Supplementary Material (ESI) for *PCCP*
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Electronic Supplementary Information (ESI) available for:

Site-dependent Effects of Methylation on the Electronic Spectra of Jet-Cooled Methylated Xanthine Compounds.

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Supporting Online Materials

FIG. S1. Charge distribution of methylated xanthine compounds calculated by B3LYP/6-311++G (d,p) using the NBO option. (a) Xanthine (XT) (b) Theophylline (TP) (c) Theobromine (TB) (d) Paraxanthine (PX) (e) Caffeine (CF).

Table S1. The HOMO-LUMO gaps of XT and methylated XT compounds. [a]Ratios with respect to the values of XT.

Table S2. Fitting parameters B and V_n (n = 3, 6, 9, 12) for TP, TB, and CF.

Table S3. The energy levels (in cm^{-1}) for the internal rotational state of methyl rotors for methylated XT compounds as obtained by treating the rotors as non-interacting.

Table S4. The allowed transitions between the combined total internal rotational states of methyl rotors for the methylated xanthine compounds, with their calculated and observed energies (in cm^{-1}) and wavefunction overlap ($\int \psi_{N_1 S_0} \psi^*_{N_1 S_1} \int \psi_{N_3 S_0} \psi^*_{N_3 S_1} \int \psi_{N_7 S_0} \psi^*_{N_7 S_1} d\tau$) for the ground and first excited states. The parameters in parentheses represent the relative energy above the 0-0 band.

Table S5. Wavefunction overlap ($\int \psi_{S_0} \psi^*_{S_1} d\tau$) for the excitation of each methyl group in methylated XT compounds.

Fig. S1.

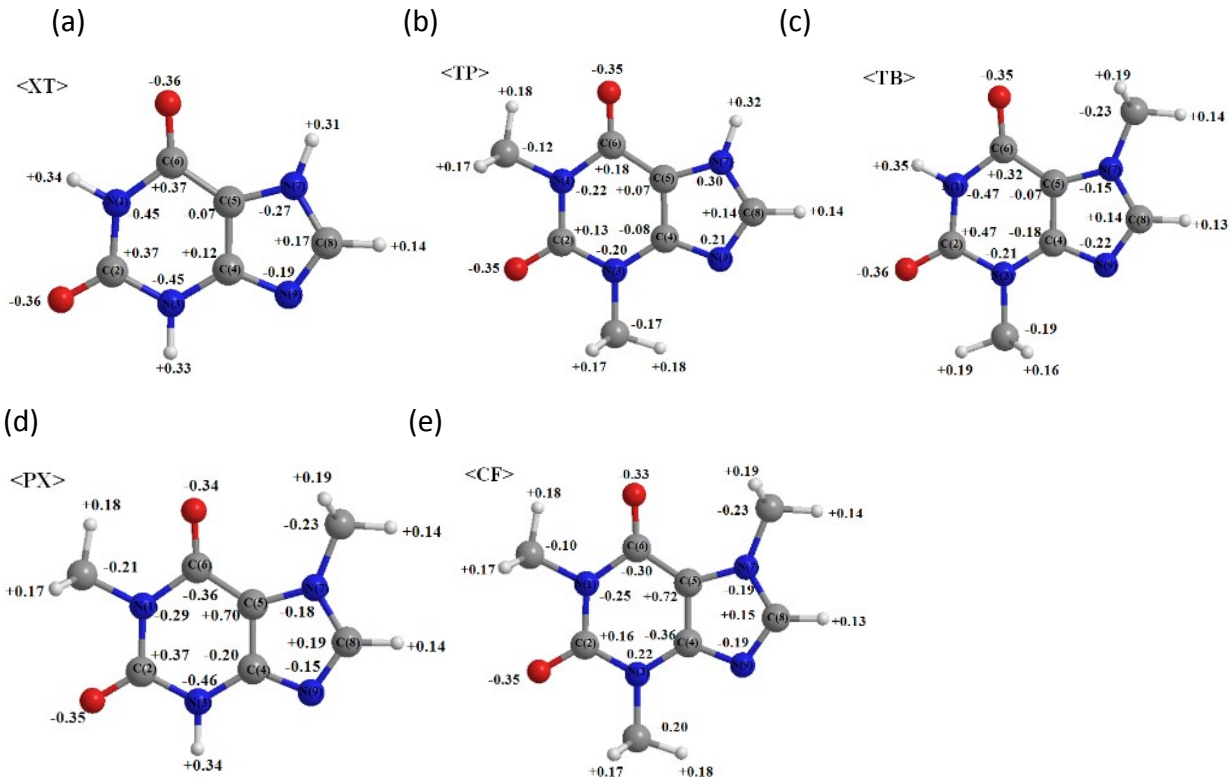

Table S1.

	XT	TP	TB	CF
HOMO-LUMO gap	5.18	5.05	4.97	5.00
R[a]	1.000	0.975	0.959	0.965

Table S2.

	TP		TB		CF		
	N1-Me	N3-Me	N3-Me	N7-Me	N1-Me	N3-Me	N7-Me
S_0 [cm^{-1}]	V_3 = 105.8 V_6 = 22.4 V_9 = -1.6 V_{12} = 0.2	V_3 = 67.1 V_6 = 8.1 V_9 = -2.8 V_{12} = 0.4	V_3 = 0.7 V_6 = 6.0 V_9 = 1.4 V_{12} = -0.2	V_3 = 143.5 V_6 = -17.5 V_9 = 3.9 V_{12} = -1.7	V_3 = 87.8 V_6 = 24.3 V_9 = 1.9 V_{12} = -0.2	V_3 = 56.6 V_6 = 9.3 V_9 = 1.1 V_{12} = -0.1	V_3 = 152.9 V_6 = 0.1 V_9 = 1.0 V_{12} = 0.5
S_1 [cm^{-1}]	V_3 = 86.4 V_6 = 13.7 V_9 = 0.1 V_{12} = 1.1	V_3 = 57.3 V_6 = -0.5 V_9 = -0.4 V_{12} = 0.1	V_3 = 110.1 V_6 = -5.3 V_9 = 1.0 V_{12} = 1.3	V_3 = 415.0 V_6 = -16.6 V_9 = -7.3 V_{12} = -1.4	V_3 = 77.6 V_6 = 12.4 V_9 = 1.4 V_{12} = 1.4	V_3 = 53.8 V_6 = -10.4 V_9 = -1.0 V_{12} = -2.6	V_3 = 447.6 V_6 = -53.2 V_9 = 0.8 V_{12} = 0.2
B	5.0	5.0	5.0	5.0	5.0	5.0	5.0

Table S3.

TP							
N1-Methyl				N3-Methyl			
S_0 state		S_1 state		S_0 state		S_1 state	
Level	Energy	Level	Energy	Level	Energy	Level	Energy
$0a_1$	0.0	$0a_1$	0.0	$0a_1$	0.0	$0a_1$	0.0
1e	0.6	1e	1.0	1e	1.5	1e	2.1
2e	57.7	2e	47.9	2e	38.7	2e	34.0
$3a_2$	69.6	$3a_2$	62.1	$3a_2$	54.9	$3a_2$	51.2
$3a_1$	83.8	$3a_1$	72.7	$3a_1$	62.4	$3a_1$	59.4
4e	109.6	4e	100.6	4e	91.6	4e	89.4
5e	152.8	5e	144.3	5e	134.9	5e	133.8
$6a_2$	206.4	$6a_2$	198.3	$6a_2$	188.1	$6a_2$	188.5
$6a_1$	207.2	$6a_1$	199.0	$6a_1$	188.7	$6a_1$	188.5
7e	271.2	7e	263.3	7e	251.9	7e	253.3
TB							
N3-Methyl				N7-Methyl			
S_0 state		S_1 state		S_0 state		S_1 state	
Level	Energy	Level	Energy	Level	Energy	Level	Energy
$0a_1$	0.0	$0a_1$	0.0	$0a_1$	0.0	$0a_1$	0.0
1e	5.0	1e	0.7	1e	0.4	1e	0.0
2e	20.0	2e	52.2	2e	59.5	2e	115.7
$3a_1$	43.5	$3a_2$	61.3	$3a_2$	65.0	$3a_2$	115.9
$3a_2$	46.5	$3a_1$	86.0	$3a_1$	103.1	$3a_1$	223.9
4e	80.1	4e	108.6	4e	121.4	4e	226.7
5e	125.0	5e	151.5	5e	164.7	5e	311.6
$6a_2$	180.0	$6a_2$	205.1	$6a_2$	214.8	$6a_2$	331.2
$6a_1$	180.1	$6a_1$	205.3	$6a_1$	219.0	$6a_1$	368.6
7e	245.0	7e	269.5	7e	280.7	7e	408.3

CF											
N1-Methyl				N3-Methyl				N7-Methyl			
S_0 state		S_1 state		S_0 state		S_1 state		S_0 state		S_1 state	
Level	Energy	Level	Energy	Level	Energy	Level	Energy	Level	Energy	Level	Energy
$0a_1$	0.0	$0a_1$	0.0	$0a_1$	0.0	$0a_1$	0.0	$0a_1$	0.0	$0a_1$	0.0
1e	0.9	1e	1.2	1e	2.0	1e	2.3	1e	0.3	1e	0.0
2e	50.8	2e	44.1	2e	35.0	2e	31.4	2e	67.7	2e	110.6
$3a_2$	66.3	$3a_2$	59.7	$3a_2$	54.1	$3a_2$	47.7	$3a_2$	73.1	$3a_2$	110.7
$3a_1$	73.1	$3a_1$	67.9	$3a_1$	57.7	$3a_1$	59.4	$3a_1$	109.8	$3a_1$	219.6
4e	102.4	4e	97.1	4e	89.7	4e	88.2	4e	128.4	4e	221.4
5e	146.1	5e	141.1	5e	134.2	5e	132.5	5e	170.3	5e	318.0
$6a_2$	200.4	$6a_2$	195.4	$6a_2$	188.9	$6a_2$	186.6	$6a_2$	222.1	$6a_2$	330.8
$6a_1$	200.5	$6a_1$	195.8	$6a_1$	189.0	$6a_1$	187.9	$6a_1$	223.3	$6a_1$	387.6
7e	265.1	7e	260.3	7e		7e	252.1	7e	286.4	7e	420.1

Table S4.

TP									
S_0 level	**S_1 level**	**Cal. E**	**Overlap**	**Obs. E**	**S_0 level**	**S_1 level**	**Cal. E**	**Overlap**	**Obs. E**
$0a_1 0a_1$ (0.0)	**$0a_1 0a_1$**	0.0	0.70	0.0	**1e1e (continued)**	**1e5e**	132.6	0.08	135.8
	$0a_1 3a_1$	59.4	0.70	52.8		**2e4e**	135.1	0.01	135.8
	$3a_1 0a_1$	72.7	0.00			**2e5e**	179.5	0.00	
	$3a_1 3a_1$	132.1	0.00			**4e4e**	187.9	-0.01	186.4
	$0a_1 6a_1$	188.5	-0.10	186.4	**$1e3a_2$ (56.3)**	**$1e3a_2$**	-4.1	0.98	-1.9
$0a_1 1e$ (1.6)	**$0a_1 1e$**	0.5	1.00	0.0		**$2e3a_2$**	42.8	-0.03	46.4
	$0a_1 2e$	32.4	-0.41	34.3		**$4e3a_2$**	95.6	0.04	
	$3a_1 1e$	73.2	0.00			**$1e6a_2$**	133.2	0.23	135.8
	$0a_1 4e$	87.9	0.17	89.1		**$2e6a_2$**	180.1	-0.01	181.3
	$3a_1 2e$	105.1	0.00		**$2e0a_1$ (57.7)**	**$1e0a_1$**	-56.7	-0.01	52.8
	$0a_1 5e$	132.2	-0.08	142.2		**$2e0a_1$**	-9.8	-0.70	-10.8
	$3a_1 5e$	160.5	0.00			**$1e3a_1$**	2.7	-0.01	0.0
$0a_1 3a_2$ (55.7)	**$0a3a_2$**	-4.5	-0.98	-1.9		**$4e0a_1$**	42.9	-0.04	46.4
	$3a_1 3a_2$	68.2	0.00			**$2e3a_1$**	49.5	-0.70	46.4
	$0a6a_2$	132.8	-0.23	142.2		**$4e3a_1$**	102.3	-0.04	
$1e0a_1$ (0.6)	**$1e0a_1$**	0.4	-0.70	0.0		**$1e6a_1$**	131.8	0.00	
	$2e\ 0a_1$	47.3	0.02	46.4		**$2e6a_1$**	178.6	0.10	172.3
	$1e3a_1$	59.8	-0.70	52.8	**2e1e (59.2)**	**1e1e**	-56.2	0.00	-54.5
	$5e0a_1$	100.0	-0.02			**1e2e**	-24.2	0.01	-24.8
	$2e3a_1$	106.6	0.02			**2e1e**	-9.3	0.21	-10.8
	$4e3a_1$	159.4	-0.03			**2e2e**	22.6	0.41	17.8
	$1e6a_1$	188.9	0.10	186.4		**1e4e**	31.2	0.00	
1e1e (2.2)	**1e1e**	0.9	0.21	0.0		**4e1e**	43.5	0.01	46.4
	1e2e	32.8	0.41	34.3		**4e2e**	75.4	0.02	
	2e1e	47.7	-0.01			**1e5e**	75.6	0.00	
	2e2e	79.6	-0.01			**2e4e**	78.1	-0.17	
	1e4e	88.2	-0.17	89.1		**2e5e**	122.5	0.08	120.0
	4e1e	100.5	0.01			**4e4e**	130.9	-0.01	135.8
	4e2e	132.4	0.02	135.8		**4e5e**	175.2	0.00	

TB									
S_0 level	S_1 level	Cal. E	Overlap	Obs. E	S_0 level	S_1 level	Cal. E	Overlap	Obs. E
$0a_10a_1$ (0.0)	$0a_10a_1$	0.0	-0.10	0.0	1e1e (Continued)	2e5e	340.9	0.04	340.7
	$3a_10a_1$	86.0	-0.06	81.9		4e5e	397.3	-0.03	400.1
	$0a_13a_1$	223.9	-0.27	216.8	$2e0a_1$ (5.0)	$1e0a_1$	-19.3	0.07	-22.2
	$3a_13a_1$	309.9	-0.16	309.2		$2e0a_1$	32.2	0.09	30.4
	$0a_16a_1$	331.2	0.31	340.7		$4e0a_1$	88.6	-0.02	
	$3a_16a_1$	417.2	0.18	400.1		$1e3a_1$	204.7	0.18	210.5
$0a_11e$ (0.4)	$0a_11e$	0.0	0.03	0.0		$2e3a_1$	256.2	0.25	249.4
	$3a_11e$	86.0	0.02			$4e3a_1$	312.6	-0.04	309.2
	$0a_12e$	115.7	-0.07	110.6	$2e1e$ (5.4)	1e1e	-19.7	-0.02	-22.2
	$3a_12e$	201.6	-0.04			2e1e	31.8	-0.02	
	$0a_14e$	226.7	-0.07	235.0		4e1e	88.2	0.00	
	$0a_15e$	311.6	-0.07	309.2		1e2e	96.0	0.05	96.2
	$3a_14e$	312.6	-0.04	309.2		2e2e	147.5	0.07	140.0
	$3a_15e$	397.6	-0.04	400.1		4e2e	203.9	-0.01	
$0a_12e$ (59.5)	$0a_11e$	-59.5	-0.12	-60.0		1e4e	207.0	0.05	210.5
	$3a_11e$	26.5	-0.07	30.4		2e4e	258.5	0.07	262.6
	$0a_12e$	56.2	-0.07			1e5e	292.0	0.05	297.2
	$3a_12e$	142.2	-0.04	140.0		4e4e	314.9	-0.01	309.2
	$0a_14e$	167.2	0.13	168.0		2e5e	343.5	0.07	340.7
	$0a_15e$	252.2	0.13	249.4		4e5e	399.9	-0.01	400.1
	$3a_14e$	253.2	0.08		$3a_10a_1$ (46.5)	$0a_10a_1$	-43.5	-0.06	-47.0
	$3a_15e$	338.1	0.08	340.7		$3a_10a_1$	42.5	0.10	40.3
$1e0a_1$ (0.0)	$1e0a_1$	-22.2	-0.1	-22.2		$0a_13a_1$	180.4	-0.16	
	$2e0a_1$	29.3	0.06	30.4		$3a_13a_1$	266.4	0.26	
	$4e0a_1$	85.7	-0.04		$3a_11e$ (46.9)	$0a_11e$	-43.9	0.02	-47.0
	$1e3a_1$	201.8	-0.25	194.9		$3a_11e$	42.1	-0.03	40.3
	$2e3a_1$	253.3	0.16	249.4		$0a_12e$	71.8	-0.04	67.0
	$4e3a_1$	309.7	-0.11	309.2		$3a_12e$	157.7	0.07	

1e1e (0.4)	**1e1e**	-22.2	0.02	-22.2		**$0a_14e$**	182.8	-0.04	179.8
	2e1e	29.3	-0.02			**$0a_15e$**	267.7	-0.04	262.6
	4e1e	85.7	0.01			**$3a_14e$**	268.7	0.07	272.0
	1e2e	93.5	-0.07	96.2		**$3a_15e$**	353.7	0.07	359.0
	2e2e	145	0.04		**$3a_20a_1$ (43.5)**	**$3a_20a_1$**	14.8	-0.06	11.1
	4e2e	201.4	-0.03			**$3a_23a_1$**	238.7	-0.16	235.0
	1e4e	204.5	-0.07	210.5	**$3a_21e$ (43.9)**	**$3a_21e$**	14.4	0.02	11.1
	2e4e	256.0	0.04			**$3a_22e$**	130.0	-0.04	140.0
	1e5e	289.4	-0.34	297.2		**$3a_24e$**	241.0	-0.04	240.6
	4e4e	312.4	-0.03	309.2		**$3a_25e$**	326.0	-0.04	324.3

CF

S_0 level	S_1 level	Cal. E	Overlap	Obs. E	S_0 level	S_1 level	Cal. E	Overlap	Obs. E
$0a_10a_10a_1$ (0 . 0)	**$0a_10a_10a_1$**	0.0	-0.17	0.0	**$1e1e0a_1$ (2 . 8)**	**$1e1e0a_1$**	0.7	0.05	0.0
	$0a_13a_10a_1$	59.4	-0.14	61.6		**$2e1e0a_1$**	43.6	0.00	
	$3a_10a_10a_1$	67.9	-0.01			**$2e2e0a_1$**	72.7	0.00	71.6
	$3a_13a_10a_1$	127.4	-0.01			**$1e1e3a_1$**	220.3	-0.13	221.3
	$0a_10a_13a_1$	219.6	0.42	221.3		**$1e2e3a_1$**	249.4	0.22	252.7
	$0a_13a_13a_1$	279.0	0.36	271.0		**$2e1e3a_1$**	263.1	0.00	
	$3a_10a_13a_1$	287.5	0.02	289.3		**$2e2e3a_1$**	292.2	0.00	289.3
	$3a_13a_13a_1$	347.0	0.02	346.2	**$1e1e1e$ (3 . 1)**	**1e1e1e**	0.4	-0.01	0.0
$0a_10a_11e$ (0 . 3)	**$0a_10a_11e$**	-0.3	0.04	0.0		**1e2e1e**	29.5	0.02	28.6
	$0a_13a_11e$	59.2	0.03	61.6		**2e1e1e**	43.3	0.00	
	$3a_10a_11e$	67.7	0.00			**2e2e1e**	72.4	0.00	
	$0a_10a_12e$	110.3	-0.12	102.8		**1e1e2e**	111.0	0.04	
	$3a_13a_11e$	127.1	0.00			**1e2e2e**	140.1	-0.06	134.7
	$0a_13a_12e$	169.7	-0.10	174.1		**2e1e2e**	153.8	0.00	156.0
	$3a_10a_12e$	178.2	-0.01			**2e2e2e**	182.9	0.00	182.9
	$3a_13a_12e$	237.7	-0.01	239.5	**$1e2e0a_1$ (35 . 9)**	**$1e1e0a_1$**	-32.3	-0.09	
$0a_11e0a_1$ (2. 0)	**$0a_11e0a_1$**	0.4	0.05	0.0		**$1e2e0a_1$**	-3.2	0.06	-4.3
	$0a_12e0a_1$	29.5	-0.09	28.6		**$2e1e0a_1$**	10.5	0.00	
	$3a_11e0a_1$	68.3	0.00	71.6		**$2e2e0a_1$**	39.6	0.00	
	$3a_12e0a_1$	97.4	0.00			**$1e1e3a_1$**	187.2	0.24	182.9

	$0a_1 1e 3a_1$	219.9	-0.13	221.3		$1e 2e 3a_1$	216.3	-0.14	215.0
	$0a_1 2e 3a_1$	249.0	0.22	252.7		$2e 1e 3a_1$	230.1	0.00	
	$3a_1 1e 3a_1$	287.9	-0.01	289.3		$2e 2e 3a_1$	259.2	0.00	
	$3a_1 2e 3a_1$	317.0	0.01	317.2		$1e 1e 1e$	-32.6	0.02	
	$0a_1 1e 1e$	0.1	-0.01	0.0		$1e 2e 1e$	-3.5	-0.01	-4.3
	$0a_1 2e 1e$	29.2	0.02	28.6		$2e 1e 1e$	10.2	0.00	
	$3a_1 1e 1e$	68.0	-0.01	61.6	$1e 2e 1e$	$2e 2e 1e$	39.3	0.00	
$0a_1 1e 1e$	$3a_1 2e 1e$	97.1	0.00		(36 . 2)	$1e 1e 2e$	77.9	-0.07	71.6
(2. 3)	$0a_1 1e 2e$	110.7	0.04	104.0		$1e 2e 2e$	107.0	0.04	104.0
	$0a_1 2e 2e$	139.8	-0.06	134.7		$2e 1e 2e$	120.8	0.00	120.3
	$3a_1 1e 2e$	178.6	0.00			$2e 2e 2e$	149.9	0.00	149.0
	$3a_1 2e 2e$	207.7	0.00	207.4		$1e 0a_1 0a_1$	-49.6	0.00	
	$0a_1 1e 0a_1$	-32.7	-0.09			$2e 0a_1 0a_1$	-6.7	-0.17	-8.1
	$0a_1 2e 0a_1$	-3.6	0.06	-4.3		$1e 3a_1 0a_1$	9.9	0.00	
	$3a_1 1e 0a_1$	35.3	0.00	35.4	$2e 0a_1 0a_1$	$2e 3a_1 0a_1$	52.7	-0.14	61.6
$0a_1 2e 0a_1$	$3a_1 2e 0a_1$	64.4	0.00		(50 . 8)	$1e 0a_1 3a_1$	170	-0.01	
(35. 0)	$0a_1 1e 3a_1$	186.9	0.24	182.9		$2e 0a_1 3a_1$	212.9	0.42	215.0
	$0a_1 2e 3a_1$	216.0	-0.14	215.0		$1e 3a_1 3a_1$	229.5	-0.01	
	$3a_1 1e 3a_1$	254.8	0.01	252.7		$2e 3a_1 3a_1$	272.3	0.36	271.0
	$3a_1 2e 3a_1$	283.9	-0.01	289.3		$1e 0a_1 1e$	-49.9	0.00	
	$0a_1 1e 1e$	-33.0	0.02			$2e 0a_1 1e$	-7	0.04	-8.1
	$0a_1 2e 1e$	-3.9	-0.01	-4.3		$1e 3a_1 1e$	9.6	0.00	
	$3a_1 1e 1e$	35.0	0.00	35.4	$2e 0a_1 1e$	$2e 3a_1 1e$	52.4	0.03	
$0a_1 2e 1e$	$3a_1 2e 1e$	64.1	0.00	61.6	(51 . 1)	$1e 0a_1 2e$	60.7	0.00	61.6
(35 . 3)	$0a_1 1e 2e$	77.6	-0.07	71.6		$2e 0a_1 2e$	103.6	-0.12	104.0
	$0a_1 2e 2e$	106.7	0.04	104.0		$1e 3a_1 2e$	120.2	0.00	120/3
	$3a_1 1e 2e$	145.5	0.00			$2e 3a_1 2e$	163.0	-0.10	161.6
	$1e 0a_1 0a_1$	0.3	-0.17	0.0		$1e 1e 0a_1$	-49.2	0.00	
	$2e 0a_1 0a_1$	43.2	0.00			$1e 2e 0a_1$	-20.1	0.00	
	$1e 3a_1 0a_1$	59.8	-0.14	61.6	$2e 1e 0a_1$	$2e 1e 0a_1$	-6.4	0.05	-8.1
$1e 0a_1 0a_1$	$2e 3a_1 0a_1$	102.6	0.00	102.8		$2e 2e 0a_1$	22.7	-0.09	27.4
(0 . 9)	$1e 0a_1 3a_1$	219.9	0.42	221.3	(52 . 7)	$1e 1e 3a_1$	170.4	0.00	
	$2e 0a_1 3a_1$	262.8	0.01			$1e 2e 3a_1$	199.5	0.00	201.8
	$1e 3a_1 3a_1$	279.4	0.36	271.0		$2e 1e 3a_1$	213.2	-0.13	215.0

	$2e3a_1 3a_1$	322.2	0.01			**$2e2e3a_1$**	242.3	0.22	239.5
$1e0a_1 1e$ **(1 . 2)**	**$1e0a_1 1e$**	0.1	0.04	0.0	**2e1e1e** **(53 . 0)**	**1e1e1e**	-49.5	0.00	
	$2e0a_1 1e$	42.9	0.00			**1e2e1e**	-20.4	0.00	
	$1e3a_1 1e$	59.5	0.03	61.6		**2e1e1e**	-6.6	-0.01	-8.1
	$2e3a_1 1e$	102.4	0.00	102.8		**2e2e1e**	22.5	0.02	27.4
	$1e0a_1 2e$	110.6	-0.12	102.8		**1e1e2e**	61.1	0.00	61.6
	$2e0a_1 2e$	153.5	0.00	156.0		**1e2e2e**	90.2	0.00	
	$1e3a_1 2e$	170.1	-0.10	174.2		**2e1e2e**	103.9	0.04	104.0
	$2e3a_1 2e$	212.9	0.00			**2e2e2e**	133.0	-0.06	134.7

Table S5.

TP							
$\int \psi_{S_o}\psi^*_{S_1}$	**$0a_1$-$0a_1$**	**$0a_1$-$3a_1$**	**1e-1e**	**1e-2e**	**1e-5e**	**2e-1e**	**2e-2e**
N1	1.00	0.00	-1.00	0.03	-0.04	-0.02	-1.00
N3	0.70	0.70	-0.21	-0.41	0.17	-0.42	0.22
	2e-5e	**$3a_2$-$3a_2$**	**$3a_1$-$0a_1$**	**$3a_1$-$3a_1$**	**4e-1e**	**4e-2e**	**4e-4e**
N1	-0.05	1.00	0.06	-1.00	-0.04	-0.05	1.00
N3	0.10	-0.98	0.71	-0.67	0.17	0.10	0.45
TB							
$\int \psi_{S_o}\psi^*_{S_1}$	**$0a_1$-$0a_1$**	**$0a_1$-$3a_1$**	**1e-1e**	**1e-2e**	**1e-5e**	**2e-1e**	**2e-2e**
N3	-0.43	-0.25	-0.40	0.25	-0.17	0.29	0.39
N7	0.24	0.63	-0.06	0.17	0.17	0.27	0.16
	2e-5e	**$3a_2$-$3a_2$**	**$3a_1$-$0a_1$**	**$3a_1$-$3a_1$**	**4e-1e**	**4e-2e**	**4e-4e**
N3	-0.07	-0.25	-0.25	0.42	-0.10	0.16	0.45
N7	-0.30	-0.71	0.85	0.22	0.29	0.30	0.01
CF							
$\int \psi_{S_o}\psi^*_{S_1}$	**$0a_1$-$0a_1$**	**$0a_1$-$3a_1$**	**1e-1e**	**1e-2e**	**1e-5e**	**2e-1e**	**2e-2e**
N1	1.00	0.05	1.00	0.02	-0.03	-0.02	1.00
N3	0.75	0.65	-0.24	0.40	0.17	0.42	-0.25
N7	-0.22	0.56	0.05	-0.16	-0.15	0.27	-0.15
	2e-5e	**$3a_2$-$3a_2$**	**$3a_1$-$0a_1$**	**$3a_1$-$3a_1$**	**4e-1e**	**4e-2e**	**4e-4e**
N1	-0.00	1.00	-0.05	1.00	0.03	0.00	1.00
N3	0.06	0.98	0.66	-0.73	0.14	0.12	-0.46
N7	0.30	0.77	-0.87	0.25	0.31	-0.29	0.01