Electronic Supplementary Information:

Excess and excited-state dipole moments of real-life dyes: A comparison between wave-function, BSE/*GW*, and TD-DFT values

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S1. ADDITIONAL DATA FOR BSE/*GW* CALCULATIONS

S1.1. Finite-field calculations

The ES dipole moments at the BSE/*GW* level were determined using the finite-field (FF, numerical difference) and approximated analytical gradients (AA) methods. For the FF approach, the electric field was applied along each Cartesian axes (x, y, and z) using positive and negative point charges of ±125e and ±250e placed at 1000 Bohr from the origin, which results in electric fields of ±0.00025 a.u. or ±0.0005 a.u., respectively (the sign obviously depends on how the positive and negative charges are placed). This was done for the ground-state calculations using ORCA 5.1 program and the obtained Kohn-Sham eigenstates were used in the following BSE/*GW* calculations.

We estimated the BSE/GW dipole moments using the finite difference method to approximate the first-order derivatives. First using the usual central difference formula:

$$\mu^{\mathrm{ES}} \approx \frac{E^{\mathrm{ES}}_{\mathrm{tot}}(+E^{\mathrm{F}}) - E^{\mathrm{ES}}_{\mathrm{tot}}(-E^{\mathrm{F}})}{2E^{\mathrm{F}}}$$

where $\pm E^{\mathrm{F}}$ is the applied electric field, in our case, it is ±0.00025 a.u. or ±0.0005 a.u.; and also with the five-point formula, which removes the contribution from the next high-order derivative:

$$\mu^{\mathrm{ES}} \approx \frac{E^{\mathrm{ES}}_{\mathrm{tot}}(-2E^{\mathrm{F}}) - 8E^{\mathrm{ES}}_{\mathrm{tot}}(-E^{\mathrm{F}}) + 8E^{\mathrm{ES}}_{\mathrm{tot}}(+E^{\mathrm{F}}) - E^{\mathrm{ES}}_{\mathrm{tot}}(+2E^{\mathrm{F}})}{12E^{\mathrm{F}}}$$

where $E^{\mathrm{F}} = 0.00025$ a.u. The differences between these schemes provide a hint of the stability of the numerical derivatives. In our case, on average variation of *c.a.* 0.0075 Debye was found between various estimates which is irrelevant for our purposes. We used the μ^{ES} obtained with the second formula in the graphs and in the calculation of the $\Delta\mu$ listed in this work.

S1.2. *GW* energy correction levels

During the calculations, we observed that adding the electric field can lead to a switch between some close-lying DFT orbitals and consequently to a change in the *GW* levels, which results in inconsistent *GW* energy correction windows that in turn influence the BSE transition energies and lead to numerical instability of the computed ES dipole moments. In

order to avoid these switching of the GW levels we reduced the number of corrected highest occupied and lowest unoccupied eigenvalues. For the DMABN case, we corrected 3 highest occupied and 5 lowest unoccupied eigenvalues (later simply 3&5) for BSE/evGW/PBE0, while for BSE/evGW/PBEh we used 3&3. Higher/lower levels are shifted rigidly following the correction obtained for the highest/lowest explicitly corrected level.[1] Such choice is reasonable since higher orbitals do not play any significant role in the investigated excited states. We nevertheless note that when PBE0 is used as a starting point for the GW calculations, we observed that, for DMABN structures with 0° and 10°, the addition of the electric field leads to a small non-negligible participation of a higher unoccupied orbital in the first lowest transition. However, we do not correct this higher unoccupied level as the increase of corrected unoccupied eigenvalues yields less numerically stable results. For the dyes, we applied the 5&5 correction scheme, except in a few cases where it led to unstable dipoles: for compounds **4**, **13**, **18**, and **20** we used the 3&3 correction scheme; for compounds **6** and **16** we used 2&2; and finally, for molecule **8** we applied 1&4 correction. In all cases, we checked that the key contributing orbitals for the S_1 transition (usually HOMO-LUMO) are indeed corrected. In the calculation with AA, the problem of switching of GW levels does not arise, so we corrected all the occupied and virtual states within a 10 eV gap.

S1.3. Optimally tuned PBEα

For the dyes, we used two global hybrid functionals, namely PBE0 and the optimally tuned PBEα (only with AA scheme) as starting points. The optimal tuning was done in a usual way, where we search for the optimum percentage of exact exchange, α, that leads to the equality between the -ϵ_{HOMO} and total energy differences computed from neutral and anionic systems (ionization potential for a given α). The corresponding values of α for each molecule are listed in Table S1.

TABLE S1. The percentage of exact exchange (α) used in the optimally-tuned global hybrid PBEα functional for each of the molecule in the dyes set. All values are in %.

	α		α		α		α		α
1	68	**6**	69	**11**	68	**16**	62	**21**	66
2	66	**7**	70	**12**	70	**17**	67	**22**	61
3	67	**8**	68	**13**	68	**18**	66	**23**	67
4	67	**9**	62	**14**	64	**19**	67	**24**	59
5	67	**10**	68	**15**	62	**20**	62	**25**	57

S2. DMABN

S2.1. Molecular orbitals

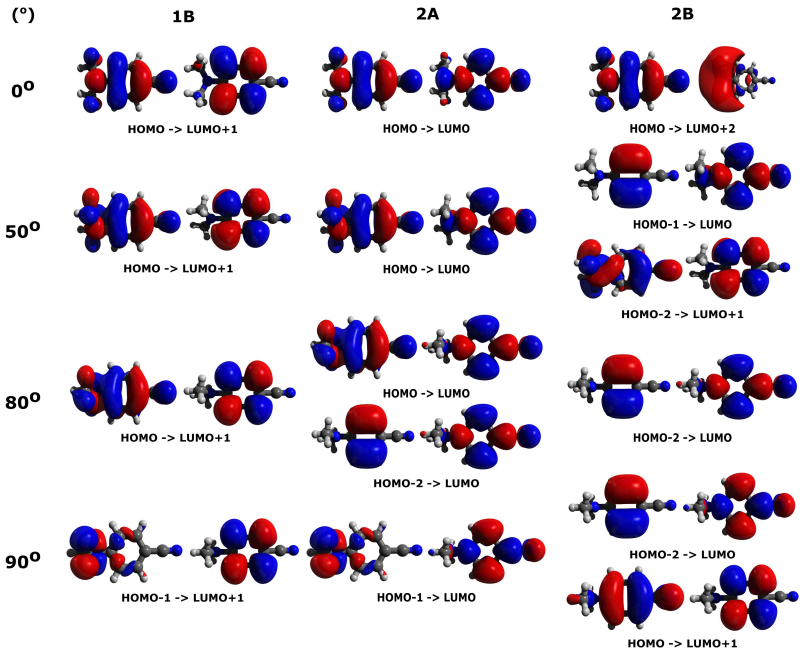


FIG. S1. Hartree-Fock MOs participating in the transitions to the 1B, 2A, and 2B ES (S_1, S_2, and S_3 respectively at the untwisted geometry) of DMABN determined at the CC2 [equivalent results were obtained with ADC(2)] method using cc-pVTZ basis set.

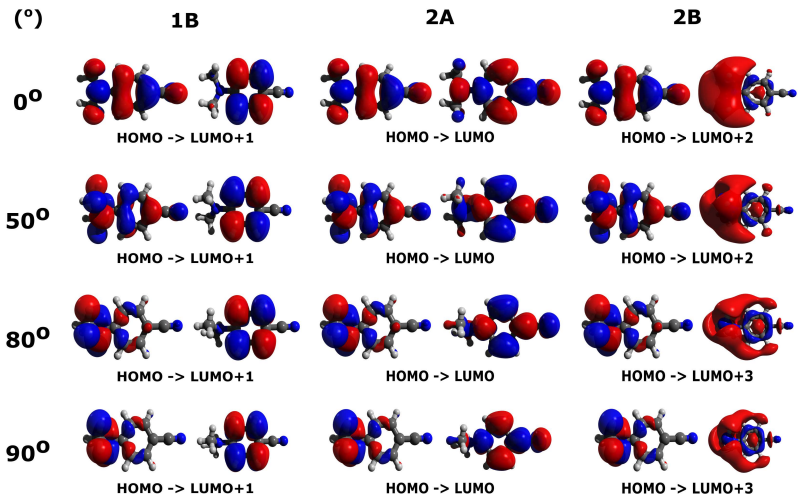


FIG. S2. PBE MOs participating in the transitions to the 1B, 2A, and 2B ES (S_1, S_2, and S_3 respectively at the untwisted geometry) of DMABN calculated at the TD-PBE/cc-pVTZ level of theory.

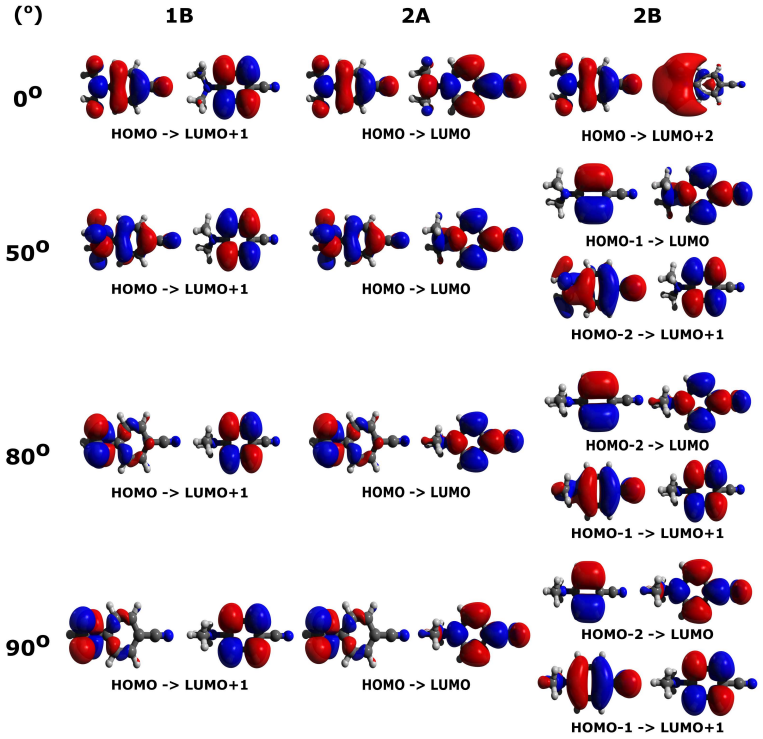


FIG. S3. PBE0 MOs participating in the transitions to the 1B, 2A, and 2B ES (S_1, S_2, and S_3 respectively at the untwisted geometry) of DMABN calculated at the TD-PBE0/cc-pVTZ level of theory.

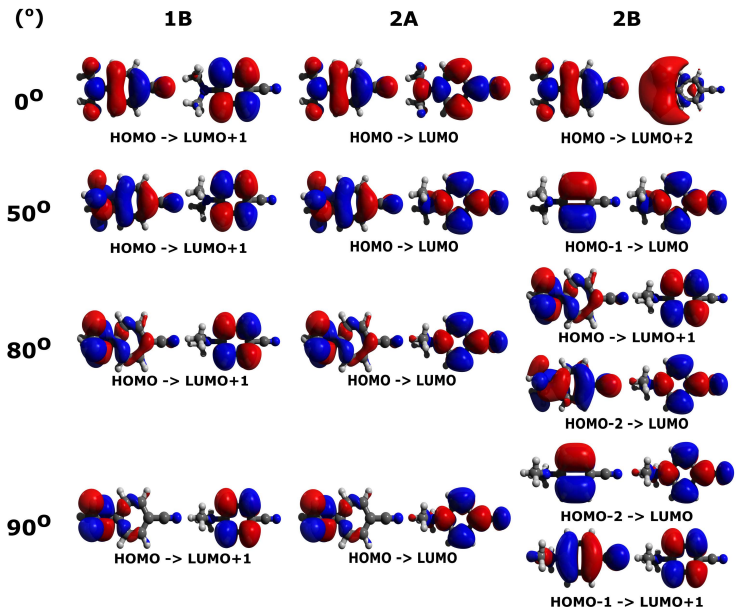


FIG. S4. PBEh MOs participating in the transitions to the 1B, 2A, and 2B ES (S_1, S_2, and S_3 respectively at the untwisted geometry) of DMABN calculated at the TD-PBEh/cc-pVTZ level of theory.

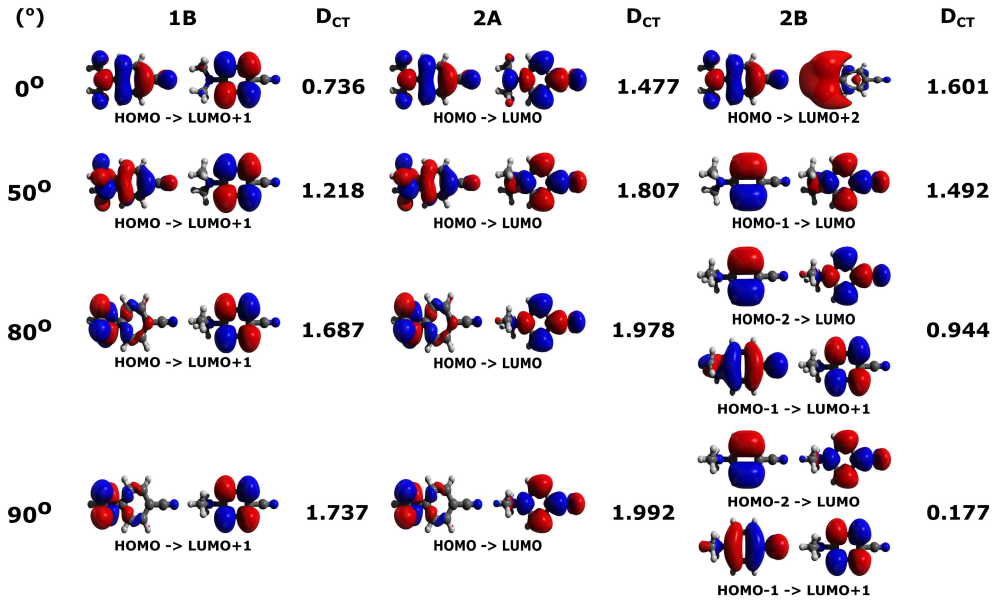


FIG. S5. CAM-B3LYP MOs participating in the transitions to the 1B, 2A, and 2B ES (S_1, S_2, and S_3 respectively at the untwisted geometry) of DMABN and D_{CT} values (in Å) calculated at the TD-CAM-B3LYP/cc-pVTZ level of theory.

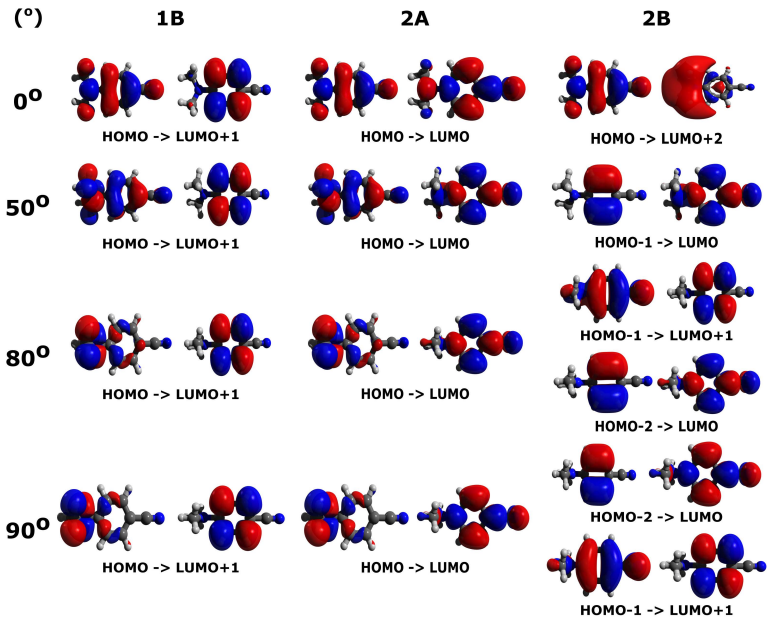


FIG. S6. PBE0 MOs participating in the transitions to the 1B, 2A, and 2B ES (S_1, S_2, and S_3 respectively at the untwisted geometry) of DMABN calculated at the BSE/evGW/PBE0/cc-pVTZ level of theory.

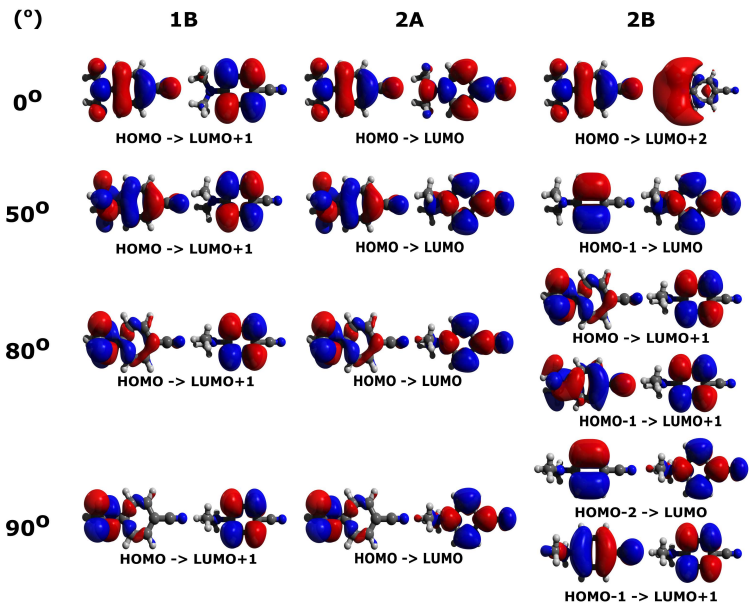
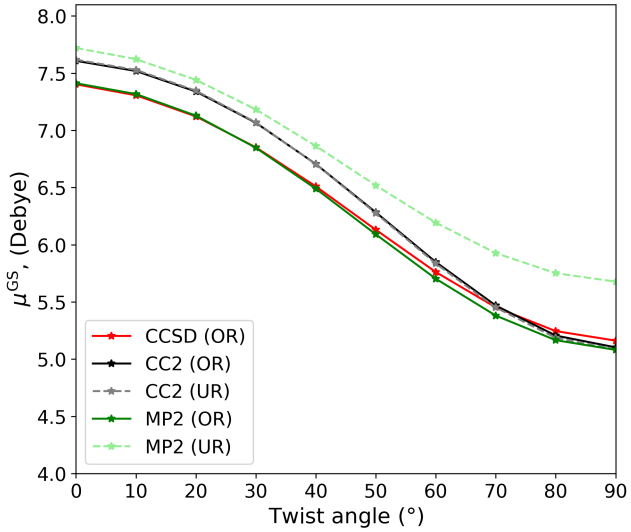
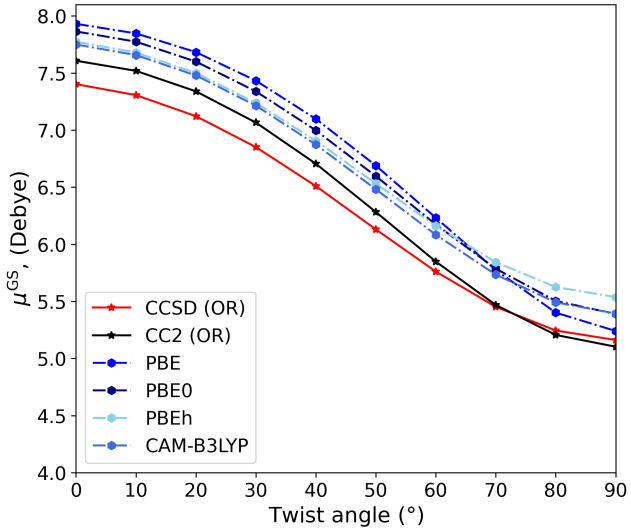


FIG. S7. PBEh MOs participating in the transitions to the 1B, 2A, and 2B ES (S_1, S_2, and S_3 respectively at the untwisted geometry) of DMABN calculated at the BSE/evGW/PBEh/cc-pVTZ level of theory.

S2.2. Ground-state dipoles



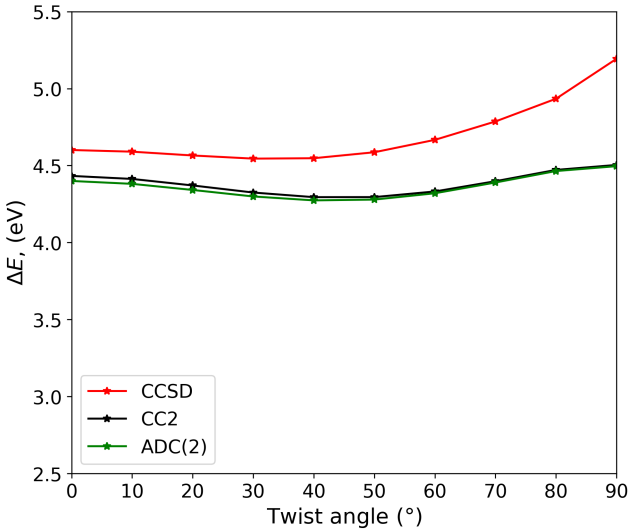
(a) Wave-function methods



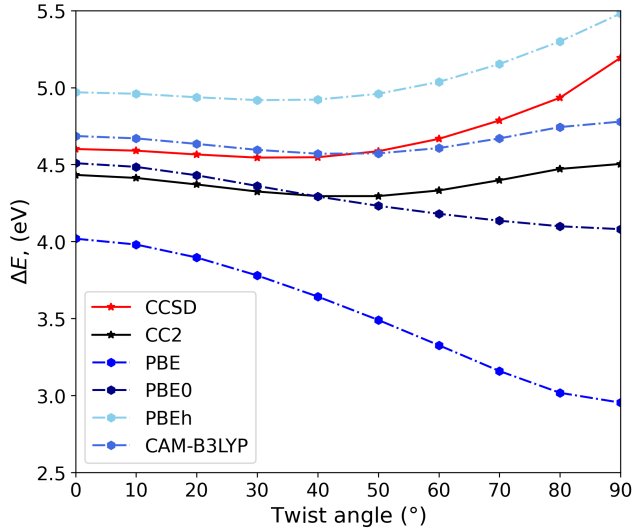
(b) TD-DFT

FIG. S8. Evolution of the μ^{GS} of DMABN with twist angle calculated with (a) wave-function methods (CCSD, CC2, and MP2) and (b) TD-DFT (PBE, PBE0, PBEh, and CAM-B3LYP functionals). OR (UR) stands for the relaxed (unrelaxed) approach used to compute the dipoles. All calculations are done using cc-pVTZ atomic basis set.

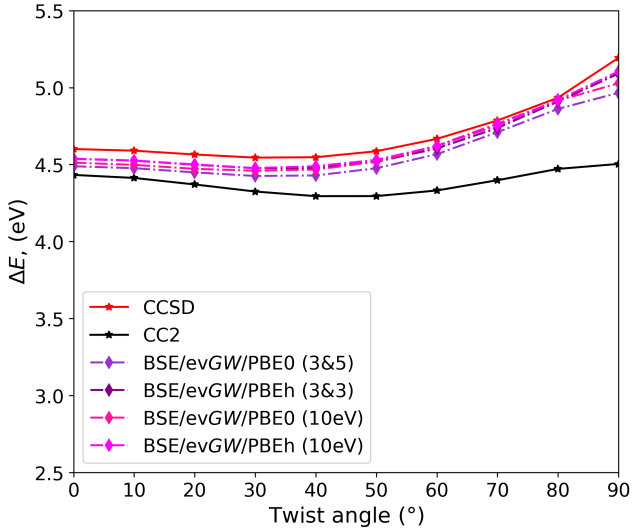
S2.3. Transition energies



(a) Wave-function methods

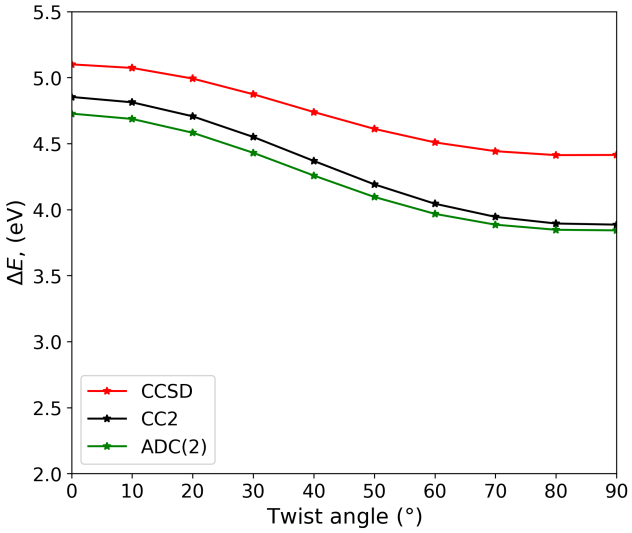


(b) TD-DFT

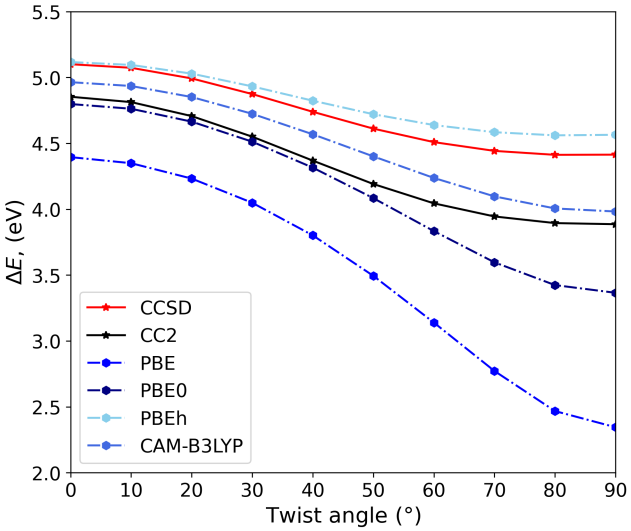


(c) BSE/evGW

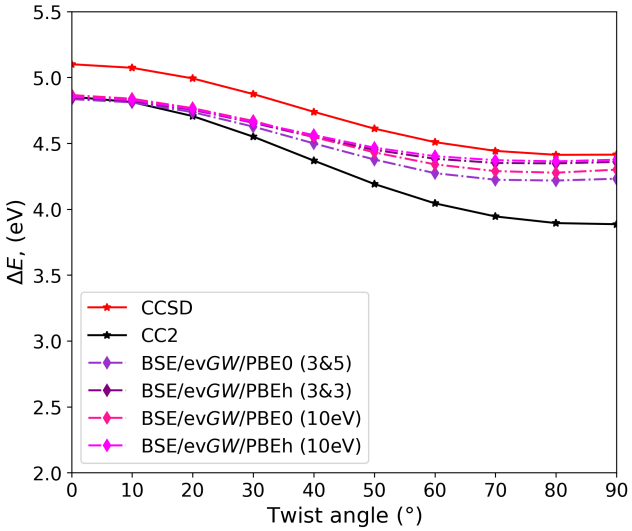
FIG. S9. Evolution of the ΔE of the **1B** ES of DMABN upon twisting calculated with the (a) wave-function methods [CCSD, CC2, and ADC(2)], (b) TD-DFT (PBE, PBE0, PBEh, and CAM-B3LYP functionals), and (c) BSE/evGW using PBE and PBEh as starting points. See the Section above for the explanation of the different correction schemes used at the GW level that are provided in the brackets. All calculations are done using cc-pVTZ atomic basis set.



(a) Wave-function methods

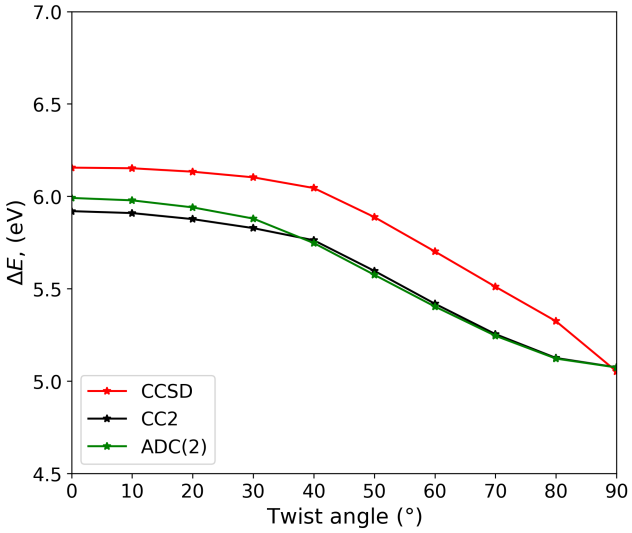


(b) TD-DFT

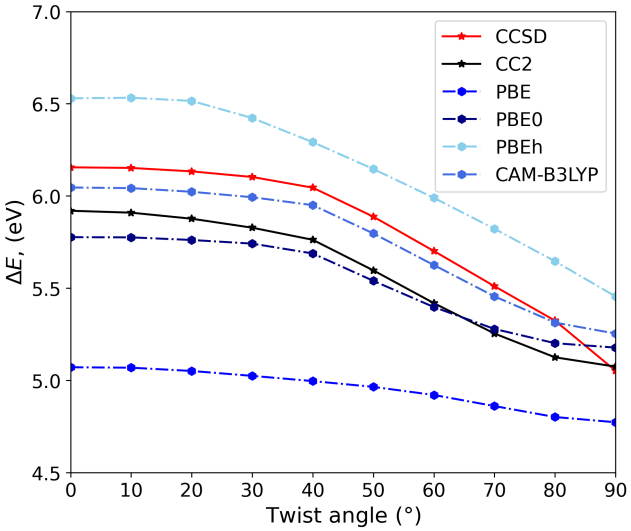


(c) BSE/evGW

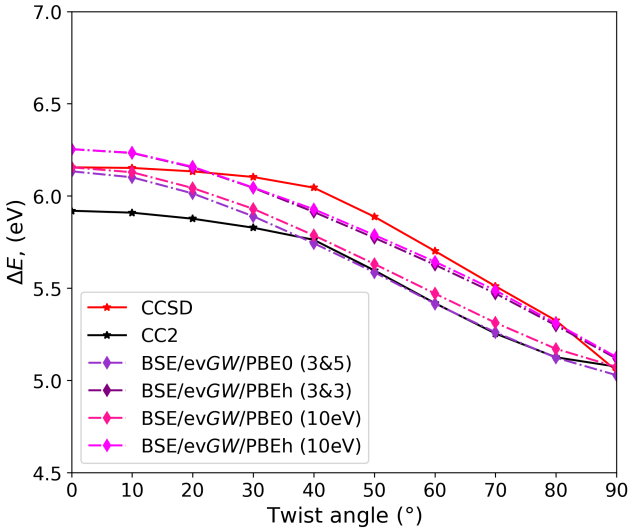
FIG. S10. Evolution of the ΔE of the **2A** ES of DMABN upon twisting obtained with (a) wave-function, (b) TD-DFT, and (c) BSE/evGW formalisms. See Figure S9 for more details.



(a) Wave-function methods



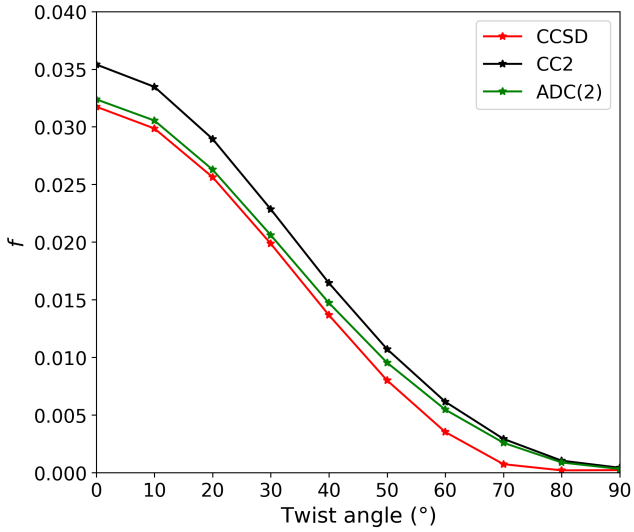
(b) TD-DFT



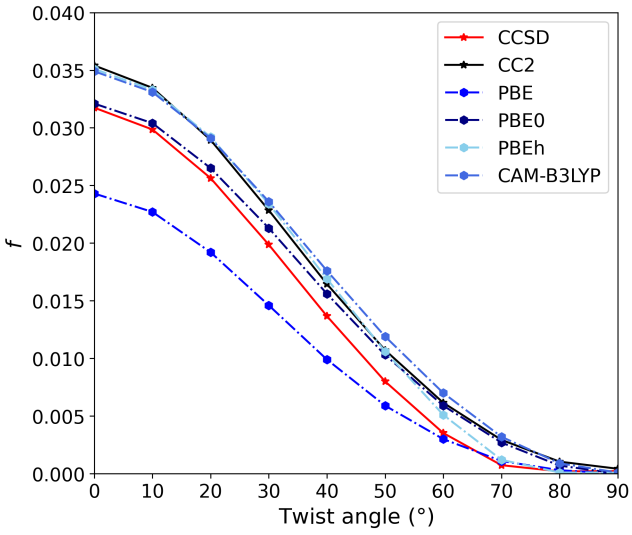
(c) BSE/evGW

FIG. S11. Evolution of the ΔE of the **2B** ES of DMABN upon twisting calculated with (a) wave-function, (b) TD-DFT, and (c) BSE/evGW formalisms. See Figure S9 for more details.

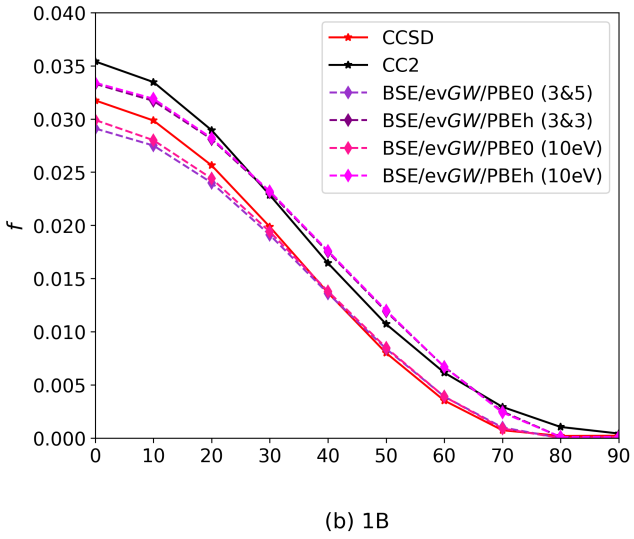
S2.4. Oscillator strength (f)



(a) Wave-function methods

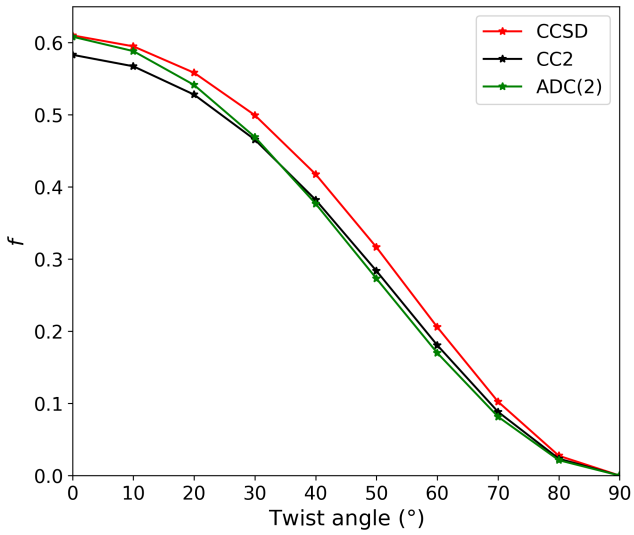


(b) TD-DFT

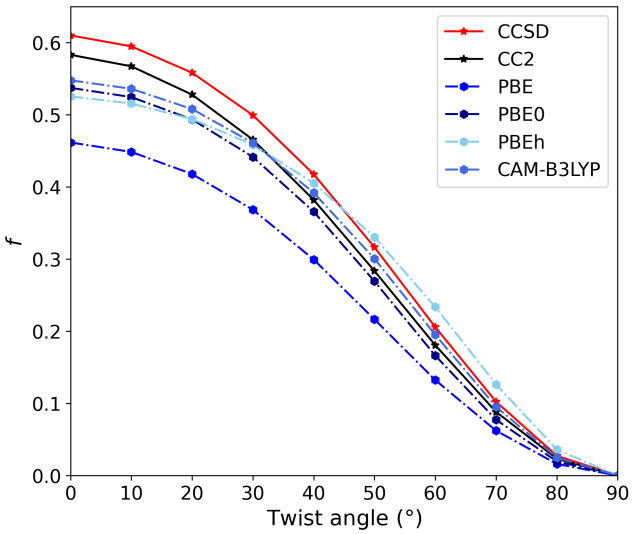


(c) BSE/evGW

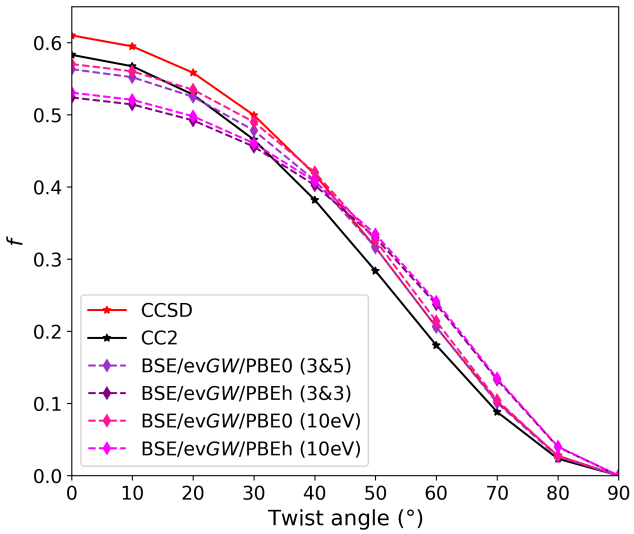
FIG. S12. Evolution of the f of the **1B** ES of DMABN upon twisting calculated with (a) wave-function, (b) TD-DFT, and (c) BSE/evGW formalisms. See Figure S9 for more details.



(a) Wave-function methods

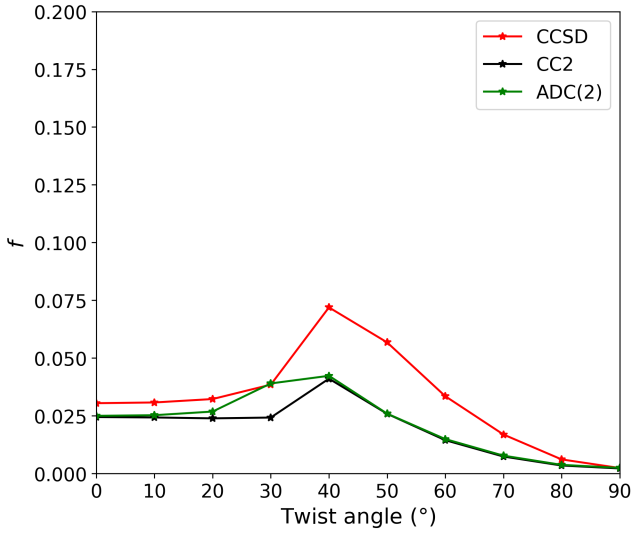


(b) TD-DFT

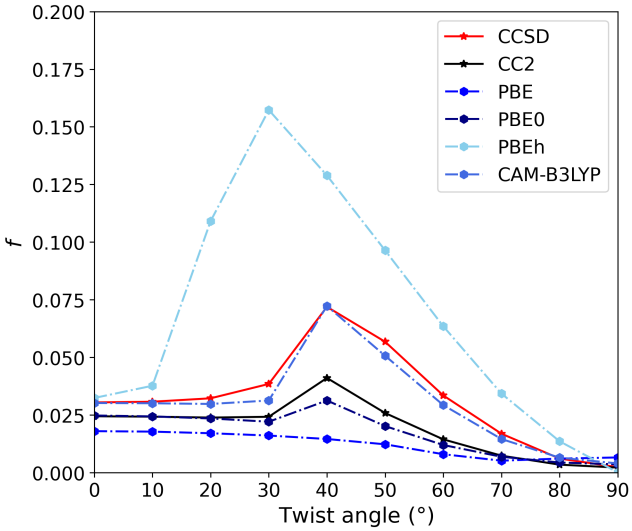


(c) BSE/evGW

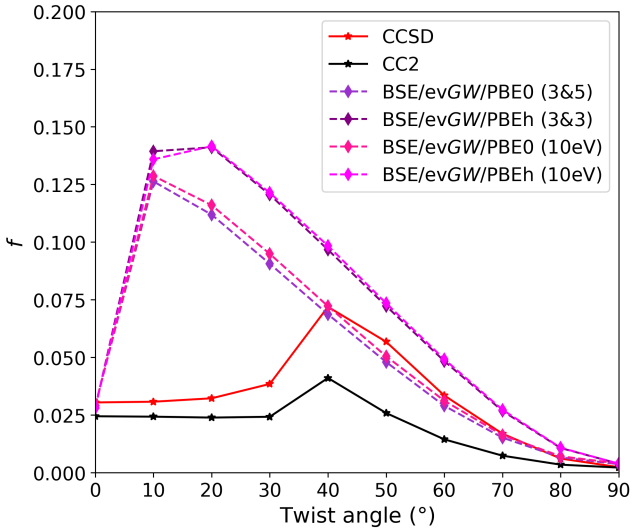
FIG. S13. Evolution of the f of the **2A** ES of DMABN upon twisting calculated with (a) wave-function, (b) TD-DFT, and (c) BSE/evGW formalisms. See Figure S9 for more details.



(a) Wave-function methods



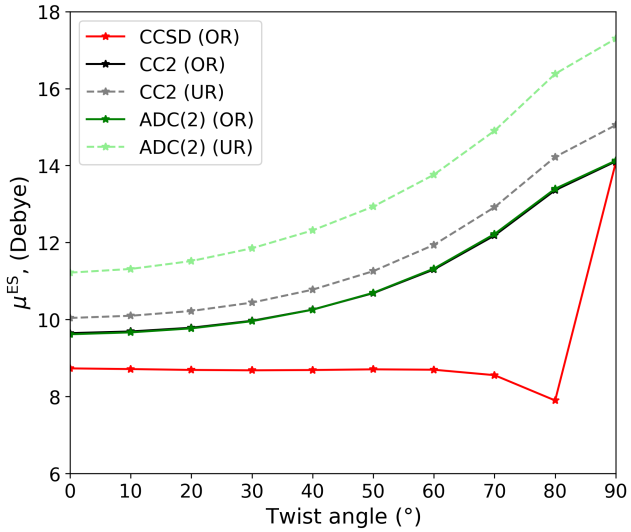
(b) TD-DFT



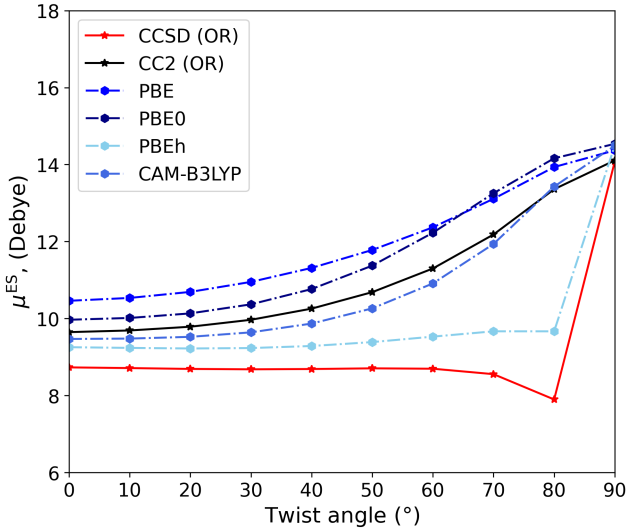
(c) BSE/evGW

FIG. S14. Evolution of the f of the **2B** ES of DMABN upon twisting calculated with (a) wave-function, (b) TD-DFT, and (c) BSE/evGW formalisms. See Figure S9 for more details.

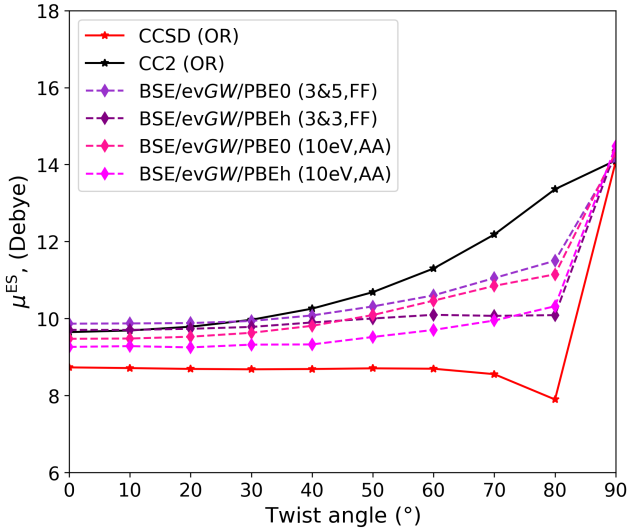
S2.5. Excited-state dipoles



(a) Wave-function methods

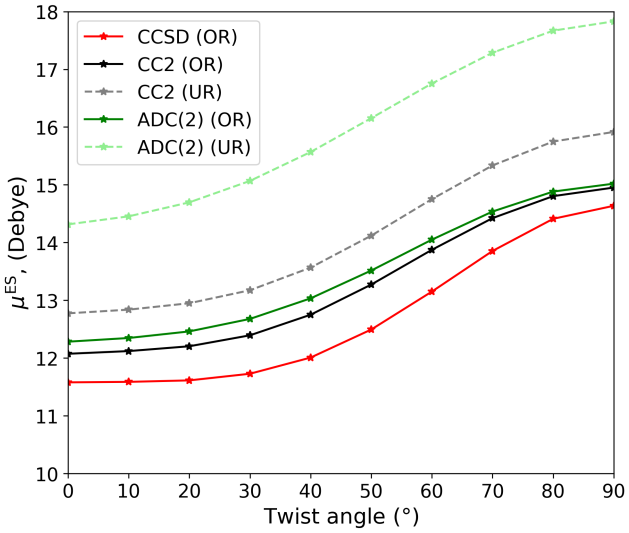


(b) TD-DFT

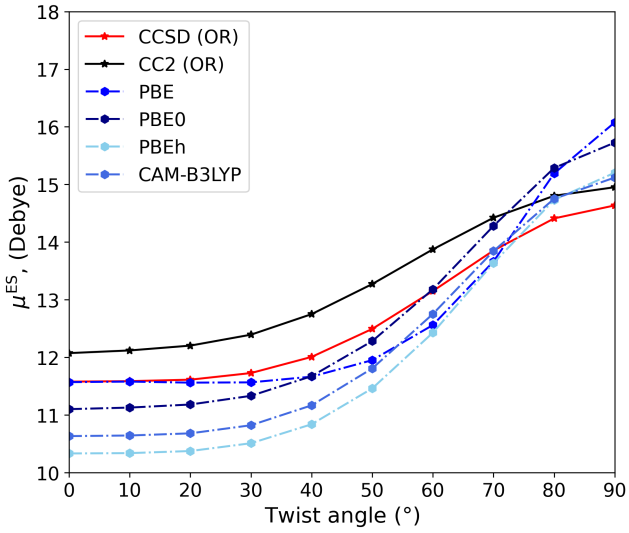


(c) BSE/evGW

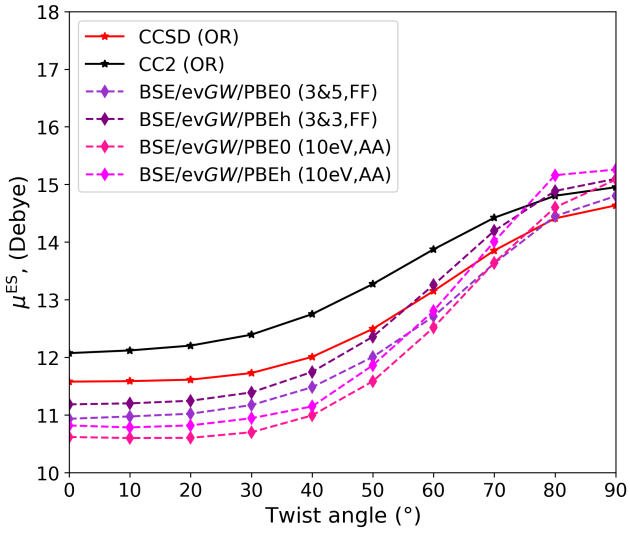
FIG. S15. Evolution of the μ^{ES} of the **1B** ES of DMABN upon twisting obtained using (a) wave-function, (b) TD-DFT, and (c) BSE/evGW formalisms. FF (AA) indicates that the dipole moments were calculated using the finite-field (approximate analytical gradients) approach. See Figure S9 for more details.



(a) Wave-function methods

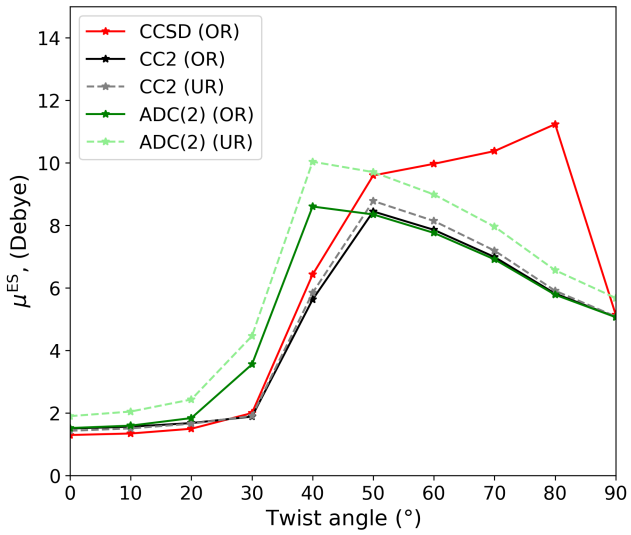


(b) TD-DFT

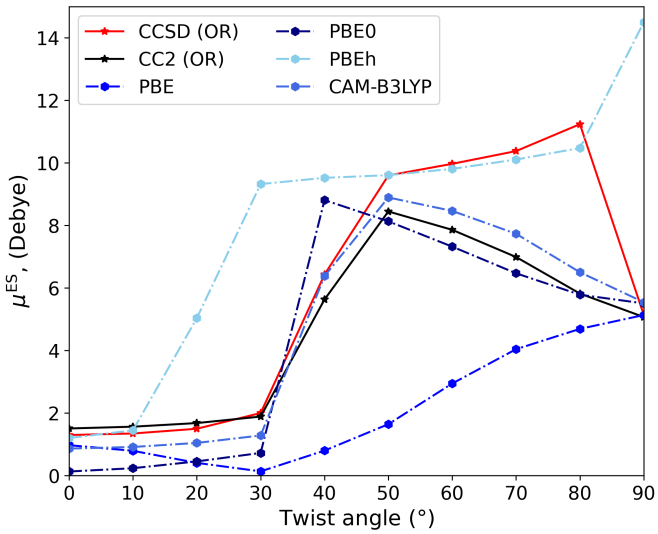


(c) BSE/evGW

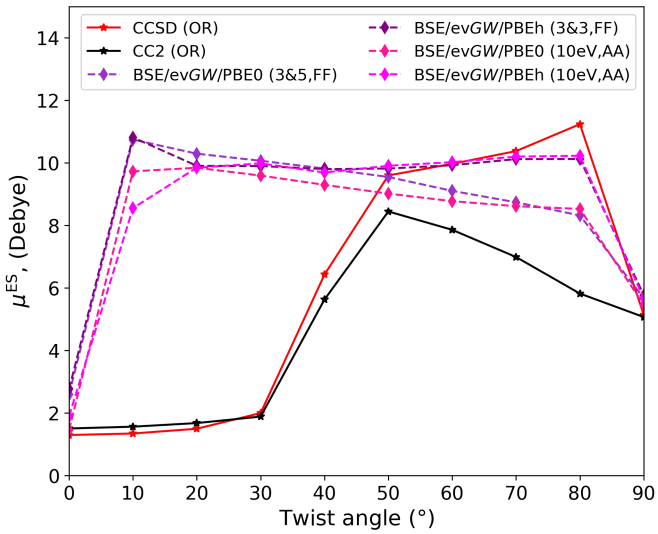
FIG. S16. Evolution of the μ^{ES} of the **2A** ES of DMABN upon twisting calculated with (a) wave-function, (b) TD-DFT, and (c) BSE/evGW formalisms. See Figure S15 for more details.



(a) Wave-function methods



(b) TD-DFT



(c) BSE/evGW

FIG. S17. Evolution of the μ^{ES} of the **2B** ES of DMABN upon twisting calculated with (a) wave-function, (b) TD-DFT, and (c) BSE/evGW formalisms. See Figure S15 for more details.

S2.6. Excess dipoles

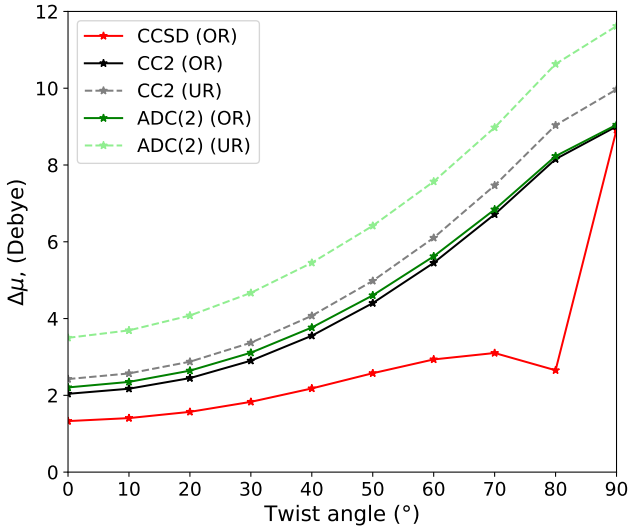


FIG. S18. Evolution of the $\Delta\mu$ of the **1B** ES of DMABN upon twisting obtained with the CCSD, CC2, and ADC(2) levels of theory. See Figure S15 for more details.

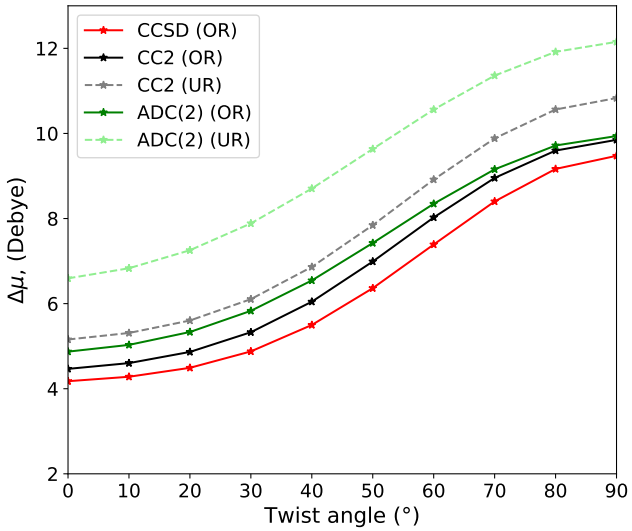
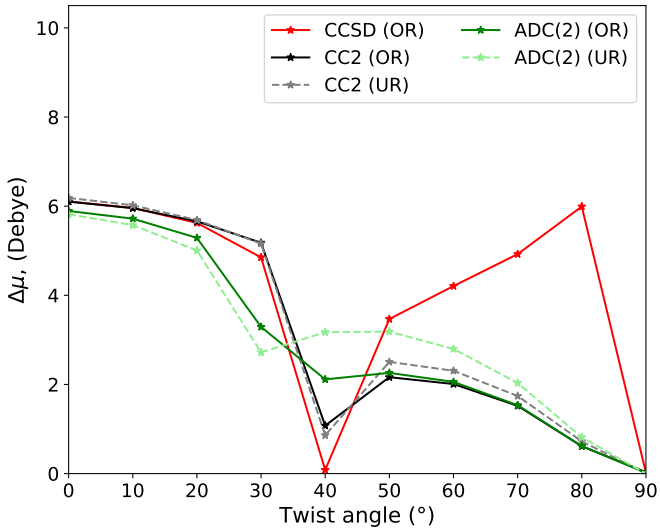
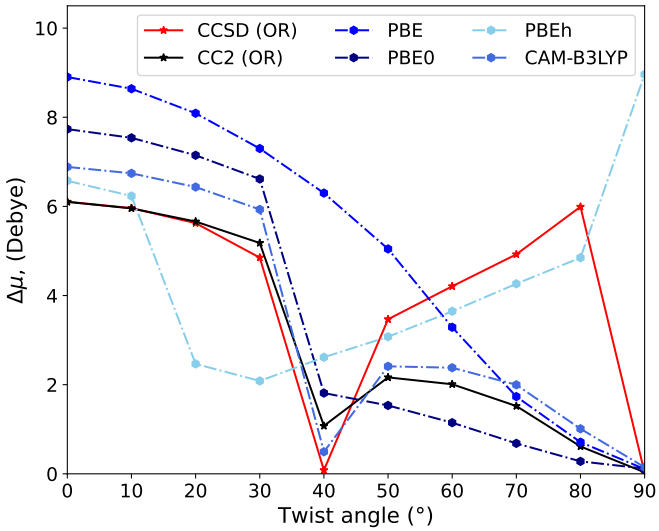


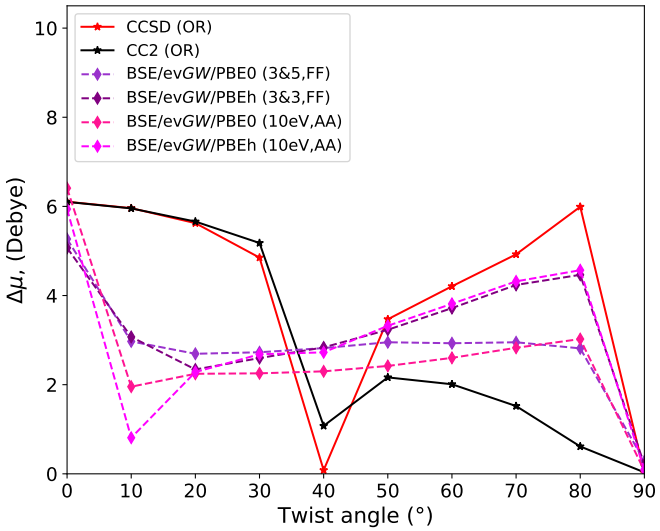
FIG. S19. Evolution of the $\Delta\mu$ of the **2A** ES of DMABN upon twisting obtained with the CCSD, CC2, and ADC(2) levels of theory. See Figure S15 for more details.



(a) Wave-function methods

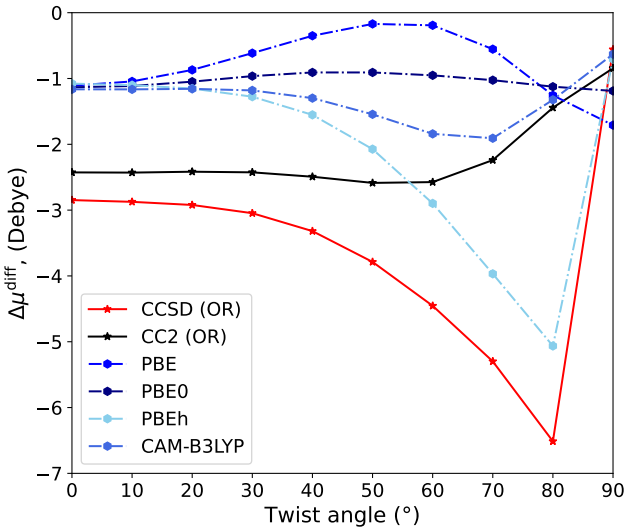


(b) TD-DFT

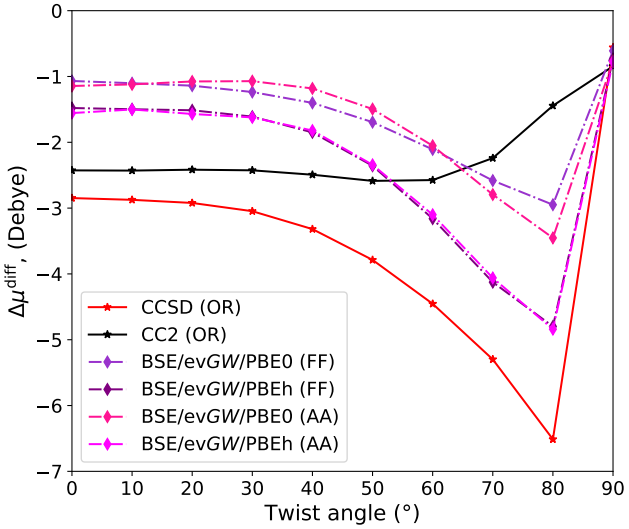


(c) BSE/evGW

FIG. S20. Evolution of the $\Delta\mu$ of the **2B** ES of DMABN upon twisting obtained with the (a) wave-function, (b) TD-DFT, and (c) BSE/evGW formalisms. See Figure S15 for more details.



(a) TD-DFT



(b) BSE/evGW

FIG. S21. Evolution of the differences in the total excess dipole moments between **1B** and **2A** states ($\Delta\mu^{\mathrm{diff}}$) obtained with (a) TD-DFT and (b) BSE/evGW methods compared to CCSD and CC2 results. See the caption of Figure S11 for more details.

S2.7. Energy differences between 2B and 1B ES

TABLE S2. The energy difference between **2B** and **1B** states (ΔE_{diff})[a] obtained at ADC(2), TD-DFT (PBE and CAM-B3LYP), and BSE/evGW/PBEh[b] levels of theory using the cc-pVTZ atomic basis set.

(°)	$\Delta E_{\text{diff}}^{\text{ADC(2)}}$	$\Delta E_{\text{diff}}^{\text{PBE}}$	$\Delta E_{\text{diff}}^{\text{CAM-B3LYP}}$	$\Delta E_{\text{diff}}^{\text{BSE/ev}GW\text{/PBEh}}$
0	1.59	1.05	1.36	1.72
10	1.60	1.09	1.37	1.71
20	1.60	1.15	1.39	1.66
30	1.58	1.25	1.40	1.57
40	1.47	1.35	1.38	1.44
50	1.30	1.47	1.22	1.26
60	1.08	1.58	1.02	1.02
70	0.86	1.59	0.79	0.73
80	0.66	1.60	0.57	0.39
90	0.58	1.61	0.48	0.03

[a] $\Delta E_{\text{diff}} = E_{\mathbf{2B}}^{\text{tot}}$ - $E_{\mathbf{1B}}^{\text{tot}}$.

[b] The results obtained with 3&3 correction scheme at evGW level.

S3. DYES

S3.1. Ground state dipoles

TABLE S3. GS dipole moments for the dyes obtained with wave-function (CCSD, CC2, and MP2) and TD-DFT (PBE, PBE0, PBEh, PBEα, M06-2X, CAM-B3LYP, and ωB97X-D) methods. OR (UR) stands for the relaxed (unrelaxed) approach used to calculate dipoles. All values are in Debye and have been obtained with the cc-pVTZ atomic basis set.

	CCSD (OR)	**CC2 (OR)**	**CC2 (UR)**	**MP2 (OR)**	**MP2 (UR)**	**PBE**	**PBE0**	**PBEh**	**PBEα**	**M06-2X**	**CAM-B3LYP**	**ωB97X-D**
1	4.56	4.53	4.47	4.52	5.01	4.87	4.89	4.94	5.02	4.84	4.83	4.80
2	4.24	3.95	3.88	4.04	4.55	3.93	4.16	4.39	4.49	4.30	4.32	4.30
3	9.51	8.25	8.29	8.81	10.59	7.13	8.27	9.43	9.79	9.08	9.16	9.31
4	4.54	4.59	4.50	4.42	5.09	4.98	5.00	5.05	5.11	4.90	4.94	4.92
5	1.83	2.00	2.03	1.95	1.73	1.95	1.89	1.80	1.80	1.85	1.84	1.85
6	1.98	1.92	1.90	1.81	2.23	1.76	1.93	2.07	2.12	2.02	1.99	2.02
7	2.05[a]	2.37	2.36	2.15	2.17	2.88	2.57	2.30	2.25	2.33	2.36	2.35
8	0.67[a]	0.91	0.82	0.72	0.83	1.32	1.10	0.94	0.85	0.85	0.90	0.87
9	9.09[a]	8.86	8.72	8.72	10.12	9.75	9.86	9.99	10.09	9.88	9.77	9.70
10	6.10[a]	5.90	5.68	5.76	7.14	6.02	6.37	6.74	6.93	6.42	6.49	6.47
11	1.81[a]	2.04	2.07	1.98	1.71	2.02	1.93	1.81	1.79	1.86	1.85	1.85
12	1.88[a]	1.88	1.83	1.98	1.89	1.83	1.87	1.89	1.92	1.87	1.90	1.89
13	4.71[a]	4.53	4.32	4.37	5.75	4.86	5.12	5.43	5.57	5.14	5.19	5.13
14	3.93[a]	4.60	4.67	4.34	3.67	4.47	4.16	3.79	3.74	3.95	3.95	3.95
15	0.26[a]	0.02	0.14	0.23	1.29	1.02	0.57	0.06	0.18	0.35	0.24	0.26
16	6.31[a]	6.79	6.75	6.45	6.69	7.22	7.07	6.88	6.94	6.91	6.84	6.81
17	8.61[a]	9.31	9.27	8.99	8.98	9.67	9.43	9.19	9.21	9.13	9.15	9.17
18	0.67[a]	0.60	0.59	0.59	0.88	0.70	0.71	0.77	0.80	0.65	0.68	0.70
19	2.06[a]	2.21	2.22	2.22	2.06	2.32	2.16	2.06	2.07	2.11	2.09	2.10
20	2.46[a]	2.61	2.59	2.63	2.35	2.66	2.59	2.48	2.50	2.55	2.56	2.53
21	2.68[a]	3.32	3.20	2.70	2.36	3.67	3.25	2.80	2.73	2.94	2.96	2.99
22	6.72[a]	7.63	7.61	7.01	7.20	8.71	7.98	7.48	7.49	7.43	7.36	7.32
23	3.33[a]	3.36	3.20	3.39	3.62	3.59	3.62	3.64	3.71	3.60	3.57	3.55
24	6.85[a]	6.10	6.08	6.49	7.68	6.87	6.93	7.03	7.33	7.00	6.84	6.76
25	3.75[a]	2.50	2.52	2.44	2.78	3.62	3.69	3.76	4.01	3.80	3.76	3.82

[a] Dipole moments were estimated using the following formula: $\mu_{\mathrm{CCSD}}^{\mathrm{cc-pVTZ}^*} = \mu_{\mathrm{CCSD}}^{\mathrm{cc-pVDZ}} + (\mu_{\mathrm{CC2}}^{\mathrm{cc-pVTZ}} - \mu_{\mathrm{CC2}}^{\mathrm{cc-pVDZ}})$

S3.2. Transition energies

TABLE S4. ES transition energies for the indicated ES of the dyes obtained with CCSD, CC2, and ADC(2) methods and the cc-pVTZ atomic basis set. Energies are in eV.

	State	CCSD	CC2	ADC(2)
1	$A\ (\pi \rightarrow \pi^*)$	4.334	4.117	4.101
2	$B_2\ (\pi \rightarrow \pi^*)$	2.904	2.915	2.791
3	$A_1\ (\pi \rightarrow \pi^*)$	3.028	2.550	2.405
	$B_1\ (\pi \rightarrow \pi^*)$	3.093	2.528	2.360
4	$A\ (\pi \rightarrow \pi^*)$	4.071	3.827	3.795
5	$A^{'}\ (\pi \rightarrow \pi^*)$	4.216	3.998	3.969
6	$A^{'}\ (\pi \rightarrow \pi^*)$	4.225	4.026	3.988
7	$A\ (\pi \rightarrow \pi^*)$		4.156	4.126
8	$A\ (\pi \rightarrow \pi^*)$		4.151	4.116
9	$A\ (\pi \rightarrow \pi^*)$		3.546	3.388
10	$A^{'}\ (\pi \rightarrow \pi^*)$		3.713	3.665
11	$A\ (\pi \rightarrow \pi^*)$		3.433	3.405
12	$A^{'}\ (\pi \rightarrow \pi^*)$		3.192	3.162
13	$A^{'}\ (\pi \rightarrow \pi^*)$		3.373	3.310
14	$A^{'}\ (\pi \rightarrow \pi^*)$		2.517	2.328
15	$B_2\ (\pi \rightarrow \pi^*)$		2.782	2.575
16	$A\ (\pi \rightarrow \pi^*)$		3.466	3.356
17	$A^{''}\ (\pi \rightarrow \pi^*)$		2.682	2.588
18	$A\ (\pi \rightarrow \pi^*)$		3.914	3.898
19	$A\ (\pi \rightarrow \pi^*)$		3.606	3.579
20	$A\ (\pi \rightarrow \pi^*)$		3.805	3.767
21	$A^{'}\ (\pi \rightarrow \pi^*)$		2.259	2.125
22	$A\ (\pi \rightarrow \pi^*)$		3.280	3.227
23	$A\ (n \rightarrow \pi^*)$		3.017	2.833
	$B\ (\pi \rightarrow \pi^*)$		3.556	3.553
24	$A\ (\pi \rightarrow \pi^*)$		2.153	1.901
25	$B_2\ (\pi \rightarrow \pi^*)$		2.117	1.886

TABLE S5. ES transition energies for the dyes obtained with TD-DFT using PBE, PBE0, PBEh, M06-2X, CAM-B3LYP, and ωB97X-D functionals.[a]

	State	PBE	PBE0	PBEh	M06-2X	CAM-B3LYP	ωB97X-D
1	A ($\pi \rightarrow \pi^*$)	3.241	3.840	4.400	4.212	4.131	4.137
2	B_2 ($\pi \rightarrow \pi^*$)	2.988	3.150	3.187	3.099	3.109	3.111
3	A_1 ($\pi \rightarrow \pi^*$)	2.567	2.590	2.930	2.922	2.882	2.979
	B_1 ($\pi \rightarrow \pi^*$)	1.572	2.142	2.911	2.800	2.755	2.892
4	A ($\pi \rightarrow \pi^*$)	3.066	3.412	3.668	3.651	3.612	3.650
5	$A^{'}$ ($\pi \rightarrow \pi^*$)	3.553	4.028	4.482	4.295	4.272	4.290
6	$A^{'}$ ($\pi \rightarrow \pi^*$)	3.026	3.512	3.832	3.800	3.764	3.796
7	A ($\pi \rightarrow \pi^*$)	3.337	3.790	4.138	4.052	4.040	4.090
8	A ($\pi \rightarrow \pi^*$)	3.408	3.766	4.041	4.007	3.959	3.996
9	A ($\pi \rightarrow \pi^*$)	2.941	3.323	3.653	3.549	3.514	3.523
10	$A^{'}$ ($\pi \rightarrow \pi^*$)	2.838	3.349	3.820	3.747	3.713	3.749
11	A ($\pi \rightarrow \pi^*$)	2.892	3.376	3.836	3.685	3.683	3.717
12	$A^{'}$ ($\pi \rightarrow \pi^*$)	2.643	2.965	3.264	3.229	3.207	3.242
13	$A^{'}$ ($\pi \rightarrow \pi^*$)	2.673	3.109	3.464	3.397	3.381	3.417
14	$A^{'}$ ($\pi \rightarrow \pi^*$)	2.421	2.669	2.851	2.773	2.755	2.759
15	B_2 ($\pi \rightarrow \pi^*$)	2.717	3.004	3.273	3.109	3.126	3.136
16	A ($\pi \rightarrow \pi^*$)	2.913	3.459	3.957	3.778	3.772	3.818
17	$A^{''}$ ($\pi \rightarrow \pi^*$)	1.814	2.501	3.161	3.046	3.016	3.060
18	A ($\pi \rightarrow \pi^*$)	2.888	3.415	3.772	3.743	3.720	3.768
19	A ($\pi \rightarrow \pi^*$)	2.778	3.238	3.595	3.542	3.542	3.606
20	A ($\pi \rightarrow \pi^*$)	2.883	3.547	4.133	3.951	3.965	4.036
21	A ($\pi \rightarrow \pi^*$)	1.977	2.295	2.667	2.514	2.513	2.521
22	A ($\pi \rightarrow \pi^*$)	2.137	2.942	3.766	3.576	3.639	3.797
23	A ($n \rightarrow \pi^*$)	2.128	2.866	3.541	3.106	3.216	3.186
	B ($\pi \rightarrow \pi^*$)	2.477	3.011	3.490	3.392	3.393	3.448
24	A ($\pi \rightarrow \pi^*$)	2.120	2.424	2.706	2.570	2.587	2.614
25	B_2 ($\pi \rightarrow \pi^*$)	2.254	2.387	2.508	2.371	2.400	2.394

[a] See caption of Table S4 for more info.

TABLE S6. ES transition energies for the dyes obtained with BSE/evGW formalisms using PBE0, PBEh, and PBEα starting points.[a]

	State	BSE/evGW/PBE0 (5&5)	BSE/evGW/PBE0 (10eV)	BSE/evGW/PBEh (10eV)	BSE/evGW/PBEα (10eV)
1	A $(\pi \rightarrow \pi^*)$	4.004	4.010	4.080	4.111
2	B_2 $(\pi \rightarrow \pi^*)$	2.789	2.774	2.797	2.806
3	A_1 $(\pi \rightarrow \pi^*)$	2.625	2.621	2.572	2.563
	B_1 $(\pi \rightarrow \pi^*)$	2.490	2.485	2.526	2.557
4	A $(\pi \rightarrow \pi^*)$	3.545	3.546	3.602	3.626
5	$A^{'}$ $(\pi \rightarrow \pi^*)$	3.974	3.989	4.059	4.116
6	$A^{'}$ $(\pi \rightarrow \pi^*)$	3.690	3.696	3.775	3.818
7	A $(\pi \rightarrow \pi^*)$	3.947	3.963	4.007	4.036
8	A $(\pi \rightarrow \pi^*)$	3.856	3.873	3.931	3.949
9	A $(\pi \rightarrow \pi^*)$	3.284	3.277	2.774	3.340
10	$A^{'}$ $(\pi \rightarrow \pi^*)$	3.469	3.475	3.556	3.592
11	A $(\pi \rightarrow \pi^*)$	3.390	3.408	3.488	3.549
12	$A^{'}$ $(\pi \rightarrow \pi^*)$	2.916	2.928	2.998	3.040
13	$A^{'}$ $(\pi \rightarrow \pi^*)$	3.118	3.137	3.190	3.226
14	$A^{'}$ $(\pi \rightarrow \pi^*)$	2.435	2.437	2.456	2.453
15	B_2 $(\pi \rightarrow \pi^*)$	2.841	2.850	2.824	2.820
16	A $(\pi \rightarrow \pi^*)$	3.599	3.652	3.617	3.621
17	$A^{''}$ $(\pi \rightarrow \pi^*)$	2.780	2.777	2.813	2.844
18	A $(\pi \rightarrow \pi^*)$	3.651	3.657	3.736	3.764
19	A $(\pi \rightarrow \pi^*)$	3.426	3.432	3.474	3.499
20	A $(\pi \rightarrow \pi^*)$	3.897	3.920	3.991	4.002
21	A $(\pi \rightarrow \pi^*)$	2.234	2.249	2.263	2.278
22	A $(\pi \rightarrow \pi^*)$	3.555	3.576	3.504	3.492
23	A $(n \rightarrow \pi^*)$	3.056	3.064	3.243	3.421
	B $(\pi \rightarrow \pi^*)$	3.354	3.357	3.459	3.502
24	A $(\pi \rightarrow \pi^*)$	2.277	2.311	2.278	2.281
25	B_2 $(\pi \rightarrow \pi^*)$	2.139	2.143	2.139	2.145

[a] See caption of Table S4 for more info.

S3.3. Oscillator strengths

TABLE S7. Oscillator strengths for the considered transitions obtained with CCSD, CC2, and ADC(2) methods and the cc-pVTZ atomic basis set. All values in a.u.

	State	CCSD	CC2	ADC(2)
1	$A\ (\pi \rightarrow \pi^*)$	0.045	0.057	0.061
2	$B_2\ (\pi \rightarrow \pi^*)$	0.545	0.422	0.433
3	$A_1\ (\pi \rightarrow \pi^*)$	0.471	0.466	0.328
	$B_1\ (\pi \rightarrow \pi^*)$	0.007	0.006	0.005
4	$A\ (\pi \rightarrow \pi^*)$	0.887	0.803	0.850
5	$A^{'}\ (\pi \rightarrow \pi^*)$	0.035	0.038	0.035
6	$A^{'}\ (\pi \rightarrow \pi^*)$	0.575	0.617	0.626
7	$A\ (\pi \rightarrow \pi^*)$		0.896	0.971
8	$A\ (\pi \rightarrow \pi^*)$		0.642	0.691
9	$A\ (\pi \rightarrow \pi^*)$		0.393	0.457
10	$A^{'}\ (\pi \rightarrow \pi^*)$		0.293	0.307
11	$A\ (\pi \rightarrow \pi^*)$		0.041	0.034
12	$A^{'}\ (\pi \rightarrow \pi^*)$		0.362	0.364
13	$A^{'}\ (\pi \rightarrow \pi^*)$		0.279	0.293
14	$A^{'}\ (\pi \rightarrow \pi^*)$		0.709	0.782
15	$B_2\ (\pi \rightarrow \pi^*)$		0.843	0.906
16	$A\ (\pi \rightarrow \pi^*)$		0.404	0.402
17	$A^{''}\ (\pi \rightarrow \pi^*)$		0.080	0.081
18	$A\ (\pi \rightarrow \pi^*)$		0.464	0.494
19	$A\ (\pi \rightarrow \pi^*)$		1.265	1.273
20	$A\ (\pi \rightarrow \pi^*)$		0.620	0.620
21	$A^{'}\ (\pi \rightarrow \pi^*)$		0.204	0.191
22	$A\ (\pi \rightarrow \pi^*)$		0.893	0.881
23	$A\ (n \rightarrow \pi^*)$		0.000	0.000
	$B\ (\pi \rightarrow \pi^*)$		1.998	2.159
24	$A\ (\pi \rightarrow \pi^*)$		0.770	0.764
25	$B_2\ (\pi \rightarrow \pi^*)$		1.463	1.641

TABLE S8. Oscillator strengths for the considered transitions of the dyes determined with TD-DFT using PBE, PBE0, PBEh, M06-2X, CAM-B3LYP, and ωB97X-D functionals.[a]

	State	PBE	PBE0	PBEh	M06-2X	CAM-B3LYP	ωB97X-D
1	$A\ (\pi \rightarrow \pi^*)$	0.046	0.065	0.083	0.061	0.068	0.065
2	$B_2\ (\pi \rightarrow \pi^*)$	0.153	0.425	0.552	0.493	0.500	0.509
3	$A_1\ (\pi \rightarrow \pi^*)$	0.408	0.387	0.444	0.438	0.426	0.440
	$B_1\ (\pi \rightarrow \pi^*)$	0.001	0.003	0.007	0.006	0.006	0.006
4	$A\ (\pi \rightarrow \pi^*)$	0.644	0.801	0.856	0.818	0.820	0.828
5	$A^{'}\ (\pi \rightarrow \pi^*)$	0.021	0.033	0.043	0.041	0.039	0.039
6	$A^{'}\ (\pi \rightarrow \pi^*)$	0.335	0.648	0.707	0.692	0.683	0.681
7	$A\ (\pi \rightarrow \pi^*)$	0.717	0.950	1.027	0.994	0.982	0.997
8	$A\ (\pi \rightarrow \pi^*)$	0.435	0.623	0.650	0.633	0.636	0.642
9	$A\ (\pi \rightarrow \pi^*)$	0.202	0.316	0.411	0.403	0.386	0.383
10	$A^{'}\ (\pi \rightarrow \pi^*)$	0.161	0.216	0.384	0.352	0.358	0.369
11	$A\ (\pi \rightarrow \pi^*)$	0.019	0.035	0.058	0.047	0.048	0.049
12	$A^{'}\ (\pi \rightarrow \pi^*)$	0.274	0.356	0.441	0.416	0.418	0.425
13	$A^{'}\ (\pi \rightarrow \pi^*)$	0.108	0.267	0.370	0.337	0.342	0.353
14	$A^{'}\ (\pi \rightarrow \pi^*)$	0.425	0.668	0.863	0.811	0.795	0.804
15	$B_2\ (\pi \rightarrow \pi^*)$	0.594	0.784	0.950	0.891	0.877	0.878
16	$A\ (\pi \rightarrow \pi^*)$	0.210	0.349	0.468	0.440	0.428	0.432
17	$A^{''}\ (\pi \rightarrow \pi^*)$	0.024	0.069	0.172	0.139	0.141	0.153
18	$A\ (\pi \rightarrow \pi^*)$	0.148	0.409	0.519	0.480	0.490	0.501
19	$A\ (\pi \rightarrow \pi^*)$	0.855	1.228	1.411	1.336	1.346	1.370
20	$A\ (\pi \rightarrow \pi^*)$	0.359	0.558	0.709	0.662	0.670	0.689
21	$A\ (\pi \rightarrow \pi^*)$	0.154	0.207	0.265	0.242	0.245	0.247
22	$A\ (\pi \rightarrow \pi^*)$	0.417	0.670	1.116	1.019	1.072	1.186
23	$A\ (n \rightarrow \pi^*)$	0.000	0.000	0.000	0.000	0.000	0.000
	$B\ (\pi \rightarrow \pi^*)$	1.107	1.743	2.297	2.085	2.147	2.209
24	$A\ (\pi \rightarrow \pi^*)$	0.464	0.722	0.982	0.900	0.895	0.906
25	$B_2\ (\pi \rightarrow \pi^*)$	1.250	1.463	1.629	1.519	1.544	1.551

[a] See caption of Table S7 for more info.

TABLE S9. Oscillator strengths for the considered transitions of the dyes obtained with BSE/evGW formalisms using PBE0, PBEh, and PBEα starting points.[a]

	State	BSE/evGW/PBE0 (5&5)	BSE/evGW/PBE0 (10eV)	BSE/evGW/PBEh (10eV)	BSE/evGW/PBEα (10eV)
1	A ($\pi \rightarrow \pi^*$)	0.055	0.055	0.062	0.064
2	B_2 ($\pi \rightarrow \pi^*$)	0.409	0.404	0.420	0.426
3	A_1 ($\pi \rightarrow \pi^*$)	0.466	0.464	0.385	0.352
	B_1 ($\pi \rightarrow \pi^*$)	0.004	0.004	0.005	0.005
4	A ($\pi \rightarrow \pi^*$)	0.876	0.880	0.820	0.796
5	$A^{'}$ ($\pi \rightarrow \pi^*$)	0.033	0.033	0.037	0.038
6	$A^{'}$ ($\pi \rightarrow \pi^*$)	0.717	0.733	0.688	0.668
7	A ($\pi \rightarrow \pi^*$)	1.004	1.013	0.962	0.935
8	A ($\pi \rightarrow \pi^*$)	0.663	0.672	0.620	0.596
9	A ($\pi \rightarrow \pi^*$)	0.324	0.322	0.314	0.310
10	$A^{'}$ ($\pi \rightarrow \pi^*$)	0.313	0.316	0.326	0.327
11	A ($\pi \rightarrow \pi^*$)	0.039	0.039	0.045	0.049
12	$A^{'}$ ($\pi \rightarrow \pi^*$)	0.362	0.364	0.360	0.359
13	$A^{'}$ ($\pi \rightarrow \pi^*$)	0.295	0.298	0.301	0.303
14	$A^{'}$ ($\pi \rightarrow \pi^*$)	0.665	0.667	0.664	0.655
15	B_2 ($\pi \rightarrow \pi^*$)	0.798	0.803	0.754	0.741
16	A ($\pi \rightarrow \pi^*$)	0.402	0.416	0.397	0.394
17	$A^{''}$ ($\pi \rightarrow \pi^*$)	0.098	0.097	0.126	0.137
18	A ($\pi \rightarrow \pi^*$)	0.523	0.529	0.513	0.506
19	A ($\pi \rightarrow \pi^*$)	1.435	1.440	1.324	1.287
20	A ($\pi \rightarrow \pi^*$)	0.736	0.752	0.720	0.706
21	A ($\pi \rightarrow \pi^*$)	0.211	0.212	0.198	0.193
22	A ($\pi \rightarrow \pi^*$)	1.249	1.258	1.078	1.049
23	A ($n \rightarrow \pi^*$)	0.000	0.000	0.000	0.000
	B ($\pi \rightarrow \pi^*$)	2.415	2.423	2.217	2.148
24	A ($\pi \rightarrow \pi^*$)	0.761	0.780	0.753	0.750
25	B_2 ($\pi \rightarrow \pi^*$)	1.348	1.353	1.248	1.277

[a] See caption of Table S7 for more info.

S3.4. Excited-state dipoles

TABLE S10. ES dipole moments (in Debye) obtained with CCSD, CC2, and ADC(2) methods and the cc-pVTZ atomic basis set. OR (UR) stands for the relaxed (unrelaxed) approach used to calculate dipoles.

	State	CCSD (OR)	CC2 (OR)	CC2 (UR)	ADC(2) (OR)	ADC(2) (UR)
1	A ($\pi \rightarrow \pi^*$)	7.26	8.36	8.89	8.25	10.22
2	B_2 ($\pi \rightarrow \pi^*$)	3.89	3.77	3.44	3.81	3.28
3	A_1 ($\pi \rightarrow \pi^*$)	1.78	4.15	5.27	4.83	7.98
	B_1 ($\pi \rightarrow \pi^*$)	3.34	5.43	7.02	5.46	8.47
4	A ($\pi \rightarrow \pi^*$)	7.61	8.67	8.98	8.52	9.61
5	$A^{'}$ ($\pi \rightarrow \pi^*$)	2.52	2.96	3.24	3.02	3.88
6	$A^{'}$ ($\pi \rightarrow \pi^*$)	1.35	0.80	1.20	0.41	1.59
7	A ($\pi \rightarrow \pi^*$)	3.83[a]	7.15	7.53	7.05	7.90
8	A ($\pi \rightarrow \pi^*$)	5.42[a]	6.35	6.72	6.24	6.58
9	A ($\pi \rightarrow \pi^*$)	13.46[a]	12.91	13.07	13.21	13.96
10	$A^{'}$ ($\pi \rightarrow \pi^*$)	5.44[a]	4.80	4.65	4.53	5.03
11	A ($\pi \rightarrow \pi^*$)	3.03[a]	3.83	4.24	3.86	5.06
12	$A^{'}$ ($\pi \rightarrow \pi^*$)	2.17[a]	2.13	2.15	2.10	2.31
13	$A^{'}$ ($\pi \rightarrow \pi^*$)	6.09[a]	6.13	6.06	5.58	5.64
14	$A^{'}$ ($\pi \rightarrow \pi^*$)	5.04[a]	5.42	6.08	5.54	7.15
15	B_2 ($\pi \rightarrow \pi^*$)	1.55[a]	1.31	1.92	1.29	1.94
16	A ($\pi \rightarrow \pi^*$)	12.28[a]	14.53	15.82	14.82	18.63
17	$A^{''}$ ($\pi \rightarrow \pi^*$)	16.80[a]	18.80	20.26	18.95	23.19
18	A ($\pi \rightarrow \pi^*$)	0.60[a]	1.42	1.50	0.95	1.26
19	A ($\pi \rightarrow \pi^*$)	6.80[a]	9.45	10.16	9.24	11.26
20	A ($\pi \rightarrow \pi^*$)	8.45[a]	11.02	11.76	11.36	12.91
21	$A^{'}$ ($\pi \rightarrow \pi^*$)	5.49[a]	6.21	6.92	6.54	8.63
22	A ($\pi \rightarrow \pi^*$)	23.85[a]	29.25	30.71	28.79	31.90
23	A ($n \rightarrow \pi^*$)	1.91[a]	1.63	0.95	1.55	0.05
	B ($\pi \rightarrow \pi^*$)	4.54[a]	4.76	4.76	4.79	5.35
24	A ($\pi \rightarrow \pi^*$)	7.45[a]	5.23	5.35	5.05	6.92
25	B_2 ($\pi \rightarrow \pi^*$)	3.85[a]	2.73	2.71	2.64	2.85

[a] Dipole moments were calculated using the following formula: $\mu_{\mathrm{CCSD}}^{\mathrm{cc-pVTZ}^*} = \mu_{\mathrm{CCSD}}^{\mathrm{cc-pVDZ}} + (\mu_{\mathrm{CC2}}^{\mathrm{cc-pVTZ}} - \mu_{\mathrm{CC2}}^{\mathrm{cc-pVDZ}})$

TABLE S11. ES dipole moments (in Debye) for the dyes calculated at TD-PBE, TD-PBE0, TD-PBEh, TD-M06-2X, TD-CAM-B3LYP, and TD-ωB97X-D levels of theory with the cc-pVTZ atomic basis set.

	State	PBE	PBE0	PBEh	M06-2X	CAM-B3LYP	ωB97X-D
1	A ($\pi \rightarrow \pi^*$)	9.45	9.39	8.67	7.80	8.74	8.63
2	B_2 ($\pi \rightarrow \pi^*$)	3.72	3.90	3.96	3.94	3.94	3.90
3	A_1 ($\pi \rightarrow \pi^*$)	2.89	2.44	0.32	0.46	0.40	0.12
	B_1 ($\pi \rightarrow \pi^*$)	0.43	1.78	3.06	2.99	2.78	2.58
4	A ($\pi \rightarrow \pi^*$)	9.70	7.70	6.71	7.06	6.79	6.60
5	$A^{'}$ ($\pi \rightarrow \pi^*$)	3.10	3.01	2.77	2.84	2.84	2.86
6	$A^{'}$ ($\pi \rightarrow \pi^*$)	7.41	2.43	0.78	0.67	0.61	0.69
7	A ($\pi \rightarrow \pi^*$)	10.78	7.45	5.09	5.86	5.51	5.24
8	A ($\pi \rightarrow \pi^*$)	5.82	5.37	3.88	4.51	4.17	3.91
9	A ($\pi \rightarrow \pi^*$)	12.03	12.11	12.14	12.45	12.19	12.12
10	$A^{'}$ ($\pi \rightarrow \pi^*$)	4.09	3.98	5.38	5.25	5.38	5.55
11	A ($\pi \rightarrow \pi^*$)	4.11	3.74	3.25	3.52	3.48	3.49
12	$A^{'}$ ($\pi \rightarrow \pi^*$)	1.89	1.92	1.93	1.91	1.95	1.95
13	$A^{'}$ ($\pi \rightarrow \pi^*$)	5.29	5.66	5.99	5.90	5.89	5.86
14	$A^{'}$ ($\pi \rightarrow \pi^*$)	4.06	4.14	4.09	4.39	4.30	4.35
15	B_2 ($\pi \rightarrow \pi^*$)	2.30	1.91	1.40	1.68	1.56	1.61
16	A ($\pi \rightarrow \pi^*$)	12.80	12.86	11.90	12.23	11.93	11.73
17	$A^{''}$ ($\pi \rightarrow \pi^*$)	19.66	18.61	16.50	16.99	16.98	16.70
18	A ($\pi \rightarrow \pi^*$)	12.05	1.85	0.79	0.96	0.78	0.79
19	A ($\pi \rightarrow \pi^*$)	13.15	9.07	5.99	6.71	6.06	5.52
20	A ($\pi \rightarrow \pi^*$)	15.68	12.17	8.43	8.93	8.63	7.96
21	A ($\pi \rightarrow \pi^*$)	5.40	5.53	5.68	5.66	5.34	5.27
22	A ($\pi \rightarrow \pi^*$)	26.04	27.80	22.75	24.64	23.31	21.38
23	A ($n \rightarrow \pi^*$)	1.23	1.75	2.05	2.11	1.99	1.99
	B ($\pi \rightarrow \pi^*$)	4.09	4.60	4.64	4.66	4.60	4.55
24	A ($\pi \rightarrow \pi^*$)	7.66	7.65	7.45	7.62	7.41	7.33
25	B_2 ($\pi \rightarrow \pi^*$)	4.27	4.01	3.81	3.91	3.84	3.86

TABLE S12. ES dipole moments (in Debye) for the dyes obtained with the BSE/evGW formalism using PBE0, PBEh, and PBEα starting points and the cc-pVTZ atomic basis set. FF (AA) indicates that the dipole moments are calculated using the finite-field (approximated analytical gradients) approach.

	State	**BSE/evGW/PBE0 (FF)**	**BSE/evGW/PBE0 (AA)**	**BSE/evGW/PBEh (AA)**	**BSE/evGW/PBEα (AA)**
1	A ($\pi \rightarrow \pi^*$)	8.62	8.53	8.63	8.63
2	B_2 ($\pi \rightarrow \pi^*$)	3.82	3.94	3.87	3.84
3	A_1 ($\pi \rightarrow \pi^*$)	2.06	2.70	0.32	0.65
	B_1 ($\pi \rightarrow \pi^*$)	5.78	1.78	3.02	3.53
4	A ($\pi \rightarrow \pi^*$)	6.94	6.66	6.79	6.83
5	$A^{'}$ ($\pi \rightarrow \pi^*$)	2.79	2.81	2.74	2.71
6	$A^{'}$ ($\pi \rightarrow \pi^*$)	0.52	0.80	0.90	1.01
7	A ($\pi \rightarrow \pi^*$)	5.36	5.27	5.12	4.98
8	A ($\pi \rightarrow \pi^*$)	3.36	4.05	4.01	3.93
9	A ($\pi \rightarrow \pi^*$)	12.56	11.80	12.28	12.37
10	$A^{'}$ ($\pi \rightarrow \pi^*$)	5.67	5.36	5.85	6.05
11	A ($\pi \rightarrow \pi^*$)	3.59	3.45	3.21	3.09
12	$A^{'}$ ($\pi \rightarrow \pi^*$)	1.95	1.94	1.98	2.00
13	$A^{'}$ ($\pi \rightarrow \pi^*$)	6.19	5.75	6.24	6.43
14	$A^{'}$ ($\pi \rightarrow \pi^*$)	4.88	4.39	4.25	4.21
15	B_2 ($\pi \rightarrow \pi^*$)	1.78	1.85	1.76	1.73
16	A ($\pi \rightarrow \pi^*$)	12.46	11.85	12.33	12.42
17	$A^{''}$ ($\pi \rightarrow \pi^*$)	17.02	17.57	17.00	16.76
18	A ($\pi \rightarrow \pi^*$)	0.76	0.78	0.71	0.74
19	A ($\pi \rightarrow \pi^*$)	6.45	5.82	5.86	5.79
20	A ($\pi \rightarrow \pi^*$)	6.20	8.22	8.38	8.34
21	A ($\pi \rightarrow \pi^*$)	5.97	4.94	5.56	5.77
22	A ($\pi \rightarrow \pi^*$)	24.44	22.18	22.42	22.29
23	A ($n \rightarrow \pi^*$)	2.02	1.91	2.31	2.48
	B ($\pi \rightarrow \pi^*$)	4.67	4.35	4.62	4.71
24	A ($\pi \rightarrow \pi^*$)	8.04	7.85	8.07	8.10
25	B_2 ($\pi \rightarrow \pi^*$)	3.71	4.15	4.05	4.03

S3.5. Excess dipoles

TABLE S13. Excess dipole moments (in Debye) for the dyes obtained with CC2 and ADC(2) methods and the cc-pVTZ atomic basis set. OR (UR) stands for the relaxed (unrelaxed) approach used to calculate dipoles.

	State	CC2 (OR)	CC2 (UR)	ADC(2) (OR)	ADC(2) (UR)
1	A ($\pi \rightarrow \pi^*$)	3.88	4.48	3.78	5.28
2	B_2 ($\pi \rightarrow \pi^*$)	0.18	0.44	0.23	1.27
3	A_1 ($\pi \rightarrow \pi^*$)	12.40	13.56	13.63	18.57
	B_1 ($\pi \rightarrow \pi^*$)	13.68	15.31	14.27	19.06
4	A ($\pi \rightarrow \pi^*$)	5.01	5.47	5.11	5.60
5	$A^{'}$ ($\pi \rightarrow \pi^*$)	0.96	1.22	1.06	2.15
6	$A^{'}$ ($\pi \rightarrow \pi^*$)	2.59	3.02	2.05	3.69
7	A ($\pi \rightarrow \pi^*$)	4.92	5.31	5.06	5.92
8	A ($\pi \rightarrow \pi^*$)	5.55	5.99	5.65	6.04
9	A ($\pi \rightarrow \pi^*$)	4.11	4.48	4.51	4.00
10	$A^{'}$ ($\pi \rightarrow \pi^*$)	3.18	3.83	3.16	5.69
11	A ($\pi \rightarrow \pi^*$)	1.82	2.20	1.90	3.35
12	$A^{'}$ ($\pi \rightarrow \pi^*$)	0.75	0.70	0.82	0.56
13	$A^{'}$ ($\pi \rightarrow \pi^*$)	2.02	2.27	1.88	2.79
14	$A^{'}$ ($\pi \rightarrow \pi^*$)	1.47	2.27	2.17	5.09
15	B_2 ($\pi \rightarrow \pi^*$)	1.33	1.78	1.52	3.23
16	A ($\pi \rightarrow \pi^*$)	7.83	9.15	8.47	12.13
17	$A^{''}$ ($\pi \rightarrow \pi^*$)	9.50	10.99	9.97	14.22
18	A ($\pi \rightarrow \pi^*$)	1.24	1.37	0.85	0.94
19	A ($\pi \rightarrow \pi^*$)	8.72	9.51	8.56	11.40
20	A ($\pi \rightarrow \pi^*$)	8.55	9.29	8.89	10.71
21	$A^{'}$ ($\pi \rightarrow \pi^*$)	2.89	3.72	3.84	6.29
22	A ($\pi \rightarrow \pi^*$)	21.62	23.09	21.78	24.70
23	A ($n \rightarrow \pi^*$)	1.73	2.25	1.84	3.66
	B ($\pi \rightarrow \pi^*$)	1.40	1.56	1.40	1.73
24	A ($\pi \rightarrow \pi^*$)	3.64	5.12	5.59	10.59
25	B_2 ($\pi \rightarrow \pi^*$)	0.23	0.19	0.20	0.08

S3.6. Statistical analysis

S3.6.1. CC2 (OR) as a reference

TABLE S14. Mean absolute error (MAE), mean signed error (MSE), standard deviation of the errors (σ), maximal positive [Max(+)] and negative [Max(-)] deviations, Pearson correlation coefficient (R), Spearman rank-order correlation coefficient (ρ), and linear determination coefficient (R^2) of the ES transition energies calculated from the data presented in Tables S4, S5, and S6. The CC2 data are used as a reference for the statistical analysis.

	ADC(2)	**PBE**[a]	**PBE0**	**PBEh**	**M06-2X**	**CAM-B3LYP**	**ωB97X-D**	**BSE/evGW PBE0 (5&5)**	**BSE/evGW PBE0 (10eV)**	**BSE/evGW PBEh (10eV)**	**BSE/evGW PBEα (10eV)**
MAE	0.09	0.61	0.26	0.29	0.20	0.20	0.22	0.15	0.16	0.13	0.13
MSE	-0.09	-0.59	-0.17	0.24	0.12	0.11	0.15	-0.09	-0.08	-0.04	-0.01
σ	0.07	0.38	0.25	0.24	0.19	0.21	0.21	0.16	0.17	0.15	0.15
Max(+)	0.00	0.14	0.27	0.55	0.42	0.43	0.52	0.27	0.30	0.23	0.40
Max(−)	-0.25	-1.14	-0.55	-0.19	-0.23	-0.26	-0.23	-0.34	-0.33	-0.25	-0.21
R	1.00	0.80	0.93	0.93	0.96	0.96	0.95	0.97	0.97	0.97	0.97
ρ	1.00	0.83	0.93	0.91	0.94	0.94	0.92	0.95	0.95	0.95	0.96
R^2	1.00	0.64	0.87	0.87	0.93	0.92	0.91	0.94	0.94	0.95	0.94

[a] The problematic case of molecule **18** (state mixing) was removed from the data set for the statistical analysis with the PBE functional.

TABLE S15. Statistical analysis of the oscillator strength presented in Tables S7, S8, and S9. The CC2 data are used as a reference for the statistical analysis.[a]

	ADC(2)	**PBE**[a]	**PBE0**	**PBEh**	**M06-2X**	**CAM-B3LYP**	**ωB97X-D**	**BSE/evGW/ PBE0 (5&5)**	**BSE/evGW/ PBE0 (10eV)**	**BSE/evGW/ PBEh (10eV)**	**BSE/evGW/ PBEα (10eV)**
MAE	0.04	0.20	0.05	0.09	0.05	0.05	0.06	0.07	0.07	0.05	0.05
MSE	0.02	-0.20	-0.04	0.09	0.05	0.05	0.06	0.04	0.05	0.01	0.00
σ	0.06	0.19	0.07	0.08	0.04	0.05	0.07	0.11	0.12	0.08	0.07
Max(+)	0.18	0.00	0.05	0.30	0.13	0.18	0.29	0.42	0.42	0.22	0.16
Max(−)	-0.14	-0.89	-0.26	-0.02	-0.03	-0.04	-0.03	-0.12	-0.11	-0.22	-0.19
R	1.00	0.96	0.99	1.00	1.00	1.00	0.99	0.98	0.98	0.99	0.99
ρ	0.99	0.97	0.99	0.99	0.99	0.99	0.99	0.99	0.99	0.99	0.98
R^2	0.99	0.92	0.98	0.99	0.99	0.99	0.99	0.97	0.97	0.97	0.98

[a] See caption of the Table S14 for more details.

[b] The problematic case of molecule **18** (state mixing) was removed from the data set for the statistical analysis with the PBE functional.

TABLE S16. Statistical analysis of the ES dipole moments presented in Tables S10, S11, and S12. The CC2 (OR) data are used as a reference for the statistical analysis.[a]

	CC2 (UR)	**ADC(2)** (OR)	**ADC(2)** (UR)	**PBE**[b]	**PBE0**	**PBEh**	**M06-2X**	**CAM-B3LYP**	**ωB97X-D**	**BSE/*GW* PBE0**[c]	**BSE/*GW* PBE0**[d]	**BSE/*GW* PBEh**[e]	**BSE/*GW* PBEα**[f]
MAE	0.54	0.21	1.47	1.72	0.91	1.47	1.25	1.40	1.58	1.26	1.48	1.51	1.51
MSE	0.45	-0.03	1.27	0.36	-0.24	-1.10	-0.87	-1.03	-1.21	-0.80	-1.06	-1.00	-0.96
σ	0.56	0.27	1.42	2.37	1.19	1.77	1.47	1.68	2.00	1.68	1.85	1.89	1.91
Max(+)	1.60	0.68	4.39	6.61	2.41	2.22	2.39	2.18	2.09	2.81	2.62	2.84	2.87
Max(−)	-0.68	-0.55	-1.58	-5.00	-3.65	-6.50	-4.60	-5.94	-7.87	-4.82	-7.07	-6.83	-6.96
R	1.00	1.00	0.99	0.92	0.98	0.97	0.98	0.97	0.96	0.97	0.96	0.96	0.96
ρ	0.99	1.00	0.96	0.81	0.90	0.89	0.91	0.90	0.88	0.91	0.88	0.88	0.88
R^2	1.00	1.00	0.97	0.85	0.96	0.94	0.95	0.94	0.92	0.94	0.93	0.92	0.92

[a] See caption of the Table S14 for more details.

[b] The problematic case of molecule **18** (state mixing) was removed from the data set for the statistical analysis with the PBE functional.

[c] BSE/evGW/PBE0 (FF).

[d] BSE/evGW/PBE0 (AA).

[e] BSE/evGW/PBEh (AA).

[f] BSE/evGW/PBEα (AA).

TABLE S17. Statistical analysis of the excess dipole moments presented in Table S13 and in Table 2. The CC2 (OR) data are used as a reference for the statistical analysis.[a]

	CC2 (UR)	**ADC(2)** (OR)	**ADC(2)** (UR)	**PBE**[b]	**PBE0**	**PBEh**	**M06-2X**	**CAM-B3LYP**	**ωB97X-D**	**BSE/*GW* PBE0**[c]	**BSE/*GW* PBE0**[d]	**BSE/*GW* PBEh**[e]	**BSE/*GW* PBEα**[f]
MAE	0.65	0.36	2.19	2.07	1.03	1.35	1.12	1.29	1.45	1.25	1.69	1.38	1.32
MSE	0.64	0.26	2.13	0.02	-0.58	-1.33	-1.11	-1.26	-1.43	-1.21	-1.68	-1.35	-1.26
σ	0.48	0.50	1.96	3.01	1.60	1.46	1.15	1.36	1.65	1.47	1.91	1.48	1.47
Max(+)	1.63	1.95	6.95	6.31	1.81	0.25	0.18	0.20	0.21	0.37	0.04	0.34	0.46
Max(−)	-0.05	-0.54	-0.30	-8.16	-6.57	-6.35	-4.41	-5.67	-7.56	-5.16	-7.42	-6.75	-6.82
R	1.00	1.00	0.96	0.80	0.95	0.98	0.99	0.99	0.98	0.96	0.97	0.98	0.97
ρ	0.99	0.98	0.94	0.83	0.95	0.96	0.98	0.98	0.97	0.96	0.96	0.96	0.95
R^2	1.00	0.99	0.93	0.63	0.90	0.96	0.98	0.97	0.96	0.93	0.94	0.96	0.95

[a] See caption of the Table S14 for more details.

[b] The problematic case of molecule **18** (state mixing) was removed from the data set for the statistical analysis with the PBE functional.

[c] BSE/evGW/PBE0 (FF).

[d] BSE/evGW/PBE0 (AA).

[e] BSE/evGW/PBEh (AA).

[f] BSE/evGW/PBEα (AA).

S3.6.2. CCSD (OR) as a reference

TABLE S18. Statistical analysis of the GS dipole moments presented in Tables S3. The CCSD (OR) data are used as a reference for the statistical analysis.[a]

	CC2 (OR)	**CC2** (UR)	**MP2** (OR)	**MP2** (UR)	**PBE**	**PBE0**	**PBEh**	**PBEα**	**M06-2X**	**CAM-B3LYP**	**ωB97X-D**
MAE	0.37	0.39	0.25	0.46	0.54	0.38	0.28	0.34	0.24	0.23	0.22
MSE	0.01	-0.03	-0.08	0.31	0.29	0.26	0.24	0.31	0.21	0.20	0.19
σ	0.52	0.52	0.36	0.50	0.74	0.44	0.30	0.32	0.26	0.24	0.22
Max(+)	0.91	0.89	0.40	1.08	1.99	1.26	0.89	1.00	0.79	0.67	0.60
Max(−)	-1.26	-1.24	-1.31	-0.98	-2.38	-1.24	-0.20	-0.19	-0.43	-0.35	-0.19
R	0.98	0.98	0.99	0.99	0.96	0.99	1.00	1.00	1.00	1.00	1.00
ρ	0.97	0.97	0.98	0.99	0.97	0.99	0.99	0.99	0.99	1.00	0.99
R^2	0.96	0.96	0.98	0.98	0.92	0.97	0.99	0.99	0.99	0.99	0.99

[a] See caption of the Table S14 for more details.

TABLE S19. Statistical analysis of the ES dipole moments presented in Tables S10, S11, and S12. The CCSD (OR) data are used as a reference for the statistical analysis.[a]

	CC2 (OR)	**CC2** (UR)	**ADC(2)** (OR)	**ADC(2)** (UR)	**PBE**[b]	**PBE0**	**PBEh**	**M06-2X**	**CAM-B3LYP**	**ωB97X-D**	**BSE/*GW* PBE0**[c]	**BSE/*GW* PBE0**[d]	**BSE/*GW* PBEh**[e]	**BSE/*GW* PBEα**[f]
MAE	1.29	1.76	1.35	2.50	1.93	1.09	0.70	0.46	0.51	0.64	0.63	0.66	0.54	0.55
MSE	0.87	1.32	0.84	2.14	1.22	0.63	-0.24	-0.01	-0.16	-0.34	0.07	-0.19	-0.13	-0.09
σ	1.55	1.98	1.60	2.62	2.63	1.45	0.99	0.64	0.69	0.84	0.93	0.82	0.72	0.72
Max(+)	5.40	6.86	4.94	8.05	7.23	3.95	2.74	2.03	1.68	1.41	2.44	1.44	1.37	1.37
Max(−)	-2.21	-2.09	-2.40	-1.86	-2.91	-1.56	-2.49	-1.32	-1.38	-2.47	-2.25	-1.67	-1.46	-1.56
R	0.98	0.97	0.97	0.95	0.90	0.97	0.98	0.99	0.99	0.99	0.98	0.99	0.99	0.99
ρ	0.90	0.87	0.90	0.84	0.80	0.93	0.94	0.97	0.97	0.97	0.95	0.96	0.97	0.97
R^2	0.95	0.93	0.95	0.91	0.81	0.95	0.96	0.99	0.98	0.98	0.97	0.98	0.98	0.98

[a] See caption of the Table S14 for more details.

[b] The problematic case of molecule **18** (state mixing) was removed from the data set for the statistical analysis with the PBE functional.

[c] BSE/evGW/PBE0 (FF).

[d] BSE/evGW/PBE0 (AA).

[e] BSE/evGW/PBEh (AA).

[f] BSE/evGW/PBEα (AA).

TABLE S20. Statistical analysis of the excess dipole moments with CC2 and ADC(2) methods presented in Tables S13 and 2. The CCSD (OR) data are used as a reference for the statistical analysis.[a]

	CC2 (OR)	**CC2 (UR)**	**ADC(2) (OR)**	**ADC(2) (UR)**
MAE	1.03	1.59	1.21	3.11
MSE	0.93	1.57	1.19	3.06
σ	1.15	1.40	1.16	2.40
Max(+)	4.49	5.96	4.65	7.57
Max(−)	-0.77	-0.20	-0.11	-0.38
R	0.98	0.98	0.99	0.96
ρ	0.93	0.93	0.95	0.91
R^2	0.96	0.97	0.97	0.93

[a] See caption of the Table S14 for more details.

S3.7. CC2 dipoles with cc-pVDZ basis set

TABLE S21. GS, ES, and excess dipole moments (in Debye) for the dyes obtained with CC2 (OR)/cc-pVDZ level of theory.

	μ^{GS}	**State**	μ^{ES}	$\Delta\mu$
7	2.53	A ($\pi \rightarrow \pi^*$)	7.90	5.51
8	0.82	A ($\pi \rightarrow \pi^*$)	6.22	5.49
9	8.66	A ($\pi \rightarrow \pi^*$)	12.64	4.06
10	5.66	$A^{'}$ ($\pi \rightarrow \pi^*$)	4.46	3.16
11	2.10	A ($\pi \rightarrow \pi^*$)	3.98	1.93
12	1.81	$A^{'}$ ($\pi \rightarrow \pi^*$)	2.04	0.78
13	4.17	$A^{'}$ ($\pi \rightarrow \pi^*$)	5.46	1.82
14	4.74	$A^{'}$ ($\pi \rightarrow \pi^*$)	5.73	1.71
15	0.01	B_2 ($\pi \rightarrow \pi^*$)	1.38	1.37
16	6.39	A ($\pi \rightarrow \pi^*$)	14.11	7.81
17	8.86	$A^{''}$ ($\pi \rightarrow \pi^*$)	18.49	9.63
18	0.52	A ($\pi \rightarrow \pi^*$)	1.58	1.40
19	2.29	A ($\pi \rightarrow \pi^*$)	9.74	8.99
20	2.46	A ($\pi \rightarrow \pi^*$)	10.95	8.64
21	3.14	A ($\pi \rightarrow \pi^*$)	6.21	3.07
22	7.36	A ($\pi \rightarrow \pi^*$)	29.00	21.64
23	3.11	A ($n \rightarrow \pi^*$)	1.45	1.65
		B ($\pi \rightarrow \pi^*$)	4.50	1.40
24	6.34	A ($\pi \rightarrow \pi^*$)	5.23	3.69
25	2.58	B_2 ($\pi \rightarrow \pi^*$)	2.81	0.23

S3.8. Basis set benchmark

TABLE S22. GS and ES dipole moments (in Debye) for the dyes obtained with CC2 (OR), TD-M06-2X, and CAM-B3LYP level of theory using cc-pVDZ, cc-pVTZ, aug-cc-pVDZ, and aug-cc-pVTZ basis sets.

	Basis set	CC2 (OR)		M06-2X		CAM-B3LYP	
		μ^{GS}	μ^{ES}	μ^{GS}	μ^{ES}	μ^{GS}	μ^{ES}
8	cc-pVDZ	0.82	6.22	0.77	4.55	0.82	4.12
	aug-cc-pVDZ	0.87	6.24	0.79	4.53	0.85	4.18
	cc-pVTZ	0.91	6.35	0.85	4.51	0.90	4.17
	aug-cc-pVTZ	0.87	6.23	0.83	4.46	0.87	4.12
9	cc-pVDZ	8.66	12.64	9.72	12.28	9.53	11.91
	aug-cc-pVDZ	9.17	13.34	9.95	12.63	9.98	12.51
	cc-pVTZ	8.86	12.91	9.88	12.45	9.77	12.19
	aug-cc-pVTZ	9.15	13.30	9.96	12.60	9.95	12.44
10	cc-pVDZ	5.66	4.46	6.14	4.86	6.19	4.97
	aug-cc-pVDZ	6.06	5.11	6.41	5.37	6.61	5.64
	cc-pVTZ	5.90	4.80	6.42	5.25	6.49	5.38
	aug-cc-pVTZ	6.06	5.13	6.51	5.45	6.62	5.62

S4. CARTESIAN COORDINATES

S4.1. DMABN

The CCSD(T)-interpolated set of the ground-state (GS) geometries of DMABN with a twist angle from 0° and 90° and a step of 10° was taken from the previous work.[2] Cartesian coordinates are given in a.u.

0° twist angle

N	0.00000000	0.00000000	-4.53730762
C	0.00000000	0.00000000	-1.96082123
C	2.27890066	0.00000000	-0.58294421
C	-2.27890066	0.00000000	-0.58294421
H	4.06467185	0.00000000	-1.55102730
H	-4.06467185	0.00000000	-1.55102730
C	0.00000000	0.00000000	3.37433145
C	2.26709804	0.00000000	2.02802650
C	-2.26709804	0.00000000	2.02802650
H	4.03366985	0.00000000	3.04098312
H	-4.03366985	0.00000000	3.04098312
C	0.00000000	0.00000000	6.06795463
C	2.36483881	0.00000000	-5.90183665
C	-2.36483881	0.00000000	-5.90183665
H	1.96835533	0.00000000	-7.91288508
H	-1.96835533	0.00000000	-7.91288508
H	3.49549259	-1.67110793	-5.47000455
H	3.49549259	1.67110793	-5.47000455
H	-3.49549259	1.67110793	-5.47000455
H	-3.49549259	-1.67110793	-5.47000455
N	0.00000000	0.00000000	8.26378470

10° twist angle

N	-0.00000000	0.00000000	-4.54252023
C	-0.00000000	0.00000000	-1.95697215
C	2.27359527	-0.14451680	-0.58297208
C	-2.27359527	0.14451680	-0.58297208
H	4.05253431	-0.25759171	-1.55837367
H	-4.05253431	0.25759171	-1.55837367
C	-0.00000000	0.00000000	3.37225998
C	2.26434477	-0.14392881	2.02908254
C	-2.26434477	0.14392881	2.02908254
H	4.02605581	-0.25590865	3.04417038
H	-4.02605581	0.25590865	3.04417038
C	-0.00000000	0.00000000	6.06685502
C	2.35334946	0.26243148	-5.89971807
C	-2.35334946	-0.26243148	-5.89971807
H	1.96559068	0.21919094	-7.91254616
H	-1.96559068	-0.21919094	-7.91254616
H	3.66295004	-1.27271590	-5.46626211
H	3.29260374	2.04835772	-5.46626211
H	-3.66295004	1.27271590	-5.46626211
H	-3.29260374	-2.04835772	-5.46626211
N	-0.00000000	0.00000000	8.26249554

20° twist angle

N	0.00000000	-0.00000000	-4.54773564
C	0.00000000	-0.00000000	-1.95312588
C	-2.25946893	0.28570567	-0.58299948
C	2.25946893	-0.28570567	-0.58299948
H	-4.02466997	0.50891207	-1.56570903
H	4.02466997	-0.50891207	-1.56570903
C	0.00000000	-0.00000000	3.37018571
C	-2.25278788	0.28486086	2.03013822
C	2.25278788	-0.28486086	2.03013822
H	-4.00281100	0.50614805	3.04735559
H	4.00281100	-0.50614805	3.04735559
C	0.00000000	-0.00000000	6.06575259
C	-2.31215209	-0.52502382	-5.89759580
C	2.31215209	0.52502382	-5.89759580
H	-1.93784688	-0.44002978	-7.91218369
H	1.93784688	0.44002978	-7.91218369
H	-3.78610299	0.85336104	-5.46251396
H	-3.04626803	-2.40479771	-5.46251396
H	3.78610299	-0.85336104	-5.46251396
H	3.04626803	2.40479771	-5.46251396
N	0.00000000	-0.00000000	8.26120358

30° twist angle

N	0.00000000	-0.00000000	-4.55295386
C	0.00000000	-0.00000000	-1.94928240
C	-2.23780139	0.41923050	-0.58302639
C	2.23780139	-0.41923050	-0.58302639
H	-3.98338878	0.74624945	-1.57303325
H	3.98338878	-0.74624945	-1.57303325
C	0.00000000	-0.00000000	3.36810864
C	-2.23367531	0.41845752	2.03119355
C	2.23367531	-0.41845752	2.03119355
H	-3.96618281	0.74302608	3.05053878
H	3.96618281	-0.74302608	3.05053878
C	0.00000000	-0.00000000	6.06464738
C	-2.23942025	-0.78814911	-5.89546991
C	2.23942025	0.78814911	-5.89546991
H	-1.88333190	-0.66282618	-7.91179769
H	1.88333190	0.66282618	-7.91179769
H	-3.86254858	0.41129616	-5.45876015
H	-2.75354585	-2.73978673	-5.45876015
H	3.86254858	-0.41129616	-5.45876015
H	2.75354585	2.73978673	-5.45876015
N	0.00000000	-0.00000000	8.25990881

40° twist angle

N	-0.00000000	0.00000000	-4.55817486
C	-0.00000000	0.00000000	-1.94544172
C	-2.21120191	0.53921411	-0.58305279
C	2.21120191	-0.53921411	-0.58305279
H	-3.93336008	0.95917213	-1.58034616
H	3.93336008	-0.95917213	-1.58034616
C	-0.00000000	0.00000000	3.36602878
C	-2.20958915	0.53882083	2.03224854
C	2.20958915	-0.53882083	2.03224854
H	-3.92077993	0.95610439	3.05371993
H	3.92077993	-0.95610439	3.05371993
C	-0.00000000	0.00000000	6.06353937
C	-2.13111434	-1.05305723	-5.89334044
C	2.13111434	1.05305723	-5.89334044

H	-1.79836616	-0.88863486	-7.91138819
H	1.79836616	0.88863486	-7.91138819
H	-3.88723182	-0.05807088	-5.45500074
H	-2.40761524	-3.05243056	-5.45500074
H	3.88723182	0.05807088	-5.45500074
H	2.40761524	3.05243056	-5.45500074
N	-0.00000000	0.00000000	8.25861126

50° twist angle

N	-0.00000000	0.00000000	-4.56339863
C	-0.00000000	0.00000000	-1.94160380
C	-2.18448624	0.63625224	-0.58307866
C	2.18448624	-0.63625224	-0.58307866
H	-3.88316327	1.13100797	-1.58764764
H	3.88316327	-1.13100797	-1.58764764
C	-0.00000000	0.00000000	3.36394615
C	-2.18533043	0.63649812	2.03330318
C	2.18533043	-0.63649812	2.03330318
H	-3.87513336	1.12866918	3.05689905
H	3.87513336	-1.12866918	3.05689905
C	-0.00000000	0.00000000	6.06242859
C	-1.97872140	-1.32270396	-5.89120745
C	1.97872140	1.32270396	-5.89120745
H	-1.67543716	-1.11996937	-7.91095522
H	1.67543716	1.11996937	-7.91095522
H	-3.84968800	-0.56497325	-5.45123581
H	-1.99386119	-3.34122882	-5.45123581
H	3.84968800	0.56497325	-5.45123581
H	1.99386119	3.34122882	-5.45123581
N	-0.00000000	0.00000000	8.25731094

60° twist angle

N	-0.00000000	0.00000000	-4.56862517
C	-0.00000000	0.00000000	-1.93776865
C	-2.16651379	0.69254692	-0.58310398
C	2.16651379	-0.69254692	-0.58310398
H	-3.84853732	1.23022189	-1.59493754
H	3.84853732	-1.23022189	-1.59493754
C	-0.00000000	0.00000000	3.36186076
C	-2.16977140	0.69358825	2.03435748
C	2.16977140	-0.69358825	2.03435748
H	-3.84496571	1.22908019	3.06007615
H	3.84496571	-1.22908019	3.06007615
C	-0.00000000	0.00000000	6.06131505
C	-1.76335974	-1.60301682	-5.88907100
C	1.76335974	1.60301682	-5.88907100
H	-1.49812707	-1.36190185	-7.91049880
H	1.49812707	1.36190185	-7.91049880
H	-3.72622388	-1.13125946	-5.44746539
H	-1.48030006	-3.60183344	-5.44746539
H	3.72622388	1.13125946	-5.44746539
H	1.48030006	3.60183344	-5.44746539
N	-0.00000000	0.00000000	8.25600786

70° twist angle

N	0.00000000	-0.00000000	-4.57385445
C	0.00000000	-0.00000000	-1.93393625
C	-2.17319604	0.66873262	-0.58312872

C	2.17319604	-0.66873262	-0.58312872
H	-3.85769532	1.18708422	-1.60221572
H	3.85769532	-1.18708422	-1.60221572
C	0.00000000	-0.00000000	3.35977262
C	-2.17889449	0.67048614	2.03541146
C	2.17889449	-0.67048614	2.03541146
H	-3.85854875	1.18734683	3.06325122
H	3.85854875	-1.18734683	3.06325122
C	0.00000000	-0.00000000	6.06019877
C	-1.43941956	-1.90297078	-5.88693115
C	1.43941956	1.90297078	-5.88693115
H	-1.22701984	-1.62216977	-7.91001898
H	1.22701984	1.62216977	-7.91001898
H	-3.45582390	-1.80189449	-5.44368957
H	-0.79340881	-3.81576271	-5.44368957
H	3.45582390	1.80189449	-5.44368957
H	0.79340881	3.81576271	-5.44368957
N	0.00000000	-0.00000000	8.25470202

80° twist angle

N	0.00000000	0.00000000	-4.57908647
C	0.00000000	0.00000000	-1.93010659
C	-2.22323388	0.47304498	-0.58315288
C	2.22323388	-0.47304498	-0.58315288
H	-3.94371757	0.83911811	-1.60948204
H	3.94371757	-0.83911811	-1.60948204
C	0.00000000	0.00000000	3.35768174
C	-2.23155336	0.47481515	2.03646511
C	2.23155336	-0.47481515	2.03646511
H	-3.94915983	0.84027608	3.06642427
H	3.94915983	-0.84027608	3.06642427
C	0.00000000	0.00000000	6.05907974
C	-0.89538995	-2.21484501	-5.88478796
C	0.89538995	2.21484501	-5.88478796
H	-0.76581730	-1.89433289	-7.90951577
H	0.76581730	1.89433289	-7.90951577
H	-2.86857125	-2.64305532	-5.43990839
H	0.22584147	-3.89402594	-5.43990839
H	2.86857125	2.64305532	-5.43990839
H	-0.22584147	3.89402594	-5.43990839
N	0.00000000	0.00000000	8.25339345

90° twist angle

N	0.00000000	0.00000000	-4.58432122
C	0.00000000	0.00000000	-1.92627965
C	2.27223933	0.00000000	-0.58317642
C	-2.27223933	0.00000000	-0.58317642
H	4.02775652	0.00000000	-1.61673635
H	-4.02775652	0.00000000	-1.61673635
C	0.00000000	0.00000000	3.35558814
C	2.28329002	0.00000000	2.03751845
C	-2.28329002	0.00000000	2.03751845
H	4.03802035	0.00000000	3.06959530
H	-4.03802035	0.00000000	3.06959530
C	0.00000000	0.00000000	6.05795799
C	0.00000000	2.39190414	-5.88264149
C	0.00000000	-2.39190414	-5.88264149
H	0.00000000	2.05256971	-7.90898921
H	0.00000000	-2.05256971	-7.90898921
H	1.66857006	3.52917345	-5.43612191

H	-1.66857006	3.52917345	-5.43612191
H	-1.66857006	-3.52917345	-5.43612191
H	1.66857006	-3.52917345	-5.43612191
N	0.00000000	0.00000000	8.25208215

S4.2. Dyes

Below we provide the Cartesian coordinates of the dyes studied in this work. These geometries were taken from the previous work[3] and are given in Å.

1

C	1.237443	1.029399	-0.010403
C	-0.063072	0.573643	-0.006031
C	-0.384557	-0.780804	-0.002150
C	0.616959	-1.740659	-0.003223
C	1.938677	-1.306089	-0.007218
C	2.265971	0.065922	-0.009164
H	1.458323	2.093481	-0.019139
H	0.375546	-2.799292	-0.000464
H	2.745509	-2.034357	-0.014886
C	-1.340822	1.359341	-0.000750
C	-1.864970	-0.917001	0.005185
O	-2.547962	-1.912713	0.010940
O	-1.492386	2.557188	-0.000158
N	3.589626	0.463597	-0.067146
H	4.281691	-0.206590	0.239646
H	3.793394	1.409103	0.227631
N	-2.351172	0.400180	0.004797
H	-3.337271	0.627794	0.008562

2

C	0.000000	1.214223	1.109890
C	0.000000	-1.214223	1.109890
C	0.000000	0.000000	1.786939
C	0.000000	2.550733	1.582712
C	0.000000	3.374118	0.469203
C	0.000000	2.524326	-0.659917
H	0.000000	0.000000	2.873398
H	0.000000	2.844299	2.624326
H	0.000000	4.454395	0.446062
H	0.000000	2.781633	-1.711711
B	0.000000	0.000000	-1.229799
F	1.141999	0.000000	-2.008760
F	-1.141999	0.000000	-2.008760
N	0.000000	1.247454	-0.278502
N	0.000000	-1.247454	-0.278502
C	0.000000	-2.550733	1.582712
H	0.000000	-2.844299	2.624326
C	0.000000	-2.524326	-0.659917
H	0.000000	-2.781633	-1.711711
C	0.000000	-3.374118	0.469203
H	0.000000	-4.454395	0.446062

3

C	0.000000	0.714710	-1.742030
C	0.000000	-0.714710	-1.742030
C	0.000000	-1.434003	-2.951532
C	0.000000	-0.709772	-4.128212
C	0.000000	0.709772	-4.128212
C	0.000000	1.434003	-2.951532
C	0.000000	0.000000	0.205790
H	0.000000	-2.520135	-2.949107
H	0.000000	-1.233699	-5.079986
H	0.000000	1.233699	-5.079986
H	0.000000	2.520135	-2.949107
C	0.000000	-1.179114	2.304029
C	0.000000	1.179114	2.304029
C	0.000000	-1.200543	3.685635
H	0.000000	-2.052139	1.661265
C	0.000000	1.200543	3.685635
H	0.000000	2.052139	1.661265
C	0.000000	0.000000	4.393898
H	0.000000	-2.157670	4.193972
H	0.000000	2.157670	4.193972
H	0.000000	0.000000	5.478875
N	0.000000	-1.158000	-0.445599
N	0.000000	1.158000	-0.445599
N	0.000000	0.000000	1.642060

4

C	-1.403894	0.228690	0.087805
C	-0.837767	1.483878	0.130462
C	0.577524	1.457504	0.133262
C	1.088155	0.178634	0.094908
S	-0.185775	-1.000949	0.036195
H	-1.427056	2.393239	0.180108
H	1.205503	2.341428	0.172543
C	-2.813783	-0.126287	0.080156
C	-3.399966	-1.310197	0.455842
S	-4.009922	1.014544	-0.450324
C	-4.818143	-1.294621	0.323644
H	-2.834571	-2.154801	0.835548
C	-5.285865	-0.101050	-0.147555
H	-5.459860	-2.130527	0.575815
H	-6.310698	0.187089	-0.338498
C	2.464782	-0.238418	0.094803
C	3.112661	-1.607983	0.067343
C	3.654547	0.408792	0.116993
H	2.912611	-2.230290	0.945160
H	2.923954	-2.189590	-0.840384
C	4.483757	-0.857904	0.093223
H	5.088487	-1.037111	0.986596
H	5.099922	-0.995979	-0.799637
C	3.986542	1.791203	0.150029
N	4.249552	2.920971	0.177094

5

C	-0.002731	1.412780	-3.036713
C	-0.008523	0.060697	-3.417644
C	-0.001581	-0.960023	-2.473878
C	0.016187	-0.594314	-1.124979
C	0.012564	0.762943	-0.724254
C	0.006190	1.768996	-1.693457
H	-0.009496	2.183805	-3.800711

H	-0.022695	-0.195485	-4.472987
H	-0.017118	-2.000866	-2.782547
H	0.005479	2.815312	-1.399711
C	0.016187	-0.594314	1.124979
C	-0.001581	-0.960023	2.473878
C	-0.008523	0.060697	3.417644
C	-0.002731	1.412780	3.036713
C	0.006190	1.768996	1.693457
C	0.012564	0.762943	0.724254
H	-0.017118	-2.000866	2.782547
H	-0.022695	-0.195485	4.472987
H	-0.009496	2.183805	3.800711
H	0.005479	2.815312	1.399711
C	-0.002173	-2.841639	0.000000
H	-1.031300	-3.220520	0.000000
H	0.517797	-3.219778	-0.883278
H	0.517797	-3.219778	0.883278
N	0.038521	-1.400045	0.000000

6

C	-2.477437	-3.093011	0.000000
C	-1.413009	-3.938888	0.000000
C	-1.053761	-1.113669	0.000000
C	-2.308293	-1.677058	0.000000
H	0.622933	-5.439386	0.000000
H	-3.474847	-3.518473	0.000000
H	-1.533589	-5.018247	0.000000
C	0.919389	-4.394418	0.000000
C	1.644004	-1.645691	0.000000
H	-3.196038	-1.048455	0.000000
C	2.592654	-2.626877	0.000000
C	2.221514	-4.011665	0.000000
H	1.963198	-0.605303	0.000000
H	3.654873	-2.389369	0.000000
H	2.984777	-4.782360	0.000000
C	-0.893821	0.302101	0.000000
C	-0.724939	1.506015	0.000000
C	-0.511820	2.904791	0.000000
C	-1.449679	3.911945	0.000000
S	1.100379	3.560822	0.000000
C	-0.867324	5.209808	0.000000
H	-2.514559	3.712327	0.000000
C	0.499644	5.172120	0.000000
H	-1.438704	6.130650	0.000000
H	1.187781	6.006759	0.000000
B	0.173794	-2.037991	0.000000
N	-0.113077	-3.474433	0.000000

7

C	-4.668140	-1.081332	-0.303998
C	-3.288936	-1.269998	-0.272369
C	-2.417011	-0.212254	0.024076
C	-2.976791	1.042716	0.312465
C	-4.353536	1.233813	0.279465
C	-5.207558	0.174122	-0.031545
H	-5.321354	-1.916287	-0.540982
H	-2.873546	-2.251709	-0.488715
H	-2.330995	1.873120	0.583088
H	-4.764808	2.212947	0.508310
H	-6.282661	0.325567	-0.052234

C	-0.968256	-0.461978	0.026701
C	-0.006599	0.475542	-0.003546
H	-0.685780	-1.514306	0.024394
H	-0.298126	1.524056	-0.066216
C	1.441857	0.244373	0.007478
C	2.310635	1.310486	-0.263573
C	2.024161	-1.003229	0.282487
C	3.689824	1.147228	-0.279410
H	1.892829	2.292798	-0.473125
C	3.398947	-1.178976	0.268990
H	1.393449	-1.853566	0.525884
C	4.257285	-0.104701	-0.013324
H	4.335298	1.993138	-0.503539
H	3.821702	-2.157946	0.482707
N	5.637281	-0.295723	-0.081164
H	6.194767	0.536012	0.067315
H	5.989940	-1.081351	0.450843

8

C	3.811954	-0.130557	-0.009403
C	4.382173	-1.305652	-0.433624
C	5.801842	-1.234197	-0.517216
C	2.403438	0.164572	0.203601
C	1.851978	1.128268	1.022292
C	-0.064162	0.160353	0.155432
C	0.438067	1.125776	0.993956
C	-1.455740	-0.162593	-0.132606
O	-2.300220	0.685220	0.579493
O	-1.868893	-1.018742	-0.864529
C	-4.255457	-0.639859	0.995023
C	-4.247276	0.893776	-0.806105
C	-5.629521	-0.746433	0.355583
C	-5.624272	0.251617	-0.816359
H	-5.774096	-1.781609	0.038019
H	-6.385946	-0.521598	1.111774
H	-5.766219	-0.226070	-1.788469
H	-6.377611	1.037399	-0.718565
O	-3.760373	1.667380	-1.585645
O	-3.775771	-1.288316	1.885444
N	-3.609601	0.409280	0.337892
S	1.186775	-0.743423	-0.622402
S	5.023535	1.076900	0.282639
C	6.285071	-0.009173	-0.153776
H	2.447779	1.793639	1.637233
H	-0.193737	1.792247	1.568902
H	3.804218	-2.196711	-0.655345
H	6.433453	-2.058646	-0.825865
H	7.314787	0.320210	-0.121754

9

C	-1.123799	0.853443	-0.021762
C	-2.551030	0.761168	-0.017734
C	-3.141529	-0.542880	0.003862
C	-2.304777	-1.627173	0.019120
C	-0.888539	-1.530564	0.014637
C	-0.251354	-0.298420	-0.005081
H	-2.764198	-2.610267	0.034873
H	-0.309237	-2.445893	0.026249
N	-0.781946	2.115964	-0.042335
N	-3.030623	1.986393	-0.036194

O	-1.939783	2.789132	-0.050897
N	-4.575151	-0.725703	0.009070
O	-5.008543	-1.869841	0.028457
O	-5.260063	0.282164	-0.006387
N	1.080338	-0.104389	-0.008395
H	1.430976	0.845856	-0.035296
C	2.040996	-1.198020	0.001553
H	1.866764	-1.819068	0.890849
H	1.879732	-1.829972	-0.882409
C	3.445955	-0.651043	0.008612
C	4.136536	-0.458929	-1.189858
C	4.052561	-0.289439	1.214367
C	5.419933	0.084708	-1.184339
H	3.667403	-0.738986	-2.130363
C	5.334733	0.255275	1.222301
H	3.517503	-0.438750	2.149733
C	6.019784	0.442068	0.022058
H	5.950978	0.226661	-2.120701
H	5.800006	0.529963	2.164113
H	7.020516	0.863429	0.027586

10

C	-1.337395	-3.692601	0.000000
C	-1.691498	-2.326299	0.000000
C	-0.710379	-1.357603	0.000000
C	0.665178	-1.719723	0.000000
C	1.018622	-3.094621	0.000000
C	-0.014403	-4.069014	0.000000
C	-1.038647	0.060962	0.000000
C	1.695846	-0.738120	0.000000
C	1.370522	0.710538	0.000000
C	3.021383	-1.115361	0.000000
C	3.373253	-2.482160	0.000000
C	2.393940	-3.447804	0.000000
H	2.661282	-4.501648	0.000000
H	4.420722	-2.765595	0.000000
H	-2.118728	-4.445766	0.000000
H	-2.733063	-2.019370	0.000000
H	0.259304	-5.120998	0.000000
O	2.188561	1.604522	0.000000
H	3.783409	-0.341660	0.000000
N	-0.001316	0.995331	0.000000
C	-0.611914	2.248367	0.000000
C	-1.989866	1.972750	0.000000
N	-2.222513	0.604438	0.000000
C	-2.884521	3.042373	0.000000
C	-2.322200	4.313316	0.000000
H	-3.958031	2.888899	0.000000
H	-2.965908	5.189022	0.000000
C	-0.138606	3.560421	0.000000
H	0.921206	3.790040	0.000000
N	-1.001574	4.573352	0.000000

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C	-1.719059	-0.798286	-0.009454
C	-2.336297	0.474094	-0.006951
C	-3.725596	0.607547	0.016721
C	-4.486947	-0.558214	0.024194
C	-3.888935	-1.826382	0.013186
C	-2.502861	-1.951072	-0.001952

C	-0.284916	-0.563323	-0.015074
C	-0.111746	0.860177	-0.015469
H	-2.036435	-2.932683	-0.005355
C	0.816239	-1.387048	-0.013982
C	1.135346	1.443648	0.000866
C	2.115760	-0.824150	-0.007305
C	2.273312	0.599811	0.002390
C	3.279792	-1.644710	-0.004924
C	3.593325	1.135862	0.016000
C	4.535098	-1.095406	0.006714
C	4.691783	0.316082	0.017611
N	-1.359751	1.459029	-0.031883
H	1.266807	2.522290	0.019045
H	3.713795	2.216730	0.024254
H	5.689562	0.745177	0.027163
H	5.412633	-1.734905	0.008106
H	3.150471	-2.724645	-0.012465
H	0.705329	-2.469289	-0.014604
H	-4.206302	1.580638	0.035546
H	-5.570069	-0.479737	0.042712
H	-4.512839	-2.714411	0.020649
C	-1.582765	2.882291	0.006675
H	-0.859197	3.383343	-0.642919
H	-1.486493	3.281147	1.023943
H	-2.583251	3.103059	-0.369796

12

C	2.420942	1.482631	0.000000
C	1.255350	0.737383	0.000000
C	0.001155	1.426171	0.000000
C	-0.019809	2.850484	0.000000
C	1.204427	3.566477	0.000000
C	2.399680	2.892334	0.000000
H	3.386844	0.989516	0.000000
C	-1.238486	0.720789	0.000000
C	-1.265965	3.529752	0.000000
H	1.177632	4.653216	0.000000
H	3.338413	3.437889	0.000000
C	-2.446162	2.827243	0.000000
C	-2.430987	1.417948	0.000000
H	-1.266407	4.617013	0.000000
H	-3.396486	3.352490	0.000000
H	-3.357971	0.854586	0.000000
C	1.263301	-0.741550	0.000000
C	0.018526	-1.443846	0.000000
C	2.429231	-1.487828	0.000000
C	-1.233700	-0.754730	0.000000
C	-0.007767	-2.863638	0.000000
C	2.403746	-2.898049	0.000000
H	3.396465	-0.998002	0.000000
C	-1.272808	-3.502522	0.000000
C	1.213604	-3.582559	0.000000
H	3.344353	-3.441114	0.000000
C	-2.407260	-2.731176	0.000000
H	-1.335731	-4.586820	0.000000
H	1.190699	-4.668897	0.000000
H	-3.392493	-3.190333	0.000000
N	-2.397435	-1.379163	0.000000

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C	-2.251300	-2.595930	0.000000
C	-2.352997	-1.202668	0.000000
C	-1.209914	-0.409599	0.000000
C	0.060140	-1.029812	0.000000
C	0.127499	-2.429726	0.000000
C	-1.012216	-3.225185	0.000000
C	-1.274474	1.067491	0.000000
C	1.303022	-0.283829	0.000000
C	1.225955	1.189985	0.000000
C	-0.057339	1.821479	0.000000
C	2.366460	1.972869	0.000000
C	2.472772	-0.975823	0.000000
C	2.525748	-2.427861	0.000000
H	-0.905484	-4.305781	0.000000
C	-2.479119	1.744655	0.000000
C	-2.540846	3.153617	0.000000
C	-1.386368	3.892172	0.000000
C	-0.123172	3.245343	0.000000
H	-3.509299	3.643969	0.000000
H	-1.418379	4.978578	0.000000
C	2.296644	3.378601	0.000000
H	3.213539	3.959437	0.000000
C	1.074428	4.003424	0.000000
H	1.005332	5.088265	0.000000
H	-3.413880	1.195724	0.000000
H	-3.350986	-0.782671	0.000000
H	3.446262	-0.503663	0.000000
H	3.345938	1.507425	0.000000
O	3.528136	-3.096644	0.000000
O	1.312840	-3.089661	0.000000
O	-3.417977	-3.290404	0.000000
H	-3.242262	-4.242340	0.000000

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C	-4.138496	-1.348099	0.000000
C	-2.838608	-1.763099	0.000000
C	-1.777249	-0.817462	0.000000
C	-2.126259	0.560173	0.000000
C	-3.429216	1.004672	0.000000
C	-4.461598	0.047528	0.000000
C	0.154185	1.091188	0.000000
C	0.458278	-0.309152	0.000000
C	1.862042	-0.696844	0.000000
C	2.868714	0.295941	0.000000
C	2.477437	1.702702	0.000000
C	1.122711	2.070502	0.000000
H	-4.947046	-2.072671	0.000000
H	-2.578006	-2.816640	0.000000
H	-3.639764	2.068986	0.000000
H	0.825675	3.113948	0.000000
N	-0.495082	-1.218989	0.000000
N	-5.753606	0.428024	0.000000
H	-6.500670	-0.251528	0.000000
H	-6.018592	1.402558	0.000000
O	-1.129831	1.480413	0.000000
N	3.408829	2.662295	0.000000
H	4.397376	2.461724	0.000000
H	3.145838	3.638558	0.000000
C	2.221496	-2.053695	0.000000
C	4.218975	-0.103671	0.000000
C	3.553972	-2.422403	0.000000
C	4.558372	-1.443259	0.000000

H	1.435006	-2.800288	0.000000
H	3.824033	-3.473518	0.000000
H	5.603421	-1.734527	0.000000
H	5.023582	0.624796	0.000000

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C	0.000000	3.635796	-1.247143
C	0.000000	2.494159	-1.986235
C	0.000000	1.212197	-1.358709
C	0.000000	1.183154	0.063514
C	0.000000	2.327635	0.835357
C	0.000000	3.579916	0.189274
C	0.000000	0.000000	-2.046535
C	0.000000	-1.183154	0.063514
C	0.000000	-1.212197	-1.358709
C	0.000000	-2.494159	-1.986235
H	0.000000	-2.542664	-3.071456
C	0.000000	-3.635796	-1.247143
C	0.000000	-3.579916	0.189274
C	0.000000	-2.327635	0.835357
H	0.000000	0.000000	-3.135218
H	0.000000	4.606828	-1.733468
H	0.000000	2.542664	-3.071456
H	0.000000	2.236890	1.914619
H	0.000000	-4.606828	-1.733468
H	0.000000	-2.236890	1.914619
N	0.000000	4.727188	0.886930
N	0.000000	-4.727188	0.886930
C	0.000000	4.801792	2.336803
C	0.000000	-4.801792	2.336803
H	0.000000	5.594304	0.367410
H	0.000000	-5.594304	0.367410
O	0.000000	0.000000	0.719083
H	0.000000	5.850867	2.629645
H	0.893535	4.323161	2.751245
H	-0.893535	4.323161	2.751245
H	-0.893535	-4.323161	2.751245
H	0.000000	-5.850867	2.629645
H	0.893535	-4.323161	2.751245

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C	-1.918040	2.409891	0.011443
C	-1.204905	1.077637	-0.005985
C	-1.901945	-0.149754	-0.017504
N	-3.284857	-0.158097	0.005452
C	-3.995694	1.070895	-0.311088
C	-3.375139	2.245094	0.430411
C	0.186018	1.045803	-0.012010
C	0.926918	-0.144320	-0.012330
C	0.204241	-1.349699	-0.014545
C	-1.174769	-1.376407	-0.027286
C	2.363834	-0.016756	-0.012126
C	2.963582	1.191081	-0.015545
C	2.170623	2.419739	-0.020016
O	0.805455	2.264346	-0.018901
C	-4.001107	-1.394681	-0.264940
C	-3.331432	-2.565292	0.438568
C	-1.901837	-2.702972	-0.072464
C	3.211920	-1.265756	-0.008506

O	2.619129	3.536937	-0.024771
H	-5.026781	-1.264386	0.094705
H	-4.053963	-1.586911	-1.351300
H	0.738921	-2.295350	-0.016221
H	4.038640	1.317031	-0.015303
F	2.963558	-2.027514	-1.088803
F	4.522066	-0.994839	-0.006804
F	2.959909	-2.024192	1.073133
H	-3.982316	1.258016	-1.399396
H	-5.039765	0.933433	-0.013103
H	-1.348736	-3.444815	0.513129
H	-1.924005	-3.072170	-1.106994
H	-3.332737	-2.378005	1.518701
H	-3.899683	-3.482423	0.255288
H	-3.939681	3.159025	0.221961
H	-3.439084	2.050704	1.507231
H	-1.396479	3.095751	0.685402
H	-1.861395	2.866287	-0.985957

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C	0.433847	-0.042019	3.532424
C	-0.778104	-0.075246	2.851166
C	-0.793466	-0.071020	1.452292
C	0.429925	-0.034735	0.715466
C	1.652795	0.000583	1.438676
C	1.640699	-0.003467	2.838802
C	-1.983568	-0.105631	0.675546
C	0.429925	-0.034735	-0.715466
C	-0.793466	-0.071020	-1.452292
C	-1.983568	-0.105631	-0.675546
C	-0.778104	-0.075246	-2.851166
H	-1.720441	-0.104658	-3.389446
C	0.433847	-0.042019	-3.532424
C	1.640699	-0.003467	-2.838802
C	1.652795	0.000583	-1.438676
C	2.886846	0.038219	-0.685470
C	2.886846	0.038219	0.685470
H	0.441914	-0.045318	4.617765
H	-1.720441	-0.104658	3.389446
H	2.580787	0.023251	3.381838
H	0.441914	-0.045318	-4.617765
H	2.580787	0.023251	-3.381838
O	-3.260934	-0.176211	1.154061
O	-3.260934	-0.176211	-1.154061
C	-4.115092	0.015528	0.000000
C	-4.625615	1.443296	0.000000
H	-5.232052	1.621088	-0.891989
H	-5.232052	1.621088	0.891989
H	-3.779594	2.136818	0.000000
C	-5.191542	-1.042435	0.000000
H	-5.816181	-0.933599	0.890402
H	-5.816181	-0.933599	-0.890402
H	-4.732640	-2.033496	0.000000
C	4.130708	0.075477	1.406235
N	5.113025	0.105009	2.017357
C	4.130708	0.075477	-1.406235
N	5.113025	0.105009	-2.017357

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C	5.516433	-2.544408	0.021683

C	5.926315	-1.331367	-0.452413
C	4.857231	-0.394025	-0.551387
C	3.651515	-0.912220	-0.148611
S	3.828997	-2.559382	0.369399
H	6.110731	-3.431922	0.191469
H	6.951063	-1.113283	-0.729338
H	4.968153	0.617852	-0.926694
C	2.350043	-0.262424	-0.117367
C	1.108854	-0.835151	-0.170456
S	2.230415	1.466462	-0.013254
C	0.032986	0.109555	-0.154002
H	0.962407	-1.904344	-0.284238
C	0.496358	1.410842	-0.090807
C	-0.244543	2.664988	-0.049497
C	0.082612	3.848280	-0.667534
S	-1.672565	2.859016	0.924967
C	-0.825293	4.904623	-0.371434
H	0.938091	3.944653	-1.327653
C	-1.826280	4.511746	0.471239
H	-0.742594	5.906825	-0.775307
H	-2.652678	5.100327	0.846456
C	-1.380982	-0.247374	-0.258452
C	-1.883094	-1.456254	0.044115
H	-2.045678	0.541482	-0.603424
H	-1.213376	-2.218994	0.441543
C	-3.290282	-1.863626	-0.070895
C	-3.691476	-3.079597	0.500234
C	-4.258752	-1.089135	-0.729406
C	-5.015589	-3.505232	0.432751
H	-2.952138	-3.694128	1.008861
C	-5.581044	-1.512212	-0.797116
H	-3.975164	-0.154549	-1.204629
C	-5.967544	-2.721092	-0.214941
H	-5.302604	-4.449700	0.885871
H	-6.314528	-0.899467	-1.313294
H	-7.000961	-3.049603	-0.272624

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C	1.835835	-0.696774	0.000476
C	1.362577	0.622551	0.000712
C	-0.003313	0.845939	0.000624
C	-0.889845	-0.241647	0.000286
C	-0.301303	-1.516237	0.000082
N	1.006811	-1.747540	0.000170
H	-0.378489	1.865759	0.000834
H	2.075028	1.439323	0.000971
H	-0.940728	-2.398643	-0.000170
C	3.295596	-0.984413	0.000569
C	3.766543	-2.303430	0.000363
N	4.122414	0.067173	0.000858
C	5.136295	-2.520344	0.000465
H	3.054918	-3.120907	0.000130
C	5.434296	-0.163024	0.000951
C	6.014876	-1.433437	0.000767
H	5.529069	-3.535318	0.000310
H	6.071240	0.721031	0.001185
C	7.508646	-1.616201	0.000891
H	7.837311	-2.174144	0.884089
H	7.837493	-2.173826	-0.882442
H	8.023451	-0.651427	0.001115
C	-2.347788	-0.132169	0.000140
C	-3.058701	1.011046	0.000084

H	-2.883773	-1.080782	0.000049
H	-2.527984	1.961702	0.000114
C	-4.506385	1.085947	-0.000016
C	-5.477502	0.091674	0.000178
N	-5.166829	2.299359	-0.000354
C	-6.741673	0.720795	-0.000054
H	-5.286377	-0.972768	0.000480
C	-6.515150	2.082767	-0.000385
H	-7.709498	0.239877	0.000017
H	-7.204540	2.915555	-0.000636
C	-4.540781	3.606890	-0.000653
H	-3.923486	3.744006	0.891941
H	-3.923304	3.743507	-0.893197
H	-5.325829	4.364241	-0.000943

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N	1.705485	-0.002760	-0.000521
C	2.462012	-1.201767	-0.011773
C	3.611667	-1.318173	0.778242
C	2.070618	-2.278474	-0.816349
C	4.358732	-2.492348	0.755849
H	3.914600	-0.482990	1.403361
C	2.813697	-3.455248	-0.818731
H	1.182431	-2.185919	-1.435006
C	3.963148	-3.569004	-0.037208
H	5.249324	-2.568415	1.373006
H	2.497687	-4.283079	-1.446959
H	4.544420	-4.485727	-0.047014
C	2.373698	1.247857	0.010362
C	1.914808	2.288671	0.826347
C	3.503025	1.451217	-0.791139
C	2.571362	3.515836	0.828957
H	1.042441	2.128454	1.453658
C	4.163996	2.675950	-0.768773
H	3.858127	0.643463	-1.424837
C	3.700878	3.716528	0.035952
H	2.203802	4.315053	1.466141
H	5.039869	2.819768	-1.394846
H	4.214777	4.672658	0.045726
C	0.295993	-0.053328	0.005300
C	-0.456021	0.890422	-0.707277
C	-0.380674	-1.045614	0.728624
C	-1.843408	0.839920	-0.694161
H	0.055123	1.660322	-1.277550
C	-1.767755	-1.092214	0.732202
H	0.189596	-1.772885	1.298912
C	-2.526698	-0.154117	0.018522
H	-2.404234	1.568735	-1.274279
H	-2.273105	-1.848861	1.325993
C	-3.991910	-0.233987	0.020444
C	-4.785220	-1.346833	0.120295
S	-5.013808	1.162525	-0.103086
H	-4.409722	-2.361582	0.184927
C	-6.400358	0.127737	-0.014634
H	-7.401804	0.539302	-0.056409
N	-6.141361	-1.137582	0.102201

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C	0.246150	4.797895	0.699720
C	0.246150	4.797895	-0.699720

C	0.131341	3.602183	1.396714
C	0.131341	3.602183	-1.396714
C	0.016622	2.396252	0.697992
C	0.016622	2.396252	-0.697992
C	-0.105938	1.125096	1.461659
C	-0.105938	1.125096	-1.461659
C	-0.212458	-0.137280	0.720669
C	-0.212458	-0.137280	-0.720669
C	-0.311429	-1.351384	1.441018
C	-0.311429	-1.351384	-1.441018
C	-0.400919	-2.555109	0.682196
C	-0.400919	-2.555109	-0.682196
H	0.127653	3.574859	2.481407
H	0.127653	3.574859	-2.481407
H	0.335842	5.734577	1.242123
H	0.335842	5.734577	-1.242123
H	-0.471926	-3.506487	1.197184
H	-0.471926	-3.506487	-1.197184
O	-0.109412	1.182880	2.696830
O	-0.109412	1.182880	-2.696830
N	-0.340395	-1.412799	2.801109
N	-0.340395	-1.412798	-2.801109
H	-0.247388	-0.522433	3.277268
H	-0.247388	-0.522433	-3.277268
C	-0.344592	-2.635417	3.577834
H	-0.660276	-2.361020	4.588235
H	-1.111913	-3.319412	3.194634
C	-0.344592	-2.635417	-3.577834
H	-1.111913	-3.319411	-3.194634
H	-0.660276	-2.361020	-4.588235
C	1.018670	-3.327815	3.635277
H	0.959104	-4.249352	4.223670
H	1.378833	-3.581562	2.633431
H	1.757813	-2.667370	4.097742
C	1.018670	-3.327815	-3.635277
H	1.378833	-3.581562	-2.633431
H	0.959104	-4.249352	-4.223670
H	1.757813	-2.667369	-4.097742

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C	0.000000	0.000000	0.700257
C	-1.196818	0.136580	-0.022626
C	-1.201662	0.134221	-1.409557
C	0.000000	0.000000	-2.117278
C	1.201662	-0.134221	-1.409557
C	1.196818	-0.136580	-0.022626
C	0.000000	0.000000	2.177110
C	-1.046396	-0.573706	2.910173
C	-1.055406	-0.579468	4.296836
C	0.000000	0.000000	5.037529
C	1.055406	0.579468	4.296836
C	1.046396	0.573706	2.910173
H	-2.131478	0.274355	0.513398
H	-2.130819	0.248428	-1.958118
H	2.130819	-0.248428	-1.958118
H	2.131478	-0.274355	0.513398
H	-1.870293	-1.050974	2.385374
H	-1.898226	-1.034562	4.803843
H	1.898226	1.034562	4.803843
H	1.870293	1.050974	2.385374
N	0.000000	0.000000	6.415198
C	0.000000	0.000000	-3.587077

C	-1.095977	0.125394	-5.538723
C	1.095977	-0.125394	-5.538723
N	0.000000	0.000000	-6.277232
N	1.175814	-0.133923	-4.224054
N	-1.175814	0.133923	-4.224054
Cl	-2.580384	0.296165	-6.408490
Cl	2.580384	-0.296165	-6.408490
C	-1.015349	-0.708412	7.176181
C	1.015349	0.708412	7.176181
C	-2.275346	0.124249	7.415668
C	2.275346	-0.124249	7.415668
H	-0.568273	-0.990369	8.136272
H	-1.258278	-1.649103	6.670901
H	0.568273	0.990369	8.136272
H	1.258278	1.649103	6.670901
H	2.031270	-1.032629	7.976141
H	3.015070	0.444118	7.988929
H	2.728613	-0.428724	6.467626
H	-3.015070	-0.444118	7.988929
H	-2.031270	1.032629	7.976141
H	-2.728613	0.428724	6.467626

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C	-0.143287	0.763820	-1.021638
C	0.143287	-0.763820	-1.021638
C	0.030067	-1.198937	0.419517
C	0.000000	0.000000	1.300990
C	-0.030067	1.198937	0.419517
O	0.000000	0.000000	2.519904
C	-0.024326	-2.442119	0.931588
C	0.009711	-3.666662	0.160691
H	-0.097168	-2.525576	2.016936
H	0.088297	-3.574262	-0.921327
C	-0.046054	-4.881747	0.742027
H	-0.119625	-4.916663	1.829715
C	0.024326	2.442119	0.931588
C	-0.009711	3.666662	0.160691
H	0.097168	2.525576	2.016936
H	-0.088297	3.574262	-0.921327
C	0.046054	4.881747	0.742027
H	0.119625	4.916663	1.829715
C	-0.016851	-6.188408	0.077591
C	0.065261	-6.339242	-1.316471
C	-0.073633	-7.345736	0.867815
C	0.090059	-7.602936	-1.893284
H	0.109538	-5.463072	-1.956574
C	-0.048859	-8.612747	0.291411
H	-0.137620	-7.244925	1.948716
C	0.033265	-8.746146	-1.092719
H	0.153728	-7.699573	-2.973211
H	-0.093577	-9.494641	0.923563
H	0.052764	-9.732039	-1.547434
C	0.016851	6.188408	0.077591
C	-0.065261	6.339242	-1.316471
C	0.073633	7.345736	0.867815
C	-0.090059	7.602936	-1.893284
H	-0.109538	5.463072	-1.956574
C	0.048859	8.612747	0.291411
H	0.137620	7.244925	1.948716
C	-0.033265	8.746146	-1.092719
H	-0.153728	7.699573	-2.973211
H	0.093577	9.494641	0.923563

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H	-0.547932	-1.303319	-1.676710
H	1.156769	-0.958412	-1.394242
H	-1.156769	0.958412	-1.394242
H	0.547932	1.303319	-1.676710

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C	-1.705242	-4.147340	0.317485
C	-0.343088	-4.193386	-0.137272
C	0.303642	-3.023910	-0.585494
C	-0.436554	-1.867125	-0.559341
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C	-2.418026	-2.980762	0.332797
H	-2.167205	-5.070258	0.654359
H	1.330561	-3.031121	-0.933525
H	-3.446004	-2.960339	0.678702
C	-0.996327	0.232298	-0.778867
C	-1.047104	1.580694	-1.029690
C	-2.266600	2.246688	-0.746557
C	-3.367164	1.513615	-0.220407
C	-2.119466	-0.448895	-0.262429
O	0.029227	-0.646985	-0.956203
N	0.307278	-5.374528	-0.128570
H	-0.142047	-6.220413	0.190672
H	1.265050	-5.451445	-0.439403
O	-3.258054	0.163028	0.006946
C	0.134555	2.350243	-1.588679
F	0.494535	3.326909	-0.745863
F	-0.191229	2.918681	-2.756680
F	1.187763	1.564859	-1.788250
C	-2.495435	3.636526	-0.950363
C	-3.695668	4.216988	-0.657234
H	-1.696012	4.255695	-1.341086
H	-3.800477	5.282425	-0.815416
C	-4.586870	2.073829	0.082214
C	-4.796508	3.458752	-0.126521
H	-5.363633	1.418703	0.454118
N	-5.972593	4.047665	0.161907
C	-6.240948	5.456492	-0.144273
C	-5.786438	6.393196	0.971602
H	-7.320565	5.543330	-0.297737
H	-5.778876	5.713173	-1.100810
H	-6.024684	7.429553	0.716767
H	-6.291559	6.148460	1.910852
H	-4.707930	6.317766	1.139734
C	-7.064728	3.310922	0.801029
C	-7.945481	2.579875	-0.209535
H	-7.655308	4.041990	1.360780
H	-6.646919	2.624916	1.543326
H	-8.753992	2.052209	0.303989
H	-8.393741	3.287986	-0.912846
H	-7.368574	1.851766	-0.787510

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C	0.000000	3.881093	-1.850088
C	0.000000	4.985732	0.240238
C	0.000000	3.730745	0.907779
C	0.000000	2.486980	0.144103
C	0.000000	2.645311	-1.265379
H	0.000000	7.144322	0.493465

H	0.000000	3.974138	-2.927312
C	0.000000	6.182252	0.988031
C	0.000000	3.741771	2.320622
H	0.000000	1.789226	-1.926808
C	0.000000	4.914948	3.042629
C	0.000000	6.143824	2.366831
H	0.000000	2.804142	2.861412
H	0.000000	4.887014	4.126997
H	0.000000	7.074356	2.925419
C	0.000000	1.226010	0.770148
C	0.000000	0.000000	0.110449
H	0.000000	1.181795	1.853085
H	0.000000	0.000000	-0.976588
C	0.000000	-1.226010	0.770148
H	0.000000	-1.181795	1.853085
N	0.000000	5.034723	-1.151266
C	0.000000	6.351123	-1.826153
C	0.000000	6.297608	-3.344343
H	0.885143	6.893643	-1.479821
H	-0.885143	6.893643	-1.479821
H	0.000000	7.327373	-3.709923
H	0.892809	5.808729	-3.743691
H	-0.892809	5.808729	-3.743691
C	0.000000	-2.486980	0.144103
C	0.000000	-3.730745	0.907779
C	0.000000	-2.645311	-1.265379
C	0.000000	-3.741771	2.320622
C	0.000000	-4.985732	0.240238
C	0.000000	-3.881093	-1.850088
H	0.000000	-1.789226	-1.926808
C	0.000000	-4.914948	3.042629
H	0.000000	-2.804142	2.861412
C	0.000000	-6.182252	0.988031
H	0.000000	-3.974138	-2.927312
C	0.000000	-6.143824	2.366831
H	0.000000	-4.887014	4.126997
H	0.000000	-7.144322	0.493465
H	0.000000	-7.074356	2.925419
N	0.000000	-5.034723	-1.151266
C	0.000000	-6.351123	-1.826153
C	0.000000	-6.297608	-3.344343
H	-0.885143	-6.893643	-1.479821
H	0.885143	-6.893643	-1.479821
H	0.000000	-7.327373	-3.709923
H	-0.892809	-5.808729	-3.743691
H	0.892809	-5.808729	-3.743691

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