---->	3b2g	9.4155	8.7229	7	0.00000	0.00000	0.00000	0.00000
1b3u	---->	3b2g	9.7579	8.8677	8	0.39633	0.00000	0.00000	0.00581
3b3u	---->	2b1g	5.6840	5.0088	9	0.00000	4.29888	0.00000	0.39840
1au	---->	2b1g	7.2625	5.7979	10	4.71454	0.00000	0.00000	0.61224
1b1g	---->	2b1g	7.3133	5.8048	11	0.00000	0.00000	0.00000	0.00000
2b2g	---->	2b1g	7.1914	6.5558	12	0.00000	0.00000	0.00000	0.00000
2b3u	---->	2b1g	9.0306	8.6096	13	0.00000	-2.06490	0.00000	0.14604
1b2g	---->	2b1g	10.9008	10.0571	14	0.00000	0.00000	0.00000	0.00000
1b3u	---->	2b1g	11.2948	10.6841	15	0.00000	-0.50748	0.00000	0.01103
3b3u	---->	2au	5.6617	5.0163	16	0.00000	0.00000	0.00000	0.00000
1au	---->	2au	7.3144	5.8058	17	0.00000	0.00000	0.00000	0.00000
1b1g	---->	2au	7.2767	5.8127	18	4.67121	0.00000	0.00000	0.60222
2b2g	---->	2au	7.2235	6.5638	19	0.00000	-4.37626	0.00000	0.52470
2b3u	---->	2au	9.0359	8.6177	20	0.00000	0.00000	0.00000	0.00000
1b2g	---->	2au	10.9141	10.0650	21	0.00000	-0.08731	0.00000	0.00032
1b3u	---->	2au	11.2968	10.6916	22	0.00000	0.00000	0.00000	0.00000
3b3u	---->	4b3u	6.0109	4.7883	23	0.00000	0.00000	0.00000	0.00000
1au	---->	4b3u	7.0464	6.3983	24	0.00000	0.00000	0.00000	0.00000
1b1g	---->	4b3u	7.0796	6.4051	25	0.00000	4.44760	0.00000	0.53115
2b2g	---->	4b3u	7.6212	6.2199	26	3.00592	0.00000	0.00000	0.26118
2b3u	---->	4b3u	9.1099	8.4577	27	0.00000	0.00000	0.00000	0.00000
1b2g	---->	4b3u	11.0224	10.1777	28	-0.30508	0.00000	0.00000	0.00389
1b3u	---->	4b3u	11.3911	10.6331	29	0.00000	0.00000	0.00000	0.00000
3b3u	---->	4b2g	7.7592	6.5861	30	0.36103	0.00000	0.00000	0.00384
1au	---->	4b2g	8.9095	8.4522	31	0.00000	2.16301	0.00000	0.15810
1b1g	---->	4b2g	8.9135	8.4592	32	0.00000	0.00000	0.00000	0.00000
2b2g	---->	4b2g	9.2244	8.4041	33	0.00000	0.00000	0.00000	0.00000
2b3u	---->	4b2g	11.1013	9.7141	34	1.08155	0.00000	0.00000	0.04925
1b2g	---->	4b2g	12.8332	12.3342	35	0.00000	0.00000	0.00000	0.00000
1b3u	---->	4b2g	13.1609	12.4514	36	0.10862	0.00000	0.00000	0.00059
3b3u	---->	5b3u	9.1860	8.4904	37	0.00000	0.00000	0.00000	0.00000
1au	---->	5b3u	10.5312	9.6775	38	0.00000	0.00000	0.00000	0.00000
1b1g	---->	5b3u	10.5429	9.6843	39	0.00000	-0.02281	0.00000	0.00002
2b2g	---->	5b3u	10.7966	9.9700	40	-0.34860	0.00000	0.00000	0.00498
2b3u	---->	5b3u	12.5719	12.1355	41	0.00000	0.00000	0.00000	0.00000
1b2g	---->	5b3u	14.4311	13.6984	42	-0.18826	0.00000	0.00000	0.00194
1b3u	---->	5b3u	14.8413	14.2546	43	0.00000	0.00000	0.00000	0.00000
3b3u	---->	5b2g	9.6442	8.7146	44	0.96822	0.00000	0.00000	0.03429
1au	---->	5b2g	10.9817	10.4034	45	0.00000	0.54765	0.00000	0.01249
1b1g	---->	5b2g	10.9825	10.4099	46	0.00000	0.00000	0.00000	0.00000
2b2g	---->	5b2g	11.2668	10.4671	47	0.00000	0.00000	0.00000	0.00000
2b3u	---->	5b2g	12.9386	12.2276	48	0.34892	0.00000	0.00000	0.00597
1b2g	---->	5b2g	14.9117	14.2938	49	0.00000	0.00000	0.00000	0.00000
1b3u	---->	5b2g	15.2032	14.4657	50	-0.13679	0.00000	0.00000	0.00108

SINGLET STATE EIGENVECTORS (VERTICAL)

The highlights indicate significant entries

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.0000	0.9888	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0341	0.0000	0.0000	0.0000	0.0019	0.0000	0.0000	-0.0871
3	0.0000	0.0000	-0.6319	0.0000	0.0000	0.0000	0.0000	0.7030	0.0000	0.0000	-0.3118	0.0000	0.0000	0.0000	0.0006	0.0000
4	0.0000	0.0000	0.0000	0.6323	0.0000	0.0000	-0.6975	0.0000	0.0000	0.0000	0.0000	-0.3231	0.0000	0.0191	0.0000	0.0000
5	0.0000	0.0000	0.0000	0.0000	-0.4182	0.8327	0.0000	0.0000	0.0000	-0.3174	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6	0.0000	0.0463	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2000	0.0000	0.0000	0.0000	0.7261	0.0000	0.0000	-0.1266

7	0.0000	0.0000	0.0000	0.0000	-0.0084	0.0487	0.0000	0.0000	0.0000	-0.0479	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8	0.0000	-0.0259	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0060	0.0000	0.0000	0.0000	0.0942	0.0000	0.0000	0.0237
9	0.0000	0.0000	-0.5940	0.0000	0.0000	0.0000	0.0000	-0.6982	0.0000	0.0000	-0.3790	0.0000	0.0000	0.0000	-0.0781	0.0000
10	0.0000	-0.0144	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6589	0.0000	0.0000	0.0000	-0.0295	0.0000	0.0000	0.2329
11	0.0000	0.0000	0.0000	0.0000	-0.2960	0.0915	0.0000	0.0000	0.0000	0.6329	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12	0.0000	0.0000	0.0000	-0.3357	0.0000	0.0000	-0.1146	0.0000	0.0000	0.0000	0.0000	-0.4490	0.0000	-0.7587	0.0000	0.0000
13	0.0000	0.0000	0.0762	0.0000	0.0000	0.0000	0.0000	-0.0497	0.0000	0.0000	-0.2240	0.0000	0.0000	0.0000	-0.2135	0.0000
14	0.0000	0.0000	0.0000	-0.0091	0.0000	0.0000	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0175	0.0000	-0.0080	0.0000	0.0000
15	0.0000	0.0000	0.0156	0.0000	0.0000	0.0000	0.0000	-0.0161	0.0000	0.0000	-0.0114	0.0000	0.0000	0.0000	-0.0133	0.0000
16	0.0000	0.0000	0.0000	0.5908	0.0000	0.0000	0.7010	0.0000	0.0000	0.0000	0.0000	-0.3712	0.0000	-0.1103	0.0000	0.0000
17	0.0000	0.0000	0.0000	0.0000	-0.2952	0.0933	0.0000	0.0000	0.0000	0.6323	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18	0.0000	-0.0156	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6507	0.0000	0.0000	0.0000	-0.0299	0.0000	0.0000	0.2315
19	0.0000	0.0000	0.3345	0.0000	0.0000	0.0000	0.0000	0.0926	0.0000	0.0000	-0.4638	0.0000	0.0000	0.0000	-0.7532	0.0000
20	0.0000	0.0000	0.0000	-0.0770	0.0000	0.0000	0.0443	0.0000	0.0000	0.0000	0.0000	-0.2162	0.0000	-0.2205	0.0000	0.0000
21	0.0000	0.0000	0.0084	0.0000	0.0000	0.0000	0.0000	-0.0026	0.0000	0.0000	0.0144	0.0000	0.0000	0.0000	-0.0022	0.0000
22	0.0000	0.0000	0.0000	-0.0149	0.0000	0.0000	0.0103	0.0000	0.0000	0.0000	0.0000	-0.0114	0.0000	-0.0180	0.0000	0.0000
23	0.0000	0.0000	0.0000	0.0000	-0.8005	-0.4850	0.0000	0.0000	0.0000	-0.3010	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24	0.0000	0.0000	0.0000	-0.3532	0.0000	0.0000	0.0407	0.0000	0.0000	0.0000	0.0000	-0.6584	0.0000	0.5852	0.0000	0.0000
25	0.0000	0.0000	0.3501	0.0000	0.0000	0.0000	0.0000	-0.0128	0.0000	0.0000	-0.6473	0.0000	0.0000	0.0000	0.6006	0.0000
26	0.0000	0.1243	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.2563	0.0000	0.0000	0.0000	-0.0624	0.0000	0.0000	0.8909
27	0.0000	0.0000	0.0000	0.0000	-0.0087	-0.1713	0.0000	0.0000	0.0000	-0.0366	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28	0.0000	0.0157	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0068	0.0000	0.0000	0.0000	0.0888	0.0000	0.0000	0.0076
29	0.0000	0.0000	0.0000	0.0000	-0.0031	-0.0115	0.0000	0.0000	0.0000	-0.0117	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30	0.0000	0.0434	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1878	0.0000	0.0000	0.0000	-0.6504	0.0000	0.0000	-0.2482
31	0.0000	0.0000	0.0842	0.0000	0.0000	0.0000	0.0000	0.0797	0.0000	0.0000	-0.2714	0.0000	0.0000	0.0000	0.1384	0.0000
32	0.0000	0.0000	0.0000	-0.0852	0.0000	0.0000	-0.0712	0.0000	0.0000	0.0000	0.0000	-0.2730	0.0000	0.1373	0.0000	0.0000
33	0.0000	0.0000	0.0000	0.0000	0.0826	0.1280	0.0000	0.0000	0.0000	-0.0341	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34	0.0000	0.0092	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0038	0.0000	0.0000	0.0000	-0.0038	0.0000	0.0000	0.1033
35	0.0000	0.0000	0.0000	0.0000	0.0069	0.0453	0.0000	0.0000	0.0000	-0.0176	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36	0.0000	-0.0081	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0070	0.0000	0.0000	0.0000	0.0590	0.0000	0.0000	0.0164
37	0.0000	0.0000	0.0000	0.0000	-0.0417	-0.0355	0.0000	0.0000	0.0000	-0.0513	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38	0.0000	0.0000	0.0000	-0.0034	0.0000	0.0000	0.0010	0.0000	0.0000	0.0000	0.0000	0.0159	0.0000	0.0242	0.0000	0.0000
39	0.0000	0.0000	0.0024	0.0000	0.0000	0.0000	0.0000	0.0019	0.0000	0.0000	0.0156	0.0000	0.0000	0.0000	0.0172	0.0000
40	0.0000	0.0190	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0041	0.0000	0.0000	0.0000	-0.1029	0.0000	0.0000	-0.0109
41	0.0000	0.0000	0.0000	0.0000	-0.0203	-0.0485	0.0000	0.0000	0.0000	-0.0163	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42	0.0000	-0.0008	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0037	0.0000	0.0000	0.0000	-0.0014	0.0000	0.0000	0.0041
43	0.0000	0.0000	0.0000	0.0000	-0.0129	-0.0129	0.0000	0.0000	0.0000	-0.0065	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44	0.0000	-0.0280	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0010	0.0000	0.0000	0.0000	-0.0933	0.0000	0.0000	0.0329
45	0.0000	0.0000	0.0161	0.0000	0.0000	0.0000	0.0000	0.0217	0.0000	0.0000	-0.0252	0.0000	0.0000	0.0000	0.0254	0.0000
46	0.0000	0.0000	0.0000	-0.0157	0.0000	0.0000	-0.0152	0.0000	0.0000	0.0000	0.0000	-0.0280	0.0000	0.0295	0.0000	0.0000
47	0.0000	0.0000	0.0000	0.0000	0.0129	0.0038	0.0000	0.0000	0.0000	-0.0067	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48	0.0000	-0.0073	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0090	0.0000	0.0000	0.0000	-0.0677	0.0000	0.0000	0.0211
49	0.0000	0.0000	0.0000	0.0000	-0.0041	0.0162	0.0000	0.0000	0.0000	-0.0074	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50	0.0000	-0.0117	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0024	0.0000	0.0000	0.0000	-0.0002	0.0000	0.0000	0.0045

	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32
1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.0000	0.0025	-0.1071	0.0000	0.0000	0.0000	0.0000	-0.0012	0.0000	0.0000	0.0000	0.0000	-0.0407	0.0000	0.0000	0.0000
3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0726	0.0000	0.0000	0.0528	0.0000	0.0000	0.0000	0.0000	0.0000	0.0241	0.0000
4	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0723	0.0000	0.0000	0.0529	0.0000	0.0000	0.0000	-0.0224	0.0000	-0.0221
5	0.0014	0.0000	0.0000	0.0037	-0.0336	0.0000	0.0000	0.0000	0.0000	0.0000	-0.1665	-0.0293	0.0000	0.0000	0.0000	0.0000
6	0.0000	-0.0070	0.6167	0.0000	0.0000	0.0000	0.0000	-0.0853	0.0000	0.0000	0.0000	0.0000	-0.0373	0.0000	0.0000	0.0000
7	-0.0077	0.0000	0.0000	0.2412	-0.5929	0.0000	0.0000	0.0000	0.0000	0.0000	0.3303	0.6272	0.0000	0.0000	0.0000	0.0000
8	0.0000	0.0033	0.0117	0.0000	0.0000	0.0000	0.0000	0.6000	0.0000	0.0000	0.0000	0.0000	-0.6963	0.0000	0.0000	0.0000
9	0.0000	0.0000	0.0000	0.0000	0.0000	0.0379	0.0000	0.0000	-0.0888	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0013	0.0000
10	0.0000	-0.7014	-0.1341	0.0000	0.0000	0.0000	0.0000	0.0152	0.0000	0.0000	0.0000	0.0000	0.0126	0.0000	0.0000	0.0000
11	0.7068	0.0000	0.0000	-0.0310	-0.0505	0.0000	0.0000	0.0000	0.0000	0.0000	0.0070	0.0024	0.0000	0.0000	0.0000	0.0000
12	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.1883	0.0000	0.0000	-0.2243	0.0000	0.0000	0.0000	-0.0703	0.0000	0.0745
13	0.0000	0.0000	0.0000	0.0000	0.0000	-0.3954	0.0000	0.0000	0.8123	0.0000	0.0000	0.0000	0.0000	0.0000	-0.1870	0.0000
14	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.1901	0.0000	0.0000	-0.2081	0.0000	0.0000	0.0000	0.2476	0.0000	-0.6776
15	0.0000	0.0000	0.0000	0.0000	0.0000	0.0835	0.0000	0.0000	-0.0170	0.0000	0.0000	0.0000	0.0000	0.0000	-0.2604	0.0000
16	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0370	0.0000	0.0000	-0.0888	0.0000	0.0000	0.0000	0.0005	0.0000	0.0193
17	-0.7073	0.0000	0.0000	-0.0444	-0.0424	0.0000	0.0000	0.0000	0.0000	0.0000	0.0020	0.0016	0.0000	0.0000	0.0000	0.0000
18	0.0000	0.7127	-0.1151	0.0000	0.0000	0.0000	0.0000	0.0154	0.0000	0.0000	0.0000	0.0000	0.0179	0.0000	0.0000	0.0000
19	0.0000	0.0000	0.0000	0.0000	0.0000	0.1904	0.0000	0.0000	-0.2244	0.0000	0.0000	0.0000	0.0000	0.0000	0.0747	0.0000
20	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3924	0.0000	0.0000	0.8134	0.0000	0.0000	0.0000	0.1869	0.0000	-0.1653
21	0.0000	0.0000	0.0000	0.0000	0.0000	0.1888	0.0000	0.0000	-0.2065	0.0000	0.0000	0.0000	0.0000	0.0000	-0.2629	0.0000
22	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0830	0.0000	0.0000	-0.0189	0.0000	0.0000	0.0000	0.2522	0.0000	-0.5895
23	-0.0016	0.0000	0.0000	0.0160	0.0254	0.0000	0.0000	0.0000	0.0000	0.0000	0.1650	-0.0660	0.0000	0.0000	0.0000	0.0000
24	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.2623	0.0000	0.0000	0.1002	0.0000	0.0000	0.0000	-0.1339	0.0000	-0.0230
25	0.0000	0.0000	0.0000	0.0000	0.0000	0.2641	0.0000	0.0000	0.1005	0.0000	0.0000	0.0000	0.0000	0.0000	0.1305	0.0000
26	0.0000	-0.0050	0.3209	0.0000	0.0000	0.0000	0.0000	-0.0006	0.0000	0.0000	0.0000	0.0000	0.0253	0.0000	0.0000	0.0000
27	-0.0001	0.0000	0.0000	-0.2196	-0.6998	0.0000	0.0000	0.0000	0.0000	0.0000	-0.5942	-0.2166	0.0000	0.0000	0.0000	0.0000
28	0.0000	0.0000	0.0788	0.0000	0.0000	0.0000	0.0000	-0.2590	0.0000	0.0000	0.0000	0.0000	0.2657	0.0000	0.0000	0.0000
29	0.0010	0.0000	0.0000	-0.1434	0.1150	0.0000	0.0000	0.0000	0.0000	0.0000	-0.1504	-0.1861	0.0000	0.0000	0.0000	0.0000
30	0.0000	-0.0083	0.6670	0.0000	0.0000	0.0000	0.0000	0.0092	0.0000	0.0000	0.0000	0.0000	-0.0630	0.0000	0.0000	0.0000
31	0.0000	0.0000	0.0000	0.0000	0.0000	-0.7504	0.0000	0.0000	-0.4659	0.0000	0.0000	0.0000	0.0000	0.0000	-0.2960	0.0000
32	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7511	0.0000	0.0000	-0.4639	0.0000	0.0000	0.0000	0.2989	0.0000	0.0383
33	0.0014	0.0000	0.0000	-0.5060	-0.3015	0.0000	0.0000	0.0000	0.0000	0.0000	0.6427	-0.4365	0.0000	0.0000	0.0000	0.0000
34	0.0000	-0.0021	0.0725	0.0000	0.0000	0.0000	0.0000	-0.0127	0.0000	0.0000	0.0000	0.0000	-0.1603	0.0000	0.0000	0.0000
35	-0.0017	0.0000	0.0000	-0.0329	0.0316	0.0000	0.0000	0.0000	0.0000	0.0000	0.1019	-0.0084	0.0000	0.0000	0.0000	0.0000
36	0.0000	0.0015	0.0104	0.0000	0.0000	0.0000	0.0000	-0.0040	0.0000	0.0000	0.0000	0.0000	-0.0137	0.0000	0.0000	0.0000
37	0.0087	0.0000	0.0000	-0.7618	0.1637	0.0000	0.0000	0.0000	0.0000	0.0000	-0.1090	0.5456	0.0000	0.0000	0.0000	0.0000
38	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.3379	0.0000	0.0000	0.0892	0.0000	0.0000	0.0000	0.6269	0.0000	0.3131
39	0.0000	0.0000	0.0000	0.0000	0.0000	0.3341	0.0000	0.0000	0.0918	0.0000	0.0000	0.0000	0.0000	0.0000	-0.6226	0.0000
40	0.0000	-0.0009	0.1211	0.0000	0.0000	0.0000	0.0000	0.2876	0.0000	0.0000	0.0000	0.0000	0.0000	0.2444	0.0000	0.0000
41	0.0017	0.0000	0.0000	0.0177	-0.0508	0.0000	0.0000	0.0000	0.0000	0.0000	-0.1256	0.0271	0.0000	0.0000	0.0000	0.0000
42	0.0000	0.0025	0.0227	0.0000	0.0000	0.0000	0.0000	-0.0009	0.0000	0.0000	0.0000	0.0000	0.0144	0.0000	0.0000	0.0000
43	-0.0022	0.0000	0.0000	-0.0055	-0.0161	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0404	-0.0271	0.0000	0.0000	0.0000	0.0000
44	0.0000	0.0038	-0.0431	0.0000	0.0000	0.0000	0.0000	-0.6944	0.0000	0.0000	0.0000	0.0000	-0.5920	0.0000	0.0000	0.0000
45	0.0000	0.0000	0.0000	0.0000	0.0000	0.1168	0.0000	0.0000	-0.0255	0.0000	0.0000	0.0000	0.0000	0.0000	-0.5742	0.0000
46	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.1176	0.0000	0.0000	-0.0244	0.0000	0.0000	0.0000	0.5783	0.0000	0.2443
47	-0.0013	0.0000	0.0000	0.1790	-0.1338	0.0000	0.0000	0.0000	0.0000	0.0000	0.0792	-0.1700	0.0000	0.0000	0.0000	0.0000
48	0.0000	0.0013	0.0161	0.0000	0.0000	0.0000	0.0000	-0.0036	0.0000	0.0000	0.0000	0.0000	-0.0122	0.0000	0.0000	0.0000
49	0.0021	0.0000	0.0000	-0.0035	-0.0019	0.0000	0.0000	0.0000	0.0000	0.0000	0.0353	-0.0349	0.0000	0.0000	0.0000	0.0000
50	0.0000	-0.0018	0.0086	0.0000	0.0000	0.0000	0.0000	-0.0026	0.0000	0.0000	0.0000	0.0000	0.0059	0.0000	0.0000	0.0000

NO	EV	KK	NM	SX	SY	SZ	OSC	LOGEPS
2	4.232512	34.1394	292.9	9.975403	0.000000	0.000000	1.597407	4.938741
3	4.553103	36.7253	272.3	0.000000	0.261534	0.000000	0.001181	1.807645
4	4.559092	36.7736	271.9	0.000000	0.000000	0.000000	0.000000	0.000000
5	5.767301	46.5191	215.0	0.000000	0.000000	0.000000	0.000000	0.000000
6	5.815358	46.9067	213.2	0.000000	0.000000	0.000000	0.000000	0.000000
7	5.968857	48.1448	207.7	0.000000	0.000000	0.000000	0.000000	0.000000
8	6.033895	48.6694	205.5	0.000000	-6.168478	0.000000	0.870784	4.675236
9	6.466011	52.1548	191.7	5.750459	0.000000	0.000000	0.810957	4.644324
10	6.946413	56.0298	178.5	0.000000	0.000000	0.000000	0.000000	0.000000

11	6.950880	56.0658	178.4	0.000000	-1.282061	0.000000	0.043333	3.372140
12	6.951980	56.0747	178.3	0.000000	0.000000	0.000000	0.000000	0.000000
13	7.287062	58.7774	170.1	-0.806394	0.000000	0.000000	0.017972	2.989930
14	7.478643	60.3227	165.8	0.000000	0.000000	0.000000	0.000000	0.000000
15	7.533659	60.7665	164.6	0.000000	6.389746	0.000000	1.166621	4.802255
16	7.640213	61.6260	162.3	4.079606	0.000000	0.000000	0.482279	4.418624
17	7.890435	63.6443	157.1	0.000000	0.000000	0.000000	0.000000	0.000000
18	7.890532	63.6450	157.1	0.033511	0.000000	0.000000	0.000034	0.261775
19	8.103547	65.3632	153.0	-1.096124	0.000000	0.000000	0.036928	3.302677
20	8.704655	70.2117	142.4	0.000000	0.000000	0.000000	0.000000	0.000000
21	8.846967	71.3596	140.1	0.000000	0.000000	0.000000	0.000000	0.000000
22	8.912864	71.8912	139.1	0.000000	-0.614224	0.000000	0.012753	2.840953
23	8.916604	71.9213	139.0	0.000000	0.000000	0.000000	0.000000	0.000000
24	9.091363	73.3309	136.4	-0.330665	0.000000	0.000000	0.003770	2.311688
25	9.184892	74.0853	135.0	0.000000	-1.852982	0.000000	0.119612	3.813099
26	9.188068	74.1110	134.9	0.000000	0.000000	0.000000	0.000000	0.000000
27	9.442684	76.1647	131.3	0.000000	0.000000	0.000000	0.000000	0.000000
28	9.597037	77.4097	129.2	0.000000	0.000000	0.000000	0.000000	0.000000
29	9.874976	79.6516	125.5	-1.401346	0.000000	0.000000	0.073550	3.601909
30	9.908260	79.9200	125.1	0.000000	0.000000	0.000000	0.000000	0.000000
31	9.908596	79.9227	125.1	0.000000	-0.253870	0.000000	0.002422	2.119519
32	10.354837	83.5221	119.7	0.000000	0.000000	0.000000	0.000000	0.000000
33	10.376106	83.6937	119.5	0.000000	0.769878	0.000000	0.023326	3.103160
34	10.817211	87.2516	114.6	0.274616	0.000000	0.000000	0.003094	2.225849
35	11.043812	89.0794	112.3	-0.288918	0.000000	0.000000	0.003496	2.278951
36	11.194024	90.2910	110.8	0.000000	0.000000	0.000000	0.000000	0.000000
37	11.244186	90.6956	110.3	0.319400	0.000000	0.000000	0.004351	2.373879
38	11.404955	91.9924	108.7	0.000000	0.000000	0.000000	0.000000	0.000000
39	11.717748	94.5154	105.8	0.000000	0.194151	0.000000	0.001675	1.959404
40	11.719721	94.5313	105.8	0.000000	0.000000	0.000000	0.000000	0.000000
41	12.050123	97.1963	102.9	0.000000	-0.191628	0.000000	0.001678	1.960190
42	12.051071	97.2039	102.9	0.000000	0.000000	0.000000	0.000000	0.000000
43	12.692453	102.3773	97.7	0.000000	0.000000	0.000000	0.000000	0.000000
44	12.807028	103.3015	96.8	-0.360129	0.000000	0.000000	0.006300	2.534648
45	13.071901	105.4380	94.8	0.000000	0.000000	0.000000	0.000000	0.000000
46	13.480778	108.7360	92.0	0.012313	0.000000	0.000000	0.000008	0.000000
47	14.101294	113.7410	87.9	0.096608	0.000000	0.000000	0.000499	1.433572
48	14.219290	114.6928	87.2	0.000000	0.000000	0.000000	0.000000	0.000000
49	15.832835	127.7076	78.3	0.000000	0.000000	0.000000	0.000000	0.000000
50	15.896631	128.2222	78.0	0.004059	0.000000	0.000000	0.000001	0.000000

CALCULATION OF MCD B TERMS FOR PI-PI* TRANSITIONS

PI MOLECULAR ORBITAL COEFFICIENTS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	0.3424	0.3055	0.1357	0.4049	0.0000	0.0000	-0.3160	0.2717	0.0000	0.0000	-0.4216	-0.1770	-0.2945	-0.3710
2	0.3337	0.0907	0.4936	0.1698	0.0000	0.0000	0.3557	0.3867	0.0000	0.0000	0.1233	0.4553	0.0573	0.3259
3	0.3337	-0.0907	0.4936	-0.1698	0.0000	0.0000	0.3557	-0.3867	0.0000	0.0000	0.1233	-0.4553	0.0573	-0.3259
4	0.3424	-0.3055	0.1357	-0.4049	0.0000	0.0000	-0.3160	-0.2717	0.0000	0.0000	-0.4216	0.1770	-0.2945	0.3710
5	0.2616	-0.2881	-0.0730	-0.1615	0.3548	-0.3545	-0.2522	0.2653	-0.3523	0.3526	0.1802	0.0747	0.2832	-0.2549
6	0.2166	-0.2799	-0.2514	0.2179	0.3523	-0.3526	0.1209	0.1041	0.3548	-0.3545	0.2056	-0.2637	-0.2881	0.2093
7	0.2018	-0.2753	-0.3175	0.4002	0.0000	0.0000	0.3424	-0.3381	0.0000	0.0000	-0.3969	0.3334	0.2892	-0.1965
8	0.2166	-0.2799	-0.2514	0.2179	-0.3523	0.3526	0.1209	0.1041	-0.3548	0.3545	0.2056	-0.2637	-0.2881	0.2093
9	0.2616	-0.2881	-0.0730	-0.1615	-0.3548	0.3545	-0.2522	0.2653	0.3523	-0.3526	0.1802	0.0747	0.2832	-0.2549
10	0.2616	0.2881	-0.0730	0.1615	-0.3548	-0.3545	-0.2522	-0.2653	0.3523	0.3526	0.1802	-0.0747	0.2832	0.2549
11	0.2166	0.2799	-0.2514	-0.2179	-0.3523	-0.3526	0.1209	-0.1041	-0.3548	-0.3545	0.2056	0.2637	-0.2881	-0.2093
12	0.2018	0.2753	-0.3175	-0.4002	0.0000	0.0000	0.3424	0.3381	0.0000	0.0000	-0.3969	-0.3334	0.2892	0.1965
13	0.2166	0.2799	-0.2514	-0.2179	0.3523	0.3526	0.1209	-0.1041	0.3548	0.3545	0.2056	0.2637	-0.2881	-0.2093
14	0.2616	0.2881	-0.0730	0.1615	0.3548	0.3545	-0.2522	-0.2653	-0.3523	-0.3526	0.1802	-0.0747	0.2832	0.2549

CONTRIBUTIONS TO MCD B-TERMS B(F) DUE TO MIXING OF I'TH STATE WITH GROUNDSTATE

I\F	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4	0.0000	0.0369	-0.0002	0.0000	0.0000	0.0000	0.0000	-0.1074	0.0171	0.0000	0.0017	0.0000	-0.0002	0.0000	0.0708	-0.0076
5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7	0.0000	-0.0948	-0.1159	0.0000	0.0000	0.0000	0.0000	-0.4156	0.0608	0.0000	1.1320	0.0000	-0.0913	0.0000	-0.5764	0.0803
8	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
11	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12	0.0000	-0.1102	0.0024	0.0000	0.0000	0.0000	0.0000	1.1662	-0.1339	0.0000	-0.0336	0.0000	-0.0018	0.0000	-1.0742	-0.0193
13	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
14	0.0000	0.0500	0.0664	0.0000	0.0000	0.0000	0.0000	-0.5367	0.1407	0.0000	-0.9082	0.0000	-0.0306	0.0000	1.2217	0.0078
15	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23	0.0000	0.0049	0.0010	0.0000	0.0000	0.0000	0.0000	-0.0661	-0.1105	0.0000	0.0218	0.0000	-0.0016	0.0000	0.3334	-0.0241
24	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26	0.0000	-0.0039	0.0060	0.0000	0.0000	0.0000	0.0000	0.0103	0.0756	0.0000	0.1300	0.0000	-0.0140	0.0000	-0.3438	0.0218
27	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30	0.0000	-0.0028	-0.0005	0.0000	0.0000	0.0000	0.0000	-0.0175	0.0496	0.0000	0.0013	0.0000	0.0000	0.0000	0.0278	0.0130
31	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32	0.0000	0.0025	-0.0028	0.0000	0.0000	0.0000	0.0000	0.0130	-0.0478	0.0000	-0.0038	0.0000	-0.0023	0.0000	0.0100	-0.0119
33	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0041	0.0020	0.0000	-0.0016	0.0000	-0.0001	0.0000	-0.0059	0.0000
41	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

42	0.0000	-0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0025	-0.0013	0.0000	-0.0009	0.0000	0.0000	0.0000	0.0073	-0.0001
43	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32
1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4	0.0000	0.0001	-0.0048	0.0000	0.0000	0.0011	0.0000	0.0000	0.0076	0.0000	0.0000	0.0000	-0.0113	0.0000	-0.0004	0.0000
5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7	0.0000	0.0002	0.0211	0.0000	0.0000	-0.0682	0.0000	0.0713	0.0089	0.0000	0.0000	0.0000	-0.0232	0.0000	-0.0178	0.0000
8	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
11	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12	0.0000	-0.0004	0.0119	0.0000	0.0000	0.0283	0.0000	0.0013	0.1772	0.0000	0.0000	0.0000	0.0010	0.0000	0.0015	0.0000
13	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
14	0.0000	0.0001	0.0028	0.0000	0.0000	0.3290	0.0000	0.0211	-0.3944	0.0000	0.0000	0.0000	0.0000	0.0000	0.0220	0.0000
15	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23	0.0000	-0.0002	0.0015	0.0000	0.0000	-0.0205	0.0000	0.0001	-0.1172	0.0000	0.0000	0.0000	0.0001	0.0000	-0.0076	0.0000
24	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26	0.0000	0.0002	-0.0027	0.0000	0.0000	-0.1051	0.0000	0.0000	0.2137	0.0000	0.0000	0.0000	0.0001	0.0000	-0.0358	0.0000
27	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30	0.0000	-0.0001	0.0029	0.0000	0.0000	-0.0094	0.0000	-0.0002	-0.0478	0.0000	0.0000	0.0000	-0.0023	0.0000	-0.0037	0.0000
31	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32	0.0000	0.0001	-0.0024	0.0000	0.0000	-0.0178	0.0000	-0.0008	0.0521	0.0000	0.0000	0.0000	0.0029	0.0000	-0.0072	0.0000
33	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40	0.0000	0.0002	-0.0002	0.0000	0.0000	0.0028	0.0000	-0.0003	0.0053	0.0000	0.0000	0.0000	-0.0010	0.0000	0.0019	0.0000
41	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42	0.0000	-0.0001	0.0001	0.0000	0.0000	0.0008	0.0000	-0.0002	-0.0065	0.0000	0.0000	0.0000	0.0009	0.0000	0.0004	0.0000
43	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

CONTRIBUTIONS TO MCD B-TERMS B(F) DUE TO MIXING OF I'TH STATE WITH F'TH STATE

The highlights indicate significant entries

I\F	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.0000	0.0000	0.9991	0.0000	0.0000	0.0000	0.0000	-0.3446	0.0000	0.0000	-0.2420	0.0000	0.0000	0.0000	0.1050	0.0000
3	0.0000	-0.9991	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.1455	0.0000	0.0000	0.0000	-0.0016	0.0000	0.0000	0.0151
4	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8	0.0000	0.3446	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7168	0.0000	0.0000	0.0000	0.3981	0.0000	0.0000	-0.4792
9	0.0000	0.0000	0.1455	0.0000	0.0000	0.0000	0.0000	-0.7168	0.0000	0.0000	-1.5289	0.0000	0.0000	0.0000	0.1791	0.0000
10	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
11	0.0000	0.2420	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.5289	0.0000	0.0000	0.0000	0.0450	0.0000	0.0000	0.6149
12	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13	0.0000	0.0000	0.0016	0.0000	0.0000	0.0000	0.0000	-0.3981	0.0000	0.0000	-0.0450	0.0000	0.0000	0.0000	-0.2107	0.0000
14	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15	0.0000	-0.1050	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.1791	0.0000	0.0000	0.0000	0.2107	0.0000	0.0000	-8.8461
16	0.0000	0.0000	-0.0151	0.0000	0.0000	0.0000	0.0000	0.4792	0.0000	0.0000	-0.6149	0.0000	0.0000	0.0000	8.8461	0.0000
17	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18	0.0000	0.0000	-0.0001	0.0000	0.0000	0.0000	0.0000	-0.0012	0.0000	0.0000	0.0048	0.0000	0.0000	0.0000	-0.0028	0.0000
19	0.0000	0.0000	-0.0061	0.0000	0.0000	0.0000	0.0000	0.1339	0.0000	0.0000	0.0826	0.0000	0.0000	0.0000	-0.0033	0.0000
20	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22	0.0000	-0.0046	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2188	0.0000	0.0000	0.0000	0.0065	0.0000	0.0000	0.1161
23	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24	0.0000	0.0000	-0.0010	0.0000	0.0000	0.0000	0.0000	0.0829	0.0000	0.0000	0.0035	0.0000	0.0000	0.0000	0.0695	0.0000
25	0.0000	0.0052	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0155	0.0000	0.0000	0.0000	0.0633	0.0000	0.0000	-0.0342
26	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29	0.0000	0.0000	-0.0081	0.0000	0.0000	0.0000	0.0000	0.0723	0.0000	0.0000	0.0064	0.0000	0.0000	0.0000	0.0684	0.0000
30	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0631	0.0000	0.0000	0.0000	-0.0005	0.0000	0.0000	-0.0212
32	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33	0.0000	0.0019	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0031	0.0000	0.0000	0.0000	0.0005	0.0000	0.0000	-0.0032
34	0.0000	0.0000	-0.0002	0.0000	0.0000	0.0000	0.0000	-0.0106	0.0000	0.0000	-0.0132	0.0000	0.0000	0.0000	0.0589	0.0000
35	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0170	0.0000	0.0000	0.0012	0.0000	0.0000	0.0000	-0.0670	0.0000
36	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37	0.0000	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	-0.0064	0.0000	0.0000	0.0056	0.0000	0.0000	0.0000	0.0040	0.0000
38	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39	0.0000	-0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0036	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0002
40	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

43	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	-0.0003	0.0000	0.0000	0.0004	0.0000	0.0000	0.0000	0.0007	0.0000
45	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0001	0.0000	0.0000	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
48	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32
1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.0000	0.0000	0.0000	0.0000	0.0000	0.0046	0.0000	0.0000	-0.0052	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0003	0.0000
3	0.0000	0.0001	0.0061	0.0000	0.0000	0.0000	0.0000	0.0010	0.0000	0.0000	0.0000	0.0000	0.0081	0.0000	0.0000	0.0000
4	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8	0.0000	0.0012	-0.1339	0.0000	0.0000	0.0000	0.0000	-0.0829	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0723	0.0000	0.0000
9	0.0000	0.0000	0.0000	0.0000	0.0000	-0.2188	0.0000	0.0000	0.0155	0.0000	0.0000	0.0000	0.0000	0.0000	0.0631	0.0000
10	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
11	0.0000	-0.0048	-0.0826	0.0000	0.0000	0.0000	0.0000	-0.0035	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0064	0.0000	0.0000
12	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0065	0.0000	0.0000	-0.0633	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000
14	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15	0.0000	0.0028	0.0033	0.0000	0.0000	0.0000	0.0000	-0.0695	0.0000	0.0000	0.0000	0.0000	-0.0684	0.0000	0.0000	0.0000
16	0.0000	0.0000	0.0000	0.0000	0.0000	-0.1161	0.0000	0.0000	0.0342	0.0000	0.0000	0.0000	0.0000	0.0000	0.0212	0.0000
17	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18	0.0000	0.0000	0.0000	0.0000	0.0000	0.0020	0.0000	0.0000	-0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000
19	0.0000	0.0000	0.0000	0.0000	0.0000	0.0500	0.0000	0.0000	-0.0602	0.0000	0.0000	0.0000	0.0000	0.0000	0.0080	0.0000
20	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22	0.0000	-0.0020	-0.0500	0.0000	0.0000	0.0000	0.0000	0.0021	0.0000	0.0000	0.0000	0.0000	0.0287	0.0000	0.0000	0.0000
23	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0021	0.0000	0.0000	0.1216	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0036	0.0000
25	0.0000	0.0005	0.0602	0.0000	0.0000	0.0000	0.0000	-0.1216	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0573	0.0000	0.0000
26	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0287	0.0000	0.0000	0.0573	0.0000	0.0000	0.0000	0.0000	0.0000	-0.7980	0.0000
30	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31	0.0000	-0.0004	-0.0080	0.0000	0.0000	0.0000	0.0000	0.0036	0.0000	0.0000	0.0000	0.0000	0.7980	0.0000	0.0000	0.0000
32	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33	0.0000	0.0000	0.0038	0.0000	0.0000	0.0000	0.0000	0.0168	0.0000	0.0000	0.0000	0.0000	-0.0920	0.0000	0.0000	0.0000
34	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0061	0.0000	0.0000	0.0118	0.0000	0.0000	0.0000	0.0000	0.0000	0.0017	0.0000
35	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0046	0.0000	0.0000	0.0117	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0019	0.0000
36	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0052	0.0000	0.0000	0.0104	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0043	0.0000
38	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39	0.0000	0.0004	0.0001	0.0000	0.0000	0.0000	0.0000	0.0008	0.0000	0.0000	0.0000	0.0000	0.0045	0.0000	0.0000	0.0000
40	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41	0.0000	-0.0001	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0008	0.0000	0.0000	0.0000	0.0000	-0.0044	0.0000	0.0000	0.0000
42	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44	0.0000	0.0000	0.0000	0.0000	0.0000	0.0082	0.0000	0.0000	-0.0211	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0011	0.0000
45	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000	-0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0009	0.0000
48	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

WAVENUMBERS IN KK = 1000CM-1,
MCD B-TERMS IN (BOHR-MAGNETON DEBYE2)/KK,**
ELECTRIC TRANSITION MOMENTS IN DEBYES
TRANSITION MOMENT ANGLES IN DEG
OSCILLATOR STRENGTHS OSC

F	W	BG	+	BF	=	B	M(X)	M(Y)	PHI(X-->Y)	OSC	TERM	LEADING CONFIGURATIONS
2	34.139	-0.117330		-0.514619		-0.631949	-9.975403	0.000000	0.000000	1.597407	1 B1u	98%[3b3u->3b2g]
3	36.724	-0.043660		1.115914		1.072254	0.000000	-0.261534	90.000000	0.001181	1 B2u	40%[1au->3b2g], 35%[3b3u->2b1g]
4	36.773	0.000000		0.000000		0.000000	0.000000	0.000000	0.000000	0.000000	1 B3g	40%[1b1g->3b2g], 35%[3b3u->2au]
5	46.518	0.000000		0.000000		0.000000	0.000000	0.000000	0.000000	0.000000	2 Ag	64%[3b3u->4b3u], 17%[2b2g->3b2g]
6	46.906	0.000000		0.000000		0.000000	0.000000	0.000000	0.000000	0.000000	3 Ag	69%[2b2g->3b2g], 24%[3b3u->4b3u]
7	48.144	0.000000		0.000000		0.000000	0.000000	0.000000	0.000000	0.000000	2 B3g	49%[1b1g->3b2g], 49%[3b3u->2au]
8	48.668	0.047721		-0.692769		-0.645048	0.000000	6.168478	90.000000	0.870784	2 B2u	49%[1au->3b2g], 49%[3b3u->2b1g]
9	52.154	0.052179		2.055680		2.107860	-5.750459	0.000000	0.000000	0.810957	2 B1u	43%[1au->2b1g], 42%[1b1g->2au]
10	56.028	0.000000		0.000000		0.000000	0.000000	0.000000	0.000000	0.000000	4 Ag	40%[1b1g->2b1g], 40%[1au->2au]
11	56.064	0.338495		-2.339737		-2.001242	0.000000	1.282061	90.000000	0.043333	3 B2u	42%[1b1g->4b3u], 22%[2b2g->2au]
12	56.073	0.000000		0.000000		0.000000	0.000000	0.000000	0.000000	0.000000	3 B3g	43%[1au->4b3u], 20%[2b2g->2b1g]
13	58.776	-0.141768		0.721982		0.580214	0.806394	0.000000	0.000000	0.017972	3 B1u	53%[2b3u->3b2g], 42%[3b3u->4b2g]
14	60.321	0.000000		0.000000		0.000000	0.000000	0.000000	0.000000	0.000000	4 B3g	58%[2b2g->2b1g], 34%[1au->4b3u]
15	60.765	-0.329182		9.047968		8.718786	0.000000	-6.389746	90.000000	1.166621	4 B2u	57%[2b2g->2au], 36%[1b1g->4b3u]
16	61.624	0.059980		-8.637913		-8.577933	-4.079606	0.000000	0.000000	0.482279	4 B1u	79%[2b2g->4b3u], 6%[3b3u->4b2g]
17	63.643	0.000000		0.000000		0.000000	0.000000	0.000000	0.000000	0.000000	5 Ag	50%[1b1g->2b1g], 50%[1au->2au]
18	63.643	-0.000029		-0.002427		-0.002456	-0.033511	0.000000	0.000000	0.000034	5 B1u	51%[1b1g->2au], 49%[1au->2b1g]
19	65.362	0.030214		-0.201065		-0.170851	1.096124	0.000000	0.000000	0.036928	6 B1u	44%[3b3u->4b2g], 38%[2b3u-->3b2g]
20	70.210	0.000000		0.000000		0.000000	0.000000	0.000000	0.000000	0.000000		
21	71.358	0.000000		0.000000		0.000000	0.000000	0.000000	0.000000	0.000000		
22	71.889	0.140903		-0.323148		-0.182245	0.000000	0.614224	90.000000	0.012753	5 B2u	
23	71.920	0.000000		0.000000		0.000000	0.000000	0.000000	0.000000	0.000000		
24	73.329	0.092206		-0.252447		-0.160242	0.330665	0.000000	0.000000	0.003770	7 B1u	
25	74.083	-0.100990		0.111480		0.010490	0.000000	1.852982	90.000000	0.119612	6 B2u	
26	74.109	0.000000		0.000000		0.000000	0.000000	0.000000	0.000000	0.000000		
27	76.163	0.000000		0.000000		0.000000	0.000000	0.000000	0.000000	0.000000		
28	77.408	0.000000		0.000000		0.000000	0.000000	0.000000	0.000000	0.000000		
29	79.650	-0.032775		0.538540		0.505765	1.401346	0.000000	0.000000	0.073550	8 B1u	
30	79.918	0.000000		0.000000		0.000000	0.000000	0.000000	0.000000	0.000000		

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