Supporting Information

Vibrational Structure in Magnetic Circular Dichroism Spectra of Polycyclic Aromatic Hydrocarbons

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Content

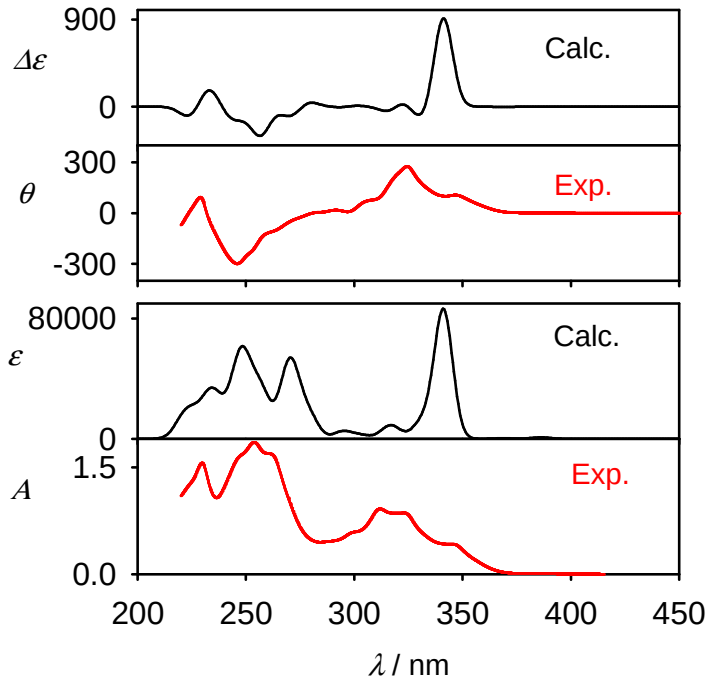


Figure S1. ECD (top) and absorption (bottom) spectra of (P)-(+)-PAH6, B3LYP/6-311++G** calculation and experiment in hexane solution.

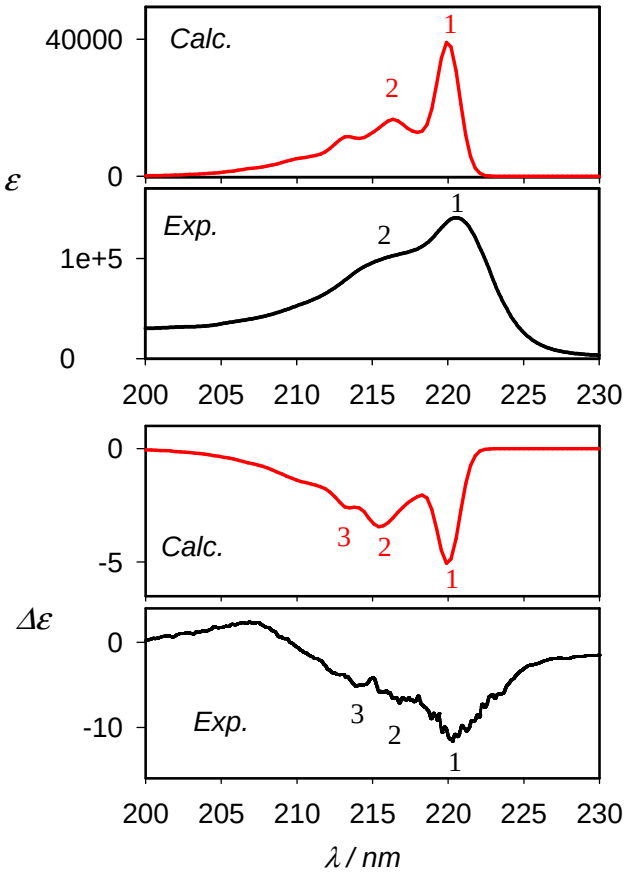


Figure S2. Calculated and experimental absorption and MCD band of the 9th (B_{1u}) naphthalene transition. The calculated spectrum was shifted by 5 nm left.

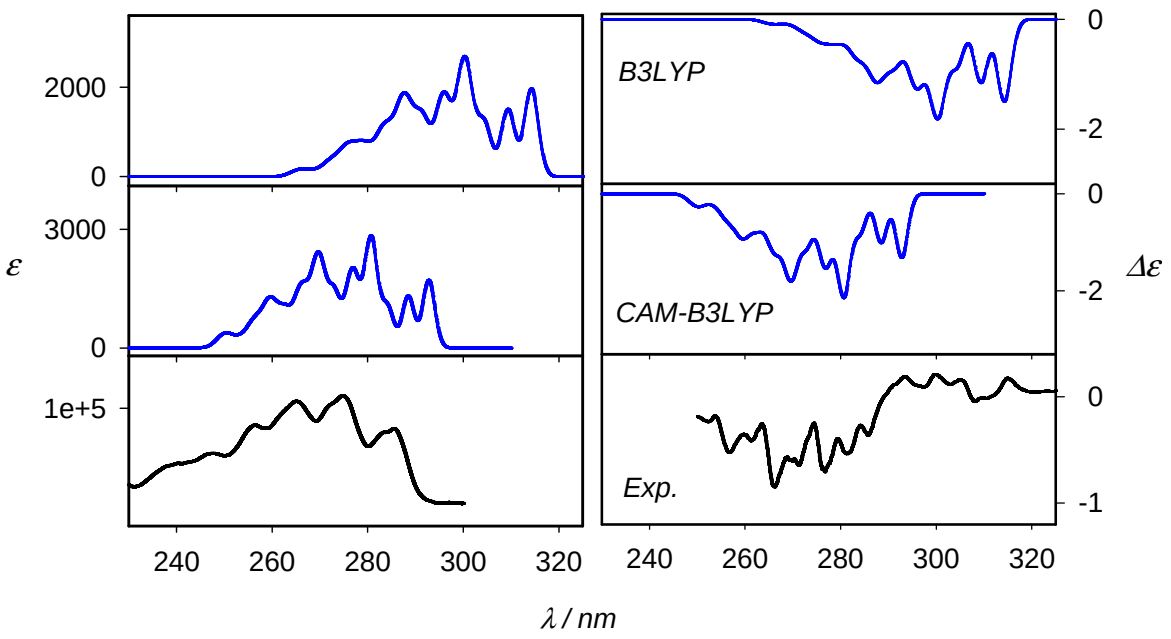


Figure S3. Naphtalene vibrational absorption and MCD of the first B_{3u} electronic state obtained with the B3LYP and CAM-B3LYP functionals.

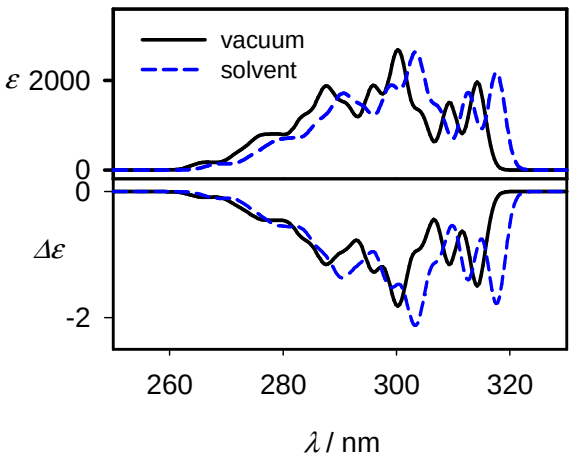


Figure S4. Naphthalene B_{3u} absorption and MCD simulated in vacuum and with the PCM (n-hexane) solvent, B3LYP calculation.

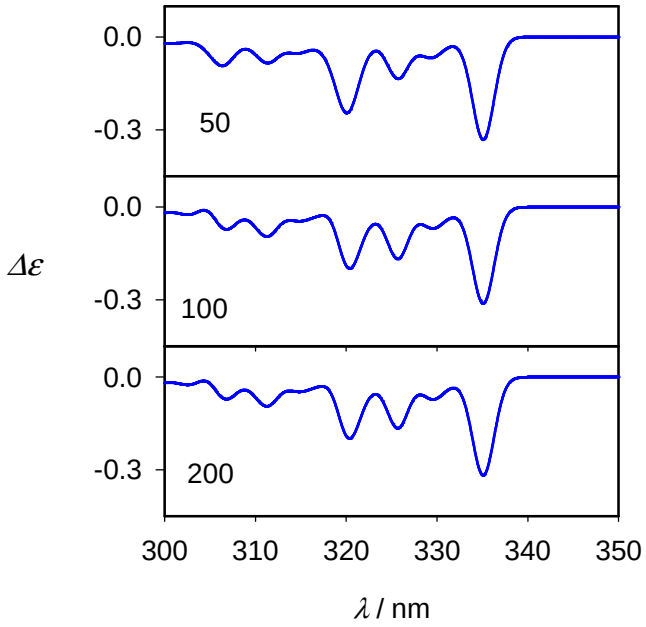


Figure S5. Phenanthrene MCD spectrum of the $S_0 \rightarrow S_1$ transition simulated with 50, 100 and 200 excited electronic states.

	dipole	MD tensor
I	*FC*	*FC*
II	*FC*+*HT*	*FC*
III	*FC*	*FC*+*HT*
IV (full mode)	*FC*+*HT*	*FC*+*HT*

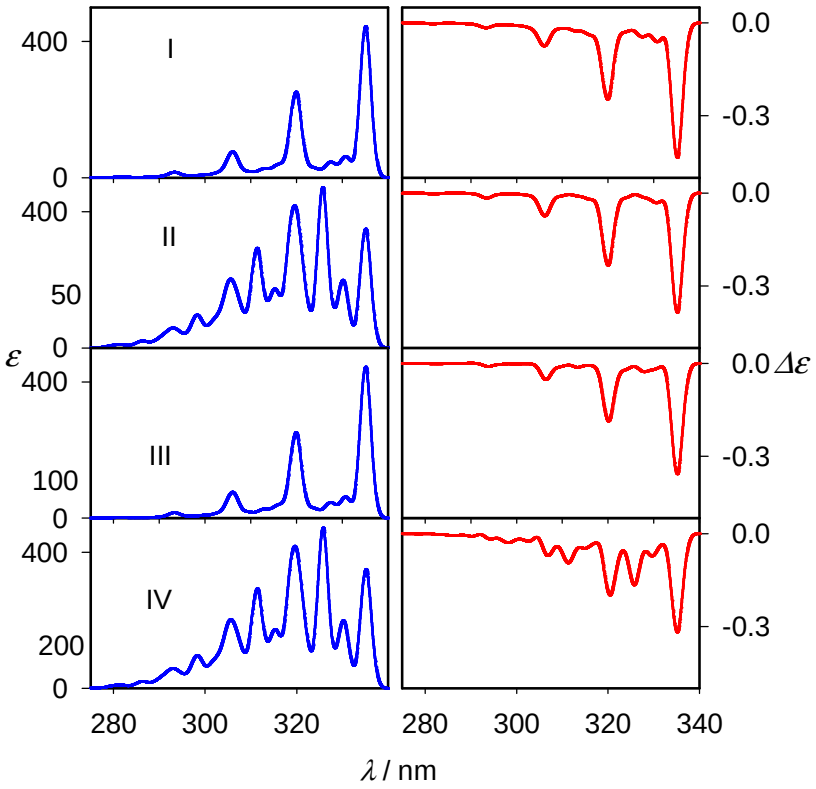


Figure S6. Absorption (left) and MCD (right) phenanthrene spectra simulated at different approximations as defined in the table at the top. The Franck-Condon (*FC*) and the Herzberg-Teller (*HT*) contributions refer to the first and second terms in formula (3) ($X(R) = FC + HT$).

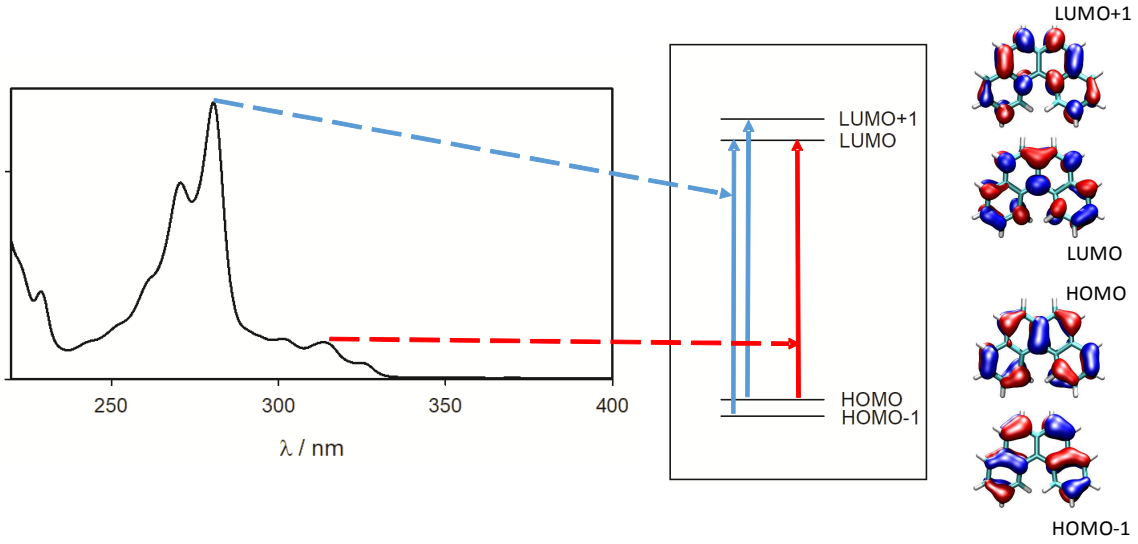


Figure S7. Orbitals dominant in the second (HOMO→LUMO) and fourth (HOMO-1→LUMO and HOMO→LUMO+1) lowest-energy PAH4 transitions.

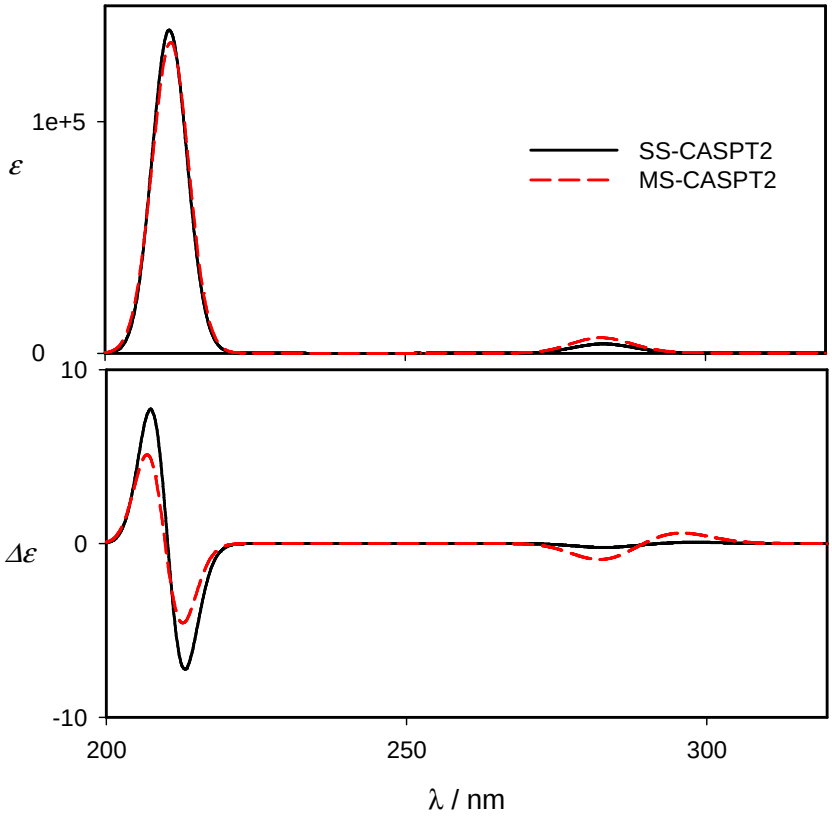


Figure S8. Comparison of the single- and multi-state CASPT2 approaches, for absorption and MCD naphthalene spectra.

Table S1. Summary of Experimental Conditions

	Range, nm	Path length, cm	Concentration, mol/L
naphtalene	195-300	0.1	2.5×10^{-4}
	230-350	1.0	5×10^{-4}
anthracene	190-300	0.1	5×10^{-5}
	270-400	1.0	2.5×10^{-4}
phenanthrene	190-350	0.1	2.5×10^{-4}
	300-400	1.0	5×10^{-3}
PAH4	220-400	0.1	2.5×10^{-4}
PAH5	220-400	0.1	5×10^{-4}
PAH6	220-500	0.1	5×10^{-4}

n-hexane was used as a solvent.

Table S2. Lowest-energy electronic transitions, energies (*E*/eV) and oscillator strengths (*f*) calculated by different methods.

		B3LYP vacuum		B3LYP CPCM		ωB97XD CPCM		LC-BLYP CPCM		exp., lit.	exp., this work
		E	*f*	*E*	*f*	*E*	*f*	*E*	*f*	*E*	*E*
Benzene:											
1	B_{2u}	5.39 (5.09)[1]	0							4.90[2]	(4.63)[1]
Anthracene:											
1	B_{1u}	3.21 (2.90)	0.06	3.18	0.08	3.53	0.12	3.79	0.15	3.38[3]	3.31
2	B_{2u}	3.84	0.00	3.84	0.00	4.04	0.00	4.13	0.00	3.57[3]	
3	B_{3G}	4.50	0.00	4.50	0.00	5.13	0.00	5.38	0.00		
4	B_{2G}	4.76	0.00	4.80	0.00	5.49	0.00	5.67	0.00		
5	B_{3G}	4.83	0.00	4.80	0.00	5.46	0.00	6.21	0.00		
6	A_u	4.96	0.00	5.02	0.00	5.87	0.00	6.09	0.00		
7	B_{3u}	4.98	0.00	5.06	0.02	5.81	0.00	6.01	0.00		
8	B_{1u}	5.05	0.00	5.04	0.00	5.63	0.00	5.88	0.00		
9	B_{2u}	5.14	1.99	4.89	2.26	5.14	2.38	5.33	2.47	4.86[3]	4.92
10	B_{2g}	5.44	0.00	5.50	0.00	6.33	0.00	6.56	0.00		
11	B_{1g}	5.47	0.00	5.54	0.00	6.36	0.00	6.58	0.00		
12	A_g	5.49	0.00	5.49	0.00	5.81	0.00	6.15	0.00		
13	B_{1u}	5.73	0.08	5.71	0.13	6.06	0.22	6.25	0.30		5.82
14	B_{1u}	5.83	0.01	5.81	0.01	6.36	0.04	6.99	0.04		
15	A_g	5.88	0.00	5.88	0.00	6.96	0.00	7.14	0.00		
16	B_{3u}	5.97	0.01	6.03	0.02	6.43	0.04	6.94	0.05		
17	B_{1g}	5.99	0.00	6.04	0.00	6.82	0.00	7.06	0.00		
18	A_u	6.00	0.00	6.07	0.00	6.74	0.00	7.17	0.00		
19	B_{2g}	6.04	0.00	6.03	0.00	6.65	0.00	6.82	0.00		
20	B_{3u}	6.05	0.00	6.04	0.00	6.86	0.00	7.10	0.00		
Phenanthrene:											
1	A_1	3.94 (3.70)	0.00	3.94	0.00	4.25	0.00	4.45	0.00	3.63[3]	3.59
2	B_2	4.19 (3.87)	0.06	4.17	0.11	4.51	0.14	4.71	0.11	4.23[3]	4.24
3	A_1	4.68	0.10	4.64	0.15	5.20	0.28	5.65	0.36	4.93[3]	4.82
4	B_2	4.88	0.62	4.76	0.89	5.14	1.20	5.36	1.29	5.30[4]	4.94
5	A_1	5.05	0.03	5.04	0.04	5.75	0.19	5.98	0.33		
6	B_2	5.11	0.10	5.09	0.06	5.38	0.09	5.57	0.15		
7	B_1	5.23	0.00	5.28	0.01	5.99	0.01	6.22	0.01		
8	B_1	5.46	0.00	5.53	0.00	6.35	0.01	6.61	0.01		
9	A_2	5.48	0.00	5.53	0.00	6.30	0.00	6.55	0.00		
10	A_2	5.55	0.00	5.61	0.00	6.51	0.00	6.57	0.00		
11	B_2	5.66	0.00	5.66	0.01	6.24	0.43	6.44	0.46		
12	A_1	5.72	0.13	5.66	0.19	6.05	0.05	7.24	0.35		
13	B_1	5.76	0.01	5.83	0.01	6.68	0.03	6.93	0.04		
14	A_2	5.79	0.00	5.87	0.00	6.75	0.00	6.78	0.00		
15	B_2	5.82	0.63	5.75	0.64	6.64	0.03	7.37	0.00		
16	A_1	5.96	0.00	5.96	0.00	6.81	0.00	7.40	0.01		
17	B_1	5.98	0.01	6.04	0.01	6.97	0.00	7.25	0.00		
18	A_2	5.99	0.00	6.07	0.00	6.97	0.00	7.03	0.00		
19	B_2	6.24	0.03	6.19	0.02	6.90	0.02	7.54	0.02		
20	A_2	6.25	0.00	6.32	0.00	7.13	0.00	7.28	0.00		

PAH4:

1	*B*	3.61 (3.37)	0.00	3.61	0.00	3.94	0.00	4.16	0.00	3.38[3]	
2	*A*	3.70 (3.49)	0.02	3.69	0.03	4.09	0.03	4.32	0.02	3.84[3]	
3	*B*	4.35 (4.02)	0.82	4.23	1.07	4.61	1.31	4.90	1.44	4.48[3]	4.42
4	*A*	4.40	0.10	4.37	0.16	4.84	0.05	5.03	0.01		4.58
5	*A*	4.59	0.00	4.59	0.01	5.03	0.40	5.45	0.75		
6	*B*	4.62	0.00	4.62	0.00	5.18	0.02	5.41	0.01		
7	*B*	4.85	0.09	4.83	0.07	5.66	0.02	6.06	0.07		4.75
8	*A*	4.89	0.00	4.89	0.00	5.77	0.23	6.05	0.30		
9	*B*	5.07	0.00	5.10	0.00	5.86	0.03	6.18	0.33		
10	*B*	5.10	0.00	5.11	0.00	5.90	0.00	6.20	0.00		
11	*A*	5.15	0.06	5.14	0.12	5.90	0.30	6.26	0.00		
12	*A*	5.26	0.00	5.32	0.00	6.04	0.01	6.42	0.00		
13	*B*	5.29	0.00	5.36	0.00	5.94	0.22	6.46	0.00		
14	*A*	5.37	0.00	5.42	0.02	6.25	0.01	6.57	0.07		
15	*A*	5.51	0.02	5.50	0.13	6.33	0.02	6.66	0.48		
16	*A*	5.55	0.01	5.60	0.01	6.40	0.34	6.71	0.06		
17	*B*	5.57	0.01	5.64	0.00	6.25	0.00	6.50	0.00		
18	*B*	5.62	0.08	5.57	0.12	6.34	0.01	6.79	0.00		
19	*B*	5.69	0.01	5.70	0.01	6.53	0.00	6.90	0.05		
20	*B*	5.71	0.02	5.77	0.02	6.66	0.04	7.05	0.10		
21	*A*	5.72	0.03	5.78	0.00	6.47	0.02	6.97	0.00		
22	*A*	5.75	0.38	5.67	0.51	6.59	0.19	7.00	0.05		
23	*B*	5.90	0.00	5.93	0.01	6.81	0.14	7.10	0.05		
24	*A*	5.93	0.04	5.93	0.02	6.76	0.03	7.12	0.00		
25	*A*	5.98	0.00	6.05	0.00	6.81	0.00	7.25	0.01		
26	*B*	6.00	0.00	6.04	0.00	6.84	0.04	7.14	0.01		
27	*B*	6.04	0.00	6.06	0.00	6.89	0.01	7.26	0.02		
28	*A*	6.10	0.03	6.11	0.10	6.87	0.00	7.31	0.00		
29	*B*	6.14	0.02	6.14	0.04	6.97	0.08	7.38	0.02		
30	*B*	6.20	0.21	6.18	0.29	7.05	0.03	7.41	0.02		

PAH5:

1	*A*	3.35 (3.11)	0.00	3.35	0.00	3.71	0.00	3.94	0.00	3.20	
2	*B*	3.57 (3.31)	0.01	3.56	0.01	3.97	0.02	4.17	0.02		3.78
3	*B*	3.83 (3.67)	0.34	3.76	0.50	4.22	0.78	4.53	0.87		4.12
4	*A*	3.96	0.06	3.93	0.11	4.51	0.14	4.89	0.08		
5	*B*	4.03	0.02	4.03	0.02	4.47	0.00	4.70	0.00		
6	*A*	4.15	0.00	4.15	0.00	4.84	0.46	5.18	0.87		
7	*A*	4.36	0.10	4.34	0.17	5.17	0.01	5.49	0.04		
8	*B*	4.49	0.36	4.45	0.42	5.13	0.52	5.58	0.68		4.66
9	*B*	4.63	0.00	4.63	0.00	5.58	0.01	5.85	0.23		
10	*A*	4.70	0.02	4.70	0.04	5.26	0.07	5.88	0.14		
11	*B*	4.93	0.08	4.92	0.09	5.67	0.17	6.17	0.00		5.38
12	*A*	5.03	0.00	5.08	0.00	5.71	1.14	6.00	0.75		
13	*A*	5.15	0.00	5.15	0.01	5.86	0.06	6.10	0.22		
14	*B*	5.16	0.03	5.14	0.07	5.89	0.02	6.26	0.00		
15	*B*	5.17	0.01	5.21	0.01	6.02	0.00	6.28	0.01		
16	*B*	5.21	0.02	5.22	0.01	6.04	0.00	6.53	0.02		
17	*B*	5.24	0.01	5.29	0.00	6.10	0.00	6.62	0.03		
18	*A*	5.27	0.00	5.29	0.83	5.95	0.01	6.45	0.11		
19	*A*	5.33	0.06	5.33	0.00	6.24	0.10	6.55	0.01		
20	*B*	5.38	0.01	5.44	0.01	6.37	0.01	6.74	0.02		

21	*A*	5.40	0.23	5.35	0.28	6.29	0.03	6.59	0.00	
22	*A*	5.43	0.29	5.48	0.00	6.40	0.02	6.70	0.00	
23	*A*	5.51	0.07	5.50	0.07	6.46	0.00	6.73	0.00	
24	*B*	5.51	0.08	5.49	0.15	6.38	0.03	6.78	0.00	
25	*A*	5.55	0.20	5.55	0.06	6.48	0.07	6.88	0.18	
26	*B*	5.56	0.04	5.61	0.00	6.41	0.04	6.90	0.09	
27	*B*	5.61	0.00	5.62	0.01	6.52	0.00	6.94	0.01	
28	*A*	5.62	0.00	5.68	0.00	6.52	0.19	7.00	0.00	
29	*A*	5.69	0.02	5.72	0.11	6.63	0.01	7.09	0.00	
30	*B*	5.72	0.01	5.76	0.01	6.66	0.08	6.99	0.03	
31	*A*	5.74	0.07	5.76	0.00	6.72	0.00	7.18	0.00	
32	*B*	5.77	0.01	5.83	0.02	6.69	0.05	7.10	0.00	
33	*B*	5.83	0.00	5.87	0.00	6.74	0.00	7.17	0.01	
34	*A*	5.87	0.03	5.89	0.04	6.75	0.01	7.23	0.01	
35	*A*	5.90	0.03	5.90	0.06	6.83	0.00	7.29	0.03	
36	*B*	5.92	0.01	5.91	0.01	6.84	0.09	7.23	0.01	
37	*A*	5.92	0.00	5.97	0.02	6.89	0.01	7.32	0.00	
38	*B*	5.94	0.01	5.98	0.13	6.89	0.01	7.26	0.00	
39	*A*	5.96	0.02	5.99	0.12	6.91	0.03	7.36	0.00	
40	*B*	5.98	0.05	6.01	0.03	6.91	0.00	7.39	0.03	
PAH6:										
1	*B*	3.21 (2.99)	0.00	3.21	0.01	3.58	0.00	3.81	0.00	
2	*A*	3.36 (3.06)	0.00	3.35	0.00	3.80	0.00	4.03	0.00	
3	*B*	3.63 (3.48)	0.34	3.57	0.45	4.01	0.58	4.32	0.64	3.99
4	*A*	3.74	0.05	3.73	0.09	4.23	0.02	4.48	0.01	
5	*B*	3.86	0.00	3.86	0.01	4.43	0.02	4.69	0.01	
6	*A*	3.92	0.04	3.91	0.06	4.46	0.42	4.90	0.85	
7	*A*	4.08	0.01	4.08	0.02	5.03	0.81	5.39	0.54	
8	*B*	4.10	0.00	4.09	0.00	4.88	0.04	5.13	0.01	
9	*B*	4.20	0.02	4.20	0.02	4.96	0.10	5.50	1.03	
10	*A*	4.22	0.01	4.22	0.02	5.09	0.00	5.62	0.55	
11	*B*	4.44	0.09	4.43	0.16	5.14	0.52	5.77	0.07	
12	*A*	4.58	0.26	4.53	0.51	5.27	0.16	5.82	0.24	4.86
13	*B*	4.63	0.09	4.62	0.11	5.32	0.09	5.91	0.09	
14	*B*	4.80	0.03	4.79	0.05	5.71	0.17	6.05	0.04	
15	*A*	4.83	0.19	4.80	0.30	5.50	0.56	5.99	0.01	
16	*A*	4.98	0.08	4.96	0.19	5.62	0.01	6.04	0.00	
17	*A*	4.99	0.10	5.03	0.01	5.81	0.01	6.11	0.06	
18	*B*	5.00	0.20	4.97	0.21	5.88	0.00	6.12	0.01	4.90
19	*B*	5.04	0.01	5.09	0.00	5.90	0.03	6.39	0.01	
20	*A*	5.09	0.10	5.07	0.08	5.87	0.01	6.20	0.07	
21	*A*	5.17	0.00	5.17	0.01	6.03	0.00	6.25	0.00	
22	*A*	5.19	0.01	5.22	0.11	6.16	0.01	6.55	0.00	
23	*B*	5.19	0.00	5.25	0.03	6.13	0.07	6.55	0.00	
24	*A*	5.24	0.00	5.27	0.04	6.21	0.00	6.65	0.05	
25	*A*	5.27	0.13	5.30	0.00	6.28	0.01	6.74	0.03	5.40
26	*B*	5.27	0.01	5.27	0.14	6.18	0.09	6.59	0.08	
27	*B*	5.30	0.00	5.29	0.03	6.29	0.04	6.63	0.10	
28	*B*	5.32	0.10	5.36	0.01	6.32	0.03	6.71	0.00	
29	*A*	5.44	0.06	5.43	0.06	6.29	0.10	6.85	0.02	
30	*B*	5.44	0.00	5.46	0.00	6.34	0.00	6.73	0.05	
31	*B*	5.46	0.00	5.49	0.01	6.40	0.04	6.89	0.06	
32	*A*	5.52	0.02	5.52	0.07	6.37	0.00	6.94	0.00	
33	*A*	5.54	0.02	5.59	0.00	6.50	0.04	6.97	0.03	
34	*B*	5.55	0.05	5.55	0.10	6.46	0.03	6.95	0.03	

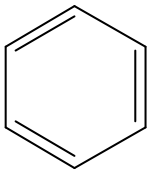
35	*A*	5.58	0.01	5.62	0.00	6.54	0.14	6.99	0.01
36	*B*	5.61	0.01	5.66	0.02	6.49	0.03	7.04	0.05
37	*B*	5.62	0.02	5.68	0.02	6.56	0.02	7.06	0.12
38	*A*	5.63	0.00	5.65	0.00	6.59	0.01	7.01	0.04
39	*B*	5.64	0.03	5.68	0.00	6.63	0.11	7.08	0.01
40	*A*	5.69	0.00	5.73	0.00	6.68	0.00	7.09	0.00

Table S4. Naphthalene transition energies (eV) and oscillator strengths obtained from the ωB97X functional using standard TDDFT, and simplified Grimme and Tamm-Dancoff approaches and 6-311++G basis set.**

	standard		simplified			
			Grimme		Tamm-Dancoff	
	E	*f*	*E*	*f*	*E*	*f*
B_{3u}	4.88	0.08	3.97	0.05	4.26	0.05
B_{2u}	4.72	0.00	4.94	0.00	4.61	0.00
A_u	6.30	0.00	4.73	0.00	4.73	0.00
B_{1g}	6.74	0.00	5.21	0.03	5.60	0.00
B_{2g}	6.79	0.00	4.86	0.00	4.93	0.00
B_{3g}	6.97	0.00	4.54	0.00	4.86	0.00
B_{2u}	6.21	1.36	6.07	1.18	6.41	1.23
B_{3u}	7.42	0.02	5.67	0.00	6.46	0.35
B_{1u}	4.88	0.08	5.33	0.00	5.21	0.03
A_g	6.62	0.00	6.15	0.00	6.20	0.00
B_{1u}	6.51	0.33	5.53	0.00	5.65	0.00
A_u	6.30	0.00	6.09	0.00	6.15	0.00
B_{1g}	7.26	0.00	6.39	0.00	6.44	0.00
B_{3g}	6.32	0.00	5.96	0.00	5.96	0.00
B_{2g}	7.44	0.00	5.69	0.02	5.89	0.00
B_{3g}	7.83	0.00	6.96	0.10	5.67	0.00
A_u	7.36	0.00	6.16	0.00	6.77	0.00
B_{3g}	8.86	0.00	7.36	0.0	5.69	0.00
A_g	7.90	0.00	7.15	0.01	7.16	0.01
B_{2g}	7.71	0.00	6.09	0.27	6.53	0.01
Δ	0.54		0.38		0.28	

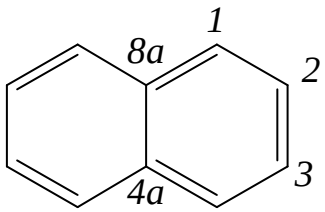
Δ - average error with respect to experimental values

Table S3. Examples of bond length variations in the ground and excited electronic states of PAHs as obtained by the B3LYP/6-311++G calculations.**

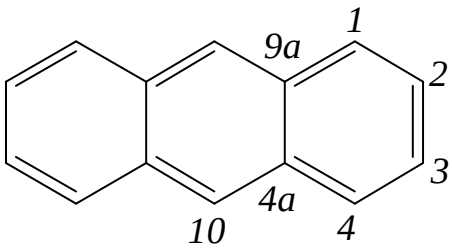


State	d_{CC}	d_{CH}
S_0, ground	1.394	1.084
S_1	1.425	1.082
S_2	1.384	1.088

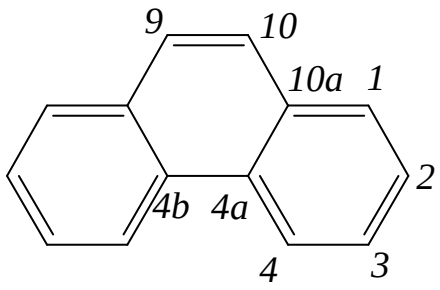
(Benzene from J. Chem. Phys 2017, 146, 144301)



State	$d_{1,2}$	$d_{2,3}$	$d_{1,8a}$	$d_{4a,8a}$	CH_1	CH_2
S_0, ground	1.375	1.415	1.420	1.432	1.085	1.084
S_1	1.428	1.376	1.414	1.438	1.085	1.083
S_2	1.400	1.426	1.413	1.486	1.085	1.083



State	$d_{1,2}$	$d_{2,3}$	$d_{4,4a}$	$d_{4a,10}$	$d_{4a,9a}$	CH_1	CH_2	CH_{10}
S_0, ground	1.368	1.425	1.429	1.399	1.443	1.085	1.084	1.086
S_1	1.409	1.388	1.408	1.414	1.442	1.085	1.084	1.086
S_2	1.385	1.430	1.414	1.406	1.480	1.085	1.083	1.086



State	$d_{1,2}$	$d_{2,3}$	$d_{3,4}$	$d_{4,4a}$	$d_{4a,4b}$	$d_{4a,10a}$	$d_{9,10}$	$d_{10,10a}$	$d_{1,10a}$
S_0, ground	1.378	1.406	1.381	1.413	1.456	1.425	1.358	1.434	1.413
S_1	1.401	1.403	1.396	1.423	1.429	1.460	1.396	1.410	1.409
S_2	1.383	1.402	1.410	1.395	1.466	1.453	1.421	1.396	1.435

State	CH_1	CH_2	CH_3	CH_4	CH_{10}
S_0, ground	1.085	1.084	1.084	1.082	1.085
S_1	1.085	1.083	1.084	1.081	1.085
S_2	1.085	1.084	1.083	1.083	1.084

Table S4. Most intense absorption vibrational subbands wavelength (λ/nm), dipole strength (D/debye^2) and relative weight (w/%) of the transition specified in the last column

a) Napthalene – B_{2u}

	λ	D	w	modes excited
1	314.24	0.0851	12.	
2	309.34	0.0616	21	9
3	301.04	0.0483	32	32
4	296.54	0.0334	49	9 32
5	299.18	0.0294	37	40
6	304.59	0.0213	41	9 9
7	294.73	0.0211	53	9 40
8	287.19	0.0167	62	32 40
9	304.15	0.0139	23	25
10	288.91	0.0135	59	32 32

b) Napthalene – B_{3u}

	λ	D	w	modes excited
1	314.24	0.0851	12.	
2	309.34	0.0616	21	9
3	301.04	0.0483	32	32
4	296.54	0.0334	49	9 32
5	299.18	0.0294	37	40
6	304.59	0.0213	41	9 9
7	294.73	0.0211	53	9 40
8	287.19	0.0167	62	32 40
9	304.15	0.0139	23	25
10	288.91	0.0135	59	32 32

c) Antracene - $S_0 \rightarrow S_1$

	λ	D	w	modes excited	
1	428	0.1806	20		
2	404	0.1111	44	46	
3	421	0.0803	29	8	
4	398	0.0478	61	8	46
5	382	0.0352	71	46	46
6	401	0.0330	52	55	
7	402	0.0297	48	52	
8	379	0.0205	76	46	55
9	402	0.0199	48	53	
10	380	0.0184	73	46	52

c) Phenantrene - $S_0 \rightarrow S_1$

	λ	D	w	modes excited	
1	326	0.0344	48	26	
2	335	0.0286	39		
3	330	0.0124	45	9	
4	312	0.0104	82	26	45
5	320	0.0090	63	45	
6	319	0.0088	74	55	
7	320	0.0068	68	48	
8	322	0.0043	76	8	26
9	310	0.0041	82	26	53
10	316	0.0038	79	9	45

c) Phenantrene - $S_0 \rightarrow S_2$

	λ	D	w	modes excited	
1	321	0.3409	19		
2	317	0.1416	28	9	
3	306	0.0975	46	51	
4	307	0.0482	36	46	
5	302	0.0345	61	9	51
6	320	0.0288	50	1	1
7	313	0.0271	53	9	9
8	309	0.0211	32	40	
9	303	0.0210	56	9	46
10	308	0.0199	33	44	

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