Electronic Supplementary Information for: Enhanced inverted singlet-triplet gaps in azaphenalenes and non-alternant hydrocarbons

Marc H. Garner[‡],* J. Terence Blaskovits[‡], and Clémence Corminboeuf*

Laboratory for Computational Molecular Design, Institute of Chemical Sciences and Engineering, Ecole Polytechnique federale de Lausanne (EPFL), 1015 Lausanne, Switzerland.

[‡] *These authors contributed equally to this work.*

E-mail: marc.garner@epfl.ch; clemence.corminboeuf@epfl.ch

Additional figures and tables

All molecules that have been examined at the EOM-CCSD level are listed in Table S1, along with computations at the second-order approximate coupled-cluster level (CC2) level carried out using Turbomole 7.1.[1] The CC2 method is computationally more feasible than EOM-CCSD and thus enables us to assess larger molecules with the aug-cc-pVDZ basis set. Compared to EOM-CCSD, singlet-triplet gaps are systematically underestimated (more negative) at the CC2/aug-cc-pVDZ level,[2,3] which we also see in the current dataset (Table S1). Both EOM-CCSD and CC2 computations reveal that there is little basis set dependence in the studied molecules upon increasing the basis set size from cc-pVDZ to aug-cc-pVDZ. Note that mol15 is cyclopenta[*ef*]heptalene, mol62 is benzo[*f*]cyclopenta[*cd*]azulene, and mol151 is azuleno[2,1,8-*kla*]heptalene. All optimized structures are available as supporting files in xyz-format.

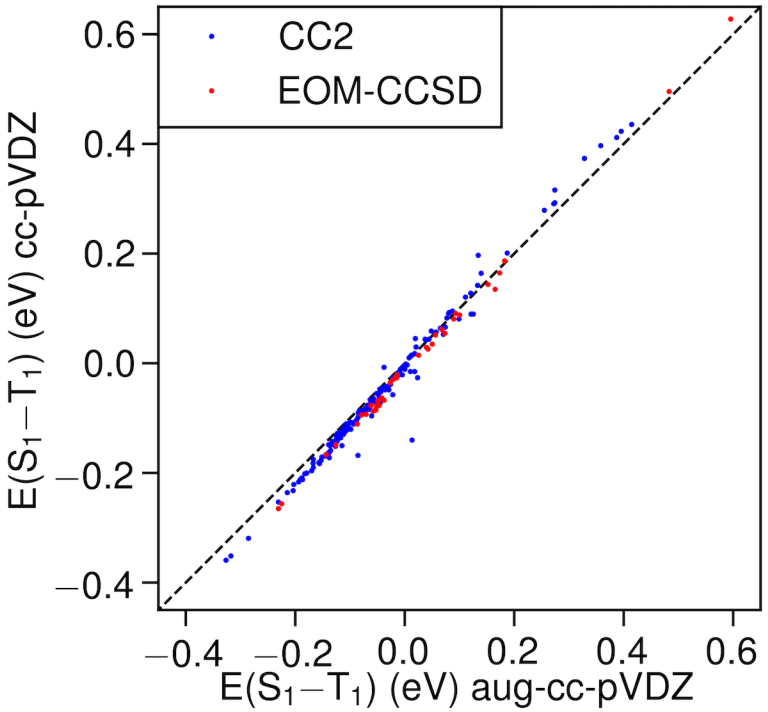

Figure S1: Singlet-triplet gaps computed with EOM-CCSD and CC2 methods using the aug-cc-PVDZ cc-PVDZ basis sets. All values from Table S1 where both aug-cc-PVDZ and cc-PVDZ data are available are included in this plot.

We have examined the possible inversion of the singlet-triplet gap in azulene because it has a small $E(S_1-T_1)$ (Figure S2). We find several substituted azulene derivatives that exhibit higher-lying Hund's rule violations. There is always another triplet that is lower than that corresponding to S_1 because close-lying molecular orbitals switch order, which has also been reported in other contexts.[4,5] All substituted azulenes are included in Table S1.

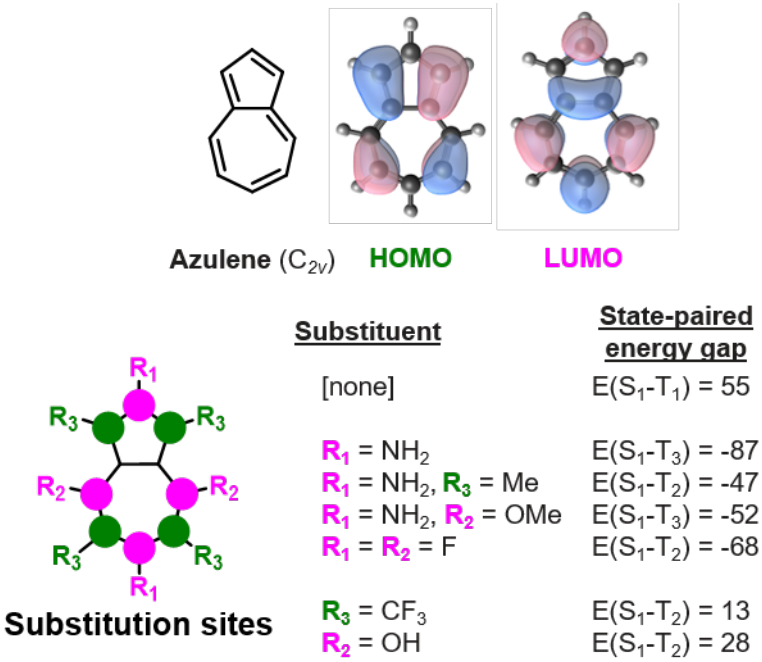

Figure S2: Structure and computed singlet-triplet gaps in substituted azulenes. R groups are H unless otherwise stated. Energies are provided in meV.

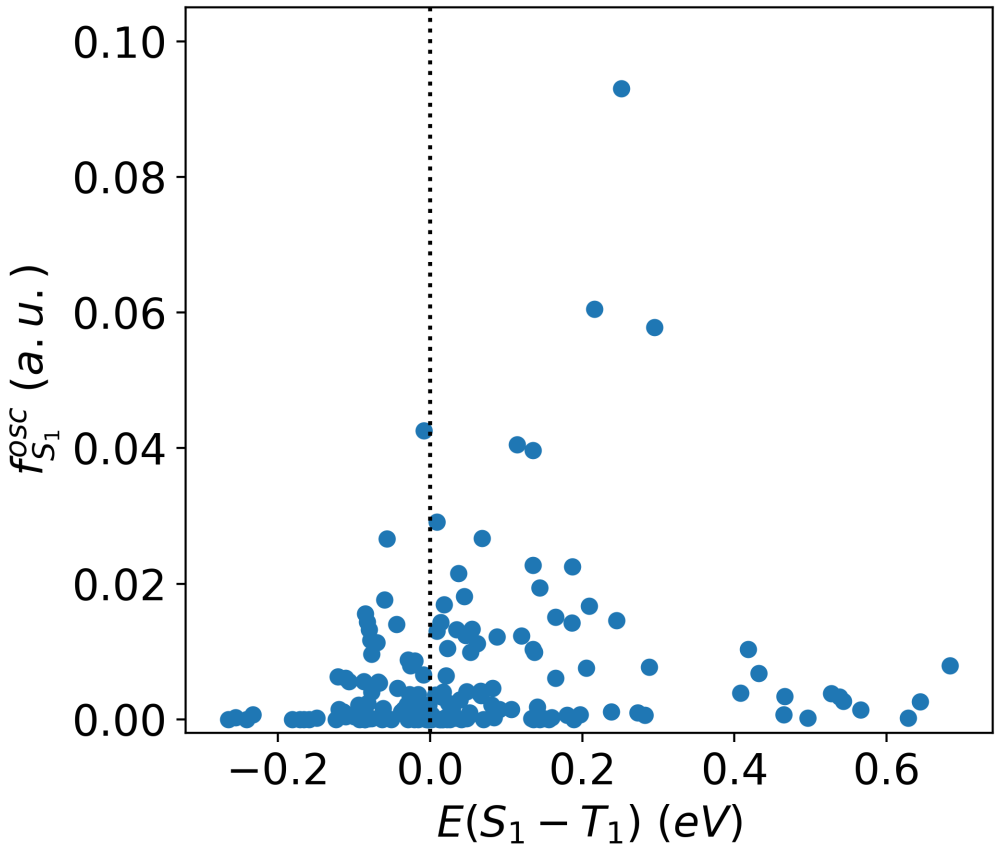

Figure S3: Comparison of the excited-state singlet-triplet gap ($E(\mathrm{S}_1{-}\mathrm{T}_1)$, *x-axis*) and the oscillator strength of the lowest singlet excited state (f_{S1}^{osc}, *y-axis*) for bare and substituted compounds studied in this work. Energies computed at the EOM-CCSD/cc-pVDZ level (see Table S1 for values). Oscillator strengths computed using Tamm-Dancoff-approximated time-dependent density functional theory at the ωB97X-D/def2-TZVP level (see Table S2 for values).

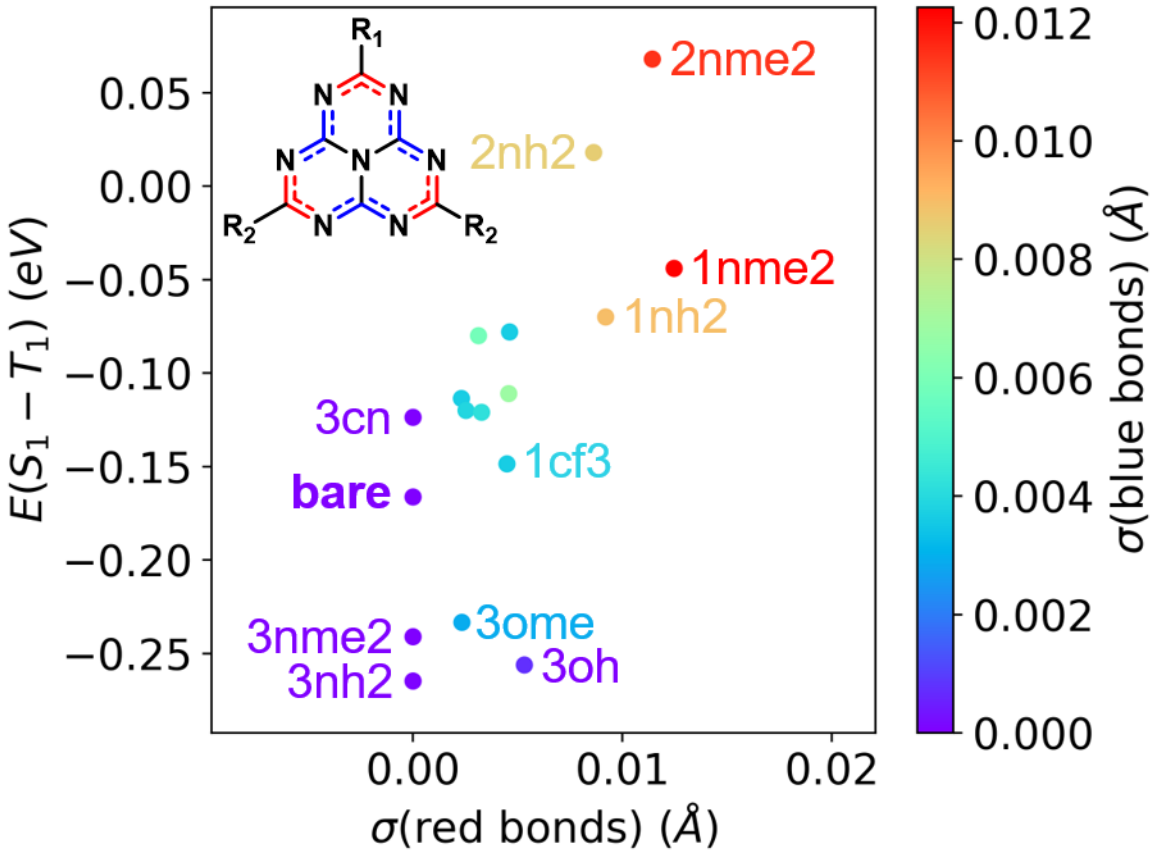

Figure S4: Comparison of excited-state singlet-triplet gap ($E(S_1-T_1)$, *y-axis*) and the standard deviation σ of bond lengths indicated in red and blue (*x-axis* and *color axis*, respectively) in heptazine derivatives. Labels correspond to the number and nature of R-group substituents, as indicated in the compound names provided in Table S1 *e.g.*, $3nh2$ corresponds to heptazine functionalized with 3 NH_2 groups (*heptazine_3nh2*). $3cn$ and $1cf3$ are listed as *heptazine_3cn_lumo* and *heptazine_1cf3_lumo* in Table S1. Threefold substitutions preserve the local symmetry and equivalent bond lengths of heptazine ($\sigma = 0$), while one- and two-fold substitutions induce deformations in the overall symmetry of the molecular core, leading to variations in bond lengths and larger σ. No trend was identified with respect to the singlet-triplet gap and the absolute bond lengths (Figure S5). Energies computed at the EOM-CCSD/cc-pVDZ level (see Table S1 for values). Geometries obtained at the ωB97X-D/def2-TZVP level.

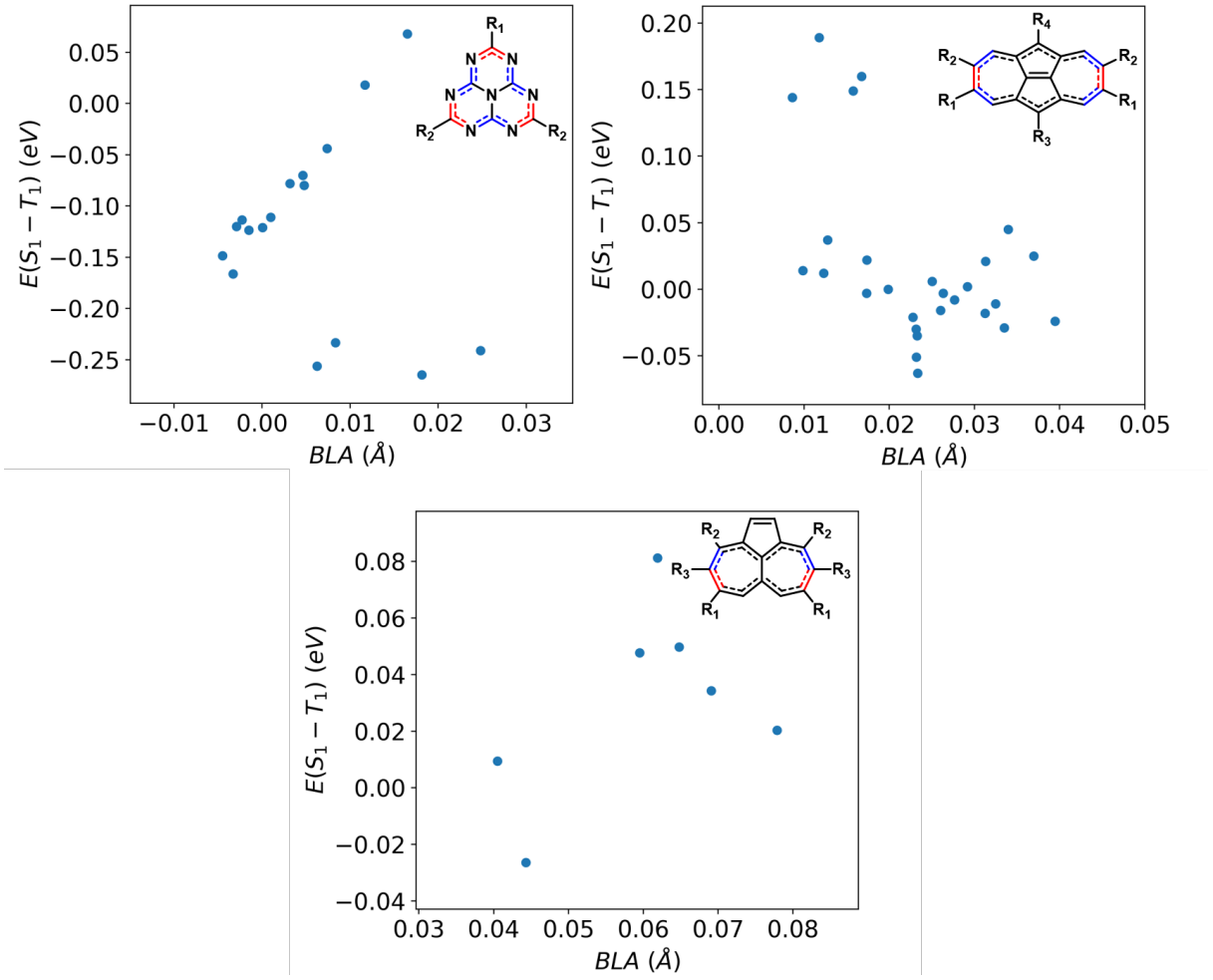

Figure S5: Comparison of the bond-length alternation between selected bonds (BLA, *x-axis*) and the excited-state singlet-triplet gap ($E(\mathrm{S}_1{-}\mathrm{T}_1)$, *y-axis*) in three representative compounds, shown in insets. The BLA is defined as the difference between the length of the bonds marked in red and those marked in blue in the insets. In each unsubstituted parent compound, all red (and blue) bonds are of equal lengths. In some substituted derivatives, electronic and steric effects lead to small differences in bond lengths of each color. In these cases, the bond length taken for the calculation of the BLA was the average for all bonds of a given color. Energies computed at the EOM-CCSD/cc-pVDZ level (see Table S1 for values). Geometries obtained at the ωB97X-D/def2-TZVP level.

Table S1: Singlet-triplet gaps computed using different methods; T_x is the triplet state with the same electron configuration as S_1. Energies are given in eV. The rightmost column indicates if the gap follows the expected trend based on the position of the substituents.

	CC2		EOM-CCSD				
	aug-cc-pVDZ	cc-pVDZ	aug-cc-pVDZ	aug-cc-pVDZ	cc-pVDZ	cc-pVDZ	
Name	S_1-T_1 gap	S_1-T_1 gap	S_1-T_1 gap	S_1-T_x gap	S_1-T_1 gap	S_1-T_x gap	Trend
azulene	-0.005	-0.021	0.073	0.073	0.055	0.055	
azulene_2nh2	0.387	0.412	0.595	-0.073	0.628	-0.087	✓
azulene_2nh2_4me	0.134	0.197			0.465	-0.047	✓
azulene_2nh2_alt	0.002	-0.001	0.152	0.098	0.144	0.095	×
azulene_2oh_2me	-0.010	-0.020			0.047	0.009	✓
azulene_2oh_2nh2	0.328	0.374			0.527	0.019	✓
azulene_2oh_alt	-0.028	-0.039	0.100	0.040	0.088	0.028	✓
azulene_2ome_2nh2	0.395	0.423			0.566	-0.052	✓
azulene_2ome_alt	-0.026	-0.038	0.050	0.050	0.035	0.035	✓
azulene_4cf3	-0.057	-0.064			0.137	0.013	✓
azulene_4f_homo	0.080	0.091	0.182	0.182	0.187	0.187	✓
azulene_4f_lumo	0.133	0.142			0.408	-0.068	✓
azulene_4me_lumo	-0.034	-0.042	0.173	0.048	0.165	0.040	×
azulene_4nh2	0.274	0.316			0.466	0.071	×
azulene_4oh	0.274	0.293	0.483	-0.055	0.496	-0.074	✓
azupyrene	-0.047	-0.061	0.042	0.042	0.026	0.026	
azupyrene_2cf3	-0.056	-0.068			0.016	0.016	✓
azupyrene_2nh2	-0.039	-0.044			0.053	0.053	×
azupyrene_2oh	-0.072	-0.082			0.007	0.007	✓
azupyrene_2oh_1cf3	-0.068	-0.076			0.015	0.015	✓
azupyrene_2ome	-0.068	-0.081			0.011	0.011	✓
azupyrene_2ome_1cf3	-0.062	-0.073			0.017	0.017	✓
azupyrene_4cn	-0.077	-0.088			-0.002	-0.002	✓
azupyrene_4nh2	0.020	0.030			0.070	-0.127	✓
azupyrene_4oh	0.018	-0.015			-0.003	-0.120	✓
azupyrene_4oh_2cf3	0.017	0.017			0.041	-0.149	✓
azupyrene_4oh_4me	0.070	0.053			0.017	-0.116	✓
azupyrene_4oh_6f	0.139	0.164			0.156	-0.080	✓
azupyrene_4ome	1.769	-0.005			0.013	-0.099	✓
cyclazine	-0.124	-0.142	-0.071	-0.071	-0.093	-0.093	
cyclazine_1cf3	-0.120	-0.136			-0.081	-0.081	×
cyclazine_1cf3_lumo	-0.058	-0.068	0.026	0.026			✓
cyclazine_1cn	-0.086	-0.099			-0.030	-0.030	×
cyclazine_1cn_lumo	-0.084	-0.096			-0.038	-0.038	✓
cyclazine_1nh2_homo	0.087	0.094			0.238	0.238	✓
cyclazine_1nme2_homo	0.012	-0.019			0.084	0.084	✓
cyclazine_1oh_homo	0.111	0.121			0.273	0.273	✓
cyclazine_1ome_homo	0.120	0.128			0.282	0.282	✓
cyclazine_2cf3_side	-0.131	-0.148			-0.095	-0.095	✓
cyclazine_2cf3_tip	-0.119	-0.136			-0.080	-0.080	×
cyclazine_2cn_lumo	-0.060	-0.068			0.002	0.002	✓
cyclazine_2cn_side	-0.108	-0.123	-0.049	-0.049	-0.068	-0.068	×
cyclazine_2cn_tip	-0.102	-0.118	-0.042	-0.042	-0.063	-0.063	×
cyclazine_2nh2	-0.127	-0.141	-0.062	-0.062	-0.077	-0.077	×
cyclazine_2nh2_homo	0.008	0.010			0.133	0.133	✓
cyclazine_2nh2_homo_alt	-0.004	-0.007			0.107	0.107	✓
cyclazine_2oh	-0.137	-0.150	-0.079	-0.079	-0.094	-0.094	✓
cyclazine_2oh_2cf3	-0.116	-0.127			-0.062	-0.062	×
cyclazine_2oh_homo	0.048	0.059			0.197	0.197	✓
cyclazine_2oh_homo_alt	0.037	0.044			0.180	0.180	✓
cyclazine_2ome	-0.117	-0.136			-0.082	-0.082	×
cyclazine_2ome_homo	0.012	0.014			0.138	0.138	✓
cyclazine_2ome_homo_alt	0.011	0.013			0.141	0.141	✓
cyclazine_3cn					-0.005	-0.005	×
cyclazine_3cn_lumo					0.136	0.136	✓
cyclazine_3nh2	-0.204	-0.232			-0.181	-0.181	✓
cyclazine_3nme2	-0.194	-0.216			-0.159	-0.159	✓
cyclazine_3oh					-0.171	-0.171	✓
cyclazine_3ome					-0.086	-0.086	×
heptazine	-0.231	-0.253	-0.144	-0.144	-0.166	-0.166	
heptazine_1cf3_lumo	-0.215	-0.236	-0.126	-0.126	-0.149	-0.149	✓
heptazine_1cn_lumo	-0.188	-0.209			-0.120	-0.120	✓
heptazine_1nh2	-0.168	-0.182			-0.070	-0.070	×
heptazine_1nme2	-0.138	-0.162			-0.044	-0.044	×
heptazine_1oh	-0.203	-0.221			-0.121	-0.121	×
heptazine_1ome	-0.191	-0.212			-0.111	-0.111	×
heptazine_2cn_lumo	-0.183	-0.201			-0.114	-0.114	✓
heptazine_2nh2	-0.116	-0.127			0.018	0.018	×
heptazine_2nme2	-0.061	-0.096			0.068	0.068	×
heptazine_2oh	-0.179	-0.200			-0.078	-0.078	×
heptazine_2ome	-0.187	-0.212			-0.080	-0.080	×
heptazine_3cn_lumo	-0.192				-0.124	-0.124	✓
heptazine_3nh2		-0.363	-0.231	-0.231	-0.265	-0.265	✓
heptazine_3nme2	-0.327	-0.359			-0.241	-0.241	✓
heptazine_3oh	-0.318	-0.351	-0.225	-0.225	-0.256	-0.256	✓
heptazine_3ome	-0.286	-0.319			-0.233	-0.233	✓

	CC2		EOM-CCSD				
	aug-cc-pVDZ	cc-pVDZ	aug-cc-pVDZ	aug-cc-pVDZ	cc-pVDZ	cc-pVDZ	
Name	**S_1-T_1 gap**	**S_1-T_1 gap**	**S_1-T_1 gap**	**S_1-T_x gap**	**S_1-T_1 gap**	**S_1-T_x gap**	**Trend**
isopyrene	-0.123	-0.132	-0.014	-0.014	-0.021	-0.021	
isopyrene_1cf3	-0.136	-0.145			-0.030	-0.030	✓
isopyrene_1cn_1	-0.139	-0.148	-0.027	-0.027	-0.035	-0.035	✓
isopyrene_1cn_1_2nh2_3_9	-0.104	-0.120			-0.011	-0.011	×
isopyrene_1cn_2	-0.045	-0.072			0.000	-0.103	n/a
isopyrene_1cn_3	-0.073	-0.086			0.006	0.006	✓
isopyrene_1cn_6_2NH2_2_10	-0.099	-0.108			0.014	0.014	×
isopyrene_1cn_6_2nh2_3_9	-0.029	-0.048			0.045	0.045	×
isopyrene_2cf3	-0.167	-0.175			-0.051	-0.051	✓
isopyrene_2cf3_lumo	-0.123	-0.131			-0.016	-0.016	✓
isopyrene_2cn_1_6	-0.138	-0.172			-0.063	-0.063	✓
isopyrene_2cn_1_6_2nh2_3_9	-0.036	-0.048			-0.011	-0.011	×
isopyrene_2cn_2_10	-0.022	-0.057			-0.003	-0.003	n/a
isopyrene_2cn_2_7	0.010	-0.015			0.022	0.022	n/a
isopyrene_2cn_lumo	-0.112	-0.120			-0.003	-0.003	✓
isopyrene_2nh2	-0.100	-0.107			0.021	0.021	×
isopyrene_2nh2_2_10	-0.068	-0.080			0.037	0.037	n/a
isopyrene_2nh2_homo	0.038	0.042			0.189	0.189	✓
isopyrene_2oh	-0.117	-0.125			-0.008	-0.008	×
isopyrene_2oh_homo	0.012	0.015			0.149	0.149	✓
isopyrene_2ome	-0.125	-0.134			-0.018	-0.018	×
isopyrene_2ome_homo	0.018	0.018			0.160	0.160	✓
isopyrene_4cn_2_5_7_10	0.121	0.090			0.012	0.012	n/a
isopyrene_4cn_3_4_8_9	-0.112	-0.118			0.002	0.002	✓
isopyrene_4me	-0.133	-0.142	-0.021	-0.021	-0.029	-0.029	✓
isopyrene_4nh2_2_5_7_10	-0.038	-0.007			0.144	-0.060	n/a
isopyrene_4oh	0.013	-0.140			0.025	-0.062	✓
isopyrene_4oh_2cn	-0.086	-0.168			-0.024	-0.024	✓
mol8	-0.023	-0.026	0.093	0.093	0.091	0.091	
mol8_2cf3	-0.046	-0.047			0.082	0.082	✓
mol8_2cn	-0.051	-0.055	0.067	0.067	0.062	0.062	✓
mol8_2nh2	-0.068	-0.076			0.048	0.048	✓
mol8_2oh	-0.071	-0.082	0.039	0.039	0.029	0.029	✓
mol8_2ome	-0.083	-0.093	0.025	0.025	0.015	0.015	✓
mol8_4oh	-0.108	-0.121	0.056	0.056	0.052	0.052	✓
mol8_4ome	-0.088	-0.103			0.039	0.039	✓
mol15	-0.012	-0.017	0.089	0.089	0.081	0.081	
mol15_2cn	-0.040	-0.046			0.048	0.048	✓
mol15_2nh2	-0.079	-0.086			0.020	0.020	✓
mol15_2oh	-0.063	-0.067			0.034	0.034	✓
mol15_2ome	-0.044	-0.052			0.050	0.050	✓
mol15_4nh2	-0.071	-0.085			0.009	0.009	✓
mol15_4oh	-0.106	-0.115	-0.015	-0.015	-0.026	-0.026	✓
mol62	0.077	0.083			0.205	0.205	
mol62_2cf3	-0.105	-0.112			0.024	0.024	✓
mol62_4nh2	-0.107	-0.110			0.067	0.067	✓
mol62_4oh	-0.124	-0.128			-0.002	-0.002	✓
mol76	0.057	0.057			0.186	0.186	
mol76_4nh2	0.099	0.081			0.295	0.295	×
mol77	0.019	0.045			0.418	0.107	
mol77_2oh	0.187	0.201			0.432	0.432	×
mol86	0.065	0.064					
mol86_3nh2	0.081	0.093			0.288	0.288	
mol86_3oh	0.044	0.044			0.165	0.165	
mol98	-0.010	-0.016			0.245	0.068	
mol98_3oh	0.358	0.397			0.683	0.028	✓
mol136	0.004	-0.003			0.135	0.135	
mol136_2nh2	0.414	0.436			0.644	0.644	×
mol136_2oh	0.255	0.279			0.543	0.543	×
mol143	0.000	-0.011			0.120	0.073	
mol143_2oh	0.272	0.291			0.538	0.029	✓
mol151	-0.009	-0.013			0.066	0.066	
mol151_2cf3	-0.013	-0.017			0.065	0.065	✓
mol151_3nh2	-0.083	-0.087			-0.009	-0.009	✓
mol151_3oh	-0.085	-0.090			-0.016	-0.016	✓

	CC2		EOM-CCSD				
	aug-cc-pVDZ	cc-pVDZ	aug-cc-pVDZ	aug-cc-pVDZ	cc-pVDZ	cc-pVDZ	
Name	**S_1-T_1 gap**	**S_1-T_1 gap**	**S_1-T_1 gap**	**S_1-T_x gap**	**S_1-T_1 gap**	**S_1-T_x gap**	**Trend**
pentaazaphenalene	-0.127	-0.151	-0.038	-0.038	-0.067	-0.067	
pentaazaphenalene_1cf3	-0.146	-0.169	-0.058	-0.058	-0.087	-0.087	✓
pentaazaphenalene_1cf3_lumo	-0.099	-0.120			-0.029	-0.029	✓
pentaazaphenalene_1cn	-0.136	-0.159	-0.047	-0.047	-0.077	-0.077	✓
pentaazaphenalene_1cn_lumo	-0.064	-0.084			0.009	0.009	✓
pentaazaphenalene_1nh2	-0.152	-0.171			-0.086	-0.086	✓
pentaazaphenalene_1nme2	-0.140	-0.165	-0.051	-0.051	-0.077	-0.077	✓
pentaazaphenalene_1oh	-0.167	-0.190	-0.087	-0.087	-0.111	-0.111	✓
pentaazaphenalene_1ome	-0.157	-0.181			-0.100	-0.100	✓
pentaazaphenalene_2cf3		-0.186			-0.107	-0.107	✓
pentaazaphenalene_2cf3_lumo	-0.112	-0.129			-0.043	-0.043	✓
pentaazaphenalene_2cn	-0.141	-0.164	-0.053	-0.053	-0.083	-0.083	✓
pentaazaphenalene_2cn_lumo	-0.094	-0.111			-0.027	-0.027	✓
pentaazaphenalene_2nh2	0.074	0.066			0.216	0.216	×
pentaazaphenalene_2nh2_homo	0.082				0.209	0.209	✓
pentaazaphenalene_2nme2	0.125	0.090			0.251	0.251	×
pentaazaphenalene_2oh		0.002	0.165	0.165	0.135	0.135	×
pentaazaphenalene_2ome	0.023	-0.026			0.114	0.114	×
pentaazaphenalene_2oh_homo		0.013			0.135	0.135	✓
pentaazaphenalene_2ome_homo	-0.052	-0.075			0.023	0.023	✓
pentaazaphenalene_3cn_lumo	-0.092	-0.107			-0.020	-0.020	✓
pentaazaphenalene_3nh2	-0.156	-0.183			-0.057	-0.057	×
pentaazaphenalene_3nme2	-0.115	-0.150			-0.008	-0.008	×
pentaazaphenalene_3oh	-0.170	-0.196	-0.053	-0.053	-0.085	-0.085	✓
pentaazaphenalene_3ome	-0.153	-0.177			-0.060	-0.060	×

Table S2: Oscillator strengths and excitation energies for select molecules computed using Tamm-Dancoff approximated time-dependent density functional theory at the ωB97X-D/def2-TZVP level. Energies are given in eV.

Name	$E(S_1)$	$E(T_1)$	$f(S_1)$
azulene_2nh2	3.039	2.266	0.0002
azulene_2nh2_alt	3.174	2.667	0.0194
azulene_2nh2_4me	2.776	2.259	0.0007
azulene_2oh_2me	2.696	2.246	0.0124
azulene_2oh_2nh2	3.294	2.601	0.0038
azulene_2oh_alt	2.922	2.480	0.0122
azulene_2ome_2nh2	3.235	2.484	0.0014
azulene_2ome_alt	2.831	2.406	0.0132
azulene_4cf3	2.713	2.293	0.0099
azulene_4f_homo	1.938	1.289	0.0225
azulene_4f_lumo	3.150	2.677	0.0039
azulene_4me_lumo	2.748	2.328	0.0151
azulene_4nh2	3.423	2.788	0.0034
azulene_4oh	3.418	2.787	0.0002
azupyrene_2cf3	2.236	1.985	0.0000
azupyrene_2nh2	2.563	2.201	0.0099
azupyrene_2oh	2.464	2.181	0.0036
azupyrene_2oh_cf3	2.513	2.231	0.0038
azupyrene_2ome	2.435	2.150	0.0036
azupyrene_2ome_cf3	2.491	2.205	0.0040
azupyrene_4cn	2.157	1.907	0.0000
azupyrene_4nh2	3.077	2.713	0.0000
azupyrene_4oh	2.821	2.530	0.0000
azupyrene_4oh_2cf3	3.099	2.755	0.0000
azupyrene_4oh_4me	2.696	2.380	0.0000
azupyrene_4oh_6f	2.641	2.224	0.0000
azupyrene_4ome	2.748	2.457	0.0000
cyclazine	1.367	1.160	0.0000
cyclazine_1cf3	1.494	1.281	0.0001
cyclazine_1cf3_lumo	1.365	1.101	0.0003
cyclazine_1cn	1.551	1.318	0.0004
cyclazine_1cn_lumo	1.218	0.963	0.0011
cyclazine_1nh2_homo	1.526	1.156	0.0011
cyclazine_1nme2_homo	1.464	1.174	0.0003
cyclazine_1oh_homo	1.534	1.144	0.0010
cyclazine_1ome_homo	1.594	1.197	0.0006
cyclazine_2cf3_side	1.577	1.369	0.0003
cyclazine_2cf3_tip	1.620	1.403	0.0001
cyclazine_2cn_lumo	1.123	0.852	0.0007
cyclazine_2cn_side	1.584	1.352	0.0055
cyclazine_2cn_tip	1.641	1.415	0.0007
cyclazine_2nh2	1.965	1.731	0.0040
cyclazine_2nh2_homo	1.219	0.917	0.0001
cyclazine_2nh2_homo_alt	1.215	0.909	0.0015
cyclazine_2oh	1.864	1.648	0.0021
cyclazine_2oh_2cf3	2.123	1.895	0.0016
cyclazine_2oh_homo	1.320	0.980	0.0007
cyclazine_2oh_homo_alt	1.300	0.962	0.0006
cyclazine_2ome	1.819	1.601	0.0024
cyclazine_2ome_homo	1.206	0.898	0.0001
cyclazine_2ome_homo_alt	1.229	0.905	0.0018
cyclazine_3cn	1.732	1.502	0.0000
cyclazine_3cn_lumo	1.133	0.813	0.0000
cyclazine_3nh2	2.239	2.100	0.0000
cyclazine_3nme2	2.278	2.145	0.0000
cyclazine_3oh	2.117	1.965	0.0000
cyclazine_3ome	2.150	1.955	0.0000
heptazine	3.220	2.982	0.0000
heptazine_1cf3_lumo	3.189	2.937	0.0002
heptazine_1cn_lumo	3.108	2.826	0.0015
heptazine_1nh2	3.600	3.261	0.0113
heptazine_1nme2	3.655	3.285	0.0140
heptazine_1oh	3.515	3.225	0.0063
heptazine_1ome	3.513	3.217	0.0061
heptazine_2cn_lumo	3.022	2.743	0.0011
heptazine_2nh2	3.957	3.534	0.0169
heptazine_2nme2	4.032	3.552	0.0267
heptazine_2oh	3.811	3.473	0.0117
heptazine_2ome	3.797	3.464	0.0132
heptazine_3cn_lumo	2.955	2.692	0.0000
heptazine_3nh2	4.327	4.183	0.0000
heptazine_3nme2	4.411	4.242	0.0000
heptazine_3oh	4.131	3.971	0.0003
heptazine_3ome	4.091	3.930	0.0007

Name	$E(S_1)$	$E(T_1)$	$f(S_1)$
isopyrene_1cf3	2.284	2.083	0.0022
isopyrene_1cn_1	2.276	2.085	0.0015
isopyrene_1cn_1_2nh2_3_9	2.446	2.242	0.0014
isopyrene_1cn_2	2.166	1.940	0.0002
isopyrene_1cn_3	2.114	1.889	0.0001
isopyrene_1cn_6_2nh2_2_10	2.290	2.021	0.0143
isopyrene_1cn_6_2nh2_3_9	2.408	2.088	0.0181
isopyrene_2cf3	2.371	2.205	0.0000
isopyrene_2cf3_lumo	2.037	1.833	0.0000
isopyrene_2cn_1_6	2.338	2.184	0.0000
isopyrene_2cn_2_10	2.124	1.909	0.0000
isopyrene_2cn_2_7	2.109	1.848	0.0000
isopyrene_2cn_lumo	2.038	1.828	0.0003
isopyrene_2nh2	2.314	2.050	0.0064
isopyrene_2nh2_2_10	2.156	1.841	0.0215
isopyrene_2nh2_homo	1.611	1.289	0.0000
isopyrene_2oh	2.267	2.039	0.0015
isopyrene_2oh_homo	1.714	1.408	0.0001
isopyrene_2ome	2.174	1.954	0.0018
isopyrene_2ome_homo	1.740	1.435	0.0003
isopyrene_4cn_2_5_7_10	2.072	1.844	0.0000
isopyrene_4cn_3_4_8_9	1.878	1.672	0.0000
isopyrene_4me	2.168	1.973	0.0000
isopyrene_4oh	2.354	2.146	0.0007
isopyrene_4oh_2cn	2.521	2.361	0.0010
isopyrene_4nh2_2_5_7_10	2.202	1.725	0.0000
mol136_2nh2	2.860	2.073	0.0026
mol136_2oh	2.891	2.264	0.0027
mol143_2oh	2.782	2.111	0.0033
mol15_2cn	1.755	1.485	0.0001
mol15_2nh2	2.122	1.866	0.0003
mol15_2oh	2.000	1.731	0.0002
mol15_2ome	1.868	1.588	0.0004
mol15_4nh2	2.610	2.288	0.0291
mol15_4oh	2.392	2.127	0.0079
mol151_2cf3	1.292	0.983	0.0038
mol151_3nh2	1.768	1.532	0.0066
mol151_3oh	1.647	1.408	0.0037
mol62_2cf3	1.534	1.279	0.0024
mol62_4nh2	1.873	1.533	0.0035
mol62_4oh	1.760	1.471	0.0021
mol76_4nh2	2.418	1.971	0.0578
mol77_2oh	2.696	2.085	0.0068
mol8_2cf3	2.145	1.861	0.0046
mol8_2cn	2.059	1.773	0.0112
mol8_2nh2	2.303	1.996	0.0041
mol8_2oh	2.180	1.892	0.0015
mol8_2ome	2.070	1.783	0.0033
mol8_4oh	2.424	2.151	0.0010
mol8_4ome	2.258	1.968	0.0029
mol86_3nh2	2.589	2.136	0.0077
mol86_3oh	2.473	2.123	0.0061
mol98_3oh	2.357	1.505	0.0079
pentaazaphenalene	2.624	2.301	0.0054
pentaazaphenalene_1cf3	2.671	2.366	0.0056
pentaazaphenalene_1cf3_lumo	2.561	2.188	0.0088
pentaazaphenalene_1cn	2.636	2.324	0.0096
pentaazaphenalene_1cn_lumo	2.483	2.053	0.0130
pentaazaphenalene_1nh2	2.956	2.694	0.0000
pentaazaphenalene_1nme2	2.963	2.698	0.0001
pentaazaphenalene_1oh	2.858	2.607	0.0004
pentaazaphenalene_1ome	2.856	2.600	0.0004
pentaazaphenalene_2cf3	2.721	2.437	0.0056
pentaazaphenalene_2cf3_lumo	2.580	2.254	0.0046
pentaazaphenalene_2cn	2.635	2.331	0.0144
pentaazaphenalene_2cn_lumo	2.406	2.093	0.0037
pentaazaphenalene_2nh2	3.300	2.629	0.0605
pentaazaphenalene_2nh2_homo	2.165	1.609	0.0167
pentaazaphenalene_2nme2	3.349	2.637	0.0930
pentaazaphenalene_2oh	3.198	2.610	0.0397
pentaazaphenalene_2oh_homo	2.281	1.788	0.0103
pentaazaphenalene_2ome	3.142	2.582	0.0405
pentaazaphenalene_2ome_homo	2.421	2.019	0.0105
pentaazaphenalene_3cn_lumo	2.323	1.976	0.0086
pentaazaphenalene_3nh2	3.613	3.244	0.0266
pentaazaphenalene_3nme2	3.655	3.251	0.0426
pentaazaphenalene_3oh	3.446	3.102	0.0156
pentaazaphenalene_3ome	3.425	3.079	0.0176

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