Supplementary information (May 30, 2011)

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

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

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

^{*a*} Wavenumber in 10^3 cm⁻¹.

^b Oscillator strength.

^c The notation (i,-j) indicates an excited singlet configuration derived from the ground configuration by promotion of an electron from the *i*'th highest occupied to the *j*'th lowest unoccupied MO.

	Term	\widetilde{v}^{a}	f^{b}	Leading configurations ^{<i>c</i>}
1	$1 {}^{1}B_{1}$	30.2	0.60	76% (1,-1), 14% (2,-2)
2	$2^{1}A$	30.8	0	71% (2,-1), 17% (1,-2)
3	$3^{1}A$	33.3	0	63% (1,-2), 16% (2,-1)
4	$1 {}^{1}B_{2}$	38.5	$2 \cdot 10^{-4}$	49% (1,-3), 40% (3,-1)
5	$1 {}^{1}B_{3}$	38.5	$1 \cdot 10^{-4}$	49% (1,-4), 40% (4,-1)
6	$2^{1}B_{1}$	40.5	1.40	72% (2,-2), 7% (1,-1)
7	$4^{1}A$	42.9	0	49% (5,-1), 42% (1,-5)
8	$2 {}^{1}B_{3}$	43.2	0.01	42% (1,-4), 40% (4,-1)
9	$2 {}^{1}B_{2}$	43.2	0.07	42% (1,-3), 40% (3,-1)
10	$5^{1}A$	44.9	0	38% (1,-5), 32% (5,-1)
11	$3 {}^{1}B_{3}$	45.2	$5 \cdot 10^{-3}$	66% (2,-3), 18% (3,-2)
12	$3 {}^{1}B_{2}$	45.2	0.01	66% (2,-4), 18% (4,-2)
13	$4 {}^{1}B_{2}$	46.1	$1 \cdot 10^{-4}$	90% (1,-6)
14	$3^{1}B_{1}$	46.5	0.05	58% (5,-2), 29% (2,-5)
15	$4^{1}B_{3}$	47.5	0.01	63% (3,-2), 15% (2,-3)
16	$5 {}^{1}B_{2}$	47.5	0.08	66% (4,-2), 15% (2,-4)
17	$5 {}^{1}B_{3}$	47.6	0.01	86% (1,-7)
18	$4 {}^{1}B_{1}$	47.8	0.13	50% (6,-1), 33% (2,-5)
19	$5 {}^{1}B_{1}$	50.0	0.14	42% (1,-11), 22% (6,-1)
20	$6 {}^{1}B_{2}$	50.6	$3 \cdot 10^{-3}$	84% (1,-8)
21	$6^{1}B_{3}$	50.9	$6 \cdot 10^{-4}$	77% (2,-6), 15% (2,-8)
22	$6^{1}A$	51.4	0	94% (1,-9)
23	$6^{1}B_{1}$	52.1	0.08	86% (1,-10)
24	$7^{1}A$	52.2	0	58% (6,-2), 13% (3,-4)
25	$7 {}^{1}B_{1}$	52.5	0.97	29% (4,-4), 29% (3,-3)
26	$7^{1}B_{2}$	53.1	$2 \cdot 10^{-4}$	87% (2,-7)
27	$7^{1}B_{3}$	53.8	0.01	35% (1,-12), 32% (5,-3)
28	$8^{1}B_{2}$	53.9	0.04	51% (5,-4), 15% (4,-5)
29	$8^{1}B_{3}$	53.9	$< 10^{-4}$	48% (1,-12), 15% (3,-5)
30	$8^{1}B_{1}$	54.0	0.21	76% (7,-1), 11% (1,-11)
31	8 ¹ A	54.6	0	53% (2,-11), 17% (6,-2)
32	$9^{1}A$	54.6	0	52% (3,-4), 47% (4,-3)
33	9 $^{1}B_{1}$	54.6	$< 10^{-4}$	50% (4,-4), 50% (3,-3)
34	$10^{1}B_{1}$	55.1	1.10^{-4}	55% (3,-6), 42% (4,-7)
35	10^{-1} A	55.1	0	54% (4,-6), 42% (3,-7)
36	9 $^{1}B_{3}$	55.8	9.10^{-4}	65% (2,-8), 13% (2,-6)
37	$11^{1}A$	56.2	0	82% (2,-13), 12% (2,-10)
38	$11^{1}B_{1}$	56.3	3.10^{-4}	72% (2,-9), 11% (1,-15)
39	$9^{1}B_{2}$	56.5	$4 \cdot 10^{-4}$	89% (1,-14)
40	$12 \ ^{1}B_{1}$	56.7	0.03	55% (1,-15), 17% (2,-9)

DPDA, $\Phi = 45^{\circ}$ (D₂). TD-PBE1PBE/6-31+G*//[6-31G* (D_{2h})]

^{*a*} Wavenumber in 10³ cm⁻¹. ^{*b*} Oscillator strength.

^c The notation (i,-j) indicates an excited singlet configuration derived from the ground configuration by promotion of an electron from the *i*'th highest occupied to the *j*'th lowest unoccupied MO.

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

DPDA, $\Phi = 90^{\circ}$ (D_{2d}). TD-PBE1PBE/6-31+G*//[6-31G* (D_{2h})]

^{*a*} Wavenumber in 10³ cm⁻¹. ^{*b*} Oscillator strength.

^c The notation (i,-j) indicates an excited singlet configuration derived from the ground configuration by promotion of an electron from the *i*'th highest occupied to the *j*'th lowest unoccupied MO.

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

Center	Atomic	Atomic	Coor	dinates (Angs	stroms)	
Number	Number	Туре	X	Y	Z	
1	6	0	0.00000	0.00000	0.679461	
2	6	0	0.00000	0.000000	-0.679461	
3	6	0	0.00000	0.00000	1.899660	
4	б	0	0.00000	0.00000	-1.899660	
5	б	0	0.00000	0.00000	3.318498	
б	б	0	0.00000	0.00000	-3.318498	
7	б	0	0.00000	1.211722	4.030916	
8	б	0	0.00000	1.211722	-4.030916	
9	б	0	0.00000	-1.211722	4.030916	
10	б	0	0.00000	-1.211722	-4.030916	
11	б	0	0.00000	1.206087	5.419091	
12	б	0	0.00000	1.206087	-5.419091	
13	6	0	0.00000	-1.206087	5.419091	
14	6	0	0.00000	-1.206087	-5.419091	
15	6	0	0.00000	0.00000	6.117221	
16	6	0	0.00000	0.00000	-6.117221	
17	1	0	0.00000	2.148075	3.481442	
18	1	0	0.00000	2.148075	-3.481442	
19	1	0	0.00000	-2.148075	3.481442	
20	1	0	0.00000	-2.148075	-3.481442	
21	1	0	0.00000	2.148474	5.959837	
22	1	0	0.00000	2.148474	-5.959837	
23	1	0	0.00000	-2.148474	5.959837	
24	1	0	0.00000	-2.148474	-5.959837	
25	1	0	0.00000	0.00000	7.203732	
26	1	0	0.00000	0.00000	-7.203732	
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Excited s	tates from	<aa,bb:aa,bb></aa,bb:aa,bb>	singles matr	ix:		
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Sta	te	X 0000 0 0	Y Z		2.	
1	0.	0.000	-3.21	6/ 0.934	£2	
2	0.	0.0	0.00		10	
3	0.		0.00		0	
4	0.	0.00			10	
5	0.	0.00	40/ U.UU		13	
6	0.	0.0	0.00		10	
./	0.	0.0	0.00		10	
8	0.	0.9	οst 0.00	00 0.122	22	

Standard orientation:

9	0.0000	0.0000	0.0000	0.0000
10	0.0000	0.0000	0.0000	0.0000
11	0.0000	0.0000	0.0000	0.0000
12	0.0000	0.0000	-3.0614	1.3046
13	0.0000	0.0000	0.0000	0.0000
14	0.1630	0.0000	0.0000	0.0038
15	0.0835	0.0000	0.0000	0.0010
16	0.0000	0.0000	0.0000	0.0000
17	0.0000	0.0000	0.0000	0.0000
18	0.0000	0.0841	0.0000	0.0011
19	0.0000	0.0000	0.0000	0.0000
20	-0.0034	0.0000	0.0000	0.0000
21	0.0000	0.0000	0.0000	0.0000
22	0.0000	0.0000	0.0000	0.0000
23	0.0000	0.0000	-1.0771	0.1786
24	0.0000	0.0000	0.0000	0.0000
25	0.0000	0.0000	-1.6037	0.4041
26	0.0000	0.0000	0.0000	0.0000
27	0.0000	0.0000	0.0000	0.0000
28	0.1633	0.0000	0.0000	0.0043
29	0.0000	0.0000	2.7701	1.2587
30	0.0000	0.0000	0.0000	0.0000
31	0.0000	0.0000	-0.0583	0.0006
32	0.0000	0.0000	0.0000	0.0000
33	0.0000	-0.6044	0.0000	0.0610
34	0.0000	0.0000	0.0000	0.0000
35	0.0000	0.0000	0.0000	0.0000
36	0.0000	0.0000	0.0000	0.0000
37	0.0000	1.4718	0.0000	0.3655
38	0.0000	0.0000	0.0000	0.0000
39	0.0000	0.0000	0.0000	0.0000
40	0.0000	0.0000	-0.4017	0.0276
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Ground to ex. state 1 2 3 4 5 6 7 8 9 10 11 12 13	cited state tra X 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	nsition velo Y 0.0000 0.0000 0.0000 -0.0053 0.0000 0.0000 -0.1961 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	bcity dipole Z 0.4286 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.6306 0.0000	Moments (Au): Osc. 0.9041 0.0000 0.0000 0.0000 0.0001 0.0000 0.1311 0.0000 0.0000 0.0000 0.0000 1.2695 0.0000
Ground to example state 1 1 2 3 4 5 6 7 8 9 10 11 12 13 14	cited state tra X 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	nsition velo Y 0.0000 0.0000 0.0000 -0.0053 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	<pre>city dipole Z 0.4286 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.6306 0.0000 0.0000</pre>	Moments (Au): Osc. 0.9041 0.0000 0.0000 0.0000 0.0001 0.0000 0.0000 0.1311 0.0000 0.0000 0.0000 1.2695 0.0000 0.0008
Ground to example state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15	cited state tra X 0.0000	nsition velo Y 0.0000 0.0000 0.0000 -0.0053 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	<pre>city dipole Z 0.4286 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.6306 0.0000 0.0000 0.0000 0.0000</pre>	Moments (Au): Osc. 0.9041 0.0000 0.0000 0.0001 0.0000 0.0000 0.1311 0.0000 0.0000 0.0000 1.2695 0.0000 0.0008 0.0019
Ground to example state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16	cited state tra X 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.000000 0.00000000	nsition velo Y 0.0000 0.0000 0.0000 -0.0053 0.0000 0.0000 -0.1961 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	<pre>city dipole Z 0.4286 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.6306 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000</pre>	Moments (Au): Osc. 0.9041 0.0000 0.0000 0.0001 0.0000 0.0000 0.1311 0.0000 0.0000 0.0000 1.2695 0.0000 0.0008 0.0019 0.0000
Ground to exa state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17	cited state tra X 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000000	nsition velo Y 0.0000 0.0000 0.0000 -0.0053 0.0000 0.0000 -0.1961 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	<pre>city dipole Z 0.4286 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.6306 0.0000 0.6306 0.0000 0.0000 0.0000 0.0000 0.0000</pre>	Moments (Au): Osc. 0.9041 0.0000 0.0000 0.0001 0.0000 0.0000 0.1311 0.0000 0.0000 0.0000 1.2695 0.0000 0.0008 0.0019 0.0000 0.0000
Ground to ex. state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18	cited state tra X 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000000	nsition velo Y 0.0000 0.0000 0.0000 -0.0053 0.0000 0.0000 -0.1961 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	bcity dipole Z 0.4286 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.6306 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	Moments (Au): Osc. 0.9041 0.0000 0.0000 0.0000 0.0000 0.0000 0.1311 0.0000 0.0000 0.0000 1.2695 0.0000 0.0008 0.0019 0.0000 0.0000 0.0000 0.0000 0.0000 0.0009
Ground to ex. state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19	cited state tra X 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000000	nsition velo Y 0.0000 0.0000 0.0000 -0.0053 0.0000 0.0000 -0.1961 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 -0.0180 0.0000	<pre>city dipole Z 0.4286 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.6306 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000</pre>	Moments (Au): Osc. 0.9041 0.0000 0.0000 0.0001 0.0000 0.1311 0.0000 0.0000 0.0000 1.2695 0.0000 0.0008 0.0019 0.0000 0.0009 0.0009 0.0000
Ground to exa state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20	cited state tra X 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000000	nsition velo Y 0.0000 0.0000 0.0000 -0.0053 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	<pre>city dipole Z 0.4286 0.0000</pre>	Moments (Au): Osc. 0.9041 0.0000 0.0000 0.0001 0.0000 0.1311 0.0000 0.0000 0.0000 1.2695 0.0000 0.0000 0.0008 0.0019 0.0000 0.0009 0.0000 0.0001 0.0001
Ground to example state 1 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 21 20 21 21 20 21 20 21 20 21 20 21 20 21 20 21 20 21 20 20 21 20 20 20 20 20 20 20 20 20 20 20 20 20	cited state tra X 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.000000 0.0000000 0.00000000	nsition velo Y 0.0000 0.0000 0.0000 -0.0053 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	<pre>city dipole Z 0.4286 0.0000</pre>	Moments (Au): Osc. 0.9041 0.0000 0.0000 0.0001 0.0000 0.0000 0.1311 0.0000 0.0000 1.2695 0.0000 0.0000 0.0008 0.0019 0.0000 0.0000 0.0000 0.0000 0.0000 0.0001 0.0000 0.0001 0.0000
Ground to exa state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 22	cited state tra X 0.0000 0.	nsition velo Y 0.0000 0.0000 0.0000 -0.0053 0.0000 -0.1961 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	<pre>city dipole Z 0.4286 0.0000 0.000</pre>	Moments (Au): Osc. 0.9041 0.0000 0.0000 0.0001 0.0000 0.0000 0.1311 0.0000 0.0000 1.2695 0.0000 0.0000 0.0008 0.0019 0.0000 0.0000 0.0000 0.0000 0.0001 0.00000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
Ground to exa state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23	cited state tra X 0.0000 0.	nsition velo Y 0.0000 0.0000 0.0000 -0.0053 0.0000 -0.1961 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	<pre>city dipole Z 0.4286 0.0000</pre>	Moments (Au): Osc. 0.9041 0.0000 0.0000 0.0001 0.0000 0.0000 0.1311 0.0000 0.0000 0.0000 1.2695 0.0000 0.0008 0.0019 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000000
Ground to exa state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 57	cited state tra X 0.0000 0.	nsition velo Y 0.0000 0.0000 0.0000 -0.0053 0.0000 0.0000 -0.1961 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	<pre>city dipole Z 0.4286 0.0000 0.2561 0.0000</pre>	Moments (Au): Osc. 0.9041 0.0000 0.0000 0.0001 0.0000 0.0000 0.1311 0.0000 0.0000 0.0000 1.2695 0.0000 0.0000 0.0008 0.0019 0.00000 0.00000 0.00000 0.00000 0.0000000 0.00000 0.00000 0.00000 0.00000000
Ground to exa state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 27	cited state tra X 0.0000 0.	nsition velo Y 0.0000 0.0000 0.0000 -0.0053 0.0000 -0.1961 0.0000	<pre>city dipole Z 0.4286 0.00000 0.00000 0.00000 0.000000</pre>	Moments (Au): Osc. 0.9041 0.0000 0.0000 0.0000 0.0000 0.0000 0.1311 0.0000 0.0000 0.0000 1.2695 0.0000 0.0000 0.0008 0.0019 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000000
Ground to exa state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27	cited state tra X 0.0000 0.	nsition velo Y 0.0000 0.0000 0.0000 0.0000 -0.0053 0.0000 0.00	<pre>city dipole Z 0.4286 0.0000 0.2561 0.0000 0.3718 0.0000 0.0000 0.0000</pre>	Moments (Au): Osc. 0.9041 0.0000 0.0000 0.0000 0.0000 0.0000 0.1311 0.0000 0.0000 0.0000 1.2695 0.0000 0.0000 0.0008 0.0019 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000000
Ground to exa state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28	cited state tra X 0.0000 0.	nsition velo Y 0.0000 0.0000 0.0000 0.0000 -0.0053 0.0000 0.00	<pre>city dipole Z 0.4286 0.0000 0.2561 0.0000 0.3718 0.0000 0.0000 0.0000 0.0000 0.0000</pre>	Moments (Au): Osc. 0.9041 0.0000 0.0000 0.0000 0.0000 0.0000 0.1311 0.0000 0.0000 0.0000 1.2695 0.0000 0.0000 0.0008 0.0019 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.1894 0.0000 0.3910 0.0000 0.0000 0.0000 0.3910 0.00000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
Ground to exa state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29	cited state tra X 0.0000 0.	nsition velo Y 0.0000 0.0000 0.0000 0.0000 -0.0053 0.0000 0.00	<pre>city dipole Z 0.4286 0.0000 0.2561 0.0000 0.2561 0.0000 0.3718 0.0000 0.0000 0.0000 0.0000 0.0000</pre>	Moments (Au): Osc. 0.9041 0.0000 0.0000 0.0000 0.0000 0.0000 0.1311 0.0000 0.0000 0.0000 1.2695 0.0000 0.0000 0.0008 0.0019 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.3910 0.0000 0.0000 0.3910 0.0000 0.0000 0.0000 0.3910 0.0000 0.0000 0.0000 0.3910 0.0000 0.0000 0.0000 0.0000 0.1894 0.0000 0.0000 0.3910 0.0000 0.0000 0.0000 0.0000 0.1894 0.0000 0.0000 0.0000 0.0000 0.1894 0.00000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
Ground to exa state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30	cited state tra X 0.0000 0.	nsition velo Y 0.0000 0.0000 0.0000 -0.0053 0.0000 -0.1961 0.00000 0.00000 0.00000 0.000000	<pre>city dipole Z 0.4286 0.0000 0.2561 0.0000 0.2561 0.0000 0.3718 0.0000 0.3718 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000</pre>	Moments (Au): Osc. 0.9041 0.0000 0.0000 0.0001 0.0000 0.0000 0.1311 0.0000 0.0000 0.0000 1.2695 0.0000 0.0008 0.0019 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.1894 0.0000 0.3910 0.0000 0.0000 0.3910 0.0000 0.0002 1.2175 0.0000
Ground to exa state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31	cited state tra X 0.00000 0.00000 0.00000 0.00000000	nsition velo Y 0.0000 0.0000 0.0000 0.0000 -0.0053 0.0000 0.00	<pre>city dipole Z 0.4286 0.0000 0.2561 0.0000 0.2561 0.0000 0.2561 0.0000 0.2561 0.0000 0.2561 0.0000 0.2561 0.0000 0.2561 0.0000 0.2561 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000</pre>	Moments (Au): Osc. 0.9041 0.0000 0.0000 0.0001 0.0000 0.0000 0.1311 0.0000 0.0000 0.0000 1.2695 0.0000 0.0000 0.0008 0.0019 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.3910 0.0000 0.0000 0.0000 0.3910 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.1894 0.0000 0.0000 0.0000 0.0000 0.1894 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.1894 0.00000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000

Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics This journal is The Owner Societies 2011

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

Excitation energies and oscillator strengths:

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

Excited Stat 52 -> 5 53 -> 5	ce 1: 56 54	Singlet-B1U -0.25056 13% 0.62888 79%	29.72232 1000/cm 336.45 nm f=0.9342 [2,-3] [1,-1]
Excited Stat 52 -> 5 53 -> 5	2: 54 56	Singlet-AU 0.67975 92% -0.10508	31.24026 1000/cm 320.10 nm f=0.0000 [2,-1]
Excited Stat 52 -> 5 53 -> 5	2e 3: 54 56	Singlet-AU 0.14079 0.68361 93%	33.98577 1000/cm 294.24 nm f=0.0000 [1,-3]
Excited Stat 49 -> 5 50 -> 5 51 -> 5 53 -> 5	2e 4: 58 54 55 57	Singlet-B3G -0.14252 0.45993 42% 0.14350 0.50722 51%	38.04677 1000/cm 262.83 nm f=0.0000 [4,-1] [1,-4]
Excited Stat 49 -> 5 50 -> 5 51 -> 5 53 -> 5	55 55 54 58	Singlet-B2U -0.14309 0.14334 0.46202 43% 0.50528 51%	38.05967 1000/cm 262.75 nm f=0.0003 [3,-1] [1,-5]
Excited Stat 49 -> 5 53 -> 5	ce 6: 54 55	Singlet-AG 0.43191 37% 0.56250 63%	40.1051 1000/cm 249.34 nm f=0.0000 [5,-1] [1,-2]
Excited Stat 49 -> 5 50 -> 5 53 -> 5	ze 7: 58 54 57	Singlet-B3G -0.10146 0.48425 47% -0.45484 41%	42.85222 1000/cm 233.36 nm f=0.0000 [4,-1] [1,-4]
Excited Stat 49 -> 5 51 -> 5 53 -> 5	2e 8: 57 54 58	Singlet-B2U -0.10311 0.48206 46% -0.45653 42%	42.92319 1000/cm 232.98 nm f=0.1222 [3,-1] [1,-5]
Excited Stat 47 -> 5 49 -> 5 50 -> 5 51 -> 5 53 -> 5	2e 9: 56 54 58 57 55	Singlet-AG 0.10832 0.49331 49% 0.14551 0.14614 -0.35142 25%	43.6628 1000/cm 229.03 nm f=0.0000 [5,-1] [1,-2]
Excited Stat 47 -> 5 52 -> 5	te 10: 54 55	Singlet-B1G 0.14852 0.68324 93%	44.3516 1000/cm 225.47 nm f=0.0000 [2,-2]
Excited Stat	te 11:	Singlet-B2G	45.40012 1000/cm 220.27 nm f=0.0000

S 7

53 -> 59 0.67529 91% [1,-6] 53 -> 61 0.17456 Excited State 12: Singlet-B1U 45.82517 1000/cm 218.22 nm f=1.3046 48 -> 54 -0.37574 28% [6,-1] 52 -> 56 0.47884 46% [2,-3] 53 -> 54 0.15190 53 -> 65 0.20911 Excited State 13: Singlet-B2G 46.80595 1000/cm 213.65 nm f=0.0000 52 -> 57 0.70249 99% [2,-4] Excited State 14: Singlet-B3U 46.83095 1000/cm 213.53 nm f=0.0038 52 -> 58 0.54441 59% [2,-5] 53 -> 60 0.43602 38% [1,-7] Excited State 15: 46.87208 1000/cm 213.35 nm f=0.0010 Singlet-B3U 39% [2,-5] 52 -> 58 -0.44402 53 -> 60 0.53581 57% [1,-7] Excited State 16: Singlet-B1G 48.14563 1000/cm 207.70 nm f=0.0000 -0.12423 46 -> 56 49 -> 56 0.68537 94% [5,-3] 17: 50.00716 1000/cm 199.97 nm f=0.0000 Excited State Singlet-B2G -0.17226 53 -> 59 0.66312 53 -> 61 88% [1,-8] Singlet-B2U Excited State 18: 50.11846 1000/cm 199.53 nm f=0.0011 48 -> 58 -0.13593 -0.42341 49 -> 57 36% [5,-4] 50 -> 55 0.51047 52% [4,-2] 51 -> 54 -0.1532453 -> 58 -0.11842 Excited State 19: Singlet-B3G 50.12572 1000/cm 199.50 nm f=0.0000 48 -> 57 -0.13636 49 -> 58 -0.42109 35% [5,-5] 50 -> 54 -0.15325 51 -> 55 0.51173 52% [3,-2] 53 -> 57 -0.11783 50.58062 1000/cm 197.70 nm f=0.0000 Excited State 20: Singlet-B3U 51 -> 56 0.70450 99% [3,-3] Excited State 21: 50.58788 1000/cm 197.68 nm f=0.0000 Singlet-B2G 50 -> 56 0.70291 99% [4,-3] Excited State 22: Singlet-AU 50.59997 1000/cm 197.63 nm f=0.0000 95% [1,-9] 53 -> 62 0.69037 53 -> 66 0.11548 Excited State 23: Singlet-B1U 50.68386 1000/cm 197.30 nm f=0.1786 48 -> 54 0.50578 51% [6,-1] 52 -> 56 0.17308 53 -> 65 0.40307 32% [1,-12] 53 -> 70 -0.12021 Excited State 24: Singlet-B1G 51.5993 1000/cm 193.80 nm f=0.0000 97% [1,-10] 53 -> 63 0.69464 Excited State 25: Singlet-B1U 51.72834 1000/cm 193.32 nm f=0.4041 49 -> 55 45% [5,-2] 0.47541 50 -> 57 0.32835 22% [4,-4] 51 -> 58 0.32366 21% [3,-5]

52.45182 1000/cm 190.65 nm f=0.0000 Excited State 26: Singlet-B3G 52 -> 59 0.62537 78% [2,-6] 52 -> 61 0.29422 17% [2,-8] Excited State 27: Singlet-B1G 52.53409 1000/cm 190.35 nm f=0.0000 44 -> 54 0.10138 47 -> 54 0.66575 89% [7,-1] 52 -> 55 -0.15606 Excited State 28: Singlet-B3U 53.14142 1000/cm 188.18 nm f=0.0043 49 -> 61 0.11244 53 -> 64 0.68220 93% [1,-11] Excited State 29: Singlet-B1U 54.00121 1000/cm 185.18 nm f=1.2587 49 -> 55 0.42605 36% [5,-2] 50 -> 57 -0.22691 10% [4,-4] 51 -> 58 -0.20851 52 -> 56 -0.12939 53 -> 65 0.38379 29% [1,-12] Excited State 30: 54.25205 1000/cm 184.32 nm f=0.0000 Singlet-AG 46 -> 54 0.24696 12% [8,-1] 47 -> 56 -0.1338448 -> 55 0.16269 50 -> 58 0.35762 26% [4,-5] 51 -> 57 0.41609 35% [3,-4] 54.60129 1000/cm 183.15 nm f=0.0006 Excited State 31: Singlet-B1U 49% [4,-4] 50 -> 57 -0.49467 0.50481 51% [3,-5] 51 -> 58 Excited State 32: Singlet-AG 54.6021 1000/cm 183.14 nm f=0.0000 50 -> 58 0.52126 54% [4,-5] 51 -> 57 -0.4773346% [3,-4] Excited State 33: Singlet-B2U 54.93924 1000/cm 182.02 nm f=0.0610 49 -> 57 -0.23294 11% [5,-4] 50 -> 55 -0.20193 52 -> 60 0.60624 74% [2,-7] 52 -> 64 -0.12866 54.94569 1000/cm 182.00 nm f=0.0000 Excited State 34: Singlet-AU 52% [4,-6] 50 -> 59 0.50977 51 -> 60 0.45674 42% [3,-7] 53 -> 66 -0.12647Excited State 35: 54.95618 1000/cm 181.96 nm f=0.0000 Singlet-B1G 43% [4,-7] 50 -> 60 0.46467 54% [3,-6] 51 -> 59 0.51876 Excited State 36: Singlet-B3G 55.42155 1000/cm 180.43 nm f=0.0000 51% [5,-5] 49 -> 58 0.50405 51 -> 55 31% [3,-2] 0.39648 52 -> 59 0.10319 37: 55.54576 1000/cm 180.03 nm f=0.3655 Excited State Singlet-B2U 49 -> 57 40% [5,-4] 0.44783 50 -> 55 0.35026 25% [4,-2] 22% [2,-7] 52 -> 60 0.33401 Excited State 38: Singlet-AU 55.56592 1000/cm 179.97 nm f=0.0000 48 -> 56 0.13545 50 -> 59 0.10131 53 -> 66 0.65765 87% [1,-13]

Excited State 39: Singlet-B2G 55.92162 1000/cm 178.82 nm f=0.0000 53 -> 61 -0.1074053 -> 67 0.67979 92% [1,-14] Excited State 40: Singlet-B1U 56.40475 1000/cm 177.29 nm f=0.0276 49 -> 55 -0.14255 50 -> 57 0.13521 51 -> 58 0.13624 53 -> 65 0.17406 53 -> 70 0.61238 75% [1,-17] 53 -> 74 0.11249 Orbital symmetries: Occupied (B1U) (AG) (AG) (B1U) (AG) (B1U) (B3G) (B2U) (B1U) (AG) (B1U) (AG) (B2U) (B3G) (B1U) (AG) (AG) (B1U) (AG) (B1U) (AG) (B3G) (B2U) (B1U) (AG) (B1U) (B2U) (B3G) (AG) (B1U) (AG) (B1U) (AG) (B2U) (B3G) (B1U) (AG) (B2U) (B3G) (B3U) (B2G) (B1U) (AG) (B2U) (B3G) (B3U) (B2U) (B2G) (B3U) (AU) (B1G) (B3G) (B2G) (B3U) (B2G) (B2U) (B1G) (AU) (AG) (B1U) (AG) (B2U) Virtual (B3G) (B1U) (B3U) (B2U) (AG) (B3G) (B2G) (B3U) (B1U) (AG) (B1U) (B3U) (B2U) (B1G) (AG) (AU) (B2G) (B3G) (B1U) (B2G) (B3U) (B1G) (AG) (B3U) (AU) (B2U) (B1U) (B2G) (B3G) (AG) (B2U) (B3G) (B3U) (B3G) (B1U) (AG) (B2G) (B2U) (AG) (B1U) (B3U) (B2U) (B3G) (AG) (B2G) (B1U) (B1U) (AG) (B3G) (B2U) (B1U) (B1U) (B3G) (B2G) (AG) (B2U) (B1U) (AG) (B3G) (B2U) (B3U) (B2U) (AG) (B3G) (B1U) (B1U) (AG) (AG) (B1U) (B3G) (B2U) (B2G) (B1U) (B3G) (AG) (B2U) (B3G) (B2U) (B1U) (B3G) (AG) (B1U) (B3G) (B2U) (AG) (B1U) (AG) (B1U) (B3U) (B2G) (B3U) (AG) (B2U) (B3G) (B1G) (B2G) (AU) (AG) (B1U) (B2U) (B3U) (B3G) (B1G) (AU) (B2G) (B1U) (AG) (B2U) (B3U) (B3G) (B2U) (B1U) (AG) (B2G) (B3U) (B2G) (AG) (B1U) (B3U) (B3G) (B1U) (AG) (B2U) (B3G) (B2U) (B3G) (AG) (B2G) (B2U) (B1U) (AG) (B1U) (B2U) (B3G) (B2U) (B3G) (AG) (B1U) (AG) (B1U) (B2U) (AG) (AG) (B3G) (B3G) (B1U) (B1G) (AU) (B3U) (B1U) (B1U) (B2U) (AG) (AG) (B1U) (B3G) (B3U) (B1U) (B2G) (B1G) (AG) (B2U) (AU) (B2G) (B3U) (B3G) (B1G) (B2G) (AU) (AG) (B1G) (AU) (B2U) (B1U) (B3U) (B1U) (AG) (B3G) (B1G) (B2U) (AG) (B1U) (B2G) (B3G) (AG) (B1U) (AG) (B1U) (B2U) (AG) (B3G) (AU) (B1U) (B2U) (B3U) (B1U) (AG) (B3G) (B1G) (AU) (B2U) (AG) (B2G) (B1U) (B1U) (B3G) (B3U) (B1G) (AU) (B3U) (B2G) (B2G) (AG) (B2U) (AG) (B1U) (B1U) (AG) (B2U) (B3G) (B1G) (AU) (B1U) (B3U) (B3G) (AG) (B2U) (AG) (B3G) (B1U) (B1U) (B2U) (AG) (B3G) (B1U) (B2U) (B2G) (AG) (B3G) (B1U) (AG) (B1U) (AG) (B1U) (AG) (B2U) (B3G) (AG) (B1U) (B1U) (AG) (B2U) (B3G) (B1U) (AG) (B1U) (AG) (B1U) The electronic state is 1-AG. Alpha occ. eigenvalues -- -10.27807 -10.27807 -10.26222 -10.26165 -10.25925 occ. eigenvalues ---10.25910 -10.25749 -10.25749 -10.25748 -10.25748 Alpha occ. eigenvalues --Alpha -10.25560 -10.25560 -10.25443 -10.25443 -10.25428 -0.81684 Alpha occ. eigenvalues ---10.25428 -0.90258 -0.90218 -0.83491 -0.67347 Alpha occ. eigenvalues ---0.78882 -0.78490 -0.78490 -0.74627 -0.56537 Alpha occ. eigenvalues ---0.64788 -0.63877 -0.63873 -0.60745 Alpha occ. eigenvalues ---0.50721 -0.50331 -0.48341 -0.55554 -0.48273 Alpha occ. eigenvalues ---0.45987 -0.45843 -0.44782 -0.44779 -0.41078 Alpha occ. eigenvalues ---0.40515 -0.38133 -0.38065 -0.37601 -0.37105 -0.36448 -0.35310 Alpha occ. eigenvalues ---0.32120 -0.27919 -0.27816

Alpha	occ.	eigenvalues	 -0.27815	-0.26039	-0.22581		
Alpha	virt.	eigenvalues	 -0.06728	-0.01782	-0.01629	-0.01559	-0.01541
Alpha	virt.	eigenvalues	 0.01017	0.01275	0.03057	0.03131	0.03358
Alpha	virt.	eigenvalues	 0.04223	0.04790	0.05328	0.05516	0.06219
Alpha	virt.	eigenvalues	 0.06340	0.06354	0.06977	0.07698	0.08220
Alpha	virt.	eigenvalues	 0.08711	0.09300	0.09800	0.09818	0.09922
Alpha	virt.	eigenvalues	 0.10391	0.11743	0.11899	0.12336	0.13979
Alpha	virt.	eigenvalues	 0.14442	0.14480	0.15057	0.15267	0.15427
Alpha	virt.	eigenvalues	 0.15733	0.15886	0.15901	0.16123	0.16358
Alpha	virt.	eigenvalues	 0.16373	0.16936	0.17394	0.17436	0.17981
Alpha	virt.	eigenvalues	 0.18134	0.19859	0.19871	0.19997	0.21421
Alpha	virt.	eigenvalues	 0.21484	0.21639	0.21920	0.21940	0.22205
Alpha	virt.	eigenvalues	 0.22865	0.23341	0.23689	0.24018	0.24229
Alpha	virt.	eigenvalues	 0.24918	0.25115	0.25663	0.26098	0.26574
Alpha	virt.	eigenvalues	 0.27311	0.27607	0.28326	0.28701	0.28797
Alpha	virt.	eigenvalues	 0.29540	0.29776	0.30807	0.31028	0.32151
Alpha	virt.	eigenvalues	 0.32505	0.33934	0.34361	0.34589	0.35331
Alpha	virt.	eigenvalues	 0.35681	0.35906	0.36072	0.36445	0.39082
Alpha	virt.	eigenvalues	 0.44022	0.45498	0.47299	0.49594	0.50766
Alpha	virt.	eigenvalues	 0.55036	0.57676	0.57872	0.61239	0.61293
Alpha	virt.	eigenvalues	 0.64257	0.65561	0.67116	0.68282	0.69673
Alpha	virt.	eigenvalues	 0.69875	0.71330	0.71349	0.72800	0.72887
Alpha	virt	eigenvalues	 0 72913	0 73282	0 74029	0 74122	0 74885
Alpha	virt.	eigenvalues	 0.75754	0.75768	0.76186	0.76747	0.76977
Alpha	virt	eigenvalues	 0 77365	0 78154	0 79087	0 80184	0 81430
Alpha	virt	eigenvalues	 0 82034	0 82085	0 83502	0 84407	0 85878
Alpha	virt	eigenvalues	 0 86852	0 87049	0 88642	0 89889	0 93082
Alpha	virt.	eigenvalues	 0.00052	0.07012	0.00012	0.05005	0.95002
Alpha	virt	eigenvalues	 0.98167	0 98378	0 99180	1 01065	1 02158
Alpha	virt	eigenvalues	 1 02369	1 03964	1 04403	1 09329	1 10159
Alpha	virt	eigenvalues	 1 12654	1 12901	1 15025	1 16483	1 19629
Alpha	virt.	eigenvalues	 1 19911	1 21131	1 23354	1 23636	1 23675
Alpha	virt.	eigenvalues	 1 23842	1 23859	1 24919	1 25817	1 28371
Alpha	virt.	eigenvalues	 1 31059	1 31885	1 34108	1 34719	1 35217
Alpha	virt	eigenvalues	 1 42947	1 43751	1 43992	1 44434	1 44740
Alpha	virt.	eigenvalues	 1 45677	1 46084	1 47499	1 48443	1 48751
Alpha	virt.	eigenvalues	 1 49337	1 49845	1 50110	1 50217	1 50276
Alpha	virt.	eigenvalues	 1 59285	1 61751	1 62479	1 67810	1 67876
Alpha	virt.	eigenvalues	 1 82279	1 82510	1 84360	1 86694	1 87304
Alpha	virt	eigenvalues	 1 89813	1 90192	1 90524	1 92921	1 93215
Alpha	virt.	eigenvalues	 1 95315	1 97088	2,00162	2 00335	2 01021
Alpha	virt.	eigenvalues	 2 01136	2 02792	2.00102	2.00333	2.01021
Alpha	virt.	eigenvalues	 2.01130	2.02/92	2.00010	2.00452	2.09171
Alpha	virt.	eigenvalues	2.13500	2.14033	2.15592	2.13322	2.10295
Alpha	virt.	eigenvalues	 2.10000	2.20233	2.20030	2.21904	2.22213
Alpha	virt.	eigenvalues	 2.2/040	2.30377	2.30020	2.31203	2.31323
Alpha	virt.	eigenvalues	 2.33110	2.30014	2.39/90	2.51295	2.54509
Alpha	virt.	eigenvalues	 2.59505	2.00733	2.03039	2.03949	2.03193
Alpha	VIIC.	eigenvalues	 2.05230	2.05290	2.00700	2.70337	2.73030
Alpha	virt.	eigenvalues	 Z./019U	2./0300	2.//849	2./010/ 2.04050	2.01/90 2 15154
Alpha	virt.	eigenvalues	 2.0/049	2.00032	2.98U42 2.25501	3.04050	3.15154
Alpha	virt.	eigenvalues	 3.101// 2 77405	3.33028	3.3559L	3.41856	3.51340
Alpha	virt.	eigenvalues	 3.//405	4.22014	4.2/414	4.2/0/9	4.2//31
Alpha	virt.	ergenvarues	 4.29924	4.31868	4.33865	4.40114	4.42230
Alpha	virt.	eigenvalues	 4.44037	4.45499	4.60097	4.04UII	4.81350
Arbua	virt.	eigenvalues	 4.90386	5.64359			

Normal termination of Gaussian 03 at Sat Nov 8 10:04:25 2008.

Gaussian 03: x86-Linux-G03RevB.04 2-Jun-2003
7-Nov-2008
* * * * * * * * * * * * * * * * * * * *
#t + td(Nst-40 - conver-3) = belobe/6-31+C*
#c ca(NSC-40,CONVEL-5) pbetpbe/0 51/G
1 4-Diphenvlbuta-1 3-divne $D=45$ (based on phelphe/6-31G* D2h geo)
1,1 Deprend Date 1,5 ardine, D 15 (babea on phetphet) 516 Dan geo.)

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

Center	Atomic Number	Atomic	Coord	dinates (Angs v	stroms) Z	
				±		
1	6	0	0.00000	0.00000	0.679461	
2	б	0	0.00000	0.00000	-0.679461	
3	6	0	0.00000	0.00000	1.899660	
4	6	0	0.00000	0.00000	-1.899660	
5	6	0	0.00000	0.00000	3.318498	
б	б	0	0.00000	0.00000	-3.318498	
7	6	0	-0.463706	1.119485	4.030916	
8	6	0	0.463706	1.119485	-4.030916	
9	б	0	0.463706	-1.119485	4.030916	
10	б	0	-0.463706	-1.119485	-4.030916	
11	6	0	-0.461549	1.114279	5.419091	
12	б	0	0.461549	1.114279	-5.419091	
13	6	0	0.461549	-1.114279	5.419091	
14	б	0	-0.461549	-1.114279	-5.419091	
15	6	0	0.00000	0.00000	6.117221	
16	6	0	0.00000	0.00000	-6.117221	
17	1	0	-0.822033	1.984562	3.481442	
18	1	0	0.822033	1.984562	-3.481442	
19	1	0	0.822033	-1.984562	3.481442	
20	1	0	-0.822033	-1.984562	-3.481442	
21	1	0	-0.822185	1.984931	5.959837	
22	1	0	0.822185	1.984931	-5.959837	
23	1	0	0.822185	-1.984931	5.959837	
24	1	0	-0.822185	-1.984931	-5.959837	
25	1	0	0.00000	0.000000	7.203732	
26	1	0	0.00000	0.000000	-7.203732	
324 bas 53 alg	sis function pha electron	ns, 552 pri ns 53 b	mitive gaussia: eta electrons	ns, 324 car	rtesian basis	functio
SCF Done	E (RPBE+HI	F-PBE) = -61	4.896597490	A.U. after	26 cycles	
	Convg :	= 0.7835D-	08	-V/T = 2.00)89	
* * * * * * * * *	* * * * * * * * * * * *	* * * * * * * * * * * * *	* * * * * * * * * * * * *	* * * * * * * * * * * * *	* * * * * * * * * * * * *	
Excited a	states from	<aa,bb:aa,bb ********</aa,bb:aa,bb 	> singles matr ******	ix: ************	* * * * * * * * * * * * *	
Ground to	o excited st	tate Transiti	on electric di	pole moments	(Au):	
sta	ate	Х	Y Z	Osc	2.	
-	1 0	.0000 0.	0000 2.56	35 0.603	32	
4	2 0	.0000 0.	0000 0.00	00 0.000	00	
	3 0	.0000 0.	0000 0.00	00 0.000	00	
4	4 0	.0000 -0.	0436 0.00	00 0.000)2	
Į.	5 0	.0245 0.	0000 0.00	00 0.000)1	
é	5 0	0000 0	0000 -3.37	13 1.390	96	

Standard orientation:

/	0.0000	0.0000	0.0000	0.0000
8	-0.2764	0.0000	0.0000	0.0100
9	0.0000	0.7378	0.0000	0.0714
10	0.0000	0.0000	0.0000	0.0000
11	0.1861	0.0000	0.0000	0.0048
12	0.0000	-0.3177	0.0000	0.0139
13	0.0000	-0.0247	0.0000	0.0001
14	0.0000	0.0000	0.5966	0.0503
15	-0.2979	0.0000	0.0000	0.0128
16	0.0000	0.7568	0.0000	0.0826
17	-0.2315	0.0000	0.0000	0.0077
18	0.0000	0.0000	-0.9303	0.1256
19	0.0000	0.0000	-0.9507	0.1374
20	0.0000	0.1401	0.0000	0.0030
21	-0.0617	0.0000	0.0000	0.0006
22	0.0000	0.0000	0.0000	0.0000
23	0.0000	0.0000	0.7115	0.0801
24	0.0000	0.0000	0.0000	0.0000
25	0.0000	0.0000	-2.4722	0.9739
26	0.0000	0.0393	0.0000	0.0002
27	-0.2368	0.0000	0.0000	0.0092
28	0.0000	0.5084	0.0000	0.0423
29	-0.0147	0.0000	0.0000	0.0000
30	0.0000	0.0000	1.1417	0.2139
31	0.0000	0.0000	0.0000	0.0000
32	0.0000	0.0000	-0.0019	0.0000
33	0.0000	0.0000	0.0000	0.0000
34 2E	0.0000	0.0000	0.0277	0.0001
30	0.0000	0.0000	0.0000	0.0000
27	0.0040	0.0000	0.0000	0.0009
38	0.0000	0.0000	0.0000	0.0000
30	0.0000		0.0505	0.0003
57				0 0004
40	0 0000	0 0000	0.0000	0.0004
40 Ground to	0.0000 excited state 1	0.0000 0.0000 cransition ve	0.0000 0.4421 Clocity dipol	0.0004 0.0336 e Moments (Au):
40 Ground to stat	0.0000 excited state 1 e X	0.00433 0.0000 transition ve Y	0.0000 0.4421 locity dipol Z	0.0004 0.0336 e Moments (Au): Osc.
40 Ground to stat 1	0.0000 excited state 1 e X 0.0000	0.0000 cransition ve Y 0.0000	0.0000 0.4421 locity dipol Z -0.3475	0.0004 0.0336 e Moments (Au): Osc. 0.5848
40 Ground to stat 1 2	0.0000 excited state 1 e X 0.0000 0.0000	0.0000 cransition ve Y 0.0000 0.0000	0.0000 0.4421 locity dipol Z -0.3475 0.0000	0.0004 0.0336 e Moments (Au): Osc. 0.5848 0.0000
40 Ground to stat 1 2 3	0.0000 excited state 1 e X 0.0000 0.0000 0.0000	0.0000 cransition ve Y 0.0000 0.0000 0.0000	0.0000 0.4421 clocity dipol z -0.3475 0.0000 0.0000	0.0004 0.0336 e Moments (Au): Osc. 0.5848 0.0000 0.0000
40 Ground to stat 1 2 3 4	0.0000 excited state 1 e X 0.0000 0.0000 0.0000 0.0000	0.0000 cransition ve Y 0.0000 0.0000 0.0000 0.0055	0.0000 0.4421 clocity dipol z -0.3475 0.0000 0.0000 0.0000	0.0004 0.0336 e Moments (Au): Osc. 0.5848 0.0000 0.0000 0.0000
40 Ground to stat 1 2 3 4 5	0.0000 excited state 1 e X 0.0000 0.0000 0.0000 0.0000 -0.0013	0.0000 cransition ve Y 0.0000 0.0000 0.0000 0.0055 0.0000	0.0000 0.4421 clocity dipol Z -0.3475 0.0000 0.0000 0.0000 0.0000	0.0004 0.0336 e Moments (Au): Osc. 0.5848 0.0000 0.0000 0.0001 0.0001 0.0000
40 Ground to stat 1 2 3 4 5 6	0.0000 excited state t e X 0.0000 0.0000 0.0000 -0.0013 0.0000	0.0000 cransition ve Y 0.0000 0.0000 0.0000 0.0055 0.0000 0.0000	0.0000 0.4421 clocity dipol Z -0.3475 0.0000 0.0000 0.0000 0.0000 0.6150	0.0004 0.0336 e Moments (Au): Osc. 0.5848 0.0000 0.0000 0.0001 0.0000 1.3650
40 Ground to stat 1 2 3 4 5 6 7	0.0000 excited state t e X 0.0000 0.0000 0.0000 -0.0013 0.0000 0.0000	0.0000 cransition ve Y 0.0000 0.0000 0.0000 0.0055 0.0000 0.0000 0.0000	0.0000 0.4421 2 -0.3475 0.0000 0.0000 0.0000 0.6150 0.0000	0.0004 0.0336 e Moments (Au): Osc. 0.5848 0.0000 0.0000 0.0001 0.0000 1.3650 0.0000
40 Ground to stat 1 2 3 4 5 6 7 8	0.0000 excited state 1 e X 0.0000 0.0000 0.0000 -0.0013 0.0000 0.0000 0.0000 0.0000	0.0000 cransition ve Y 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0.0000 0.4421 2 -0.3475 0.0000 0.0000 0.0000 0.6150 0.0000 0.0000	0.0004 0.0336 e Moments (Au): Osc. 0.5848 0.0000 0.0000 0.0001 0.0000 1.3650 0.0000 0.0133
40 Ground to stat 1 2 3 4 5 6 7 8 9	0.0000 excited state 1 e X 0.0000 0.0000 0.0000 -0.0013 0.0000 0.0000 0.0000 0.0000 0.0000	0.0000 cransition ve Y 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0.0000 0.4421 2 -0.3475 0.0000 0.0000 0.0000 0.6150 0.0000 0.0000 0.0000	0.0004 0.0336 e Moments (Au): Osc. 0.5848 0.0000 0.0000 1.3650 0.0000 0.0133 0.0733
40 Ground to stat 1 2 3 4 5 6 7 8 9 10	0.0000 excited state 1 e X 0.0000 0.0000 0.0000 -0.0013 0.0000 0.0000 0.0625 0.0000 0.0000	0.0000 cransition ve Y 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 -0.1471 0.0000	0.0000 0.4421 2 -0.3475 0.0000 0.0000 0.0000 0.6150 0.0000 0.0000 0.0000 0.0000 0.0000	0.0004 0.0336 e Moments (Au): Osc. 0.5848 0.0000 0.0000 1.3650 0.0000 0.0133 0.0733 0.0000
40 Ground to stat 1 2 3 4 5 6 7 8 9 10 11	0.0000 excited state 1 e X 0.0000 0.0000 0.0000 -0.0013 0.0000 0.0000 0.0625 0.0000 0.0000 0.0000 0.0025	0.0000 cransition ve Y 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 -0.1471 0.0000 0.0000	0.0000 0.4421 Plocity dipol Z -0.3475 0.0000 0.0000 0.0000 0.6150 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0.0004 0.0336 e Moments (Au): Osc. 0.5848 0.0000 0.0000 0.0000 1.3650 0.0000 0.0133 0.0733 0.0000 0.0022
40 Ground to stat 1 2 3 4 5 6 7 8 9 10 11 12	0.0000 excited state 1 e X 0.0000 0.0000 0.0000 -0.0013 0.0000 0.0000 0.0000 0.0625 0.0000 0.0000 -0.0259 0.0000	0.0000 cransition ve Y 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0.0000 0.4421 clocity dipol Z -0.3475 0.0000 0.0000 0.0000 0.6150 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0.0004 0.0336 e Moments (Au): Osc. 0.5848 0.0000 0.0000 0.0000 1.3650 0.0000 0.0133 0.0733 0.0000 0.0022 0.0174
40 Ground to stat 1 2 3 4 5 6 7 8 9 10 11 12 13	0.0000 excited state 1 e X 0.0000 0.0000 0.0000 -0.0013 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 -0.0259 0.0000 0.0000	0.0000 cransition ve Y 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0734 -0.0005	0.0000 0.4421 Plocity dipol Z -0.3475 0.0000 0.0000 0.0000 0.6150 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0.0004 0.0336 e Moments (Au): Osc. 0.5848 0.0000 0.0000 1.3650 0.0000 0.0133 0.0733 0.0000 0.0022 0.0174 0.0000
40 Ground to stat 1 2 3 4 5 6 7 8 9 10 11 12 13 14	0.0000 excited state 1 e X 0.0000 0.0000 0.0000 -0.0013 0.0000 0.0000 0.0625 0.0000 0.0000 -0.0259 0.0000 0.0000 0.0000	0.0000 cransition ve Y 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0734 -0.0005 0.0000	0.0000 0.4421 Plocity dipol Z -0.3475 0.0000 0.0000 0.0000 0.6150 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000000	0.0004 0.0336 e Moments (Au): Osc. 0.5848 0.0000 0.0000 1.3650 0.0000 0.0133 0.0733 0.0000 0.0022 0.0174 0.0000 0.0483
40 Ground to stat 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15	0.0000 excited state 1 e X 0.0000 0.0000 0.0000 -0.0013 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0.0000 cransition ve Y 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0734 -0.0005 0.0000 0.0000	0.0000 0.4421 Plocity dipol Z -0.3475 0.0000 0.0000 0.0000 0.6150 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000000	0.0004 0.0336 e Moments (Au): Osc. 0.5848 0.0000 0.0000 1.3650 0.0000 0.0133 0.0733 0.0000 0.0022 0.0174 0.0000 0.0483 0.0125 0.0000
40 Ground to stat 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16	0.0000 excited state 1 e X 0.0000 0.0000 0.0000 -0.0013 0.0000 0.0000 0.0625 0.0000 0.0000 -0.0259 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0.0000 cransition ve Y 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0734 -0.0005 0.0000 0.0000 0.0000 0.0000	0.0000 0.4421 Plocity dipol Z -0.3475 0.0000 0.0000 0.0000 0.6150 0.00000 0.00000 0.000000 0.000000 0.000000 0.00000000	0.0004 0.0336 e Moments (Au): Osc. 0.5848 0.0000 0.0000 1.3650 0.0000 0.0133 0.0733 0.0000 0.0022 0.0174 0.0000 0.0483 0.0125 0.0868 0.0054
40 Ground to stat 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17	0.0000 excited state 1 e X 0.0000 0.0000 0.0000 -0.0013 0.0000 0.0625 0.0000 0.0625 0.0000 0.0025 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0.0000 cransition ve Y 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0734 -0.0005 0.0000 0.0000 0.0000 0.0000	0.0000 0.4421 Plocity dipol Z -0.3475 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.000000 0.00000000	0.0004 0.0336 e Moments (Au): Osc. 0.5848 0.0000 0.0000 1.3650 0.0000 0.0133 0.0733 0.0000 0.0022 0.0174 0.0000 0.022 0.0174 0.0000 0.0483 0.0125 0.0868 0.0054 0.1184
40 Ground to stat 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18	0.0000 excited state 1 e X 0.0000 0.0000 0.0000 -0.0013 0.0000 0.0000 0.0625 0.0000 0.0000 -0.0259 0.0000 0.0000 0.0000 0.0000 0.0000 0.0637 0.0000 0.0420 0.0000	0.0000 cransition ve Y 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0734 -0.0005 0.0000 0.0000 0.0000 0.0000 0.0000	0.0000 0.4421 Plocity dipol Z -0.3475 0.0000 0.0000 0.0000 0.6150 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.0000000 0.00000000	0.0004 0.0336 e Moments (Au): Osc. 0.5848 0.0000 0.0000 0.0000 1.3650 0.0000 0.0133 0.0733 0.0000 0.0022 0.0174 0.0000 0.022 0.0174 0.0000 0.0483 0.0125 0.0868 0.0054 0.1184 0.1425
40 Ground to stat 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20	0.0000 excited state 1 e X 0.0000 0.0000 0.0000 -0.0013 0.0000 0.0000 0.0000 0.0000 -0.0259 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0420 0.0000 0.0000 0.0000	0.0000 cransition ve Y 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000000	0.0000 0.4421 Plocity dipol Z -0.3475 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.0000000 0.00000000	0.0004 0.0336 e Moments (Au): Osc. 0.5848 0.0000 0.0000 0.0000 1.3650 0.0000 0.0133 0.0733 0.0000 0.0022 0.0174 0.0000 0.0483 0.0125 0.0868 0.0054 0.1184 0.1435 0.0032
40 Ground to stat 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21	0.0000 excited state 1 e X 0.0000 0.0000 0.0000 0.0000 -0.0013 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0420 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0.0000 cransition ve Y 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0734 -0.0005 0.0000 0.0000 0.0000 -0.1679 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0.0000 0.4421 Plocity dipol Z -0.3475 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000000	0.0004 0.0336 e Moments (Au): Osc. 0.5848 0.0000 0.0000 0.0000 1.3650 0.0000 0.0133 0.0733 0.0000 0.022 0.0174 0.0000 0.0483 0.0125 0.0868 0.0054 0.1184 0.1435 0.0032 0.0009
40 Ground to stat 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22	0.0000 excited state 1 e X 0.0000 0.0000 0.0000 -0.0013 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0.0000 cransition ve Y 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.0000000 0.00000000	0.0000 0.4421 Plocity dipol Z -0.3475 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.2215 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.0000000 0.00000000	0.0004 0.0336 e Moments (Au): Osc. 0.5848 0.0000 0.0000 1.3650 0.0000 1.3650 0.0000 0.0133 0.0733 0.0733 0.0000 0.0022 0.0174 0.0000 0.0483 0.0125 0.0868 0.0054 0.1184 0.1435 0.0032 0.0009 0.0000
40 Ground to stat 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23	0.0000 excited state 1 e X 0.0000 0.0000 0.0000 -0.0013 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000	0.0000 cransition ve Y 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000000	0.0000 0.4421 Plocity dipol Z -0.3475 0.0000 0.0000 0.0000 0.6150 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000000	0.0004 0.0336 e Moments (Au): Osc. 0.5848 0.0000 0.0000 1.3650 0.0000 1.3650 0.0000 0.0133 0.0733 0.0000 0.0022 0.0174 0.0000 0.022 0.0174 0.0000 0.0483 0.0125 0.0868 0.0054 0.1184 0.1435 0.0032 0.0032 0.0009 0.0000 0.0792
40 Ground to stat 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24	0.0000 excited state 1 e X 0.0000 0.0000 0.0000 -0.0013 0.0000 0.0000 0.0625 0.0000 0.0625 0.0000 0.0000 -0.0259 0.0000 0.0000 0.0000 0.0637 0.0000 0.0637 0.0000 0.0637 0.0000 0.0420 0.0000 0.0000 0.0181 0.0000 0.0000 0.0000 0.0000	0.0000 cransition ve Y 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.000000 0.00000 0.0000000 0.00000000	0.0000 0.4421 Plocity dipol Z -0.3475 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000000	0.0004 0.0336 e Moments (Au): Osc. 0.5848 0.0000 0.0000 1.3650 0.0000 0.0133 0.0733 0.0000 0.0125 0.0868 0.0054 0.1184 0.1435 0.0032 0.009 0.0009 0.0000 0.0792 0.0000
40 Ground to stat 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25	0.0000 excited state 1 e X 0.0000 0.0000 0.0000 0.0000 -0.0013 0.0000 0.0000 0.0625 0.0000 0.0000 -0.0259 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	0.0000 cransition ve Y 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000000	0.0000 0.4421 Plocity dipol 2 -0.3475 0.0000 0.1966 0.2215 0.0000 0.0000 0.1979 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000000	0.0004 0.0336 e Moments (Au): Osc. 0.5848 0.0000 0.0001 0.0000 1.3650 0.0000 0.0133 0.0733 0.0000 0.022 0.0174 0.0000 0.022 0.0174 0.0000 0.0483 0.0125 0.0868 0.0054 0.1184 0.1435 0.0032 0.0009 0.0009 0.0000 0.0792 0.0000 0.0792 0.0000 0.9439
40 Ground to stat 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26	0.0000 excited state 1 e X 0.0000 0.0000 0.0000 0.0000 -0.0013 0.0000 0.0000 0.0000 0.0000 -0.0259 0.0000	0.0000 cransition ve Y 0.00000 0.00000 0.000000 0.00000 0.0000000 0.00000 0.00000 0.00000000	0.0000 0.4421 Plocity dipol 2 -0.3475 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.1966 0.2215 0.0000 0.0000 0.0000 0.1966 0.2215 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000000	0.0004 0.0336 e Moments (Au): Osc. 0.5848 0.0000 0.0001 0.0000 1.3650 0.0000 0.0133 0.0733 0.0000 0.022 0.0174 0.0000 0.022 0.0174 0.0000 0.0483 0.0125 0.0868 0.0054 0.1184 0.1435 0.0032 0.0009 0.0009 0.0009 0.0000 0.0792 0.0000 0.9439 0.0006
40 Ground to stat 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27	0.0000 excited state 1 e X 0.00000 0.00000 0.00000 0.00000 0.000000	0.0000 cransition ve Y 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000000	0.0000 0.4421 Plocity dipol 2 -0.3475 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.2215 0.0000 0.0000 0.2215 0.0000 0.0000 0.1966 0.2215 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000	0.0004 0.0336 e Moments (Au): Osc. 0.5848 0.0000 0.0000 1.3650 0.0000 0.0133 0.0733 0.0733 0.0000 0.022 0.0174 0.0000 0.0483 0.0125 0.0868 0.0054 0.1184 0.1435 0.0032 0.0009 0.0009 0.0009 0.0000 0.0792 0.0000 0.9439 0.0006 0.0102
40 Ground to stat 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28	0.0000 excited state 1 e X 0.0000 0.0000 0.0000 0.0000 -0.0013 0.0000	0.0000 cransition ve Y 0.0000 0.00	0.0000 0.4421 Plocity dipol Z -0.3475 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.0000000 0.00000 0.000000 0.00000000	0.0004 0.0336 e Moments (Au): Osc. 0.5848 0.0000 0.0000 0.0001 0.0000 1.3650 0.0000 0.0133 0.0733 0.0000 0.022 0.0174 0.0000 0.0483 0.0125 0.0868 0.0054 0.1184 0.1435 0.0032 0.0009 0.0002 0.0009 0.0000 0.0792 0.0000 0.0792 0.0000 0.0792 0.0000 0.0792 0.0000 0.0792 0.0000 0.0792 0.0000 0.0792 0.00000 0.00000 0.00000 0.00000 0.00000000

Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics This journal is The Owner Societies 2011

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

Excitation energies and oscillator strengths:

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

Excited St 52 -> 52 ->	ate 1: 55 58	Singlet-B1 0.26193 -0.12953	14%	30.21513 1000/cm 330.96 nm f=0.6032 [2,-2]
53 ->	54	0.61636	76%	[1,-1]
Excited St 49 -> 52 ->	ate 2: 54 54	Singlet-A 0.14098 0.59583	71%	30.75229 1000/cm 325.18 nm f=0.0000
53 ->	55	0.29323	17%	[1,-2]
Excited St 49 ->	ate 3: 54	Singlet-A -0.14826		33.27519 1000/cm 300.53 nm f=0.0000
52 -> 53 ->	54 55	-0.28274 0.56068	16% 63%	[2,-1] [1,-2]
53 ->	58	-0.24551	12%	[1,-5]
Excited St 49 -> 50 ->	ate 4: 57 55	Singlet-B2 0.10876 -0.16956		38.5436 1000/cm 259.45 nm f=0.0002
51 -> 52 ->	54 57	-0.44609 -0.14927	40%	[3,-1]
53 ->	56	0.49290	49%	[1,-3]
Excited St 49 ->	ate 5: 56	Singlet-B3 0.10876		38.54522 1000/cm 259.44 nm f=0.0001
50 -> 51 ->	54 55 56	-0.44604 -0.16979	40%	[4,-1]
53 ->	57	0.49275	49%	[1,-4]
Excited St 48 ->	ate 6: 54	Singlet-B1 0.13905		40.54064 1000/cm 246.67 nm f=1.3996
52 -> 53 -> 53 ->	55 54 64	0.59853 -0.18814 0.10971	72%	[2,-2]
Excited St 49 -> 52 ->	ate 7: 54 54	Singlet-A 0.49284 -0.12593	49%	42.91835 1000/cm 233.00 nm f=0.0000 [5,-1]
53 -> 53 ->	55 58	-0.15561 -0.45582	42%	[1,-5]
Excited St 50 -> 52 -> 53 ->	ate 8: 54 56 57	Singlet-B3 0.44666 0.22330 0.46000	40% 10% 42%	43.16193 1000/cm 231.69 nm f=0.0100 [4,-1] [2,-3] [1,-4]
Excited St 51 ->	ate 9: 54	Singlet-B2 0.44540	40%	43.18613 1000/cm 231.55 nm f=0.0714 [3,-1]

10% [2,-4] 52 -> 57 0.22743 53 -> 56 0.45937 42% [1,-3] Excited State 10: Singlet-A 44.90732 1000/cm 222.68 nm f=0.0000 49 -> 54 0.39873 32% [5,-1] 50 -> 56 0.14055 51 -> 57 0.14052 52 -> 54 -0.1047753 -> 55 0.16470 53 -> 58 0.43415 38% [1,-5] Excited State 11: Singlet-B3 45.22429 1000/cm 221.12 nm f=0.0048 50 -> 54 -0.24927 12% [4,-1] 51 -> 55 0.29813 18% [3,-2] 52 -> 56 0.57487 66% [2,-3] Excited State 45.22994 1000/cm 221.09 nm f=0.0139 12: Singlet-B2 50 -> 55 0.30148 18% [4,-2] 51 -> 54 -0.25111 13% [3,-1] 52 -> 57 0.57265 66% [2,-4] 46.10021 1000/cm 216.92 nm f=0.0001 Excited State 13: Singlet-B2 90% [1,-6] 53 -> 59 0.66909 53 -> 61 0.18279 46.53494 1000/cm 214.89 nm f=0.0503 Excited State 14: Singlet-B1 0.12828 47 -> 54 48 -> 54 0.11914 49 -> 55 0.53849 58% [5,-2] 52 -> 58 0.37895 29% [2,-5] Excited State 15: Singlet-B3 47.46651 1000/cm 210.68 nm f=0.0128 49 -> 56 -0.1772751 -> 55 0.56091 63% [3,-2] 52 -> 56 -0.26981 15% [2,-3] 53 -> 57 0.13688 53 -> 60 -0.15983 Excited State 16: Singlet-B2 47.49797 1000/cm 210.54 nm f=0.0826 49 -> 57 -0.18611 50 -> 55 0.57392 66% [4,-2] -0.27711 52 -> 57 15% [2,-4] 53 -> 56 0.14375 Excited State 17: Singlet-B3 47.59637 1000/cm 210.10 nm f=0.0077 51 -> 55 0.13388 52 -> 59 -0.1733153 -> 60 0.65462 86% [1,-7] Excited State 18: Singlet-B1 47.78107 1000/cm 209.29 nm f=0.1256 0.50238 48 -> 54 50% [6,-1] 49 -> 55 0.16228 49 -> 58 -0.11015 52 -> 55 -0.1099752 -> 58 -0.4087333% [2,-5] 19: 50.02651 1000/cm 199.89 nm f=0.1374 Excited State Singlet-B1 47 -> 54 -0.13169 48 -> 54 -0.33228 22% [6,-1] 49 -> 55 0.28448 16% [5,-2] 50 -> 57 0.10001 51 -> 56 0.10016 52 -> 58 -0.1547453 -> 64 0.45647 42% [1,-11] 53 -> 68 -0.10841

Excited State 20: Singlet-B2 50.59594 1000/cm 197.64 nm f=0.0030 52 -> 60 0.17442 53 -> 59 -0.16031 53 -> 61 0.64642 84% [1,-8] 53 -> 67 0.10336 Excited State 50.91776 1000/cm 196.40 nm f=0.0006 21: Singlet-B3 52 -> 59 0.61913 77% [2,-6] 52 -> 61 0.26976 15% [2,-8] 53 -> 60 0.15923 Excited State 22: Singlet-A 51.43153 1000/cm 194.43 nm f=0.0000 53 -> 62 0.68428 94% [1,-9] 53 -> 66 0.11487 Excited State Singlet-B1 52.1171 1000/cm 191.87 nm f=0.0801 23: 50 -> 57 -0.1032451 -> 56 -0.10190 52 -> 62 -0.11040 53 -> 63 0.65431 86% [1,-10] 53 -> 64 0.12155 Excited State 52.18405 1000/cm 191.63 nm f=0.0000 24: Singlet-A -0.16718 46 -> 54 48 -> 55 0.53655 58% [6,-2] 50 -> 56 -0.24997 12% [4,-3] 51 -> 57 -0.25011 13% [3,-4] 52 -> 64 -0.11232 Excited State 25: Singlet-B1 52.46231 1000/cm 190.61 nm f=0.9739 47 -> 54 0.13580 49 -> 58 0.15059 50 -> 57 0.37769 29% [4,-4] 51 -> 56 0.37917 29% [3,-3] 52 -> 58 -0.1441553 -> 63 0.19396 53 -> 64 -0.21113 53.06561 1000/cm 188.45 nm f=0.0002 Excited State 26: Singlet-B2 87% [2,-7] 52 -> 60 0.65832 52 -> 65 -0.1101453 -> 59 0.12710 53 -> 61 -0.14381 Excited State 53.82296 1000/cm 185.79 nm f=0.0092 27: Singlet-B3 49 -> 56 0.39695 32% [5,-3] 51 -> 58 -0.3164220% [3,-5] 52 -> 61 0.13224 53 -> 65 0.41912 35% [1,-12] Excited State 28: Singlet-B2 53.877 1000/cm 185.61 nm f=0.0423 -0.10952 48 -> 56 49 -> 57 0.50631 51% [5,-4] 50 -> 58 -0.4177935% [4,-5] 51 -> 54 0.10554 Excited State 53.91733 1000/cm 185.47 nm f=0.0000 29: Singlet-B3 49 -> 56 -0.32508 21% [5,-3] 51 -> 58 0.27192 15% [3,-5] 52 -> 59 -0.11138 52 -> 61 0.17325 53 -> 65 0.48921 48% [1,-12] Excited State 30: Singlet-B1 54.01493 1000/cm 185.13 nm f=0.2139

76% [7,-1] 47 -> 54 0.61693 11% [1,-11] 53 -> 64 0.23559 Excited State 31: Singlet-A 54.58758 1000/cm 183.19 nm f=0.0000 46 -> 54 0.10478 48 -> 55 0.29114 17% [6,-2] 48 -> 58 -0.12239 50 -> 56 0.19630 51 -> 57 0.11201 52 -> 64 0.51562 53% [2,-11] Excited State 32: Singlet-B1 54.59725 1000/cm 183.16 nm f=0.0000 50 -> 57 0.49932 50% [4,-4] 51 -> 56 -0.49854 50% [3,-3] Excited State 33: Singlet-A 54.59725 1000/cm 183.16 nm f=0.0000 50 -> 56 0.48456 47% [4,-3] 51 -> 57 -0.51039 52% [3,-4] Excited State 34: 55.05054 1000/cm 181.65 nm f=0.0001 Singlet-B1 50 -> 60 0.45942 42% [4,-7] 51 -> 59 0.52248 55% [3,-6] 35: 55.05295 1000/cm 181.64 nm f=0.0000 Excited State Singlet-A 50 -> 59 0.52168 54% [4,-6] 51 -> 60 0.45919 42% [3,-7] Excited State 36: 55.83048 1000/cm 179.11 nm f=0.0009 Singlet-B3 -0.25598 13% [2,-6] 52 -> 59 52 -> 61 0.56901 65% [2,-8] 52 -> 67 0.15191 53 -> 65 -0.22940 11% [1,-12] Excited State 37: Singlet-A 56.22811 1000/cm 177.85 nm f=0.0000 52 -> 63 0.24188 12% [2,-10] 53 -> 66 0.63897 82% [1,-13] Excited State 38: Singlet-B1 56.26521 1000/cm 177.73 nm f=0.0003 0.59834 72% [2,-9] 52 -> 62 52 -> 66 0.15030 0.23075 53 -> 68 11% [1,-15] Excited State 39: Singlet-B2 56.51201 1000/cm 176.95 nm f=0.0004 52 -> 65 -0.15392 53 -> 61 -0.10236 53 -> 67 0.66618 89% [1,-14] Excited State 40: Singlet-B1 56.65639 1000/cm 176.50 nm f=0.0336 49 -> 58 0.13342 52 -> 62 -0.28738 17% [2,-9] 53 -> 63 -0.10718 53 -> 64 0.15669 53 -> 68 0.52265 55% [1,-15] 53 -> 70 -0.18167 Orbital symmetries: Occupied (A) (B1) (A) (B1) (A) (B1) (B3) (B2) (B1) (A) (A) (B1) (B2) (B3) (A) (B1) (A) (B1) (A) (B1) (A) (B3) (B2) (B1) (A) (B1) (B2) (B3) (A) (B1) (A) (B1) (A) (B2) (B3) (B1) (A) (B2) (B3) (B3) (B2) (B1) (A) (B2) (B3) (B3) (B2) (B2) (B3) (A) (B1) (B3) (B2) Virtual (B3) (B2) (A) (B1) (B2) (A) (B1) (A) (B2) (B3) (B3) (B1) (B2) (A) (B3) (B2) (B3) (B1) (A) (B1) (B3) (B2) (A) (B1) (A) (B2) (B3) (B1) (B2) (B3)

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<pre>(A) (B1) (B1) (B2) (B2) (A) (B3) (B1) (A) (B1) (A) (B1) (A) (B2) (B3) (B1) (A) (B1) (B3) (B1) (A) (B1) (A) (B1) The electronic state is 1-A. Alpha occ. eigenvalues10.27800 -10.27800 -10.26203 -10.26146 -10.25906 Alpha occ. eigenvalues10.25891 -10.25752 -10.25752 -10.25751 -10.25751 Alpha occ. eigenvalues10.25891 -10.25752 -10.25752 -10.25751 -10.2543 Alpha occ. eigenvalues10.25891 -0.2566 -0.90216 -0.83478 -0.81678 Alpha occ. eigenvalues0.78875 -0.78490 -0.78490 -0.74613 -0.67343 Alpha occ. eigenvalues0.64785 -0.63874 -0.63871 -0.60736 -0.46232 Alpha occ. eigenvalues0.46785 -0.63874 -0.63871 -0.60736 -0.44238 Alpha occ. eigenvalues0.46984 -0.45840 -0.44780 -0.44778 -0.40998 Alpha occ. eigenvalues0.36281 -0.35518 -0.31614 -0.28935 -0.27815 Alpha occ. eigenvalues0.36281 -0.35518 -0.31614 -0.28935 -0.27815 Alpha occ. eigenvalues0.36281 -0.35518 -0.31614 -0.28935 -0.27815 Alpha occ. eigenvalues 0.06386 -0.03377 -0.01551 -0.01550 0.00600 Alpha virt. eigenvalues 0.06385 0.09108 0.09805 0.09859 0.09968 Alpha virt. eigenvalues 0.06426 0.04307 0.5426 0.05512 0.05984 Alpha virt. eigenvalues 0.16676 0.11579 0.12049 0.12473 0.13923 Alpha virt. eigenvalues 0.16678 0.16808 0.1777 0.1786 0.18059 Alpha virt. eigenvalues 0.16678 0.16808 0.1777 0.17780 0.18051 Alpha virt. eigenvalues 0.16678 0.16818 0.15998 0.16116 0.16439 Alpha virt. eigenvalues 0.16167 0.12818 0.15998 0.12163 0.22210 0.22283 Alpha virt. eigenvalues 0.21617 0.21712 0.21919 0.22210 0.22283 Alpha virt. eigenvalues 0.21617 0.21712 0.21919 0.221163 0.21658 Alpha virt. eigenvalues 0.21617 0.21712 0.21919 0.22116 0.224560 Alpha virt. eigenvalues 0.21617 0.21712 0.21919 0.22116 0.22883 Alpha virt. eigenvalues 0.21617 0.27748 0.36527 0.26158 0.26430 Alpha virt. eigenvalues 0.27063 0.27628 0.27714 0.28437 0.50856 Alpha virt. eigenvalues 0.27063 0.77648 0.36527 0.26126 0.24560 Alpha virt. eigenvalues 0.73610 0.75650 0.76418 0.77002 0.77360 Alpha virt. eigenvalues -</pre>		(A) (B	1) (A)	(B2) (B3)	(A) $(B1)$	(B2) (B3) (B1)	(B2)	
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Alpha occ. eigenvalues	The elect	tronic state i	s 1-A.	10 07000	10 07000	10 00000	10 00140	10 05000
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Alpha occ. eigenvalues	Alpha o	cc eigenvalue	s s	-10.25567	-10.25752	-10.25752 -10.25443	-10.25751	-10.25751 -10.25429
Alpha occ. eigenvalues -0.78875 -0.78490 -0.78490 -0.74613 -0.67343 Alpha occ. eigenvalues -0.64785 -0.63874 -0.63871 -0.60736 -0.56533 Alpha occ. eigenvalues -0.45984 -0.45840 -0.44780 -0.44778 -0.40998 Alpha occ. eigenvalues -0.45984 -0.45840 -0.44780 -0.44778 -0.40998 Alpha occ. eigenvalues -0.42603 -0.35518 -0.31614 -0.28935 -0.37204 Alpha occ. eigenvalues -0.27814 -0.25085 -0.22887 -0.27814 -0.25085 -0.27815 -0.01550 0.00600 Alpha virt. eigenvalues 0.01053 0.01404 0.03103 0.03197 0.03366 Alpha virt. eigenvalues 0.06352 0.06449 0.07098 0.07806 0.08026 Alpha virt. eigenvalues 0.16655 0.11579 0.12249 0.13223 Alpha virt. eigenvalues 0.16678 0.14398 0.14470 0.15209 0.15790 Alpha virt. eigenvalues 0.18670 0.18980 0.21163 0.2168 0.22283 Alpha virt. eigenvalues<	Alpha o	cc. eigenvalue	s	-10.25429	-0.90256	-0.90216	-0.83478	-0.81678
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Alpha occ. eigenvalues -0.55548 -0.50719 -0.63028 -0.44330 -0.48282 Alpha occ. eigenvalues -0.45984 -0.45840 -0.44778 -0.44778 -0.44978 Alpha occ. eigenvalues -0.36281 -0.35518 -0.31614 -0.28935 -0.27815 Alpha occ. eigenvalues -0.27814 -0.25055 -0.22887 -0.01550 0.00600 Alpha virt. eigenvalues 0.06388 -0.0377 -0.01551 -0.01550 0.00600 Alpha virt. eigenvalues 0.04256 0.04307 0.05426 0.05512 0.05984 Alpha virt. eigenvalues 0.06352 0.09407 0.05426 0.07098 0.07086 0.08026 Alpha virt. eigenvalues 0.16655 0.11579 0.12049 0.12473 0.13923 Alpha virt. eigenvalues 0.16678 0.16880 0.17757 0.1778 0.15299 Alpha virt. eigenvalues 0.18675 0.22808 0.23555 0.23579 0.24168 0.24560 Alpha virt. eigenvalues 0.21617 0.21712 0.21919 0.22210 0.22283 Alpha virt. eigen	Alpha o	cc. eigenvalue	s	-0.64785	-0.63874	-0.63871	-0.60736	-0.56533
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Alpha virt. eigenvalues 0.04256 0.04307 0.05426 0.05512 0.05984 Alpha virt. eigenvalues 0.06352 0.06449 0.07098 0.07806 0.08026 Alpha virt. eigenvalues 0.08635 0.09108 0.09805 0.09859 0.09968 Alpha virt. eigenvalues 0.14357 0.14398 0.14470 0.15209 0.15590 Alpha virt. eigenvalues 0.16678 0.16880 0.17757 0.17788 0.18051 Alpha virt. eigenvalues 0.16678 0.16880 0.17757 0.17788 0.18051 Alpha virt. eigenvalues 0.16678 0.16880 0.17757 0.17788 0.18051 Alpha virt. eigenvalues 0.21617 0.21712 0.21993 0.22163 0.22283 Alpha virt. eigenvalues 0.22808 0.23555 0.23579 0.24168 0.24430 Alpha virt. eigenvalues 0.24959 0.24969 0.25520 0.26158 0.26430 Alpha virt. eigenvalues 0.35511 0.33926 0.33986 0.34929 0.35416 Alpha virt. eigenvalues 0.35514 0.36187	Alpha vi	rt. eigenvalue	s	0.01053	0.01404	0.03103	0.03197	0.03366
Alpha virt. eigenvalues 0.06352 0.06436 0.07908 0.07806 0.07806 0.08026 Alpha virt. eigenvalues 0.08635 0.09108 0.09805 0.09859 0.09968 Alpha virt. eigenvalues 0.14357 0.11579 0.12049 0.12473 0.13223 Alpha virt. eigenvalues 0.14357 0.14398 0.14470 0.15209 0.15590 Alpha virt. eigenvalues 0.16678 0.16880 0.17757 0.17788 0.18051 Alpha virt. eigenvalues 0.18165 0.19759 0.19930 0.21163 0.21268 Alpha virt. eigenvalues 0.22808 0.23555 0.23579 0.24168 0.24460 Alpha virt. eigenvalues 0.24959 0.24969 0.25520 0.26158 0.24430 Alpha virt. eigenvalues 0.23511 0.33926 0.33986 0.34929 0.35416 Alpha virt. eigenvalues 0.35511 0.3527 0.36527 0.36527 0.3652 0.39889 Alpha virt. eigenvalues 0.43511 0.45506 0.46477 0.48243 0.50856 Alpha virt. eigenvalues	Alpha vi	rt. eigenvalue	s	0.04256	0.04307	0.05426	0.05512	0.05984
Alpha virt. eigenvalues 0.008035 0.09005 0.09005 0.09005 0.09005 Alpha virt. eigenvalues 0.10605 0.11579 0.12049 0.12473 0.13923 Alpha virt. eigenvalues 0.14357 0.14398 0.14470 0.15209 0.15590 Alpha virt. eigenvalues 0.16678 0.16880 0.17757 0.17788 0.18051 Alpha virt. eigenvalues 0.18165 0.19759 0.19930 0.21163 0.2283 Alpha virt. eigenvalues 0.21617 0.21712 0.21919 0.22210 0.22283 Alpha virt. eigenvalues 0.24959 0.24959 0.25520 0.26158 0.26430 Alpha virt. eigenvalues 0.27063 0.27628 0.27714 0.28437 0.29447 Alpha virt. eigenvalues 0.35511 0.33925 0.33986 0.34929 0.35416 Alpha virt. eigenvalues 0.35914 0.36187 0.36527 0.36952 0.39889 Alpha virt. eigenvalues 0.57401 0.57804 0.61220 0.61265 0.64296 Alpha virt. eigenvalues 0.57401 0.57804	Alpha vi	rt. eigenvalue	s	0.06352	0.06449	0.07098	0.07806	0.08026
Alphavirt.Gigenvalues0.143570.143930.144700.152090.15590Alphavirt.eigenvalues0.157430.158180.159980.161160.16439Alphavirt.eigenvalues0.166780.168800.177570.177880.18051Alphavirt.eigenvalues0.181650.197590.199300.211630.21568Alphavirt.eigenvalues0.216170.217120.219190.222100.22283Alphavirt.eigenvalues0.249590.249690.255200.261580.26430Alphavirt.eigenvalues0.270630.2776280.277140.284370.29447Alphavirt.eigenvalues0.359140.361870.365270.369520.39889Alphavirt.eigenvalues0.574010.578040.612200.612650.64296Alphavirt.eigenvalues0.716330.713650.725470.728550.72862Alphavirt.eigenvalues0.734500.734840.748350.750430.75292Alphavirt.eigenvalues0.734500.734840.748350.750430.75292Alphavirt.eigenvalues0.734500.76550.764180.770200.77360Alphavirt.eigenvalues0.790610.790680.80221 <t< td=""><td>Alpha vi</td><td>rt eigenvalue</td><td>s s</td><td>0.08635</td><td>0.09108 0 11579</td><td>0.09805</td><td>0.09859</td><td>0.09908</td></t<>	Alpha vi	rt eigenvalue	s s	0.08635	0.09108 0 11579	0.09805	0.09859	0.09908
Alphavirt.eigenvalues0.157430.158180.159980.161160.16439Alphavirt.eigenvalues0.166780.168800.177570.177880.18051Alphavirt.eigenvalues0.181650.197590.199300.211630.21568Alphavirt.eigenvalues0.228080.235550.235790.241680.22283Alphavirt.eigenvalues0.249590.249690.255200.261580.26430Alphavirt.eigenvalues0.270630.276280.277140.284370.29447Alphavirt.eigenvalues0.235590.301770.309930.32684Alpha virt.eigenvalues0.359140.361870.365270.369520.39889Alpha virt.eigenvalues0.574010.578040.612200.612650.64296Alpha virt.eigenvalues0.712630.713650.725470.728550.72862Alpha virt.eigenvalues0.734500.734840.748350.750430.75292Alpha virt.eigenvalues0.790610.790680.802210.811600.81959Alpha virt.eigenvalues0.821960.840510.846380.860350.86355Alpha virt.eigenvalues0.790610.790680.802210.811600.81959Alpha virt.eigenvalue	Alpha vi	rt. eigenvalue	s	0.14357	0.14398	0.14470	0.15209	0.15590
Alpha virt.eigenvalues0.166780.168800.177570.177880.18051Alpha virt.eigenvalues0.181650.197590.199300.211630.21568Alpha virt.eigenvalues0.216170.217120.219190.222100.22283Alpha virt.eigenvalues0.240590.249690.255200.261580.26430Alpha virt.eigenvalues0.270630.276280.277140.284370.29447Alpha virt.eigenvalues0.235590.397930.301770.309930.32684Alpha virt.eigenvalues0.35110.339250.339860.349290.35416Alpha virt.eigenvalues0.435110.455060.464770.482430.50856Alpha virt.eigenvalues0.574010.578040.612200.612650.64296Alpha virt.eigenvalues0.712630.713650.725470.728550.72862Alpha virt.eigenvalues0.760340.760550.764180.770020.77360Alpha virt.eigenvalues0.734500.734840.748350.750430.75292Alpha virt.eigenvalues0.790610.790680.802210.811600.81959Alpha virt.eigenvalues0.821960.840510.846380.860350.86835Alpha virt.eigenvalues0.821960.84	Alpha vi	rt. eigenvalue	s	0.15743	0.15818	0.15998	0.16116	0.16439
Alpha virt.eigenvalues0.181650.197590.199300.211630.21568Alpha virt.eigenvalues0.216170.217120.219190.222100.22283Alpha virt.eigenvalues0.228080.235550.235790.241680.24560Alpha virt.eigenvalues0.249590.249690.255200.261580.26430Alpha virt.eigenvalues0.270630.276280.277140.284370.29447Alpha virt.eigenvalues0.355110.339250.301770.309930.32684Alpha virt.eigenvalues0.359140.361870.365270.369520.39889Alpha virt.eigenvalues0.435110.455060.464770.482430.50856Alpha virt.eigenvalues0.574010.578040.612200.612650.64296Alpha virt.eigenvalues0.712630.713650.725470.728550.72862Alpha virt.eigenvalues0.734500.734840.748350.750430.75292Alpha virt.eigenvalues0.790610.790680.802210.811600.81959Alpha virt.eigenvalues0.821960.840510.846380.860350.86835Alpha virt.eigenvalues0.821960.882110.903410.929720.93350Alpha virt.eigenvalues0.869030.8	Alpha vi	rt. eigenvalue	s	0.16678	0.16880	0.17757	0.17788	0.18051
Alpha virt.eigenvalues0.216170.217120.219190.222100.22283Alpha virt.eigenvalues0.228080.235550.235790.241680.24560Alpha virt.eigenvalues0.249590.249690.255200.261580.26430Alpha virt.eigenvalues0.270630.276280.277140.284370.29447Alpha virt.eigenvalues0.295090.297930.301770.309930.32684Alpha virt.eigenvalues0.335110.339250.339860.349290.35416Alpha virt.eigenvalues0.435110.455060.464770.482430.50856Alpha virt.eigenvalues0.574010.578040.612200.612650.64296Alpha virt.eigenvalues0.712630.713650.725470.728550.72862Alpha virt.eigenvalues0.760340.760550.764180.770020.77360Alpha virt.eigenvalues0.821960.840510.846380.860350.86835Alpha virt.eigenvalues0.821960.842110.903410.929720.93350	Alpha vi	rt. eigenvalue	s	0.18165	0.19759	0.19930	0.21163	0.21568
Alpha virt.eigenvalues0.228080.235550.235790.241680.24260Alpha virt.eigenvalues0.249590.249690.255200.261580.26430Alpha virt.eigenvalues0.270630.276280.277140.284370.29447Alpha virt.eigenvalues0.295090.297930.301770.309930.32684Alpha virt.eigenvalues0.335110.339250.339860.349290.35416Alpha virt.eigenvalues0.359140.361870.365270.369520.39889Alpha virt.eigenvalues0.574010.455060.464770.482430.50856Alpha virt.eigenvalues0.574010.578040.612200.612650.64296Alpha virt.eigenvalues0.712630.713650.725470.728550.72862Alpha virt.eigenvalues0.760340.760550.764180.770020.77360Alpha virt.eigenvalues0.821960.840510.846380.860350.86835Alpha virt.eigenvalues0.821960.840510.846380.860350.86835Alpha virt.eigenvalues0.790610.790680.890310.929720.93350Alpha virt.eigenvalues0.869030.882110.903410.929720.93350Alpha virt.eigenvalues0.869030.8	Alpha vi	rt. eigenvalue	s	0.21617	0.21712	0.21919	0.22210	0.22283
Alpha virt.eigenvalues0.270630.276280.277140.284370.29447Alpha virt.eigenvalues0.295090.297930.301770.309930.32684Alpha virt.eigenvalues0.335110.339250.339860.349290.35416Alpha virt.eigenvalues0.359140.361870.365270.369520.39889Alpha virt.eigenvalues0.435110.455060.464770.482430.50856Alpha virt.eigenvalues0.574010.578040.612200.612650.64296Alpha virt.eigenvalues0.712630.713650.725470.728550.72862Alpha virt.eigenvalues0.760340.760550.764180.770020.77360Alpha virt.eigenvalues0.821960.840510.846380.860350.86835Alpha virt.eigenvalues0.790610.790680.802210.811600.81959Alpha virt.eigenvalues0.869030.882110.903410.929720.93350Alpha virt.eigenvalues0.934810.956230.959130.976790.97819	Alpha vi	rt. eigenvalue rt. eigenvalue	s c	0.22808	0.23555	0.23579	0.24168	0.24560
Alpha virt.eigenvalues0.295090.297930.301770.309930.32684Alpha virt.eigenvalues0.335110.339250.339860.349290.35416Alpha virt.eigenvalues0.359140.361870.365270.369520.39889Alpha virt.eigenvalues0.435110.455060.464770.482430.50856Alpha virt.eigenvalues0.574010.578040.612200.612650.64296Alpha virt.eigenvalues0.654950.675090.682320.702180.70365Alpha virt.eigenvalues0.712630.713650.725470.728550.72862Alpha virt.eigenvalues0.760340.760550.764180.770020.77360Alpha virt.eigenvalues0.821960.840510.846380.860350.86835Alpha virt.eigenvalues0.821960.840510.993410.929720.9350Alpha virt.eigenvalues0.934810.956230.959130.976790.97819	Alpha vi	rt. eigenvalue	s s	0.24959 0.27063	0.27628	0.23320	0.28437	0.29447
Alpha virt. eigenvalues0.335110.339250.339860.349290.35416Alpha virt. eigenvalues0.359140.361870.365270.369520.39889Alpha virt. eigenvalues0.435110.455060.464770.482430.50856Alpha virt. eigenvalues0.574010.578040.612200.612650.64296Alpha virt. eigenvalues0.654950.675090.682320.702180.70365Alpha virt. eigenvalues0.712630.713650.725470.728550.72862Alpha virt. eigenvalues0.760340.760550.764180.770020.77360Alpha virt. eigenvalues0.790610.790680.802210.811600.81959Alpha virt. eigenvalues0.821960.840510.846380.860350.86835Alpha virt. eigenvalues0.869030.882110.903410.929720.9350Alpha virt. eigenvalues0.934810.956230.959130.976790.97819	Alpha vi	rt. eigenvalue	- s	0.29509	0.29793	0.30177	0.30993	0.32684
Alpha virt. eigenvalues0.359140.361870.365270.369520.39889Alpha virt. eigenvalues0.435110.455060.464770.482430.50856Alpha virt. eigenvalues0.574010.578040.612200.612650.64296Alpha virt. eigenvalues0.654950.675090.682320.702180.70365Alpha virt. eigenvalues0.712630.713650.725470.728550.72862Alpha virt. eigenvalues0.734500.734840.748350.750430.75292Alpha virt. eigenvalues0.760340.760550.764180.770020.77360Alpha virt. eigenvalues0.821960.840510.846380.860350.86835Alpha virt. eigenvalues0.821960.840510.903410.929720.93350Alpha virt. eigenvalues0.934810.956230.959130.976790.97819	Alpha vi	rt. eigenvalue	s	0.33511	0.33925	0.33986	0.34929	0.35416
Alpha virt. eigenvalues0.435110.455060.464770.482430.50856Alpha virt. eigenvalues0.574010.578040.612200.612650.64296Alpha virt. eigenvalues0.654950.675090.682320.702180.70365Alpha virt. eigenvalues0.712630.713650.725470.728550.72862Alpha virt. eigenvalues0.734500.734840.748350.750430.75292Alpha virt. eigenvalues0.760340.760550.764180.770020.77360Alpha virt. eigenvalues0.790610.790680.802210.811600.81959Alpha virt. eigenvalues0.821960.840510.846380.860350.86835Alpha virt. eigenvalues0.869030.882110.903410.929720.93350Alpha virt. eigenvalues0.934810.956230.959130.976790.97819	Alpha vi	rt. eigenvalue	s	0.35914	0.36187	0.36527	0.36952	0.39889
Alpha virt. eigenvalues0.574010.578040.612200.612650.64296Alpha virt. eigenvalues0.654950.675090.682320.702180.70365Alpha virt. eigenvalues0.712630.713650.725470.728550.72862Alpha virt. eigenvalues0.734500.734840.748350.750430.75292Alpha virt. eigenvalues0.760340.760550.764180.770020.77360Alpha virt. eigenvalues0.821960.840510.846380.860350.86835Alpha virt. eigenvalues0.869030.882110.903410.929720.93350Alpha virt. eigenvalues0.934810.956230.959130.976790.97819	Alpha vi	rt. eigenvalue	s	0.43511	0.45506	0.46477	0.48243	0.50856
Alpha virt. eigenvalues0.854950.875090.882320.702180.70385Alpha virt. eigenvalues0.712630.713650.725470.728550.72862Alpha virt. eigenvalues0.734500.734840.748350.750430.75292Alpha virt. eigenvalues0.760340.760550.764180.770020.77360Alpha virt. eigenvalues0.790610.790680.802210.811600.81959Alpha virt. eigenvalues0.821960.840510.846380.860350.86835Alpha virt. eigenvalues0.934810.956230.959130.976790.97819Alpha virt. eigenvalues0.934810.956230.959130.976790.97819	Alpha vi	rt. eigenvalue	s	0.57401	0.57804	0.61220	0.61265	0.64296
Alpha virt. eigenvalues 0.73450 0.73484 0.74835 0.75043 0.75292 Alpha virt. eigenvalues 0.76034 0.76055 0.76418 0.77002 0.77360 Alpha virt. eigenvalues 0.79061 0.79068 0.80221 0.81160 0.81959 Alpha virt. eigenvalues 0.82196 0.84051 0.84638 0.86035 0.86835 Alpha virt. eigenvalues 0.86903 0.88211 0.90341 0.92972 0.93350 Alpha virt. eigenvalues 0.93481 0.95623 0.95913 0.97679 0.97819	Alpha vi	rt eigenvalue	s s	0.05495 0.71263	0.0/509 0 71365	0.08232 0 72547	0.70218	0.70365 0.72862
Alpha virt. eigenvalues 0.76034 0.76055 0.76418 0.77002 0.77360 Alpha virt. eigenvalues 0.79061 0.79068 0.80221 0.81160 0.81959 Alpha virt. eigenvalues 0.82196 0.84051 0.84638 0.86035 0.86835 Alpha virt. eigenvalues 0.86903 0.88211 0.90341 0.92972 0.93350 Alpha virt. eigenvalues 0.93481 0.95623 0.95913 0.97679 0.97819	Alpha vi	rt. eigenvalue	s	0.73450	0.73484	0.74835	0.75043	0.75292
Alpha virt. eigenvalues0.790610.790680.802210.811600.81959Alpha virt. eigenvalues0.821960.840510.846380.860350.86835Alpha virt. eigenvalues0.869030.882110.903410.929720.93350Alpha virt. eigenvalues0.934810.956230.959130.976790.97819Alpha virt. eigenvalues0.988560.980661.016881.019791.02164	Alpha vi	rt. eigenvalue	s	0.76034	0.76055	0.76418	0.77002	0.77360
Alpha virt. eigenvalues 0.82196 0.84051 0.84638 0.86035 0.86835 Alpha virt. eigenvalues 0.86903 0.88211 0.90341 0.92972 0.93350 Alpha virt. eigenvalues 0.93481 0.95623 0.95913 0.97679 0.97819 Alpha virt. eigenvalues 0.93481 0.95623 0.95913 0.97679 0.97819	Alpha vi	rt. eigenvalue	s	0.79061	0.79068	0.80221	0.81160	0.81959
Alpha virt. eigenvalues 0.86903 0.88211 0.90341 0.92972 0.93350 Alpha virt. eigenvalues 0.93481 0.95623 0.95913 0.97679 0.97819 Alpha virt. eigenvalues 0.98856 0.98066 1.01688 1.01970 1.02164	Alpha vi	rt. eigenvalue	s	0.82196	0.84051	0.84638	0.86035	0.86835
Alpha virt. eigenvalues 0.93481 0.95623 0.95913 0.97679 0.97819	Alpha vi	rt. eigenvalue	s	0.86903	0.88211	0.90341	0.92972	0.93350
	Alpha vi	rt. eigenvalue	s	U.93481 0 9995 <i>6</i>	0.95623	0.95913	0.97679	U.97819 1 02164
Alpha virt. eigenvalues 1.04045 1.04121 1.09417 1.09445 1.11090	Alpha vi	rt. eigenvalue	s	1.04045	1.04121	1.09417	1.09445	1.11090

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

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

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

Center	Atomic	Atomic	Coord	dinates (Angs	stroms)	
Number	Number	Туре	Х	Y	Z	
1	 6	 0	0 00000	0 000000	0 679461	
2	6	0	0.000000	0.000000	-0.679461	
3	6	0	0.00000	0.000000	1.899660	
4	6	0	0.00000	0.00000	-1.899660	
5	6	0	0.00000	0.00000	3.318498	
6	6	0	0.00000	0.000000	-3.318498	
7	6	0	0.000000	1.211722	4.030916	
8	6	0	1.211722	0.00000	-4.030916	
9	6	0	0.00000	-1.211722	4.030916	
10	6	0	-1.211722	0.00000	-4.030916	
11	6	0	0.000000	1.206087	5.419091	
12	6	0	1.206087	0.000000	-5.419091	
13	6	0	0.00000	-1.206087	5.419091	
14	6	0	-1.206087	0.000000	-5.419091	
15	6	0	0.00000	0.00000	6.117221	
16	6	0	0.00000	0.00000	-6.117221	
17	1	0	0 000000	2 148075	3 481442	
18	1	0	2 148075	0 000000	-3 481442	
19	1	0	0 000000	-2 148075	3 481442	
20	1	0	-2.148075	0 000000	-3 481442	
21	1	0	0 000000	2 148474	5 959837	
22	1	0	2 148474	0 000000	-5 959837	
22	1	0		-2 148474	5 959837	
2.5	1	0	-2 148474	0 000000	-5 959837	
25	1	0	0 000000	0 000000	7 203732	
26	1	0	0.000000	0.000000	-7.203732	
324 bas	sis function	ns, 552 prim	nitive gaussian	ns, 324 cai	rtesian basis	function
53 alt	plia electron	1S 53 DE	eta efectrons			
SCF Done:	E (RPBE+HE	7-PBE) = -614	1.896422965	A.U. after	24 cycles	
	Convg =	= 0.5166D-0	8	-V/T = 2.00)89	
* * * * * * * * * *		· • • • • • • • • • • • • • • • • • • •	· · · · · · · · · · · · · · · · · · ·	* * * * * * * * * * * * *		
Evaited a	stated from	-77 DD·77 DD-	aingled matr			
********	**************************************	<pre><aa, <<br="" aa,="" dd="" •="">* * * * * * * * * * * * * * * * * *</aa,></pre>	**************************************	⊥∧· ***********	* * * * * * * * * * * * *	
Ground to	o excited st	ate Transitio	on electric di	pole moments	(Au):	
sta	ate	Х	Y Z	Osc	с.	
1	L 0.	.0000 0.0	0.00	00 0.000	00	
2	20.	.0000 0.0	0.00	00 0.000	00	
3	30.	.0000 0.0	0.00	00 0.000	00	
4	10.	.0000 0.0	-4.35	38 2.183	37	
<u> </u>	5 -0.	-0.0	0.00	00 0.000)2	
e	5 -0.	.0427 0.0	0.00	00 0.000)2	
5	7 0.	.0417 -0.0	0.00	00 0.000)3	
8	з О.	.0201 0.0	0.00	00 0.000)3	

Standard orientation:

9	-0.0011	0.0028	0.0000	0.0000
10	0.0028	0.0011	0.0000	0.0000
11	0 4832	0 7012	0 0000	0 1203
10	0.4052	0.7912	0.0000	0.1203
12	0./912	-0.4832	0.0000	0.1203
13	0.0000	0.0000	0.0000	0.0000
14	0.0000	0.0000	0.0000	0.0000
15	0 0033	-0 0039	0 0000	0 0000
IJ	0.0033	-0.0039	0.0000	0.0000
16	0.0039	0.0033	0.0000	0.0000
17	0.0000	0.0000	-0.0001	0.0000
18	0.000	0.0000	0.0031	0.0000
10	0 0000	0 0000	0 0000	0,0000
19	0.0000	0.0000	0.0000	0.0000
20	0.0000	0.0000	0.0000	0.0000
21	-0.1261	0.1740	0.0000	0.0070
22	-0.1740	-0.1261	0.0000	0.0070
23	0 0000	0 0000	-0 0001	0 0000
2.5	0.0000	0.0000		1.2640
24	0.0000	0.0000	-2.9250	1.3648
25	0.1291	-0.0311	0.0000	0.0028
26	0.0311	0.1291	0.0000	0.0028
27	0 0000	0 0000	0 0000	0 0000
27	0.0000	0.0000	0.0000	0.0000
28	0.0000	0.0000	0.0000	0.0000
29	0.0000	0.0000	0.0000	0.0000
30	0.0000	0.0000	-0.0277	0.0001
31	0 0000	0 0000	0 0000	0 0000
22	0.0000	0.0000	0.0000	0.0000
32	0.0000	0.0000	-0.1508	0.0038
33	0.0000	0.0000	0.0000	0.0000
34	0.0000	0.0000	0.0000	0.0000
35	0 0096	0 0851	0 0000	0 0012
20	0.0051	0.0001	0.0000	0.0012
30	-0.0851	0.0096	0.0000	0.0012
37	0.0000	0.0000	0.0014	0.0000
38	0.3569	-0.3644	0.0000	0.0445
39	-0.3644	-0.3569	0.000	0.0445
10	0 0000	0 0000	0 0000	0 0000
- U	0.0000	0.0000		
Created to a	waited atota t	wangition ma	logitu dipolo	Memorita (Au)
Ground to e	xcited state t	ransition vel	locity dipole	Moments (Au)
Ground to e state	xcited state t X	ransition vel Y	locity dipole Z	Moments (Au): Osc.
Ground to e state 1	xcited state t X 0.0000	ransition vel Y 0.0000	locity dipole Z 0.0000	e Moments (Au): Osc. 0.0000
Ground to e state 1 2	xcited state t X 0.0000 0.0000	ransition ve: Y 0.0000 0.0000	locity dipole Z 0.0000 0.0000	e Moments (Au): Osc. 0.0000 0.0000
Ground to e state 1 2 2	xcited state t X 0.0000 0.0000 0.0000	ransition ve: Y 0.0000 0.0000	0.0000 locity dipole Z 0.0000 0.0000	e Moments (Au); Osc. 0.0000 0.0000
Ground to e state 1 2 3	xcited state t X 0.0000 0.0000 0.0000	ransition vel Y 0.0000 0.0000 0.0000	0.0000 locity dipole Z 0.0000 0.0000 0.0000	e Moments (Au); Osc. 0.0000 0.0000 0.0000
Ground to e state 1 2 3 4	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0000	ransition ve: Y 0.0000 0.0000 0.0000 0.0000 0.0000	0.0000 locity dipole Z 0.0000 0.0000 0.7425	e Moments (Au); Osc. 0.0000 0.0000 0.0000 2.1270
Ground to e state 1 2 3 4 5	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019	ransition ve: Y 0.0000 0.0000 0.0000 0.0000 0.0000 0.0056	locity dipole Z 0.0000 0.0000 0.0000 0.7425 0.0000	e Moments (Au); Osc. 0.0000 0.0000 0.0000 2.1270 0.0001
Ground to e state 1 2 3 4 5 6	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056	ransition ve: Y 0.0000 0.0000 0.0000 0.0000 0.0056 -0.0019	locity dipole Z 0.0000 0.0000 0.7425 0.0000 0.0000	e Moments (Au): Osc. 0.0000 0.0000 0.0000 2.1270 0.0001 0.0001
Ground to e state 1 2 3 4 5 6 7	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013	ransition ve: Y 0.0000 0.0000 0.0000 0.0000 0.0056 -0.0019 -0.0006	0.0000 locity dipole Z 0.0000 0.0000 0.7425 0.0000 0.0000 0.0000	e Moments (Au): Osc. 0.0000 0.0000 0.0000 2.1270 0.0001 0.0001 0.0001
Ground to e state 1 2 3 4 5 6 7	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013	ransition ve: Y 0.0000 0.0000 0.0000 0.0000 0.0056 -0.0019 -0.0006	locity dipole Z 0.0000 0.0000 0.7425 0.0000 0.0000 0.0000 0.0000	e Moments (Au): Osc. 0.0000 0.0000 2.1270 0.0001 0.0001 0.0001 0.0000
Ground to e state 1 2 3 4 5 6 7 8	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006	ransition ve: Y 0.0000 0.0000 0.0000 0.0000 0.0056 -0.0019 -0.0006 0.0013	locity dipole Z 0.0000 0.0000 0.7425 0.0000 0.0000 0.0000 0.0000 0.0000	e Moments (Au): Osc. 0.0000 0.0000 2.1270 0.0001 0.0001 0.0001 0.0000 0.0000
Ground to e state 1 2 3 4 5 6 7 8 9	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009	ransition vel Y 0.0000 0.0000 0.0000 0.0000 0.0056 -0.0019 -0.0006 0.0013 -0.0023	locity dipole Z 0.0000 0.0000 0.7425 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	e Moments (Au): Osc. 0.0000 0.0000 2.1270 0.0001 0.0001 0.0001 0.0000 0.0000 0.0000
Ground to e state 1 2 3 4 5 6 7 8 9 10	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009 -0.0023	ransition ve: Y 0.0000 0.0000 0.0000 0.0000 0.0056 -0.0019 -0.0006 0.0013 -0.0023 -0.0009	locity dipole Z 0.0000 0.0000 0.7425 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	e Moments (Au): Osc. 0.0000 0.0000 2.1270 0.0001 0.0001 0.0001 0.0000 0.0000 0.0000 0.0000 0.0000
Ground to e state 1 2 3 4 5 6 7 8 9 10 11	xcited state t X 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009 -0.0023 -0.1036	ransition ve: Y 0.0000 0.0000 0.0000 0.0006 -0.0019 -0.0006 0.0013 -0.0023 -0.0029 -0.1696	locity dipole Z 0.0000 0.0000 0.7425 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	e Moments (Au): Osc. 0.0000 0.0000 2.1270 0.0001 0.0001 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
Ground to e state 1 2 3 4 5 6 7 8 9 10 11	xcited state t X 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009 -0.0023 -0.1036 0.1696	ransition ve: Y 0.0000 0.0000 0.0000 0.0000 0.0056 -0.0019 -0.0006 0.0013 -0.0023 -0.0023 -0.1696 0.1026	locity dipole Z 0.0000 0.0000 0.7425 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	e Moments (Au): Osc. 0.0000 0.0000 0.0000 2.1270 0.0001 0.0001 0.0000 0.0000 0.0000 0.0000 0.1254 0.1254
Ground to e state 1 2 3 4 5 6 7 8 9 10 11 12	xcited state t X 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009 -0.0023 -0.1036 -0.1696	ransition ve: Y 0.0000 0.0000 0.0000 0.0000 0.0056 -0.0019 -0.0006 0.0013 -0.0023 -0.0023 -0.0009 -0.1696 0.1036	locity dipole Z 0.0000 0.0000 0.7425 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	e Moments (Au): Osc. 0.0000 0.0000 2.1270 0.0001 0.0001 0.0000 0.0000 0.0000 0.0000 0.1254 0.1254
Ground to e state 1 2 3 4 5 6 7 8 9 10 11 12 13	xcited state t X 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009 -0.0023 -0.1036 -0.1696 0.0000	ransition ve: Y 0.0000 0.0000 0.0000 0.0000 0.0056 -0.0019 -0.0006 0.0013 -0.0023 -0.0009 -0.1696 0.1036 0.0000	locity dipole Z 0.0000 0.0000 0.7425 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	e Moments (Au): Osc. 0.0000 0.0000 2.1270 0.0001 0.0001 0.0000 0.0000 0.0000 0.0000 0.1254 0.1254 0.0000
Ground to e state 1 2 3 4 5 6 7 8 9 10 11 12 13 14	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009 -0.0023 -0.1036 -0.1696 0.0000 0.0000	ransition ve: Y 0.0000 0.0000 0.0000 0.0000 0.0056 -0.0019 -0.0006 0.0013 -0.0023 -0.0023 -0.0009 -0.1696 0.1036 0.0000 0.0000	locity dipole Z 0.0000 0.0000 0.7425 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	e Moments (Au): Osc. 0.0000 0.0000 0.0000 2.1270 0.0001 0.0001 0.0000 0.0000 0.0000 0.0000 0.1254 0.1254 0.1254 0.0000 0.0000
Ground to e state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009 -0.0023 -0.1036 -0.1696 0.0000 0.0000 -0.0060	ransition ve: Y 0.0000 0.0000 0.0000 0.0000 0.0056 -0.0019 -0.0006 0.0013 -0.0023 -0.0009 -0.1696 0.1036 0.0000 0.0000 0.0000 0.0070	locity dipole Z 0.0000 0.0000 0.7425 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	e Moments (Au): Osc. 0.0000 0.0000 0.0000 2.1270 0.0001 0.0001 0.0000 0.0000 0.0000 0.0000 0.1254 0.1254 0.1254 0.0000 0.0000 0.0000 0.0000
Ground to e state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009 -0.0023 -0.1036 -0.1696 0.0000 0.0000 -0.0060 -0.0070	ransition ve: Y 0.0000 0.0000 0.0000 0.0000 0.0056 -0.0019 -0.0006 0.0013 -0.0023 -0.0009 -0.1696 0.1036 0.0000 0.0000 0.0070 -0.0060	locity dipole Z 0.0000 0.0000 0.0000 0.7425 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	e Moments (Au): Osc. 0.0000 0.0000 0.0000 2.1270 0.0001 0.0001 0.0000 0.0000 0.0000 0.0000 0.1254 0.1254 0.1254 0.0000 0.0000 0.0000 0.0000 0.0003 0.0003
Ground to e state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009 -0.0023 -0.1036 -0.1696 0.0000 0.0000 -0.0060 -0.0070	ransition ve: Y 0.0000 0.0000 0.0000 0.0000 0.0056 -0.0019 -0.0006 0.0013 -0.0023 -0.0009 -0.1696 0.1036 0.0000 0.0000 0.0070 -0.0060	locity dipole Z 0.0000 0.0000 0.0000 0.7425 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	e Moments (Au): Osc. 0.0000 0.0000 0.0000 2.1270 0.0001 0.0001 0.0000 0.0000 0.0000 0.0000 0.1254 0.1254 0.1254 0.1254 0.0000 0.0000 0.0003 0.0003 0.0003
Ground to e state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009 -0.0023 -0.1036 -0.1696 0.0000 0.0000 0.0000 -0.0060 -0.0070 0.0000	ransition ve: Y 0.0000 0.0000 0.0000 0.0000 0.0056 -0.0019 -0.0006 0.0013 -0.0023 -0.0009 -0.1696 0.1036 0.0000 0.0000 0.0070 -0.0060 0.0000	locity dipole Z 0.0000 0.0000 0.0000 0.7425 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	e Moments (Au): Osc. 0.0000 0.0000 0.0000 2.1270 0.0001 0.0001 0.0000 0.0000 0.0000 0.0000 0.1254 0.1254 0.1254 0.1254 0.0000 0.0000 0.0003 0.0003 0.0003
Ground to e state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009 -0.0023 -0.1036 -0.1696 0.0000 0.0000 -0.0060 -0.0070 0.0000 0.0000	ransition vel Y 0.0000 0.0000 0.0000 0.0000 0.0056 -0.0019 -0.0006 0.0013 -0.0023 -0.0023 -0.0009 -0.1696 0.1036 0.0000 0.0000 0.0070 -0.0060 0.0000 0.0000 0.0000	locity dipole Z 0.0000 0.0000 0.0000 0.7425 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	e Moments (Au): Osc. 0.0000 0.0000 0.0000 2.1270 0.0001 0.0001 0.0000 0.0000 0.0000 0.0000 0.1254 0.1254 0.1254 0.1254 0.0000 0.0000 0.0003 0.0003 0.0003 0.0000 0.0001
Ground to e state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009 -0.0023 -0.1036 -0.1696 0.0000 0.0000 -0.0060 -0.0070 0.0000 0.0000 0.0000 0.0000	ransition vel Y 0.0000 0.0000 0.0000 0.0000 0.0056 -0.0019 -0.0006 0.0013 -0.0023 -0.0023 -0.1696 0.1036 0.0000 0.0000 0.0070 -0.0060 0.00000 0.0000 0.0000 0.0000 0.0000 0.000000 0.000000 0.00000000	locity dipole Z 0.0000 0.0000 0.0000 0.7425 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	e Moments (Au): Osc. 0.0000 0.0000 0.0000 2.1270 0.0001 0.0001 0.0000 0.0000 0.0000 0.1254 0.1254 0.1254 0.1254 0.0000 0.0000 0.0003 0.0003 0.0003 0.0001 0.0001 0.0000
Ground to e state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009 -0.0023 -0.1036 -0.1036 -0.1696 0.0000 0.0000 -0.0060 -0.0070 0.0000 0.0000 0.0000	ransition ve: Y 0.0000 0.0000 0.0000 0.0000 0.0056 -0.0019 -0.0006 0.0013 -0.0023 -0.0023 -0.0009 -0.1696 0.1036 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	locity dipole Z 0.0000 0.0000 0.0000 0.7425 0.0000	e Moments (Au): Osc. 0.0000 0.0000 0.0000 2.1270 0.0001 0.0001 0.0000 0.0000 0.0000 0.1254 0.1254 0.1254 0.1254 0.0000 0.0000 0.0003 0.0003 0.0003 0.0003 0.0001 0.0000 0.0000
Ground to e state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009 -0.0023 -0.1036 -0.1696 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	ransition ve: Y 0.0000 0.0000 0.0000 0.0000 0.0006 -0.0019 -0.0006 0.0013 -0.0023 -0.0023 -0.0023 -0.0009 -0.1696 0.1036 0.00000 0.00000 0.00000 0.00000000	locity dipole Z 0.0000 0.0000 0.0000 0.7425 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	e Moments (Au): OSC. 0.0000 0.0000 0.0000 2.1270 0.0001 0.0001 0.0000 0.0000 0.0000 0.1254 0.1254 0.1254 0.1254 0.0000 0.0000 0.0003 0.0003 0.0003 0.0001 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000000
Ground to e state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009 -0.0023 -0.1036 -0.1696 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	ransition vel Y 0.0000 0.0000 0.0000 0.0000 0.0006 -0.0019 -0.0006 0.0013 -0.0023 -0.0009 -0.1696 0.1036 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000000	locity dipole Z 0.0000 0.0000 0.0000 0.7425 0.0000	e Moments (Au): Osc. 0.0000 0.0000 0.0000 2.1270 0.0001 0.0001 0.0000 0.0000 0.0000 0.1254 0.1254 0.1254 0.1254 0.0000 0.0000 0.0003 0.0003 0.0003 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000000
Ground to e state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009 -0.0023 -0.1036 -0.1696 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	ransition ve: Y 0.0000 0.0000 0.0000 0.0000 0.0006 -0.0019 -0.0006 0.0013 -0.0023 -0.0023 -0.0009 -0.1696 0.1036 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000000	locity dipole Z 0.0000 0.0000 0.0000 0.7425 0.0000	e Moments (Au): Osc. 0.0000 0.0000 0.0000 2.1270 0.0001 0.0001 0.0000 0.0000 0.0000 0.1254 0.1254 0.1254 0.1254 0.0000 0.0000 0.0003 0.0003 0.0003 0.0003 0.0001 0.00000 0.00000 0.00000 0.000000
Ground to e state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009 -0.0023 -0.1036 -0.1696 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	ransition vel Y 0.0000 0.0000 0.0000 0.0000 0.0006 -0.0019 -0.0006 0.0013 -0.0023 -0.0023 -0.0023 -0.0023 -0.0009 -0.1696 0.1036 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000000	locity dipole Z 0.0000 0.0000 0.0000 0.7425 0.0000	e Moments (Au): Osc. 0.0000 0.0000 0.0000 2.1270 0.0001 0.0001 0.0000 0.0000 0.0000 0.1254 0.1254 0.1254 0.1254 0.1254 0.0000 0.0000 0.0003 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0001 0.0001 0.0001 0.0001 0.0001 0.0001 0.0001 0.0001 0.0000
Ground to e state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009 -0.0023 -0.1036 -0.1696 0.00000 0.0000 0.0000 0.0000 0.00000 0.0000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000	ransition ve: Y 0.0000 0.0000 0.0000 0.0000 0.0000 0.0056 -0.0019 -0.0006 0.0013 -0.0023 -0.0009 -0.1696 0.1036 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	locity dipole Z 0.0000 0.0000 0.0000 0.7425 0.0000	e Moments (Au): Osc. 0.0000 0.0000 0.0000 2.1270 0.0001 0.0000 0.0000 0.0000 0.0000 0.1254 0.1254 0.1254 0.1254 0.0000 0.0000 0.0000 0.0003 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.00000 0.00000 0.00000 0.00000000
Ground to e state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009 -0.0023 -0.1036 -0.1696 0.0000	ransition vel Y 0.0000 0.0000 0.0000 0.0000 0.0006 0.0013 -0.0023 -0.0009 -0.1696 0.1036 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000000	locity dipole Z 0.0000 0.0000 0.0000 0.7425 0.0000	e Moments (Au): Osc. 0.0000 0.0000 0.0000 2.1270 0.0001 0.0001 0.0000 0.0000 0.0000 0.1254 0.1254 0.1254 0.1254 0.1254 0.0000 0.0000 0.0000 0.0003 0.0003 0.0003 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0003 0.0000 0.0001 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000000
Ground to e state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 27	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009 -0.0023 -0.1036 -0.1696 0.00000 0.00000 0.0000 0.0000 0.000000	ransition vel Y 0.0000 0.0000 0.0000 0.0000 0.0006 -0.0019 -0.0006 0.0013 -0.0023 -0.0023 -0.0009 -0.1696 0.1036 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000000	locity dipole Z 0.0000 0.0000 0.0000 0.7425 0.0000	e Moments (Au): Osc. 0.0000 0.0000 0.0000 2.1270 0.0001 0.0001 0.0000 0.0000 0.0000 0.0000 0.1254 0.1254 0.1254 0.1254 0.0000 0.0000 0.0000 0.0003 0.0003 0.0003 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0003 0.0000 0.0001 0.00000 0.00000 0.00000 0.00000 0.00000000
Ground to e state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009 -0.0023 -0.1036 -0.1036 -0.1696 0.00000 0.00000 0.000000	ransition vel Y 0.0000 0.0000 0.0000 0.0000 0.0006 -0.0019 -0.0006 0.0013 -0.0023 -0.0023 -0.0009 -0.1696 0.1036 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000000	locity dipole Z 0.0000 0.0000 0.0000 0.7425 0.0000	e Moments (Au): OSC. 0.0000 0.0000 0.0000 2.1270 0.0001 0.0001 0.0000 0.0000 0.0000 0.1254 0.1254 0.1254 0.1254 0.0000 0.0000 0.0003 0.0003 0.0003 0.0003 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0003 0.0000 0.0001 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000000
Ground to e state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009 -0.0023 -0.1036 -0.1036 -0.1036 -0.1696 0.0000 0.0000 -0.0070 0.000000	ransition vel Y 0.0000 0.0000 0.0000 0.0000 0.0006 -0.0019 -0.0006 0.0013 -0.0023 -0.0023 -0.0023 -0.0009 -0.1696 0.1036 0.00000 0.00000 0.00000 0.00000 0.00000000	locity dipole Z 0.0000 0.0000 0.0000 0.7425 0.00000 0.00000 0.00000 0.00000 0.000000	e Moments (Au): Osc. 0.0000 0.0000 0.0000 2.1270 0.0001 0.0001 0.0000 0.0000 0.0000 0.1254 0.1254 0.1254 0.1254 0.1254 0.0000 0.0000 0.0003 0.0003 0.0003 0.0003 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.00000 0.00000 0.00000 0.00000 0.00000000
Ground to e state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009 -0.0023 -0.1036 -0.1036 -0.1036 -0.1696 0.0000 0.0000 -0.0060 -0.0070 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000	ransition vel Y 0.0000 0.0000 0.0000 0.0000 0.0006 -0.0019 -0.0006 0.0013 -0.0023 -0.0023 -0.0023 -0.0023 -0.0009 -0.1696 0.1036 0.00000 0.00000 0.00000 0.00000 0.0000000 0.00000 0.00000 0.00000 0.00000000	locity dipole Z 0.0000 0.0000 0.0000 0.7425 0.00000 0.00000 0.00000 0.00000 0.000000	e Moments (Au): Osc. 0.0000 0.0000 0.0000 2.1270 0.0001 0.0001 0.0000 0.0000 0.0000 0.1254 0.1254 0.1254 0.1254 0.1254 0.0000 0.0000 0.0003 0.0003 0.0003 0.0003 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.00000 0.00000 0.00000 0.00000000
Ground to e state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009 -0.0023 -0.1036 -0.1696 0.00000 0.00000 0.00000 0.000000	ransition vel Y 0.0000 0.0000 0.0000 0.0000 0.0006 -0.0019 -0.0006 0.0013 -0.0023 -0.0023 -0.0023 -0.0009 -0.1696 0.1036 0.00000 0.0000 0.00000 0.0000 0.0000 0.00000 0.	locity dipole Z 0.0000 0.0000 0.0000 0.7425 0.00000 0.00000 0.00000 0.00000 0.000000	e Moments (Au): Osc. 0.0000 0.0000 0.0000 2.1270 0.0001 0.0001 0.0000 0.0000 0.0000 0.1254 0.1254 0.1254 0.1254 0.1254 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0027 0.0027 0.0027 0.00000 0.00000 0.00000 0.00000 0.0000000 0.00000 0.00000 0.00000 0.00000000
Ground to e state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 20	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009 -0.0023 -0.1036 -0.1696 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	ransition ve: Y 0.0000 0.0000 0.0000 0.0000 0.0006 0.0013 -0.0023 -0.0009 -0.1696 0.1036 0.00000 0.00000 0.00000 0.000000 0.00000 0.00000 0.00000 0.00000000	locity dipole Z 0.0000 0.0000 0.0000 0.7425 0.000000	e Moments (Au): Osc. 0.0000 0.0000 0.0000 2.1270 0.0001 0.0000 0.0000 0.0000 0.0000 0.1254 0.1254 0.1254 0.1254 0.0000 0.0000 0.0000 0.0000 0.0001 0.0000 0.0001 0.0000 0.0001 0.0027 0.0027 0.0027 0.00000 0.00000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.000
Ground to e state 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30	xcited state t X 0.0000 0.0000 0.0000 0.0000 0.0019 0.0056 0.0013 0.0006 0.0009 -0.0023 -0.1036 -0.1696 0.0000	ransition vel Y 0.0000 0.0000 0.0000 0.0000 0.0006 0.0013 -0.0019 -0.0006 0.0013 -0.0023 -0.0009 -0.1696 0.1036 0.00000 0.00000 0.00000 0.00000 0.0000 0.0000 0.0	locity dipole Z 0.0000 0.0000 0.0000 0.7425 0.000000	e Moments (Au): Osc. 0.0000 0.0000 0.0000 2.1270 0.0001 0.0001 0.0000 0.0000 0.0000 0.1254 0.1254 0.1254 0.1254 0.1254 0.0000 0.0000 0.0000 0.0000 0.0001 0.0000 0.0001 0.0000 0.0027 0.0027 0.0027 0.0027 0.0027 0.00000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000

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

Excitation energies and oscillator strengths:

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

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

Excited 52 53	State -> 54 -> 55	1:	Singlet-[B1 0.47425 0.47425	L] 45% 45%	[[30.2006 2,-1] 1,-2]	51 1000/ci	m 331.12 n	m f=0.0000
Excited 52 53	State -> 54 -> 55	2:	Singlet-[A2 0.48949 -0.48949	2] 48% 48%	[30.9119 2,-1] 1,-2]	99 1000/ci	m 323.50 n	m f=0.0000
Excited 48 49 52 52 53 53	State -> 55 -> 54 -> 55 -> 61 -> 54 -> 60	3:	Singlet-[A1 0.12747 0.12747 0.45271 0.11546 0.45271 0.11546	41% 41%	[[33.0082 2,-2] 1,-1]	23 1000/c1	m 302.96 n	m f=0.0000
Excited 52 53	State -> 55 -> 54	4:	Singlet-[B2 0.43420 -0.43420	2] 38% 38%	[37.9249 2,-2] 1,-1]	97 1000/ci	m 263.68 n	m f=2.1837
Excited 50 51 51 52 52 53 53	State -> 54 -> 55 -> 54 -> 55 -> 56 -> 57 -> 56 -> 57	5:	Singlet-E 0.10878 0.32353 -0.10878 0.32356 0.34692 0.34358 0.11664 -0.11552	21% 21% 24% 24%	3]]]]	39.25418 4,-2] 3,-2] 2,-3] 2,-4]	1000/cm	254.75 nm	f=0.0002
Excited 50 51 51 52 52 53 53	State -> 54 -> 55 -> 54 -> 55 -> 56 -> 57 -> 56 -> 57	6:	Singlet-E 0.32353 -0.10878 -0.32356 -0.10878 -0.11664 -0.11552 0.34692 -0.34358	21% 21% 24% 24%	3 [[]	<pre>39.25418 4,-1] 3,-1] 1,-3] 1,-4]</pre>	1000/cm	254.75 nm	f=0.0002
Excited 52 52 53 53	State -> 56 -> 57 -> 56 -> 57	7:	Singlet-E -0.21529 0.21483 0.44534 0.44440	40% 39%	4 [[1,-3] 1,-4]	1000/cm	231.93 nm	f=0.0003
Excited	State	8:	Singlet-E		4	13.11757	1000/cm	231.93 nm	f=0.0003

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52 -> 56 0.44534 40% [2,-3] 52 -> 57 39% [2,-4] -0.4444053 -> 56 0.21529 53 -> 57 0.21483 Excited State 9: Singlet-E 44.26772 1000/cm 225.90 nm f=0.0000 50 -> 54 -0.18611 50 -> 55 0.45994 42% [4,-2] 51 -> 54 -0.18606 51 -> 55 -0.45983 42% [3,-2] Excited State 10: Singlet-E 44.26772 1000/cm 225.90 nm f=0.0000 50 -> 54 0.45994 42% [4,-1] 50 -> 55 0.18611 51 -> 54 0.45983 42% [3,-1] 51 -> 55 -0.18606 Excited State Singlet-E 46.07843 1000/cm 217.02 nm f=0.1203 11: 48 -> 56 0.10458 48 -> 57 0.10553 50 -> 54-0.1649350 -> 55 -0.27002 15% [4,-2] 51 -> 54 0.16552 51 -> 55 -0.27100 15% [3,-2] 52 -> 56 0.26721 14% [2,-3] 52 -> 57 0.27207 15% [2,-4] 53 -> 56 0.16321 53 -> 57 -0.16618 12: 46.07843 1000/cm 217.02 nm f=0.1203 Excited State Singlet-E 49 -> 56 0.10458 49 -> 57 -0.10553 50 -> 54 -0.27002 15% [4,-1] 50 -> 55 0.16493 51 -> 54 0.27100 15% [3,-1] 51 -> 55 0.16552 52 -> 56 -0.16321 52 -> 57 -0.16618 53 -> 56 0.26721 14% [1,-3] 53 -> 57 -0.27207 15% [1,-4] Excited State 13: Singlet-[A2] 46.35911 1000/cm 215.71 nm f=0.0000 46 -> 54 0.11383 47 -> 55 -0.11383 48 -> 54 0.46643 44% [6,-1] 49 -> 55 -0.46643 44% [5,-2] Excited State 46.58414 1000/cm 214.66 nm f=0.0000 14: Singlet-[B1] 44% [6,-1] 48 -> 54 0.47140 0.47140 49 -> 55 44% [5,-2] 52 -> 54 -0.10399 53 -> 55 -0.10399 Excited State Singlet-E 47.74639 1000/cm 209.44 nm f=0.0000 15: 52 -> 58 0.39060 31% [2,-5] 52 -> 59 0.20061 52 -> 62 0.10059 53 -> 58 42% [1,-5] -0.46026 53 -> 59 0.23639 11% [1,-6] 53 -> 62 -0.11854 Excited State 16: Singlet-E 47.74639 1000/cm 209.44 nm f=0.0000 52 -> 58 0.46026 42% [2,-5] 52 -> 59 0.23639 11% [2,-6] 52 -> 62 0.11854

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53 -> 58 0.39060 31% [1,-5] 53 -> 59 -0.20061 53 -> 62 0.10059 Excited State 17: Singlet-[A1] 48.51826 1000/cm 206.11 nm f=0.0000 37% [6,-2] 48 -> 55 0.42849 49 -> 54 0.42846 37% [5,-1] 50 -> 56 0.20433 51 -> 57 0.20277 Excited State 18: Singlet-[B2] 48.52794 1000/cm 206.07 nm f=0.0000 48 -> 55 0.41003 34% [6,-2] 49 -> 54 -0.4100534% [5,-1] 52 -> 61 -0.26805 14% [2,-8] 53 -> 60 0.26805 14% [1,-7] Excited State 19: 48.71506 1000/cm 205.27 nm f=0.0000 Singlet-[B1] 52 -> 60 0.46535 43% [2,-7] 53 -> 61 0.46535 43% [1,-8] Excited State 20: 49.01832 1000/cm 204.01 nm f=0.0000 Singlet-[A2] -0.46859 44% [2,-7] 52 -> 60 53 -> 61 0.46859 44% [1,-8] Excited State 49.94264 1000/cm 200.23 nm f=0.0070 21: Singlet-E 52 -> 58 -0.14350 52 -> 59 0.35340 25% [2,-6] 52 -> 62 -0.14492 53 -> 58 0.19803 0.48770 53 -> 59 48% [1,-6] 0.19999 53 -> 62 Excited State 22: Singlet-E 49.94264 1000/cm 200.23 nm f=0.0070 52 -> 58 -0.19803 52 -> 59 0.48770 48% [2,-6] 52 -> 62 -0.19999 53 -> 58 -0.14350 53 -> 59 -0.35340 25% [1,-6] 53 -> 62 -0.14492 Excited State 23: Singlet-[A1] 49.95715 1000/cm 200.17 nm f=0.0000 50 -> 56 0.14850 51 -> 57 0.14683 52 -> 61 0.45323 41% [2,-8] 53 -> 60 0.45323 41% [1,-7] Excited State 52.51393 1000/cm 190.42 nm f=1.3648 24: Singlet-B2 50 -> 57 0.39915 32% [4,-4] 51 -> 56 33% [3,-3] 0.40903 52 -> 61 0.18997 53 -> 60 -0.18997 Excited State 25: Singlet-E 52.77606 1000/cm 189.48 nm f=0.0028 52 -> 58 -0.24328 12% [2,-5] 52 -> 59 0.14223 52 -> 62 0.58450 68% [2,-9] 52 -> 65 -0.1781253 -> 62 -0.14082Excited State 26: Singlet-E 52.77606 1000/cm 189.48 nm f=0.0028 52 -> 62 0.14082 53 -> 58 -0.24328 12% [1,-5] 53 -> 59 -0.1422353 -> 62 0.58450 68% [1,-9] 53 -> 65 0.17812

Excited State 27: Singlet-[B1] 53.06561 1000/cm 188.45 nm f=0.0000 48% [2,-10] 52 -> 63 0.48748 53 -> 64 -0.4874848% [1,-11] Excited State 28: Singlet-[A2] 53.08739 1000/cm 188.37 nm f=0.0000 48% [2,-10] 52 -> 63 0.48833 53 -> 64 0.48833 48% [1,-11] Excited State 29: Singlet-A1 54.59967 1000/cm 183.15 nm f=0.0000 50 -> 56 0.50408 51% [4,-3] 51 -> 57 -0.49596 49% [3,-4] Excited State 30: Singlet-B2 54.59967 1000/cm 183.15 nm f=0.0001 50 -> 57 0.50244 50% [4,-4] 51 -> 56 -0.49709 49% [3,-3] Excited State 31: Singlet-[A1] 54.68517 1000/cm 182.87 nm f=0.0000 52 -> 64 0.47705 46% [2,-11] 52 -> 68 0.12847 53 -> 63 0.47706 46% [1,-10] 53 -> 67 0.12843 Excited State 32: 54.72146 1000/cm 182.74 nm f=0.0038 Singlet-[B2] 52 -> 64 -0.4711444% [2,-11] 52 -> 68 -0.12217 0.47113 53 -> 63 44% [1,-10] 53 -> 67 0.12220 55.00376 1000/cm 181.80 nm f=0.0000 Excited State 33: Singlet-[B2] 50 -> 59 0.47221 45% [4,-6] 51 -> 58 0.51096 52% [3,-5] Excited State 34: Singlet-B1 55.00618 1000/cm 181.80 nm f=0.0000 0.51088 52% [4,-5] 50 -> 58 51 -> 59 0.47221 45% [3,-6] Excited State 35: Singlet-E 55.72885 1000/cm 179.44 nm f=0.0012 -0.11275 48 -> 56 48 -> 57 -0.11142 53 -> 59 0.10372 53 -> 62 -0.12010 53 -> 65 0.62223 77% [1,-12] 53 -> 66 -0.17062 Excited State 36: Singlet-E 55.72885 1000/cm 179.44 nm f=0.0012 49 -> 56 0.11275 49 -> 57 -0.1114252 -> 59 0.10372 52 -> 62 0.12010 52 -> 65 0.62223 77% [2,-12] 52 -> 66 0.17061 Excited State 37: Singlet-A1 56.2886 1000/cm 177.65 nm f=0.0000 48 -> 55 -0.1423949 -> 54 -0.1422950 -> 56 26% [4,-3] 0.36149 51 -> 57 28% [3,-4] 0.37446 52 -> 61 -0.13518 53 -> 60 -0.13490 Excited State 38: Singlet-E 56.29021 1000/cm 177.65 nm f=0.0445 48 -> 56 0.28082 16% [6,-3] 48 -> 57 0.27406 15% [6,-4] 49 -> 56 -0.27508 15% [5,-3]

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49 -> 57 0.26846 14% [5,-4] 50 -> 60 -0.1719950 -> 61 0.17558 51 -> 60 0.17371 51 -> 61 0.17733 52 -> 65 0.11432 53 -> 65 0.11670 Excited State 39: Singlet-E 56.29021 1000/cm 177.65 nm f=0.0445 48 -> 56 0.27508 15% [6,-3] 48 -> 57 0.26846 14% [6,-4] 49 -> 56 0.28081 16% [5,-3] 49 -> 57 -0.2740715% [5,-4] 50 -> 60 0.17558 50 -> 61 0.17199 51 -> 60 -0.17734 51 -> 61 0.17371 52 -> 65 -0.11670 53 -> 65 0.11432 Excited State Singlet-[A2] 56.91932 1000/cm 175.69 nm f=0.0000 40: 46 -> 54 0.45203 41% [8,-1] 47 -> 55 -0.45213 41% [7,-2] 48 -> 54 -0.10242 49 -> 55 0.10243 Orbital symmetries: Occupied (B2) (A1) (A1) (B2) (A1) (B2) (E) (E) (B2) (A1) (B2) (A1) (E) (E) (B2) (A1) (A1) (B2) (A1) (B2) (A1) (E) (E) (B2) (A1) (B2) (E) (E) (A1) (B2) (A1) (B2) (A1) (E) (E) (B2) (A1) (E) (E) (E) (E) (B2) (A1) (E) (E) (E) (E) (E) (B1) (A2) (E) (E) Virtual (E) (E) (B1) (A2) (A1) (B2) (E) (E) (A1) (E) (E) (B2) (A1) (E) (E) (E) (B2) (B2) (A1) (E) (E) (B1) (A2) (A1) (E) (E) (B2) (E) (E) (B1) (B2) (E) (E) (A2) (A1) (E) (E) (A1) (E) (B2) (E) (E) (A1) (E) (E) (B2) (B2) (E) (E) (A1) (B2) (A1) (B2) (E) (E) (E) (A1) (E) (B2) (A1) (E) (E) (B2) (A1) (E) (E) (A1) (E) (E) (B2) (B2) (A1) (A1) (B2) (E) (E) (B2) (E) (E) (A1) (E) (E) (E) (E) (B2) (A1) (B2) (E) (E) (B2) (A1) (A1) (B2) (E) (E) (A1) (E) (E) (E) (B1) (A2) (A1) (B2) (E) (E) (B1) (E) (E) (A2) (B2) (A1) (E) (E) (E) (E) (B2) (A1) (E) (E) (B2) (A1) (E) (E) (E) (E) (B2) (A1) (E) (E) (E) (B2) (A1) (B2) (A1) (E) (E) (E) (E) (E) (B2) (A1) (A1) (B2) (A1) (E) (E) (A1) (B2) (B1) (A2) (B2) (B2) (E) (E) (A1) (A1) (B2) (E) (E) (B2) (E) (E) (B1) (A1) (A2) (E) (E) (E) (B1) (B2) (A2) (B1) (A2) (A1) (E) (E) (B2) (A1) (B1) (E) (E) (B2) (E) (E) (B2) (A1) (B2) (A1) (B2) (A1) (E) (E) (A2) (A1) (E) (E) (B2) (A1) (B1) (A2) (E) (E) (A1) (B2) (E) (E) (B2) (E) (E) (B1) (A2) (E) (E) (A1) (E) (E) (A1) (B2) (B2) (A1) (E) (E) (B1) (A2) (B2) (A1) (A1) (E) (E) (B2) (B2) (E) (E) (A1) (E) (E) (B2) (E) (E) (A1) (B2) (A1) (B2) (A1) (B2) (A1) (E) (E) (A1) (B2) (B2) (A1) (E) (E) (B2) (A1) (B2) (A1) (B2) The electronic state is 1-A1. Alpha occ. eigenvalues -- -10.27787 -10.27787 -10.26179 -10.26122 -10.25883 Alpha occ. eigenvalues ---10.25868 -10.25750 -10.25750 -10.25749 -10.25749 Alpha occ. eigenvalues ---10.25570 -10.25569 -10.25440 -10.25440 -10.25426 Alpha occ. eigenvalues ---10.25426 -0.90251 -0.90212 -0.83464 -0.81671 -0.78866 -0.78488 -0.78488 Alpha occ. eigenvalues ---0.74597 -0.67337

Alpha	occ.	eigenvalues	 -0.64780	-0.63868	-0.63868	-0.60725	-0.56528
Alpha	000	eigenvalues	 -0.55540	-0.50716	-0.50324	-0.48303	-0.48303
Alpha		eigenvalueg	 -0 45980	-0 45835	-0 44775	-0 44775	-0 40802
Alpha	0000.	eigenvalues	0.40000	0.40000	0.29062	0.22770	0.40002
Alpha	0000.	eigenvalues		-0.30131	-0.30003	0.37379	-0.37379
Alpha	000.	eigenvalues	 -0.35918	-0.35910	-0.30407	-0.30407	-0.2/012
Alpha	occ.	eigenvalues	 -0.2/812	-0.23768	-0.23/68	0 01 5 2 0	0 01000
Alpha	virt.	eigenvalues	 -0.05380	-0.05380	-0.01558	-0.01539	0.01090
Alpha	virt.	eigenvalues	 0.01262	0.02753	0.02753	0.03156	0.03320
Alpha	virt.	eigenvalues	 0.03320	0.04141	0.05510	0.05671	0.05671
Alpha	virt.	eigenvalues	 0.06411	0.06411	0.06970	0.07853	0.07916
Alpha	virt.	eigenvalues	 0.08814	0.08814	0.09802	0.09923	0.10006
Alpha	virt.	eigenvalues	 0.11082	0.11082	0.11841	0.12958	0.12958
Alpha	virt.	eigenvalues	 0.14448	0.14537	0.14790	0.14790	0.15268
Alpha	virt.	eigenvalues	 0.15788	0.16042	0.16042	0.16097	0.16481
Alpha	virt.	eigenvalues	 0.16481	0.17213	0.17358	0.17358	0.18099
Alpha	virt.	eigenvalues	 0.19245	0.19245	0.19339	0.20687	0.21577
Alpha	virt.	eigenvalues	 0.21577	0.21915	0.22387	0.22768	0.22817
Alpha	virt.	eigenvalues	 0.23183	0.23183	0.23863	0.23863	0.23868
Alpha	virt.	eigenvalues	 0.24699	0.24699	0.24750	0.26219	0.26730
Alpha	virt	eigenvalues	 0 26730	0 27216	0 27701	0 28583	0 28583
Alpha	virt	eigenvalues	 0 29810	0 29860	0 29860	0 30406	0 31453
Alpha	virt.	oigenvalues	 0.20010	0.22000	0.20000	0.34620	0.34620
Alpha	virt.	eigenvalues	 0.35010	0.33925	0.34059	0.34020	0.34020
Alpha	VIIL.	eigenvalues	 0.35759	0.30250	0.30250	0.30009	0.41022
Alpha	virt.	eigenvalues	 0.41622	0.45426	0.45426	0.46327	0.51019
Alpha	virt.	eigenvalues	 0.5501/	0.5/532	0.5/532	0.61242	0.61262
Alpha	virt.	eigenvalues	 0.64356	0.65484	0.68076	0.68076	0.71090
Alpha	virt.	eigenvalues	 0.71259	0.71259	0.71566	0.71566	0.72801
Alpha	virt.	eigenvalues	 0.72913	0.73771	0.74007	0.74887	0.74887
Alpha	virt.	eigenvalues	 0.75770	0.75866	0.75866	0.76187	0.77038
Alpha	virt.	eigenvalues	 0.77354	0.78993	0.78993	0.80586	0.80586
Alpha	virt.	eigenvalues	 0.81924	0.82385	0.84283	0.84283	0.86818
Alpha	virt.	eigenvalues	 0.86952	0.87198	0.87198	0.92180	0.92180
Alpha	virt.	eigenvalues	 0.92958	0.93370	0.95738	0.95738	0.97669
Alpha	virt.	eigenvalues	 0.97669	0.98921	1.00379	1.02181	1.02197
Alpha	virt.	eigenvalues	 1.04053	1.04053	1.06637	1.06637	1.10134
Alpha	virt.	eigenvalues	 1.10134	1.12798	1.12964	1.15015	1.16477
Alpha	virt.	eigenvalues	 1.19960	1.20351	1.20351	1.21156	1.23288
Alpha	virt.	eigenvalues	 1.23846	1.23862	1.25463	1.28312	1.29149
Alpha	virt	eigenvalues	 1 29149	1 32003	1 34403	1 34652	1 41041
Alpha	virt	eigenvalues	 1 41041	1 43547	1 44254	1 44254	1 44454
Alpha	virt.	eigenvalueg	 1 44997	1 46091	1 47992	1 47992	1 49026
Alpha	virt.	eigenvalues	 1 /0026	1 /035/	1 50092	1 50112	1 5020
Alpha	virt.	eigenvalues	 1 50210	1 62712	1 65140	1 65140	1 67615
Alpha	virt.	eigenvalues	 1 02575	1 94202	1 04751	1 04751	1 96401
Alpha	VIIL.	eigenvalues	 1.02575	1.04392	1.04/51	1 02025	1.00491
Alpha	virt.	eigenvalues	 1.90333	1.90333	1.91604	1.92825	1.93218
Alpha	virt.	eigenvalues	 1.94642	1.9/05/	1.988/4	2.00417	2.0041/
Alpha	virt.	eigenvalues	 2.01169	2.04454	2.07493	2.07493	2.08573
Alpha	virt.	eigenvalues	 2.13390	2.15395	2.15524	2.16331	2.16331
Alpha	virt.	eigenvalues	 2.18986	2.20462	2.21029	2.21029	2.21775
Alpha	virt.	eigenvalues	 2.29712	2.29712	2.30380	2.30629	2.31492
Alpha	virt.	eigenvalues	 2.31492	2.39113	2.51111	2.51111	2.52199
Alpha	virt.	eigenvalues	 2.54109	2.59501	2.60780	2.63391	2.63391
Alpha	virt.	eigenvalues	 2.65195	2.65232	2.65236	2.73169	2.76530
Alpha	virt.	eigenvalues	 2.76615	2.76615	2.78115	2.81554	2.83065
Alpha	virt.	eigenvalues	 2.83065	2.88118	3.02425	3.02425	3.03634
Alpha	virt.	eigenvalues	 3.30257	3.30257	3.33061	3.41792	3.51468
Alpha	virt.	eigenvalues	 3.77437	4.23486	4.27334	4.27679	4.27992
Alpha	virt.	eigenvalues	 4.27992	4.32067	4.33905	4.39882	4.42266
Alpha	virt.	eigenvalues	 4.43642	4.43642	4.59740	4.64075	4.81139
Alpha	virt.	eigenvalues	 4.90568	5.64378	-	_	-

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

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



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



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

(-4) 2 b ₁ -	-0.42	66 - 66	(1) 11 <i>e</i> –6.47 [HOMO]	
(-3) 2 <i>a</i> ₂ -	-0.42	99 - 19	(2) 11 <i>e</i> -6.47 [HOMO]	(1654)
(-2) 12 e [LUMO]	-1.46		(3) 1 <i>b</i> ₁ -7.57	
(-1) 12 e [LUMO]	-1.46	E	(4) 1 <i>a</i> ₂ -7.57	



Frontier MO energies as a function of dihedral angle Φ

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Non-linear diyne axis, in-plane distortion



Standard orientation:

Center Atomic Atomic Coordinates (Angstroms)						
Number	Number	Туре	Х	Y	Z	
	 6	 0	0 00000	-0 679401	-0 289764	
2	6	0	0.00000	0.679401	-0.289764	
3	6	0	0.000000	-1.897728	-0.225917	
4	6	0	0.000000	1.897728	-0.225917	
5	6	0	0.00000	-3.308756	-0.077610	
6	б	0	0.00000	3.308756	-0.077610	
7	б	0	0.00000	-3.890554	1.201820	
8	6	0	0.00000	4.143853	-1.208097	
9	6	0	0.00000	-4.143853	-1.208097	
10	6	0	0.00000	3.890554	1.201820	
11	6	0	0.00000	-5.271627	1.341309	
12	6	0	0.00000	5.523747	-1.057391	
13	6	0	0.00000	-5.523747	-1.057391	
14	6	0	0.00000	5.271627	1.341309	
15	6	0	0.00000	-6.091906	0.214940	
16	6	0	0.00000	6.091906	0.214940	
17	1	0	0.00000	-3.246255	2.075551	
18	1	0	0.00000	3.695338	-2.196604	
19	1	0	0.00000	-3.695338	-2.196604	
20	1	0	0.00000	3.246255	2.075551	
21	1	0	0.00000	-5.710899	2.335052	
22	1	0	0.00000	6.160035	-1.938084	
23	1	0	0.00000	-6.160035	-1.938084	
24	1	0	0.00000	5.710899	2.335052	
25	1	0	0.00000	-7.172453	0.328512	
26	1	0	0.00000	7.172453	0.328512	
324 bas	sis functions	s, 552 prim	itive gaussia:	ns, 324 ca:	rtesian basis	functi
53 alı	pha electrons	s53 be	ta electrons			
* * * * * * * * *	* * * * * * * * * * * * *	* * * * * * * * * * * * *	* * * * * * * * * * * * *	* * * * * * * * * * * * *	* * * * * * * * * * * * *	
Excited a	states from <	AA,BB:AA,BB>	singles matr	ix:		
* * * * * * * * *	* * * * * * * * * * * * *	********	* * * * * * * * * * * * *	* * * * * * * * * * * *	* * * * * * * * * * * * *	

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

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

Excitation energies and oscillator strengths:

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

Excited 52 53	State -> 56 -> 54	1:	Singlet-F -0.21581 0.67039 9	B2 90%	29.72474 [1,-1]	1000/cm	f=0.9253
Excited 52 53	State -> 54 -> 56	2:	Singlet-A 0.68719 -0.12558	A2 94%	31.24348 [2,-1]	1000/cm	f=0.0000
Excited 48 52 53	State -> 56 -> 54 -> 56	3:	Singlet-A 0.10105 0.12914 0.68596	A2 94%	33.92286	1000/cm	f=0.0000
Excited 49 50 51 53	State -> 58 -> 54 -> 55 -> 57	4:	Singlet-F -0.13516 0.45603 0.13730 0.50265	B2 42% 51%	38.05402 [4,-1] [1,-4]	1000/cm	f=0.0000

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Singlet-A1 38.06774 1000/cm Excited State 5: f=0.0002 49 -> 57 -0.13591 50 -> 55 0.13764 51 -> 54 0.45780 42% [3,-1] 53 -> 58 0.50015 50% [1,-5] Excited State 6: Singlet-A1 40.11316 1000/cm f=0.0001 49 -> 54 0.42050 35% [5,-1] 53 -> 55 0.56252 63% [1,-2] Excited State 7: Singlet-B2 42.85544 1000/cm f=0.0012 50 -> 54 0.50801 52% [4,-1] 53 -> 57 -0.47562 45% [1,-4] Excited State 8: Singlet-A1 42.92884 1000/cm f=0.1216 51% [3,-1] 51 -> 54 0.50569 53 -> 58 -0.47695 45% [1,-5] Excited State 9: 43.67168 1000/cm f=0.0034 Singlet-A1 49 -> 54 0.53712 58% [5,-1] 50 -> 58 0.13758 51 -> 57 0.13830 53 -> 55 -0.39481 31% [1,-2] 44.35483 1000/cm 10: f=0.0000 Excited State Singlet-B1 47 -> 54 -0.15058 0.68459 52 -> 55 94% [2,-2] 11: Singlet-A2 45.35899 1000/cm Excited State f=0.0000 0.67556 53 -> 59 91% [1,-6] 53 -> 61 0.15264 Excited State 12: Singlet-B2 45.7905 1000/cm f=1.3085 48 -> 54 -0.36935 27% [6,-1] 52 -> 56 0.50763 52% [2,-3] 53 -> 54 0.20020 53 -> 65 0.20044 Excited State 13: 46.80514 1000/cm Singlet-A2 f=0.0000 52 -> 57 0.70337 99% [2,-4] Excited State 14: Singlet-B1 46.84788 1000/cm f=0.0014 52 -> 58 0.69949 98% [2,-5] Excited State 15: 47.03178 1000/cm f=0.0034 Singlet-B1 -0.11541 49 -> 59 53 -> 60 0.68504 94% [1,-7] Excited State 16: Singlet-B1 48.07949 1000/cm f=0.0001 -0.12653 46 -> 56 0.68526 49 -> 56 94% [5,-3] 49.97893 1000/cm Excited State 17: f=0.0000 Singlet-A2 53 -> 59 -0.16899 53 -> 61 0.63252 80% [1,-8] 53 -> 62 0.20634 Excited State 18: 50.12169 1000/cm Singlet-A1 f=0.0011 48 -> 58 -0.13347 49 -> 57 -0.41884 35% [5,-4] 50 -> 55 0.50664 51% [4,-2] 51 -> 54 -0.1571753 -> 58 -0.12316 Excited State 19: Singlet-B2 50.12975 1000/cm f=0.0000 Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics This journal is $\ensuremath{\mathbb{O}}$ The Owner Societies 2011

48 -> 57 -0.13388 49 -> 58 -0.4156735% [5,-5] 50 -> 54 -0.15752 51 -> 55 0.50685 51% [3,-2] 53 -> 57 -0.12269 Excited State 20: Singlet-A2 50.49754 1000/cm f=0.0000 50 -> 56 0.67938 92% [4,-3] 53 -> 61 -0.10003 53 -> 62 0.15538 Excited State 21: Singlet-B1 50.49916 1000/cm f=0.0000 51 -> 56 0.70409 99% [3,-3] Excited State 22: Singlet-A2 50.61772 1000/cm f=0.0000 50 -> 56 -0.18411 53 -> 61 -0.20663 53 -> 62 0.63192 80% [1,-9] 53 -> 66 0.11469 Excited State 50.68466 1000/cm f=0.1758 23: Singlet-B2 48 -> 54 0.51435 53% [6,-1] 50 -> 57 0.10348 51 -> 58 0.10290 0.19144 52 -> 56 53 -> 65 0.38954 30% [1,-12] 53 -> 69 -0.11319 24: 51.67914 1000/cm Excited State Singlet-B1 f=0.0001 0.69322 53 -> 63 96% [1,-10] Excited State 25: Singlet-B2 51.73318 1000/cm f=0.3990 49 -> 55 0.47784 46% [5,-2] 50 -> 57 0.34923 24% [4,-4] 51 -> 58 0.34309 24% [3,-5] Excited State 26: Singlet-B2 52.39859 1000/cm f=0.0000 52 -> 59 0.62675 79% [2,-6] 52 -> 61 0.25273 13% [2,-8] 52 -> 62 0.14434 Excited State 27: Singlet-B1 52.55586 1000/cm f=0.0000 44 -> 54 0.10275 47 -> 54 0.66862 89% [7,-1] 52 -> 55 0.15379 Excited State 53.38743 1000/cm 28: Singlet-B1 f=0.0048 49 -> 61 0.10640 53 -> 64 0.68139 93% [1,-11] Excited State 29: Singlet-B2 53.99718 1000/cm f=1.2366 39% [5,-2] 49 -> 55 0.43981 50 -> 57 12% [4,-4] -0.24881 51 -> 58 -0.22885 10% [3,-5] 52 -> 56 -0.1482753 -> 65 0.38321 29% [1,-12] 53 -> 69 0.10123 Excited State 30: Singlet-A1 54.26092 1000/cm f=0.0072 46 -> 54 0.24592 12% [8,-1] 47 -> 56 0.12750 48 -> 55 0.15735 49 -> 54 -0.10885 50 -> 58 0.39084 31% [4,-5] 51 -> 57 0.45549 41% [3,-4]

Excited State 31: Singlet-B2 54.59484 1000/cm f=0.0007 50 -> 57 -0.49389 49% [4,-4] 51 -> 58 0.50529 51% [3,-5] Excited State 32: Singlet-A1 54.59645 1000/cm f=0.0001 50 -> 58 0.52566 55% [4,-5] 51 -> 57 -0.47159 44% [3,-4] Excited State 33: Singlet-A2 55.00537 1000/cm f=0.0000 50 -> 59 0.51534 53% [4,-6] 51 -> 60 0.44431 39% [3,-7] 53 -> 66 0.14498 Excited State 34: Singlet-B1 55.01908 1000/cm f=0.0000 50 -> 60 0.45551 41% [4,-7] 51 -> 59 0.52732 56% [3,-6] Excited State 35: 55.05457 1000/cm f=0.1049 Singlet-A1 49 -> 57 -0.30629 19% [5,-4] 50 -> 55 -0.26325 14% [4,-2] 0.55597 52 -> 60 62% [2,-7] 52 -> 64 -0.11823 Excited State 36: 55.4272 1000/cm f=0.0091 Singlet-B2 49 -> 58 0.53253 57% [5,-5] 51 -> 55 0.42609 36% [3,-2] 52 -> 59 0.10261 Excited State 37: 55.52479 1000/cm f=0.0000 Singlet-A2 48 -> 56 -0.12748 50 -> 59 -0.11514 51 -> 60 -0.10493 53 -> 62 -0.10356 53 -> 66 0.64604 83% [1,-13] 53 -> 67 0.10759 Excited State 38: Singlet-A1 55.60787 1000/cm f=0.3186 49 -> 57 38% [5,-4] 0.43602 50 -> 55 0.34572 24% [4,-2] 52 -> 60 0.41114 34% [2,-7] Excited State 39: Singlet-A2 55.95227 1000/cm f=0.0000 53 -> 67 0.66896 90% [1,-14] Excited State 40: 56.39103 1000/cm f=0.0293 Singlet-B2 49 -> 55 -0.15491 50 -> 57 0.15269 51 -> 58 0.15388 53 -> 65 0.18201 53 -> 69 0.60707 74% [1,-16] 53 -> 74 0.11150

Normal termination of Gaussian 03 at Tue Apr 12 14:02:43 2011.

Gaussian 03: x86-Linux-G03RevB.04 2-Jun-2003 11-Apr-2011

<pre>#t td(Nst=40,conver=3) sym=loose pbelpbe/6-31+G*</pre>
1,4-Diphenylbuta-1,3-diyne (pbelpbe/6-31+G*//~6-31G*) Non-linear diyne axis, out-of-plane distortion



		Standard	orientation	:			
Center	Atomic	Atomic	Coordinates (Angstroms)				
Number	Number	Туре	X	Y	Z		
1	 6	0	0.00000	-0.679450	0.348572		
2	6	0	0.00000	0.679450	0.348572		
3	б	0	0.00000) -1.897877	0.284716		
4	б	0	0.00000	1.897877	0.284716		
5	б	0	0.00000	-3.308904	0.136408		
6	6	0	0.00000	3.308904	0.136408		
7	6	0	1.211691	-4.012549	0.024997		
8	6	0	-1.211691	4.012549	0.024997		
9	б	0	-1.211692	-4.012518	0.024927		
10	б	0	1.211692	4.012518	0.024927		
11	б	0	1.206042	-5.383548	-0.192152		
12	б	0	-1.206042	5.383548	-0.192152		
13	б	0	-1.206066	5 -5.383515	-0.192222		
14	6	0	1.206066	5.383515	-0.192222		
15	6	0	0.00000	-6.073033	-0.301395		
16	6	0	0.00000	6.073033	-0.301395		
17	1	0	2.147989	-3.469889	0.110975		
18	1	0	-2.147989	3.469889	0.110975		
19	1	0	-2.147980	-3.469832	0.110854		
20	1	0	2.147980	3.469832	0.110854		
21	1	0	2.148417	-5.917645	-0.276719		
22	1	0	-2.148417	5.917645	-0.276719		
23	1	0	-2.148451	-5.917588	-0.276841		
24	1	0	2.148451	5.917588	-0.276841		
25	1	0	0.00000) -7.146156	-0.471367		
26	1	0	0.00000	7.146156	-0.471367		
324 bas	sis functions	 s. 552 pri	mitive gaussi	ans, 324 c	 artesian basis	function	
53 alp	pha electrons	53 k	eta electrons	5			
* * * * * * * * *	* * * * * * * * * * * * *	* * * * * * * * * * * *	* * * * * * * * * * * * *	* * * * * * * * * * * * * *	* * * * * * * * * * * * * *		
Excited a	states from «	AA,BB:AA,BE	> singles mat	rix:			
* * * * * * * * *	* * * * * * * * * * * * * *	* * * * * * * * * * * *	* * * * * * * * * * * * *	* * * * * * * * * * * * *	* * * * * * * * * * * * * * *		
Ground to	o excited sta	ate transiti	on electric d	lipole moment	s (Au):		
sta	ate	Х	Y	Z Dip	. S. Osc.		
-	1 0.0)000 3.	1983 0.0	10.2	293 0.922	9	
	2 0.0	0000 0.	0000 0.0	0.0 0.0	000 0.000	0	
-	3 0.0	0000 0.	0000 0.0	0.0 0.0	000 0.000	0	
4	4 -0.0	0.437 0.	0000 0.0	0.0 0.0	019 0.000	2	
I	5 0.0	0000 0.	0000 0.0	0.0 0.0	000 0.000	0	
(6 0.0	0000 0.	0000 0.0	0.0	013 0.000	2	
-	7 0.0	000 0.	0000 -0.0	0.0	000 0.000	0	

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

Excitation energies and oscillator strengths:

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

Excited State 52 -> 56 52 -> 58 53 -> 54	1:	Singlet-B -0.17316 -0.12752 0.67066 90%	29.70216 1000/cm	f=0.9229
Excited State 52 -> 54	2:	Singlet-A 0.68744 95%	31.23058 1000/cm [2,-1]	f=0.0000
Excited State 52 -> 54 53 -> 56 53 -> 58	3:	Singlet-A 0.12585 0.56321 63% 0.39275 31%	33.96561 1000/cm [1,-3] [1,-5]	f=0.0000
Excited State 49 -> 58 50 -> 55 51 -> 54 53 -> 57	4:	Singlet-B -0.10478 -0.13736 0.45698 42% 0.50157 50%	38.05241 1000/cm [3,-1] [1,-4]	f=0.0002
Excited State 49 -> 57 50 -> 54 51 -> 55 53 -> 56 53 -> 58	5:	Singlet-A 0.13534 0.45488 41% -0.13767 0.28150 16% -0.41759 35%	38.05322 1000/cm [4,-1] [1,-3] [1,-5]	f=0.0000
Excited State	6:	Singlet-A	40.0696 1000/cm	f=0.0002

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49 -> 54 0.41878 35% [5,-1] 53 -> 55 64% [1,-2] 0.56429 Excited State 7: Singlet-A 42.84576 1000/cm f=0.0000 50 -> 54 0.50847 52% [4,-1] 16% [1,-3] 53 -> 56 -0.27993 53 -> 58 0.38342 29% [1,-5] Excited State 8: Singlet-B 42.9111 1000/cm f=0.1216 51 -> 54 0.50678 51% [3,-1] 53 -> 57 -0.47632 45% [1,-4] Excited State 9: Singlet-A 43.63377 1000/cm f=0.0084 58% [5,-1] 49 -> 54 0.53853 50 -> 57 -0.13544 53 -> 55 -0.39284 31% [1,-2] Excited State 10: 44.31531 1000/cm f=0.0001 Singlet-B 47 -> 54 0.15010 52 -> 55 0.68451 94% [2,-2] 45.36786 1000/cm f=0.0044 Excited State 11: Singlet-B 53 -> 59 0.67522 91% [1,-6] 53 -> 61 0.17195 12: 45.78969 1000/cm Excited State Singlet-B f=1.2769 -0.36367 26% [6,-1] 48 -> 54 52 -> 56 0.45979 42% [2,-3] 52 -> 58 0.22493 10% [2,-5] 0.19757 53 -> 54 53 -> 65 -0.20124 Excited State 13: Singlet-B 46.80917 1000/cm f=0.0109 52 -> 56 -0.37409 28% [2,-3] 52 -> 58 0.58944 69% [2,-5] Excited State 14: Singlet-A 46.84062 1000/cm f=0.0017 52 -> 57 0.69791 97% [2,-4] Excited State 15: Singlet-A 47.03904 1000/cm f=0.0031 49 -> 59 -0.11694 53 -> 60 0.68692 94% [1,-7] Excited State 16: Singlet-B 48.12224 1000/cm f=0.0001 49 -> 56 0.57281 66% [5,-3] 49 -> 58 0.38005 29% [5,-5] Excited State 50.02893 1000/cm 17: Singlet-B f=0.0006 53 -> 59 -0.1703953 -> 61 0.66355 88% [1,-8] 53 -> 67 0.10085 Excited State 18: Singlet-A 50.10636 1000/cm f=0.0000 48 -> 58 -0.10265 49 -> 57 35% [5,-4] -0.41664 50 -> 54 0.15741 51 -> 55 0.50830 52% [3,-2] Excited State 19: Singlet-B 50.11766 1000/cm f=0.0012 48 -> 57 0.13313 49 -> 56 -0.20757 49 -> 58 0.36530 27% [5,-5] 50 -> 55 0.50617 51% [4,-2] 51 -> 54 0.15615 53 -> 57 0.12260

Excited State 20: Singlet-B 50.5169 1000/cm f=0.0957 48 -> 54 0.28886 17% [6,-1] 50 -> 56 0.52208 55% [4,-3] 50 -> 58 0.25918 13% [4,-5] 52 -> 58 0.10326 53 -> 65 -0.20297 Excited State 21: Singlet-A 50.58626 1000/cm f=0.0000 51 -> 56 0.57677 67% [3,-3] 51 -> 58 0.40549 33% [3,-5] Excited State 22: Singlet-A 50.59513 1000/cm f=0.0000 53 -> 62 0.69022 95% [1,-9] 53 -> 66 0.11633 Excited State 23: 50.70079 1000/cm f=0.0679 Singlet-B 36% [6,-1] 48 -> 54 0.42476 50 -> 56 -0.2922417% [4,-3] 50 -> 58-0.27016 15% [4,-5] 52 -> 56 0.10240 53 -> 65 -0.34333 24% [1,-12] Excited State 24: 51.73721 1000/cm f=0.3813 Singlet-B 0.48072 49 -> 55 46% [5,-2] 50 -> 56 0.13426 -0.32569 50 -> 58 21% [4,-5] 51 -> 57 0.34413 24% [3,-4] 25: 51.78077 1000/cm Excited State Singlet-B f=0.0000 53 -> 63 0.69384 96% [1,-10] Excited State 26: Singlet-A 52.42198 1000/cm f=0.0000 52 -> 59 0.62752 79% [2,-6] 52 -> 61 0.28941 17% [2,-8] Excited State 27: Singlet-B 52.5357 1000/cm f=0.0002 44 -> 54 0.10255 47 -> 54 0.66840 89% [7,-1] 52 -> 55 -0.15318 Excited State 28: Singlet-A 53.40356 1000/cm f=0.0048 49 -> 61 0.11752 53 -> 64 0.68198 93% [1,-11] 53 -> 71 -0.10008 Excited State 29: 53.96492 1000/cm f=1.2644 Singlet-B 49 -> 55 0.43602 38% [5,-2] 50 -> 56 -0.12630 50 -> 58 0.21383 51 -> 57 -0.24141 12% [3,-4] 52 -> 56 -0.12188 53 -> 65 -0.37762 29% [1,-12] 53 -> 68 0.10506 Excited State 30: Singlet-A 54.26254 1000/cm f=0.0143 46 -> 54 -0.24596 12% [8,-1] 47 -> 56 0.10336 48 -> 55 -0.15805 49 -> 54 0.10885 50 -> 57 0.39832 32% [4,-4] 14% [3,-3] 51 -> 56 0.26104 51 -> 58 -0.36750 27% [3,-5] Excited State 31: Singlet-B 54.60532 1000/cm f=0.0001 Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics This journal is $\ensuremath{\mathbb{C}}$ The Owner Societies 2011

50 -> 56 -0.27983 16% [4,-3] 50 -> 58 0.41285 34% [4,-5] 51 -> 57 0.50094 50% [3,-4] Excited State 32: Singlet-A 54.60694 1000/cm f=0.0000 50 -> 57 0.52033 54% [4,-4] 51 -> 56 -0.26698 14% [3,-3] 51 -> 58 0.39656 31% [3,-5] Excited State 33: Singlet-B 54.92311 1000/cm f=0.0265 49 -> 58 0.13806 50 -> 55 -0.15299 50 -> 60 0.31953 20% [4,-7] 51 -> 59 -0.38139 29% [3,-6] 52 -> 60 0.42808 37% [2,-7] Excited State 55.02553 1000/cm f=0.0000 34: Singlet-A 50 -> 59 0.51229 52% [4,-6] 51 -> 60 -0.44306 39% [3,-7] 53 -> 66 0.15300 35: 55.14894 1000/cm f=0.0997 Excited State Singlet-B 49 -> 56 -0.17031 49 -> 58 11% [5,-5] 0.23211 50 -> 55 -0.23750 11% [4,-2] 50 -> 60 20% [4,-7] -0.31405 51 -> 59 0.35417 25% [3,-6] 52 -> 60 0.33804 23% [2,-7] 55.40623 1000/cm Excited State 36: Singlet-A f=0.0000 49 -> 57 0.53147 56% [5,-4] 51 -> 55 0.42567 36% [3,-2] 52 -> 59 -0.10379 Excited State 55.56028 1000/cm f=0.0000 37: Singlet-A 48 -> 56 -0.11134 50 -> 59 -0.12541 51 -> 60 0.11327 53 -> 66 0.65104 85% [1,-13] Excited State 38: 55.61271 1000/cm f=0.3008 Singlet-B 49 -> 56 0.24326 12% [5,-3] 49 -> 58 -0.33915 23% [5,-5] 50 -> 55 0.32948 22% [4,-2] 52 -> 60 0.42700 36% [2,-7] 55.89581 1000/cm Excited State 39: Singlet-B f=0.0005 53 -> 61 -0.1094053 -> 67 0.67974 92% [1,-14] Excited State 40: 56.3757 1000/cm f=0.0276 Singlet-B -0.15236 49 -> 55 50 -> 58 -0.12300 51 -> 57 0.15299 53 -> 65 -0.17692 74% [1,-15] 53 -> 68 0.60851 53 -> 74 0.11052

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

GAUSSIAN03 reference:

Gaussian 03, Revision B.04, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven,K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Pittsburgh PA, 2003.