Excited-State Dipole and Quadrupole Moments: TD-DFT versus CC2: Supporting Information

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S1 Impact of the geometry optimization level

Table S-1: Ground-state dipole moments, μ^{GS}, and excites-state dipole moments μ^{ES} in Debye, for the three first compounds using three different GS geometries and four different levels of theory.

		BLYP/6-31+G(d) geom.				B3LYP/6-31+G(d) geom.				M06-2X/6-31+G(d) geom.			
Mol.	State	CC2	BLYP	B3LYP	M06-2X	CC2	BLYP	B3LYP	M06-2X	CC2	BLYP	B3LYP	M06-2X
						μ^{GS}							
1		4.24	4.28	4.46	4.56	4.15	4.19	4.36	4.46	4.02	4.05	4.22	4.32
2		4.27	4.70	4.72	4.60	4.29	4.68	4.70	4.57	4.22	4.59	4.60	4.47
3		2.33	2.79	2.56	2.33	2.31	2.76	2.54	2.31	2.23	2.65	2.44	2.23
						μ^{ES}							
1	B_2 ($\pi \rightarrow \pi^\star$)	4.08	4.11	4.25	4.24	3.99	4.02	4.16	4.14	3.87	3.91	4.02	4.00
2	A'($\pi \rightarrow \pi^\star$)	7.05	7.38	6.88	6.64	7.06	7.51	6.96	6.65	6.99	7.65	7.02	6.64
	A" ($n \rightarrow \pi^\star$)	1.22	1.07	0.97	0.97	1.28	1.17	1.02	0.97	1.29	1.23	1.02	0.95
3	A ($\pi \rightarrow \pi^\star$)	6.74	8.87	6.68	5.38	6.66	9.16	6.84	5.43	6.43	9.83	7.15	5.44

S2 Results for the first set of compounds

Table S-2: Ground-state dipole moments, μ^{GS}, given in Debye, for the first fifteen compounds treated.

	CC2	SVWN5	BLYP	BP86	OLYP	M06-L	M11-L	B3LYP	PBE0	M06	BMK	SOGGA11-X	M06-2X	M06-HF	CAM-B3LYP	M11	ωB97X-D
1	4.02	4.07	4.05	4.00	4.01	4.07	3.97	4.22	4.21	4.25	4.36	4.27	4.32	4.46	4.37	4.43	4.32
2	4.22	4.62	4.59	4.55	4.54	4.50	4.50	4.60	4.55	4.51	4.62	4.56	4.47	4.50	4.56	4.54	4.50
3	2.23	2.78	2.65	2.71	2.68	2.64	2.72	2.44	2.72	2.39	2.27	2.30	2.23	1.99	2.24	2.13	2.24
4	8.25	8.58	8.47	8.42	8.41	8.42	8.43	8.77	8.77	8.63	9.09	8.91	8.91	9.35	8.95	9.06	8.85
5	3.53	3.78	3.81	3.75	3.74	3.83	3.85	4.03	4.00	4.04	4.19	4.14	4.04	4.26	4.10	4.09	4.04
6	3.60	3.96	3.79	3.83	3.79	3.57	3.29	3.46	3.40	3.14	3.30	3.13	3.08	2.91	3.14	3.08	3.12
7	2.05	2.06	2.00	2.03	2.01	1.95	1.92	1.93	1.93	1.82	1.89	1.86	1.87	1.84	1.86	1.85	1.85
8	4.62	5.03	4.95	4.93	4.92	4.85	4.87	4.96	4.93	4.87	4.98	4.92	4.87	4.96	4.88	4.84	4.83
9	8.28	7.13	7.20	7.20	7.24	7.51	7.65	8.12	8.33	8.41	8.90	8.99	9.12	9.71	9.21	9.50	9.36
10	9.15	10.22	10.09	10.03	10.02	9.93	9.84	10.09	10.02	9.90	10.14	9.95	9.96	10.17	9.95	9.95	9.80
11[a]	0.00[b]	1.10	0.92	1.01	0.96	0.80	0.70	0.57	0.59	0.42	0.37	0.34	0.38	0.25	0.26	0.27	0.28
12	2.02	1.99	1.94	1.96	1.94	1.89	1.86	1.89	1.90	1.80	1.87	1.85	1.86	1.88	1.85	1.86	1.85
13	4.46	5.07	5.09	5.00	4.99	4.93	4.95	5.03	4.92	4.92	4.94	4.91	4.75	4.74	4.86	4.72	4.75
14	4.68	5.16	5.10	5.09	5.07	5.04	4.98	5.10	5.07	4.99	5.11	5.04	4.96	5.00	5.02	4.99	4.97
15	1.90	1.71	1.75	1.75	1.79	1.75	1.72	1.88	1.91	1.76	2.05	1.98	1.99	2.20	1.97	2.07	2.00

[a]Taken at the center of mass (charged molecule); [b]0.0046 D

Table S-3: Excited-state dipole moments, μ^{ES}, given in Debye, for the first fifteen compounds treated.

	State	CC2	SVWN5	BLYP	BP86	OLYP	M06-L	M11-L	B3LYP	PBE0	M06	BMK	SOGGA11-X	M06-2X	M06-HF	CAM-B3LYP	M11	ωB97X-D
1	B_2 ($\pi \rightarrow \pi^\star$)	3.87	3.92	3.91	3.84	3.87	3.93	3.79	4.02	3.98	3.99	4.07	3.98	4.00	4.05	4.03	4.02	3.97
2	$A'(\pi \rightarrow \pi^\star)$	6.99	7.87	7.65	7.62	7.60	7.41	7.05	7.02	6.90	6.78	6.81	6.71	6.64	6.49	6.60	6.43	6.43
	A" ($n \rightarrow \pi^\star$)	1.29	1.23	1.23	1.27	1.27	1.28	1.33	1.02	1.02	1.01	0.96	0.95	0.95	0.59	1.01	0.98	1.01
3	A ($\pi \rightarrow \pi^\star$)	6.43	10.27	9.83	10.15	9.51	9.94	5.20[a]	7.15	6.96	6.66[b]	5.93	5.59	5.44	4.07	5.09	4.38	4.91
4	A ($\pi \rightarrow \pi^\star$)	8.64	9.12	8.93	8.89	8.81	8.83	5.20[a]	9.21	9.19	9.00	9.56	9.26	9.38	9.80	9.37	9.48	9.25
	A ($n \rightarrow \pi^\star$)	5.79	5.77	5.61	5.58	5.54	5.55	5.19[a]	6.10	6.15	5.90	6.66	6.34	6.58	6.89	6.51	6.73	6.38
5	A ($n \rightarrow \pi^\star$)	1.31	1.89	1.84	1.92	1.92	1.92	2.05	1.10	0.99	0.96	0.15	0.37	0.29	1.43	0.16	0.58	0.22
	A ($\pi \rightarrow \pi^\star$)	4.70[c]	4.96	4.98	4.89	4.89	4.99	4.63	5.19	5.14	5.10	5.40	5.22	5.30	5.47	5.25	5.28	5.17
6	A ($\pi \rightarrow \pi^\star$)	6.39	5.54	5.52	5.54	5.58	5.60	5.52	5.62	5.66	5.50	5.74	5.72	5.77	5.95	5.50	5.56	5.39
7	A ($\pi \rightarrow \pi^\star$)	3.81	4.09	3.94	4.03	3.96	3.98	3.58	3.69	3.69	3.38	3.61	3.45	3.48	3.27	3.46	3.47	3.46
8	A ($\pi \rightarrow \pi^\star$)	8.44	9.96	9.91	9.83	9.82	9.86	9.29	9.58	9.44	9.09	9.23	8.98	8.67	8.05	8.76	8.30	8.63
9	A_1 ($\pi \rightarrow \pi^\star$)	4.31	2.32	2.17	2.19	2.09	1.68	2.31	2.49	2.25	2.31	0.83	1.11	0.20	1.52	0.11	1.02	0.12
	B_1 ($\pi \rightarrow \pi^\star$)	5.52	0.74	0.56	0.60	0.75	0.73	1.67	1.95	2.04	2.86	2.71	3.13	1.52	3.16	2.94	3.16	2.69
10	A ($\pi \rightarrow \pi^\star$)	13.31	12.63	12.48	12.36	12.31	12.21	11.82	12.37	12.30	12.05	12.61	12.25	12.60	13.13	12.44	12.65	12.28
11	B_2 ($\pi \rightarrow \pi^\star$)	1.32	2.36	2.16	2.27	2.22	2.12	2.11	1.87	1.90	1.70	1.69	1.65	1.68	1.56	1.56	1.63	1.61
12	A' ($\pi \rightarrow \pi^\star$)	3.03	3.23	3.13	3.17	3.14	3.09	3.12	3.06	3.07	2.72	2.97	2.94	2.88	2.76	2.90	2.82	2.90
13	A ($n \rightarrow \pi^\star$)	0.47	3.24	3.17	3.30	3.38	3.22	3.17	0.81	1.54[d]	0.61	1.27	0.57	0.81	0.79	0.76	0.92	0.72
	A ($\pi \rightarrow \pi^\star$)	9.11	10.36	10.30	10.21	10.25	10.13	8.89	8.47	6.39[d]	7.90	7.24	7.67	7.59	7.03	7.36	6.94	7.04
14	A ($\pi \rightarrow \pi^\star$)	8.45	9.71	9.44	9.48	9.38	9.09	7.87	7.80	7.60	7.07	7.28	7.01	7.00	6.61	6.76	6.47	6.59
15	A' ($\pi \rightarrow \pi^\star$)	0.87	7.84	7.70	7.53	7.55	6.69	6.52	3.05	2.42	1.66	1.04	0.91	0.62	0.95	0.54	0.77	0.62

[a]M11-L provides a different picture for the low-lying $\pi \rightarrow \pi^\star$ ES in these two compounds, and no direct comparison is therefore possible; [b]Average value from two nearly-degenerate ES at 3.59 eV (μ^{ES} = 10.91 D) and 3.64 eV (μ^{ES} = 2.41 D); [c]Average value from two nearly-degenerate ES at 4.11 eV (μ^{ES} = 4.71 D) and 4.12 eV (μ^{ES} = 4.69 D); [d]PBE0 foresees these two ES at almost the same energy (3.24 and 3.25 eV), and as a consequence of the lack of symmetry, they are strongly mixed.

Table S-4: Statistical analysis obtained for the compounds of Scheme 1 (Tables S-2 and S-3). MSE, MAE, Max(+) and Max(-) give the mean signed error, mean absolute error, maximal positive and negative deviations, respectively, whereas R^2 is the linear determination coefficients. The TD-DFT errors are given with respect to CC2, and are in D (but R^2).

	μ^{GS}					μ^{ES}				
	MSE	MAE	Max(+)	Max(-)	R^2	MSE	MAE	Max(+)	Max(-)	R^2
SVWN5	0.283	0.464	1.100	-1.144	0.958	0.649	1.488	6.967	-4.782	0.621
BLYP	0.225	0.406	0.937	-1.080	0.965	0.520	1.423	6.824	-4.962	0.623
BP86	0.216	0.394	1.006	-1.075	0.965	0.531	1.440	6.656	-4.916	0.619
OLYP	0.205	0.376	0.957	-1.036	0.968	0.488	1.396	6.678	-4.775	0.627
M06-L	0.177	0.334	0.791	-0.768	0.977	0.410	1.366	5.818	-4.794	0.649
M11-L[a]	0.148	0.344	0.693	-0.627	0.979	0.090	1.129	5.648	-3.850	0.649
B3LYP	0.271	0.347	0.939	-0.157	0.987	-0.124	0.775	2.176	-3.569	0.882
PBE0[a]	0.282	0.341	0.864	-0.203	0.989	-0.209	0.783	1.543	-3.481	0.859
M06	0.188	0.328	0.747	-0.459	0.989	-0.390	0.707	0.789	-2.664	0.927
BMK	0.337	0.420	0.993	-0.304	0.992	-0.415	0.896	0.919	-3.482	0.878
SOGGA11-X	0.275	0.386	0.794	-0.469	0.991	-0.511	0.793	0.625	-3.200	0.910
M06-2X	0.252	0.369	0.839	-0.525	0.991	-0.633	0.953	0.791	-4.114	0.853
M06-HF	0.347	0.519	1.436	-0.696	0.985	-0.524	0.919	1.162	-2.794	0.883
CAM-B3LYP	0.281	0.390	0.938	-0.459	0.992	-0.647	0.949	0.733	-4.204	0.874
M11	0.291	0.422	1.222	-0.518	0.990	-0.624	0.950	0.937	-3.290	0.881
ωB97X-D	0.250	0.362	1.080	-0.477	0.991	-0.732	0.982	0.610	-4.190	0.866

[a]For both M11-L and PBE0, the problematic data have been removed for the statistics of μ^{ES} (see footnotes [a] and [d] in Table S-3).

S3 Results for the second set of compounds

Table S-5: Ground-state dipole moments, μ^{GS}, given in Debye, for the second set of compounds treated.

	CC2	B3LYP	PBE0	M06	BMK	SOGGA11-X	M06-2X	M06-HF	CAM-B3LYP	M11	ωB97X-D
16	2.18	2.12	2.12	2.01	2.10	2.06	2.09	2.18	2.07	2.14	2.08
17	7.88	8.19	8.12	7.74	7.86	7.72	7.53	7.24	7.52	7.32	7.41
18	0.61	0.69	0.72	0.58	0.72	0.73	0.66	0.66	0.69	0.67	0.71
19	1.31	1.39	1.47	1.23	1.51	1.49	1.38	1.47	1.43	1.44	1.48
20	6.06	6.49	6.48	6.48	6.66	6.65	6.51	6.68	6.62	6.59	6.57
21	7.09	7.30	7.26	7.01	7.27	7.05	7.05	7.07	7.05	7.11	6.96
22	3.51	3.72	3.71	3.67	3.78	3.70	3.67	3.76	3.67	3.66	3.62
23	0.86	1.13	1.06	1.02	0.91	0.98	0.83	0.65	0.87	0.71	0.84
24	1.92	1.89	1.89	1.88	1.94	1.88	1.89	1.93	1.93	1.94	1.91
25	8.39	8.44	8.34	8.04	8.18	7.96	7.85	7.51	7.87	7.82	7.76
26	2.48	2.41	2.45	2.42	2.43	2.42	2.45	2.47	2.48	2.51	2.50
27	4.78	4.99	5.00	4.87	5.04	4.94	4.91	4.99	4.95	4.99	4.91
28	9.46	9.54	9.53	9.35	9.46	9.34	9.21	8.94	9.27	9.20	9.25
29	3.15	3.16	3.18	3.16	3.32	3.26	3.26	3.40	3.29	3.36	3.29
30	2.73	2.71	2.66	2.63	2.71	2.58	2.62	2.65	2.65	2.68	2.60
31	4.75	5.33	5.27	5.25	5.46	5.38	5.26	5.44	5.36	5.33	5.26

Table S-6: Excited-state dipole moments, μ^{ES}, given in Debye, for the second set of compounds treated.

	State	CC2	B3LYP	PBE0	M06	BMK	SOGGA11-X	M06-2X	M06-HF	CAM-B3LYP	M11	ωB97X-D
16	A ($\pi \rightarrow \pi^\star$)	8.86	9.08	8.59	7.44	7.15	6.83	6.25	4.48	5.66	4.56	5.21
17	A ($\pi \rightarrow \pi^\star$)	29.69	28.14	28.06	27.09	26.79	25.93	24.81	18.63	23.58	19.88	21.52
18	A ($\pi \rightarrow \pi^\star$)	0.63	1.50	1.47	0.85	0.95	0.86	0.80	0.61	0.71	0.62	0.73
19	A" ($\pi \rightarrow \pi^\star$)	1.53	1.52	1.61	1.31	1.64	1.60	1.52	1.61	1.55	1.58	1.60
20	A' ($\pi \rightarrow \pi^\star$)	5.14	4.13	4.19	4.32	5.15	4.84	5.85	6.71	5.62	6.28	5.74
21	A ($\pi \rightarrow \pi^\star$)	14.82	13.11	13.06	12.21	12.93	12.45	12.34	11.78	12.18	11.70	11.91
22	A ($n \rightarrow \pi^\star$)	1.82	1.74	1.82	1.74	2.13	1.98	2.16	2.25	2.09	2.24	2.06
	B ($\pi \rightarrow \pi^\star$)	4.93	4.64	4.68	4.63	4.87	4.73	4.72	4.61	4.70	4.59	4.63
23	A ($\pi \rightarrow \pi^\star$)	6.25	5.59	5.32	4.83	4.76	4.52	4.46	3.51	4.12	3.55	3.87
24	A' ($\pi \rightarrow \pi^\star$)	2.11	1.87	1.87	1.83	1.93	1.85	1.85	1.80	1.90	1.87	1.91
25	A ($\pi \rightarrow \pi^\star$)	16.71	12.99	12.98	12.47	12.96	12.67	12.73	12.61	12.54	12.39	12.19
26	A ($\pi \rightarrow \pi^\star$)	4.90	9.10	8.06	7.22	5.54	5.53	4.57	2.63	4.08	2.95	3.44
27	A" ($\pi \rightarrow \pi^\star$)	7.02	6.36	4.75[a]	4.44[a]	6.66	6.27	6.63	6.75	6.53	6.45	6.42
28	A" ($\pi \rightarrow \pi^\star$)	18.91	18.87	18.71	18.18	17.90	17.65	17.03	14.58	17.07	16.02	16.73
29	A ($\pi \rightarrow \pi^\star$)	3.18	3.32	3.19	2.90	2.94	2.78	2.70	2.60	2.71	2.56	2.66
30	A ($\pi \rightarrow \pi^\star$)	9.77	13.11	12.24	11.47	10.36	10.10	9.00	6.94	8.73	7.63	8.03
31	A' ($\pi \rightarrow \pi^\star$)	6.48	5.97	5.89	5.86	6.22	6.05	6.10	6.41	6.14	6.12	6.06

[a]Strong state-mixing with both PBE0 and M06.

Table S-7: Statistical analysis obtained for the compounds of Scheme 2 (Tables S-5 and S-6). See caption of Table S-4 for more details.

	μ^{GS}					μ^{ES}				
	MSE	MAE	Max(+)	Max(-)	R^2	MSE	MAE	Max(+)	Max(-)	R^2
B3LYP	0.148	0.170	0.583	-0.067	0.996	-0.099	1.133	4.199	-3.724	0.947
PBE0[a]	0.133	0.162	0.522	-0.071	0.997	-0.249	1.067	3.158	-3.731	0.963
M06[a]	0.012	0.156	0.503	-0.352	0.994	-0.712	1.242	2.321	-4.248	0.967
BMK	0.138	0.184	0.711	-0.205	0.993	-0.698	0.931	0.642	-3.750	0.985
SOGGA11-X	0.062	0.200	0.630	-0.431	0.991	-0.947	1.114	0.632	-4.040	0.984
M06-2X	0.001	0.185	0.516	-0.543	0.992	-1.130	1.275	0.713	-4.877	0.986
M06-HF	-0.005	0.288	0.697	-0.882	0.980	-2.013	2.257	1.565	-11.056	0.938
CAM-B3LYP	0.036	0.197	0.613	-0.517	0.990	-1.343	1.441	0.477	-6.106	0.981
M11	0.020	0.225	0.582	-0.569	0.988	-1.867	2.055	1.136	-9.810	0.952
ωB97X-D	0.000	0.212	0.508	-0.625	0.990	-1.648	1.766	0.597	-8.166	0.970

[a]For both PBE0 and M06 the problematic data have been removed for the statistics of μ^{ES} (see footnote [a] in Table S-6).

S4 Error patterns for the GS dipoles

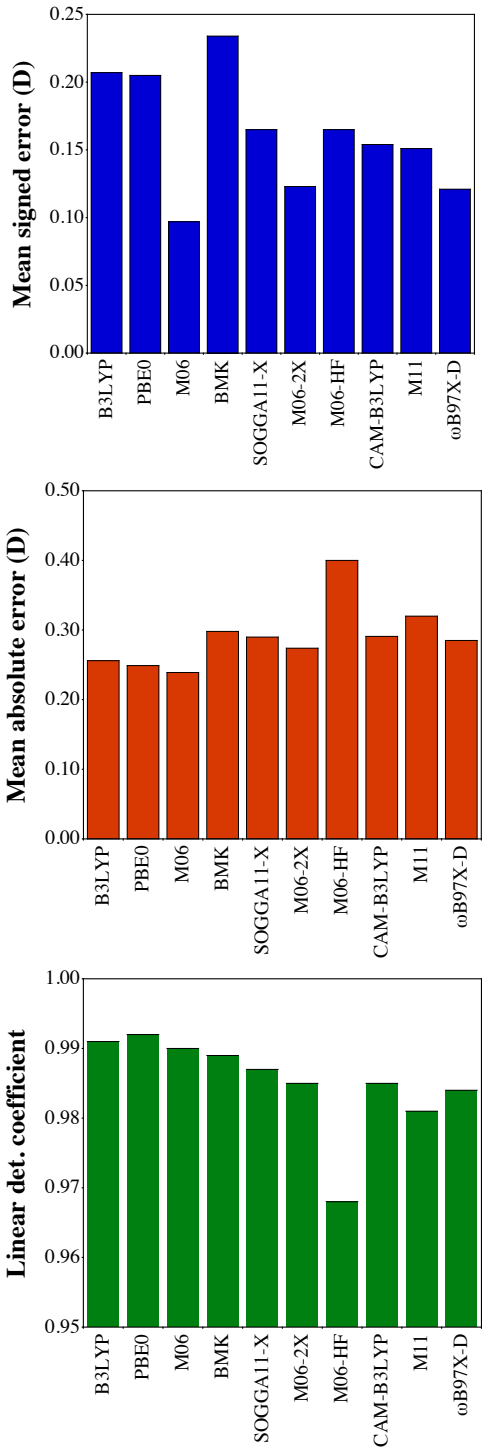

Figure S-1: MSE (top), MAE (center) and R^2 (bottom) determined for the μ^{GS} of the 31 compounds investigated here.

S5 Push-pull oligomers

S5.1 Raw values

Table S-8: Transition energies (ΔE, in eV), ground-state, excited-state and excess dipole moments (in D) for the push-pull chains. All values determined with the *aug*-cc-pVDZ atomic basis set.

	CC2				BLYP				B3LYP				CAM-B3LYP			
N	ΔE	μ^{GS}	μ^{ES}	$\Delta\mu$	ΔE	μ^{GS}	μ^{ES}	$\Delta\mu$	ΔE	μ^{GS}	μ^{ES}	$\Delta\mu$	ΔE	μ^{GS}	μ^{ES}	$\Delta\mu$
1	4.850	6.62	11.32	4.71	4.397	7.17	8.91	1.80	4.658	7.21	9.62	2.46	4.824	7.15	10.11	2.99
2	4.259	8.39	15.77	7.39	3.680	9.45	12.66	3.24	3.946	9.38	13.29	3.93	4.178	9.15	13.74	4.61
3	3.797	9.77	19.41	9.65	3.143	11.40	15.89	4.50	3.425	11.19	16.48	5.31	3.708	10.71	16.73	6.02
4	3.461	10.87	22.83	11.96	2.736	13.14	19.03	5.90	3.037	12.74	19.64	6.91	3.368	11.96	19.48	7.52
5	3.214	11.77	26.05	14.289	2.414	14.70	22.20	7.51	2.736	14.07	22.91	8.85	3.115	12.96	22.08	9.12
6	3.033	12.49	29.04	16.56	2.152	16.12	25.46	9.34	2.497	15.22	26.41	11.19	2.925	13.76	24.53	10.77
7	2.899	13.07	31.69	18.64	1.938	17.41	28.85	11.44	2.298	16.22	30.17	13.95	2.780	14.39	26.76	12.37
8	2.800	13.52	33.94	20.43	1.759	18.59	32.40	13.81	2.136	17.09	34.24	17.15	2.668	14.89	28.72	13.83
9	2.726	13.89	35.73	21.86	1.607	19.67	36.17	16.50	2.002	17.83	38.66	20.83	2.582	15.29	30.36	15.08
10	2.670	14.18	37.05	22.90	1.478	20.65	40.14	19.49	1.890	18.47	43.40	24.94	2.514	15.60	31.64	16.04
11	2.629	14.40	37.90	23.53	1.366	21.55	44.39	22.84	1.794	19.01	48.55	29.54	2.461	15.84	32.56	16.72
12	2.595	14.59	38.33	23.77	1.269	22.38	48.87	26.49	1.715	19.49	53.95	34.47	2.417	16.06	33.12	17.08
13	2.569	14.73	38.36	23.66	1.184	23.13	53.65	30.53	1.646	19.89	59.77	39.88	2.382	16.21	33.37	17.17
14	2.547	14.86	38.05	23.21	1.111	23.82	58.75	34.94	1.590	20.25	65.77	45.53	2.352	16.36	33.30	16.96
15	2.529	14.94	37.51	22.60	1.043	24.44	64.09	39.66	1.539	20.53	72.19	51.67	2.327	16.44	33.08	16.65

S5.2 Optimized geometries

Geometries of the push-pull chains used in the calculations. M06-2X/6-31+G(d) structures with C_s symmetry.

N=1

6	0.0000000	0.5963830	0.0000000
6	1.2823010	0.1763770	0.0000000
1	-0.3523430	1.6173860	0.0000000
1	1.4729810	-0.8928360	0.0000000
7	2.3701100	0.9751780	0.0000000
7	-1.0480510	-0.3763230	0.0000000
8	-2.1936620	0.0554010	0.0000000
8	-0.7633380	-1.5703030	0.0000000
1	3.2981960	0.5847920	0.0000000
1	2.2889490	1.9813260	0.0000000

N=2

6	-0.1029470	-1.1232300	0.0000000
6	0.0000000	0.2177600	0.0000000
1	-1.0137210	-1.7054230	0.0000000
1	1.0059370	0.6353930	0.0000000
6	-1.1101560	1.1224690	0.0000000
6	-0.9040420	2.4643930	0.0000000
1	-2.1222340	0.7228210	0.0000000
1	0.1130210	2.8508060	0.0000000
7	-1.8645890	3.4202890	0.0000000
7	1.0804160	-1.9430430	0.0000000
8	0.9025170	-3.1547780	0.0000000
8	2.1829960	-1.4088330	0.0000000
1	-1.6308850	4.3993920	0.0000000
1	-2.8441410	3.1768240	0.0000000

N=3

6	-0.7938060	-0.5366460	0.0000000
6	-2.1376030	-0.5518580	0.0000000
1	-0.2813750	-1.4973600	0.0000000
1	-2.7960850	0.3057820	0.0000000
6	0.0000000	0.6607350	0.0000000
6	1.3563920	0.6188930	0.0000000
1	-0.5127520	1.6213830	0.0000000

1	1.8363900	-0.3620810	0.0000000
6	2.2261740	1.7586680	0.0000000
6	3.5756350	1.6173220	0.0000000
1	1.7826380	2.7531360	0.0000000
1	4.0122230	0.6205730	0.0000000
7	4.4866670	2.6246310	0.0000000
7	-2.8567160	-1.8019860	0.0000000
8	-4.0788070	-1.7244840	0.0000000
8	-2.2315810	-2.8545440	0.0000000
1	5.4756640	2.4385960	0.0000000
1	4.1959950	3.5909980	0.0000000

N=4

6	0.0000000	0.3186620	0.0000000
6	0.4173490	-0.9721020	0.0000000
1	-1.0743340	0.5133820	0.0000000
1	1.4832700	-1.1957690	0.0000000
6	0.8638160	1.4663980	0.0000000
6	0.3906460	2.7382760	0.0000000
1	1.9395800	1.2923630	0.0000000
1	-0.6923210	2.8813830	0.0000000
6	1.1941310	3.9274450	0.0000000
6	0.6357740	5.1631800	0.0000000
1	2.2780820	3.8212870	0.0000000
1	-0.4476560	5.2646290	0.0000000
7	1.3060920	6.3467150	0.0000000
1	0.8182140	7.2266760	0.0000000
1	2.3146740	6.3748510	0.0000000
6	-0.5091980	-2.0716690	0.0000000
6	-0.1404090	-3.3633300	0.0000000
1	-1.5753490	-1.8512670	0.0000000
1	0.8696450	-3.7495690	0.0000000
7	-1.1335850	-4.4108610	0.0000000
8	-0.7090240	-5.5591490	0.0000000
8	-2.3202270	-4.1121130	0.0000000

N=5

6	-1.3549380	0.8052370	0.0000000
6	0.0000000	0.7344610	0.0000000
1	-1.9218060	-0.1281810	0.0000000
1	0.5855160	1.6537900	0.0000000
6	-2.1184940	2.0228820	0.0000000

6	-3.4749920	2.0414890	0.0000000
1	-1.5690500	2.9642640	0.0000000
1	-4.0005360	1.0838200	0.0000000
6	-4.2933020	3.2219260	0.0000000
6	-5.6468710	3.1519610	0.0000000
1	-3.8005930	4.1934020	0.0000000
1	-6.1360720	2.1799590	0.0000000
7	-6.5061840	4.2081090	0.0000000
1	-7.5032200	4.0739490	0.0000000
1	-6.1652790	5.1576190	0.0000000
6	0.7146430	-0.5125990	0.0000000
6	2.0654170	-0.6325110	0.0000000
1	0.1133190	-1.4236100	0.0000000
1	2.6874190	0.2615870	0.0000000
6	2.7172020	-1.9151040	0.0000000
6	4.0502680	-2.0761630	0.0000000
1	2.0991540	-2.8112720	0.0000000
1	4.7981930	-1.2950700	0.0000000
7	4.6308030	-3.3987480	0.0000000
8	5.8536360	-3.4523310	0.0000000
8	3.8947420	-4.3758260	0.0000000

N=6

C	0.1191890	2.8303860	0.0000000
C	0.7258100	1.6170500	0.0000000
H	-0.9723530	2.8643420	0.0000000
H	1.8147670	1.5642180	0.0000000
C	0.8046360	4.0945660	0.0000000
C	0.1583380	5.2868270	0.0000000
H	1.8946790	4.0767970	0.0000000
H	-0.9340380	5.2785390	0.0000000
C	0.7905110	6.5776420	0.0000000
C	0.0723380	7.7264540	0.0000000
H	1.8791120	6.6194330	0.0000000
H	-1.0149400	7.6824800	0.0000000
N	0.5787150	8.9915130	0.0000000
H	-0.0226360	9.7979020	0.0000000
H	1.5742370	9.1543480	0.0000000
C	0.0000000	0.3760010	0.0000000
C	0.5705780	-0.8546020	0.0000000
H	-1.0896650	0.4441620	0.0000000
H	1.6571170	-0.9417470	0.0000000
C	-0.1961720	-2.0710060	0.0000000
C	0.3347270	-3.3183500	0.0000000

H	-1.2827620	-1.9681840	0.0000000
H	1.4165590	-3.4448790	0.0000000
C	-0.4881020	-4.4992700	0.0000000
C	0.0021580	-5.7488730	0.0000000
H	-1.5700180	-4.3789820	0.0000000
H	1.0445440	-6.0370150	0.0000000
N	-0.8871710	-6.8878760	0.0000000
O	-0.3537680	-7.9892830	0.0000000
O	-2.0961680	-6.7029440	0.0000000

N=7

C	-3.4185090	2.2364870	0.0000000
C	-2.0649120	2.1532750	0.0000000
H	-3.9955370	1.3093270	0.0000000
H	-1.4743490	3.0698970	0.0000000
C	-4.1686300	3.4642620	0.0000000
C	-5.5237440	3.5051610	0.0000000
H	-3.6054980	4.3978590	0.0000000
H	-6.0659770	2.5568260	0.0000000
C	-6.3221630	4.7012120	0.0000000
C	-7.6758910	4.6591370	0.0000000
H	-5.8105380	5.6630740	0.0000000
H	-8.1853380	3.6975940	0.0000000
N	-8.5146540	5.7340540	0.0000000
H	-9.5140440	5.6202930	0.0000000
H	-8.1542160	6.6761490	0.0000000
C	-1.3511520	0.9045310	0.0000000
C	0.0000000	0.7867140	0.0000000
H	-1.9535550	-0.0060160	0.0000000
H	0.6144170	1.6873900	0.0000000
C	0.6795580	-0.4807230	0.0000000
C	2.0270410	-0.6334150	0.0000000
H	0.0532300	-1.3748130	0.0000000
H	2.6664100	0.2494310	0.0000000
C	2.6682920	-1.9209210	0.0000000
C	4.0098850	-2.1130100	0.0000000
H	2.0165450	-2.7963040	0.0000000
H	4.6785110	-1.2531540	0.0000000
C	4.5946070	-3.4287060	0.0000000
C	5.9175430	-3.6542450	0.0000000
H	3.9321050	-4.2924640	0.0000000
H	6.7027850	-2.9105630	0.0000000
N	6.4339180	-5.0045370	0.0000000
O	7.6524260	-5.1159340	0.0000000

0	5.6511570	-5.9440290	0.0000000

N=8

6	-0.2032730	5.3303320	0.0000000
6	0.5199570	4.1834790	0.0000000
1	-1.2928950	5.2573520	0.0000000
1	1.6089740	4.2408820	0.0000000
6	0.3559650	6.6565450	0.0000000
6	-0.3999730	7.7815820	0.0000000
1	1.4428880	6.7433940	0.0000000
1	-1.4867200	7.6703110	0.0000000
6	0.1079950	9.1275410	0.0000000
6	-0.7128090	10.2043970	0.0000000
1	1.1881170	9.2705390	0.0000000
1	-1.7914170	10.0603620	0.0000000
7	-0.3254960	11.5123450	0.0000000
1	-0.9989980	12.2593390	0.0000000
1	0.6505760	11.7665610	0.0000000
6	-0.0738470	2.8728700	0.0000000
6	0.6235960	1.7099590	0.0000000
1	-1.1646600	2.8269750	0.0000000
1	1.7135770	1.7427310	0.0000000
6	0.0000000	0.4135460	0.0000000
6	0.6725890	-0.7639200	0.0000000
1	-1.0914230	0.3919090	0.0000000
1	1.7628830	-0.7555250	0.0000000
6	0.0188760	-2.0452970	0.0000000
6	0.6638860	-3.2378670	0.0000000
1	-1.0726670	-2.0415720	0.0000000
1	1.7537710	-3.2574880	0.0000000
6	-0.0255550	-4.5007150	0.0000000
6	0.5852900	-5.7102030	0.0000000
1	-1.1163370	-4.4673190	0.0000000
1	1.6730750	-5.7659930	0.0000000
6	-0.1587670	-6.9433350	0.0000000
6	0.4139170	-8.1567150	0.0000000
1	-1.2462390	-6.8948680	0.0000000
1	1.4731940	-8.3750270	0.0000000
7	-0.3981320	-9.3533560	0.0000000
8	0.2079100	-10.4161510	0.0000000
8	-1.6163330	-9.2486850	0.0000000

N=9

C	-0.0274540	-6.5806610	0.0000000
C	-0.7071980	-5.4078370	0.0000000
H	1.0641400	-6.5490080	0.0000000
H	-1.7976800	-5.4252200	0.0000000
C	-0.6368110	-7.8851390	0.0000000
C	0.0746170	-9.0385330	0.0000000
H	-1.7263420	-7.9298830	0.0000000
H	1.1648890	-8.9699420	0.0000000
C	-0.4857500	-10.3640050	0.0000000
C	0.2914700	-11.4724310	0.0000000
H	-1.5707160	-10.4643180	0.0000000
H	1.3749510	-11.3713640	0.0000000
N	-0.1476110	-12.7644250	0.0000000
H	0.4956270	-13.5375780	0.0000000
H	-1.1329950	-12.9795110	0.0000000
C	-0.0666020	-4.1188730	0.0000000
C	-0.7228330	-2.9325470	0.0000000
H	1.0251310	-4.1117200	0.0000000
H	-1.8134160	-2.9283220	0.0000000
C	-0.0566440	-1.6569030	0.0000000
C	-0.6911290	-0.4587610	0.0000000
H	1.0348770	-1.6707270	0.0000000
H	-1.7813390	-0.4338920	0.0000000
C	0.0000000	0.8033490	0.0000000
C	-0.6111280	2.0135240	0.0000000
H	1.0909680	0.7681800	0.0000000
H	-1.7004220	2.0611120	0.0000000
C	0.1076490	3.2600110	0.0000000
C	-0.4759690	4.4834530	0.0000000
H	1.1975120	3.2004520	0.0000000
H	-1.5634470	4.5585490	0.0000000
C	0.2768620	5.7100110	0.0000000
C	-0.2723640	6.9483810	0.0000000
H	1.3645010	5.6212590	0.0000000
H	-1.3559700	7.0588830	0.0000000
C	0.5327120	8.1429380	0.0000000
C	0.0208940	9.3829790	0.0000000
H	1.6163860	8.0401980	0.0000000
H	-1.0262760	9.6535440	0.0000000
N	0.8914160	10.5381520	0.0000000
O	0.3385890	11.6294190	0.0000000

N=10

6	-0.8153940	7.7830720	0.0000000

6	-0.0088240	6.6939160	0.0000000
1	-1.8966200	7.6297230	0.0000000
1	1.0728690	6.8336690	0.0000000
6	-0.3553630	9.1478210	0.0000000
6	-1.1902320	10.2149240	0.0000000
1	0.7224840	9.3134280	0.0000000
1	-2.2662010	10.0260070	0.0000000
6	-0.7801610	11.5947440	0.0000000
6	-1.6748220	12.6104910	0.0000000
1	0.2870980	11.8143770	0.0000000
1	-2.7405550	12.3906000	0.0000000
7	-1.3808220	13.9434010	0.0000000
1	-2.1052840	14.6409470	0.0000000
1	-0.4251070	14.2656230	0.0000000
6	-0.4999860	5.3405110	0.0000000
6	0.2862240	4.2363650	0.0000000
1	-1.5839150	5.2100690	0.0000000
1	1.3702830	4.3563660	0.0000000
6	-0.2295240	2.8924080	0.0000000
6	0.5386060	1.7755440	0.0000000
1	-1.3154060	2.7808420	0.0000000
1	1.6244520	1.8774670	0.0000000
6	0.0000000	0.4407750	0.0000000
6	0.7497470	-0.6885350	0.0000000
1	-1.0875190	0.3474510	0.0000000
1	1.8370870	-0.6053730	0.0000000
6	0.1872380	-2.0132380	0.0000000
6	0.9164950	-3.1558630	0.0000000
1	-0.9017500	-2.0868790	0.0000000
1	2.0050880	-3.0939920	0.0000000
6	0.3267210	-4.4685680	0.0000000
6	1.0314710	-5.6262670	0.0000000
1	-0.7635410	-4.5192960	0.0000000
1	2.1209620	-5.5904640	0.0000000
6	0.4075460	-6.9233990	0.0000000
6	1.0811000	-8.0986270	0.0000000
1	-0.6834270	-6.9463860	0.0000000
1	2.1703280	-8.0970420	0.0000000
6	0.4033400	-9.3700290	0.0000000
6	1.0409100	-10.5502080	0.0000000
1	-0.6851290	-9.3798490	0.0000000
1	2.1104960	-10.7107900	0.0000000
7	0.2946900	-11.7897110	0.0000000
8	0.9578780	-12.8175390	0.0000000
8	-0.9271680	-11.7508810	0.0000000

N=11

6	-0.3116850	-9.0643640	0.0000000
6	-0.9624000	-7.8756470	0.0000000
1	0.7803400	-9.0599960	0.0000000
1	-2.0531060	-7.8674220	0.0000000
6	-0.9541960	-10.3535780	0.0000000
6	-0.2742820	-11.5253910	0.0000000
1	-2.0446220	-10.3696520	0.0000000
1	0.8174610	-11.4868070	0.0000000
6	-0.8711540	-12.8355420	0.0000000
6	-0.1261880	-13.9654630	0.0000000
1	-1.9585880	-12.9051340	0.0000000
1	0.9597520	-13.8956690	0.0000000
7	-0.6022630	-15.2450240	0.0000000
1	0.0185860	-16.0361770	0.0000000
1	-1.5933600	-15.4317180	0.0000000
6	-0.2927700	-6.6007260	0.0000000
6	-0.9233230	-5.4010450	0.0000000
1	0.7988300	-6.6175640	0.0000000
1	-2.0137440	-5.3747620	0.0000000
6	-0.2327270	-4.1375670	0.0000000
6	-0.8454690	-2.9286840	0.0000000
1	0.8583190	-4.1716810	0.0000000
1	-1.9353220	-2.8858820	0.0000000
6	-0.1353630	-1.6761920	0.0000000
6	-0.7300020	-0.4583330	0.0000000
1	0.9549530	-1.7270300	0.0000000
1	-1.8189910	-0.3985980	0.0000000
6	0.0000000	0.7825480	0.0000000
6	-0.5756010	2.0095060	0.0000000
1	1.0893220	0.7144010	0.0000000
1	-1.6633650	2.0870760	0.0000000
6	0.1752580	3.2377190	0.0000000
6	-0.3797680	4.4740960	0.0000000
1	1.2632450	3.1512040	0.0000000
1	-1.4658110	4.5711680	0.0000000
6	0.3941240	5.6877910	0.0000000
6	-0.1369320	6.9344890	0.0000000
1	1.4802440	5.5805810	0.0000000
1	-1.2203360	7.0551520	0.0000000
6	0.6659840	8.1294350	0.0000000
6	0.1659620	9.3881010	0.0000000
1	1.7490940	7.9969540	0.0000000
1	-0.9125410	9.5406530	0.0000000

6	1.0165590	10.5511840	0.0000000
6	0.5512120	11.8090970	0.0000000
1	2.0955610	10.4076810	0.0000000
1	-0.4851880	12.1184270	0.0000000
7	1.4642290	12.9316350	0.0000000
8	0.9518140	14.0422330	0.0000000
8	2.6684440	12.7215070	0.0000000

N=12

6	-1.5210940	10.1985640	0.0000000
6	-0.6615450	9.1510820	0.0000000
1	-2.5933560	9.9916620	0.0000000
1	0.4118670	9.3447820	0.0000000
6	-1.1293700	11.5849710	0.0000000
6	-2.0152470	12.6098180	0.0000000
1	-0.0609600	11.8036320	0.0000000
1	-3.0807310	12.3687080	0.0000000
6	-1.6725180	14.0083730	0.0000000
6	-2.6143310	14.9801900	0.0000000
1	-0.6169620	14.2788950	0.0000000
1	-3.6684410	14.7100680	0.0000000
7	-2.3839550	16.3261050	0.0000000
1	-3.1407490	16.9883770	0.0000000
1	-1.4446480	16.6932710	0.0000000
6	-1.0838250	7.7740180	0.0000000
6	-0.2429250	6.7113730	0.0000000
1	-2.1597850	7.5891150	0.0000000
1	0.8336940	6.8864830	0.0000000
6	-0.6884470	5.3418120	0.0000000
6	0.1369680	4.2670880	0.0000000
1	-1.7670490	5.1740940	0.0000000
1	1.2159830	4.4266360	0.0000000
6	-0.3281810	2.9041690	0.0000000
6	0.4832490	1.8188480	0.0000000
1	-1.4088860	2.7512860	0.0000000
1	1.5642230	1.9642390	0.0000000
6	0.0000000	0.4623550	0.0000000
6	0.7977330	-0.6330990	0.0000000
1	-1.0825410	0.3235080	0.0000000
1	1.8804350	-0.5017550	0.0000000
6	0.2962720	-1.9828070	0.0000000
6	1.0793120	-3.0888550	0.0000000
1	-0.7880040	-2.1071330	0.0000000
1	2.1636630	-2.9728840	0.0000000

6	0.5576530	-4.4306880	0.0000000
6	1.3234250	-5.5487740	0.0000000
1	-0.5283860	-4.5384970	0.0000000
1	2.4094250	-5.4512850	0.0000000
6	0.7772660	-6.8806770	0.0000000
6	1.5210750	-8.0133210	0.0000000
1	-0.3106080	-6.9680140	0.0000000
1	2.6086980	-7.9400540	0.0000000
6	0.9423000	-9.3316200	0.0000000
6	1.6567870	-10.4821060	0.0000000
1	-0.1471620	-9.3926690	0.0000000
1	2.7452870	-10.4422350	0.0000000
6	1.0243750	-11.7770390	0.0000000
6	1.7039580	-12.9332850	0.0000000
1	-0.0630320	-11.8256460	0.0000000
1	2.7786430	-13.0555000	0.0000000
7	1.0025760	-14.1991510	0.0000000
8	1.7024680	-15.2021610	0.0000000
8	-0.2197570	-14.2041030	0.0000000

N=13

6	-0.5829290	-11.5394830	0.0000000
6	-1.2193620	-10.3433150	0.0000000
1	0.5090700	-11.5481340	0.0000000
1	-2.3099500	-10.3223760	0.0000000
6	-1.2408290	-12.8213620	0.0000000
6	-0.5755940	-14.0013270	0.0000000
1	-2.3314170	-12.8242100	0.0000000
1	0.5165520	-13.9764080	0.0000000
6	-1.1888790	-15.3043140	0.0000000
6	-0.4586880	-16.4435940	0.0000000
1	-2.2771480	-15.3599820	0.0000000
1	0.6280700	-16.3879620	0.0000000
7	-0.9513340	-17.7173200	0.0000000
1	-0.3407140	-18.5163440	0.0000000
1	-1.9447250	-17.8911790	0.0000000
6	-0.5351710	-9.0756470	0.0000000
6	-1.1520260	-7.8691520	0.0000000
1	0.5561600	-9.1048910	0.0000000
1	-2.2421680	-7.8309350	0.0000000
6	-0.4481730	-6.6124430	0.0000000
6	-1.0488330	-5.3978260	0.0000000
1	0.6424460	-6.6577090	0.0000000
1	-2.1383510	-5.3450230	0.0000000

6	-0.3282990	-4.1506610	0.0000000
6	-0.9142760	-2.9289370	0.0000000
1	0.7615500	-4.2099030	0.0000000
1	-2.0030390	-2.8628200	0.0000000
6	-0.1784880	-1.6907640	0.0000000
6	-0.7504470	-0.4624400	0.0000000
1	0.9105130	-1.7630530	0.0000000
1	-1.8383170	-0.3835640	0.0000000
6	0.0000000	0.7668080	0.0000000
6	-0.5579200	2.0015780	0.0000000
1	1.0880410	0.6817380	0.0000000
1	-1.6447120	2.0933370	0.0000000
6	0.2074240	3.2214430	0.0000000
6	-0.3355600	4.4628840	0.0000000
1	1.2943340	3.1231540	0.0000000
1	-1.4209820	4.5685800	0.0000000
6	0.4461460	5.6721120	0.0000000
6	-0.0795620	6.9209810	0.0000000
1	1.5316150	5.5589960	0.0000000
1	-1.1630800	7.0432010	0.0000000
6	0.7219200	8.1170130	0.0000000
6	0.2181810	9.3747670	0.0000000
1	1.8053290	7.9856290	0.0000000
1	-0.8623720	9.5187760	0.0000000
6	1.0465860	10.5525310	0.0000000
6	0.5728250	11.8211150	0.0000000
1	2.1266310	10.3972870	0.0000000
1	-0.5022730	11.9960500	0.0000000
6	1.4473370	12.9666630	0.0000000
6	1.0074580	14.2335260	0.0000000
1	2.5231820	12.8012250	0.0000000
1	-0.0224320	14.5639250	0.0000000
7	1.9432270	15.3376300	0.0000000
8	1.4531820	16.4581540	0.0000000
8	3.1428040	15.1030320	0.0000000

N=14

6	2.8589820	12.4681490	0.0000000
6	1.9171830	11.4941480	0.0000000
1	3.9109840	12.1752540	0.0000000
1	0.8631900	11.7751180	0.0000000
6	2.5802730	13.8818980	0.0000000
6	3.5450020	14.8326610	0.0000000
1	1.5327490	14.1853430	0.0000000

1	4.5879220	14.5075780	0.0000000
6	3.3147520	16.2543690	0.0000000
6	4.3305920	17.1482250	0.0000000
1	2.2840230	16.6079700	0.0000000
1	5.3599100	16.7952060	0.0000000
7	4.2080200	18.5085350	0.0000000
1	5.0151550	19.1083740	0.0000000
1	3.3009730	18.9493530	0.0000000
6	2.2243700	10.0866530	0.0000000
6	1.2978450	9.0979680	0.0000000
1	3.2812430	9.8130940	0.0000000
1	0.2397240	9.3631000	0.0000000
6	1.6257170	7.6952780	0.0000000
6	0.7115440	6.6951840	0.0000000
1	2.6860760	7.4362570	0.0000000
1	-0.3497590	6.9472580	0.0000000
6	1.0566830	5.2966820	0.0000000
6	0.1537150	4.2865150	0.0000000
1	2.1199270	5.0501950	0.0000000
1	-0.9103440	4.5265990	0.0000000
6	0.5148510	2.8920800	0.0000000
6	-0.3770980	1.8722110	0.0000000
1	1.5807340	2.6575440	0.0000000
1	-1.4437350	2.1003970	0.0000000
6	0.0000000	0.4820530	0.0000000
6	-0.8804090	-0.5477800	0.0000000
1	1.0684600	0.2597230	0.0000000
1	-1.9495970	-0.3321250	0.0000000
6	-0.4864890	-1.9331770	0.0000000
6	-1.3542980	-2.9736640	0.0000000
1	0.5845940	-2.1424210	0.0000000
1	-2.4260910	-2.7717620	0.0000000
6	-0.9419520	-4.3535520	0.0000000
6	-1.7955710	-5.4057450	0.0000000
1	0.1318580	-4.5482910	0.0000000
1	-2.8700730	-5.2194350	0.0000000
6	-1.3623120	-6.7790300	0.0000000
6	-2.1993320	-7.8444850	0.0000000
1	-0.2856120	-6.9571420	0.0000000
1	-3.2767030	-7.6766190	0.0000000
6	-1.7411300	-9.2095010	0.0000000
6	-2.5575920	-10.2906350	0.0000000
1	-0.6613000	-9.3675690	0.0000000
1	-3.6380810	-10.1462120	0.0000000
6	-2.0667610	-11.6444500	0.0000000

6	-2.8558950	-12.7448200	0.0000000
1	-0.9837310	-11.7772620	0.0000000
1	-3.9393460	-12.6327040	0.0000000
6	-2.3108580	-14.0790840	0.0000000
6	-3.0658490	-15.1873510	0.0000000
1	-1.2291060	-14.2001050	0.0000000
1	-4.1462740	-15.2379960	0.0000000
7	-2.4498120	-16.4971390	0.0000000
8	-3.2145850	-17.4514520	0.0000000
8	-1.2305400	-16.5827110	0.0000000

N=15

6	-0.8489200	-14.0098190	0.0000000
6	-1.4760940	-12.8089320	0.0000000
1	0.2429730	-14.0269940	0.0000000
1	-2.5665370	-12.7798920	0.0000000
6	-1.5169990	-15.2866820	0.0000000
6	-0.8616920	-16.4720350	0.0000000
1	-2.6076060	-15.2806590	0.0000000
1	0.2306240	-16.4563600	0.0000000
6	-1.4861530	-17.7699670	0.0000000
6	-0.7662330	-18.9155980	0.0000000
1	-2.5748980	-17.8160480	0.0000000
1	0.3209840	-18.8697560	0.0000000
7	-1.2703110	-20.1851290	0.0000000
1	-0.6668400	-20.9895360	0.0000000
1	-2.2651970	-20.3500840	0.0000000
6	-0.7827760	-11.5459570	0.0000000
6	-1.3912380	-10.3353870	0.0000000
1	0.3083130	-11.5829230	0.0000000
1	-2.4811570	-10.2900070	0.0000000
6	-0.6795410	-9.0827970	0.0000000
6	-1.2730460	-7.8648690	0.0000000
1	0.4107710	-9.1346880	0.0000000
1	-2.3623320	-7.8061920	0.0000000
6	-0.5463530	-6.6209350	0.0000000
6	-1.1269060	-5.3968500	0.0000000
1	0.5431910	-6.6852880	0.0000000
1	-2.2155000	-5.3266120	0.0000000
6	-0.3871830	-4.1606180	0.0000000
6	-0.9560840	-2.9311260	0.0000000
1	0.7015890	-4.2359710	0.0000000
1	-2.0439370	-2.8504710	0.0000000
6	-0.2045910	-1.7020360	0.0000000

6	-0.7626010	-0.4675850	0.0000000
1	0.8833890	-1.7874780	0.0000000
1	-1.8496530	-0.3771530	0.0000000
6	0.0000000	0.7545720	0.0000000
6	-0.5473250	1.9938050	0.0000000
1	1.0871520	0.6594530	0.0000000
1	-1.6334810	2.0939230	0.0000000
6	0.2264080	3.2088140	0.0000000
6	-0.3097200	4.4529720	0.0000000
1	1.3126370	3.1038070	0.0000000
1	-1.3948010	4.5634120	0.0000000
6	0.4760500	5.6600380	0.0000000
6	-0.0473890	6.9096500	0.0000000
1	1.5611690	5.5441270	0.0000000
1	-1.1310730	7.0320520	0.0000000
6	0.7525830	8.1071060	0.0000000
6	0.2448640	9.3632290	0.0000000
1	1.8362300	7.9780470	0.0000000
1	-0.8368220	9.5008070	0.0000000
6	1.0631350	10.5480550	0.0000000
6	0.5764850	11.8123760	0.0000000
1	2.1445990	10.4017680	0.0000000
1	-0.5020290	11.9709590	0.0000000
6	1.4207360	12.9790440	0.0000000
6	0.9637070	14.2536180	0.0000000
1	2.4985930	12.8094140	0.0000000
1	-0.1089870	14.4427440	0.0000000
6	1.8532710	15.3877350	0.0000000
6	1.4297710	16.6600470	0.0000000
1	2.9268580	15.2082650	0.0000000
1	0.4042500	17.0038140	0.0000000
7	2.3798750	17.7521200	0.0000000
8	1.9042230	18.8787480	0.0000000
8	3.5762260	17.5019260	0.0000000

S6 Results for the quadrupolar set

Table S-9: Ground-state traceless quadrupole moment, Q^{GS}, given in Debye.Angströms.

		CC2	B3LYP	PBE0	M06	BMK	SOGGA11-X	M06-2X	M06-HF	CAM-B3LYP	M11	ωB97X-D
Q1	Q_{yy}	3.15	3.14	3.28	2.90	3.28	3.26	3.29	3.84	3.26	3.45	3.27
	Q_{zz}	4.86	4.32	4.79	4.51	4.90	4.86	5.03	6.04	4.55	5.25	4.84
Q2	Q_{yy}	3.16	3.00	3.17	2.78	3.15	3.15	3.17	3.68	3.13	3.38	3.16
	Q_{zz}	10.20	9.81	10.56	9.86	10.88	10.70	10.93	12.84	10.21	11.31	10.66
Q3	Q_{yy}	-0.54	-0.85	-0.87	-0.98	-1.04	-0.94	-0.96	-1.01	-0.81	-0.88	-0.89
	Q_{zz}	17.90	17.86	19.00	17.71	19.54	19.20	19.52	22.55	18.42	20.15	19.09
Q4	Q_{yy}	5.17	5.19	5.50	4.79	5.46	5.47	5.51	6.50	5.40	5.79	5.48
	Q_{zz}	6.04	5.26	5.87	5.56	6.06	5.96	6.21	7.52	5.58	6.52	5.95
Q5	Q_{yy}	6.38	6.55	6.91	5.94	6.83	6.86	6.88	8.16	6.79	7.22	6.87
	Q_{zz}	7.89	6.64	7.54	7.21	7.81	7.66	8.04	9.81	7.10	8.50	7.66

Table S-10: Excited-state traceless quadrupole moment, Q^{ES}, given in Debye.Angströms.

	State		CC2	B3LYP	PBE0	M06	BMK	SOGGA11-X	M06-2X	M06-HF	CAM-B3LYP	M11	ωB97X-D
Q1	B_1 ($\pi \rightarrow \pi^\star$)	Q_{yy}	2.42	2.51	2.68	1.56	2.74	2.59	2.60	3.06	2.64	2.42	2.71
		Q_{zz}	5.94	5.11	5.47	7.81	5.47	5.79	5.99	7.31	5.34	7.51	5.48
Q2	B_{3u} ($\pi \rightarrow \pi^\star$)	Q_{yy}	3.94	3.94	4.08	3.66	4.06	4.08	4.05	4.52	4.01	4.14	4.03
		Q_{zz}	7.85	7.02	7.83	7.30	8.16	8.02	8.36	10.49	7.61	8.98	8.08
Q3	B_1 ($\pi \rightarrow \pi^\star$)	Q_{yy}	0.85	1.02	0.94	0.67	0.75	0.81	2.51	0.81	0.81	1.87	0.69
		Q_{zz}	14.56	13.38	14.66	13.81	15.33	15.11	12.81	18.27	14.62	14.75	15.39
Q4	B_{2u} ($\pi \rightarrow \pi^\star$)	Q_{yy}	6.65	6.50	6.82	6.23	6.82	6.93	6.96	8.19	6.76	7.21	6.74
		Q_{zz}	4.32	3.60	4.24	3.82	4.46	4.21	4.53	5.75	3.96	4.93	4.50
Q5	B_{2u} ($\pi \rightarrow \pi^\star$)	Q_{yy}	7.77	7.81	8.17	7.30	8.14	8.26	8.26	9.69	8.11	8.57	8.08
		Q_{zz}	6.29	5.06	5.99	5.56	6.29	6.00	6.47	8.30	5.55	6.99	6.29

Table S-11: Statistical analysis obtained for the compounds of Scheme 3 (Tables S-9 and S-10). See caption of Table S-4 for definitions.

	Q^{GS}					Q^{ES}				
	MSE	MAE	Max(+)	Max(-)	R^2	MSE	MAE	Max(+)	Max(-)	R^2
B3LYP	-0.330	0.368	0.165	-1.250	0.993	-0.466	0.526	0.168	-1.230	0.985
PBE0	0.154	0.339	1.100	-0.352	0.997	0.030	0.204	0.408	-0.474	0.995
M06	-0.393	0.393	-0.187	-0.678	0.999	-0.289	0.662	1.870	-0.863	0.956
BMK	0.265	0.384	1.640	-0.503	0.998	0.161	0.276	0.762	-0.473	0.996
SOGGA11-X	0.198	0.343	1.310	-0.403	0.998	0.120	0.241	0.548	-0.291	0.997
M06-2X	0.340	0.425	1.630	-0.426	0.999	0.194	0.545	1.660	-1.750	0.976
M06-HF	1.570	1.670	4.660	-0.479	1.000	1.580	1.590	3.700	-0.044	0.996
CAM-B3LYP	-0.058	0.314	0.528	-0.789	0.995	-0.119	0.281	0.345	-0.742	0.991
M11	0.648	0.716	2.250	-0.341	0.999	0.678	0.678	1.570	0.004	0.984
ωB97X-D	0.189	0.326	1.190	-0.351	0.998	0.139	0.265	0.825	-0.464	0.996