Supplementary information: Electronic structure of small polycyclic aromatic hydrocarbons in singlet excited states

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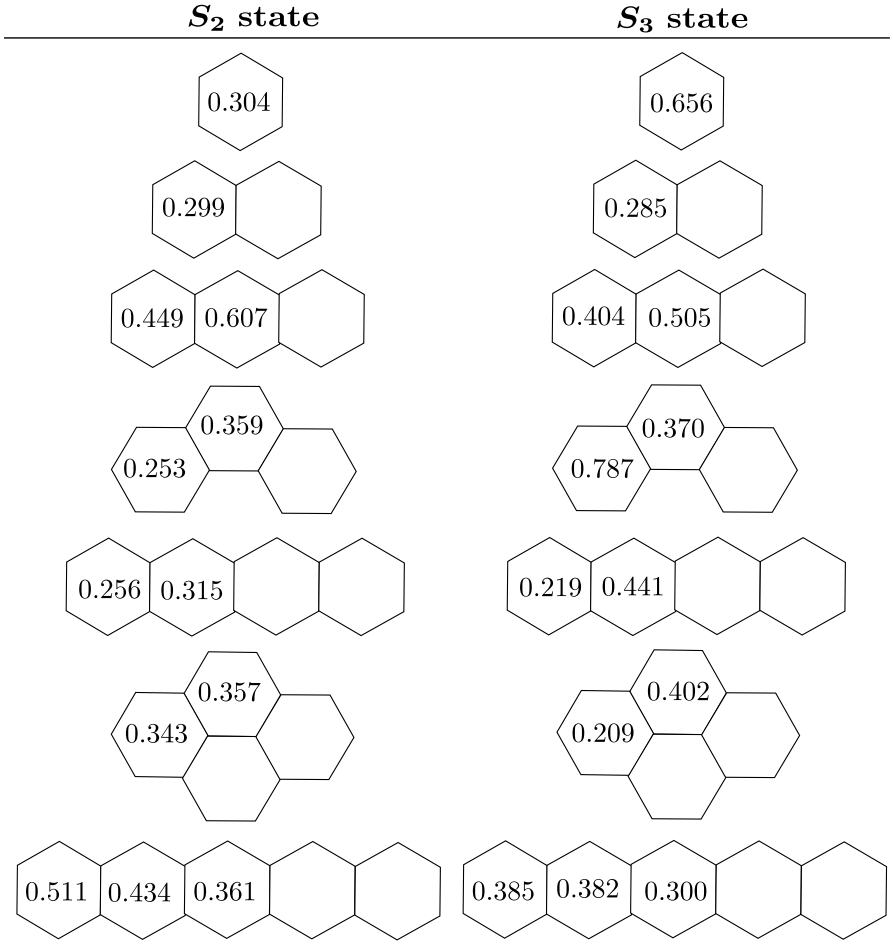

Figure S1. Aromaticity of PAHs in the S_2 and S_3 excited electronic states in terms of the θ' index.

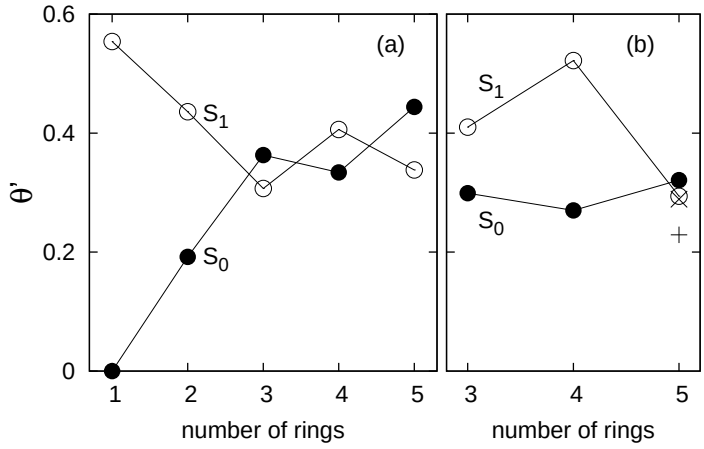

Figure S2. Aromaticity of the (a) external and (b) inner rings of acenes in the ground and first excited electronic states in terms of the θ' index. The values for the central ring in pentacene are denoted by the + and × symbols for the S_0 and S_1 states, respectively.

Table S1. Similarity indices of PAHs in the ground and excited states.

(a) $S_0 \rightarrow S_1$

molecule	D_{bcp}	D_ρ	D_ε	D_{lap}	D_δ	D_H
1	0.0569	0.0012	0.0479	0.0307	0.0860	0.0025
2	0.0542	0.0016	0.0441	0.0315	0.0643	0.0031
3	0.0613	0.0021	0.0499	0.0354	0.0579	0.0039
3b	0.0324	0.0008	0.0294	0.0215	0.0402	0.0013
4	0.0267	0.0010	0.0259	0.0190	0.0363	0.0020
4b	0.0404	0.0012	0.0315	0.0249	0.0435	0.0021
5	0.0487	0.0016	0.0395	0.0284	0.0500	0.0026

(b) $S_0 \rightarrow S_2$

molecule	D_{bcp}	D_ρ	D_ε	D_{lap}	D_δ	D_H
1	0.0410	0.0020	0.0340	0.0229	0.0388	0.0034
2	0.0711	0.0021	0.0576	0.0416	0.0778	0.0044
3	0.0424	0.0012	0.0347	0.0243	0.0472	0.0024
3b	0.0374	0.0022	0.0256	0.0364	0.0546	0.0012
4	0.0298	0.0013	0.0346	0.0250	0.0436	0.0026
4b	0.0380	0.0012	0.0309	0.0221	0.0376	0.0024
5	0.0320	0.0011	0.0247	0.0182	0.0513	0.0021

(b) $S_0 \rightarrow S_2$

molecule	D_{bcp}	D_ρ	D_ε	D_{lap}	D_δ	D_H
1	0.0769	0.0017	0.0627	0.0438	0.1069	0.0037
2	0.0747	0.0032	0.0489	0.0520	0.0727	0.0042
3	0.0665	0.0020	0.0538	0.0391	0.0677	0.0039
3b	0.0506	0.0028	0.0288	0.0446	0.1333	0.0018
4	0.0286	0.0015	0.0392	0.0285	0.0522	0.0030
4b	0.0506	0.0022	0.0389	0.0312	0.0417	0.0037
5	0.0502	0.0016	0.0408	0.0291	0.0509	0.0027