Supporting Information

Benchmarking the performance of time-dependent density functional theory methods on biochromophores

Yihan Shao,*,† Ye Mei,‡ Dage Sundholm,*,¶ and Ville R. I. Kaila*,§

†*Department of Chemistry and Biochemistry, University of Oklahoma, Norman, Oklahoma 73019, USA; Q-Chem Inc., 6601 Owens Drive, Suite 105, Pleasanton, CA 94588, USA.*

‡*State Key Laboratory of Precision Spectroscopy, Institute of Theoretical and Computational Science, East China Normal University, Shanghai 200062, China; NYU-ECNU Center for Computational Chemistry at NYU Shanghai, Shanghai, China 200062; Q-Chem Inc., 6601 Owens Drive, Suite 105, Pleasanton, CA 94588, USA.*

¶*Department of Chemistry, Faculty of Science, P.O. Box 55, FIN-00014 University of Helsinki, Finland.*

§*Department Chemie, Technische Universität München (TUM), Lichtenbergstrasse 4, D-85747 Garching, Germany.*

E-mail: yihan.shao@ou.edu; dage.sundholm@helsinki.fi; ville.kaila@ch.tum.de

Table S1: VEEs (in eV) for the lowest excited state obtained at the CC2/def2-TZVP level of theory with B3LYP/def2-SVP and MP2/def2-TZVP optimized structures.

Molecule	CC2//B3LYP	CC2//MP2
pVP	4.62	4.66
pCA	4.47	4.52
pCA^-	3.23	3.24
pCA'^-	3.35	3.28
$TMpCA^-$	3.04	3.04
pCT^-	3.04	3.04
$pHBDI^-$	2.91	2.92
pHBDI	3.67	3.71
$pHBDI^+$	3.09	3.15
$PSBT^+$	2.11	2.17
$PSB11Me_2^+$	2.10	2.17

Table S2: TDDFT and CC2 excitation energies (E, in eV) and oscillator strengths (f) for pVP with the def2-TZVP and aug-def2-TZVP basis sets.

molecule		def2-TZVP					aug-def2-TZVP				
		1a	2a	3a	4a	5a	1a	2a	3a	4a	5a
RPA	E	5.04	5.38	6.68	7.07	7.11	4.93	5.30	5.56	5.88	6.06
	f	0.31	0.08	0.59	0.47	0.00	0.29	0.08	0.01	0.00	0.00
B3LYP	E	4.48	4.80	5.60	5.76	6.16	4.41	4.72	4.76	5.16	5.37
	f	0.12	0.34	0.00	0.17	0.05	0.15	0.28	0.00	0.01	0.00
BHLYP	E	4.83	5.12	6.29	6.39	6.58	4.74	5.04	5.32	5.64	5.87
	f	0.20	0.28	0.00	0.24	0.50	0.21	0.23	0.00	0.01	0.00
CAM-B3LYP	E	4.71	5.03	6.18	6.27	6.54	4.64	4.95	5.26	5.61	5.85
	f	0.13	0.36	0.00	0.23	0.44	0.15	0.30	0.00	0.01	0.00
CAMh-B3LYP	E	4.64	4.96	6.00	6.12	6.49	4.57	4.88	5.09	5.45	5.67
	f	0.13	0.35	0.00	0.22	0.42	0.15	0.30	0.00	0.01	0.00
BP86	E	4.17	4.51	5.25	5.40	5.49	4.13	4.46	4.62	5.06	5.22
	f	0.08	0.34	0.09	0.00	0.09	0.09	0.32	0.00	0.01	0.10
PBE	E	4.18	4.52	5.20	5.26	5.48	4.11	4.45	4.45	4.91	5.11
	f	0.08	0.33	0.00	0.09	0.09	0.10	0.31	0.00	0.00	0.00
PBE0	E	4.58	4.90	5.92	5.95	6.37	4.51	4.82	5.05	5.42	5.62
	f	0.13	0.35	0.19	0.00	0.08	0.15	0.30	0.00	0.01	0.00
PBE50	E	4.87	5.16	6.43	6.61	6.65	4.79	5.10	5.58	5.89	6.11
	f	0.20	0.30	0.24	0.00	0.48	0.21	0.25	0.00	0.01	0.00
ωPBE	E	4.75	5.10	6.38	6.63	6.68	4.69	5.03	5.63	5.99	6.22
	f	0.09	0.43	0.24	0.43	0.00	0.10	0.38	0.00	0.01	0.00
ωhPBE0	E	4.66	4.97	6.08	6.19	6.52	4.59	4.90	5.22	5.56	5.76
	f	0.13	0.36	0.21	0.00	0.40	0.15	0.31	0.00	0.01	0.00
ωPBEh	E	4.74	5.06	6.27	6.50	6.59	4.67	4.98	5.42	5.75	5.95
	f	0.11	0.39	0.23	0.00	0.42	0.13	0.34	0.00	0.01	0.00
BNL	E	4.91	5.23	6.66	6.69	6.75	4.82	5.15	5.64	6.02	6.29
	f	0.14	0.36	0.00	0.18	0.64	0.15	0.31	0.00	0.01	0.00
ωB97X	E	4.82	5.13	6.49	6.62	6.87	4.76	5.08	5.87	6.21	6.49
	f	0.12	0.37	0.21	0.54	0.00	0.13	0.33	0.00	0.01	0.00
ωB97X-D	E	4.74	5.05	6.29	6.56	6.70	4.68	4.99	5.55	5.86	6.07
	f	0.12	0.38	0.23	0.44	0.00	0.14	0.32	0.00	0.01	0.00
M06-2X	E	4.78	5.11	6.28	6.31	6.66	4.70	5.03	5.19	5.54	5.73
	f	0.14	0.38	0.00	0.25	0.39	0.15	0.32	0.00	0.01	0.00
M11	E	4.87	5.17	6.47	6.50	6.66	4.77	4.96	5.08	5.30	5.45
	f	0.15	0.37	0.25	0.00	0.45	0.17	0.00	0.29	0.00	0.00
M11-L	E	4.33	4.62	5.02	5.41	5.73	3.50	3.93	4.03	4.24	4.34
	f	0.14	0.27	0.00	0.11	0.05	0.00	0.00	0.00	0.15	0.00
CC2	E	4.66	5.25	6.42	6.44	6.84	4.58	5.11	5.22	5.60	5.80
	f	0.05	0.52	0.00	0.28	0.45	0.05	0.52	0.00	0.28	0.45

Table S3: TDDFT and CC2 excitation energies (E, in eV) and oscillator strengths (f) for pCA with the def2-TZVP and aug-def2-TZVP basis sets.

molecule		def2-TZVP					aug-def2-TZVP				
		1a	2a	3a	4a	5a	1a	2a	3a	4a	5a
RPA	E	4.73	5.40	6.37	6.44	6.84	4.68	5.34	5.90	6.29	6.36
	f	0.63	0.02	0.00	0.42	0.41	0.61	0.02	0.00	0.00	0.02
B3LYP	E	4.13	4.48	4.53	5.26	5.67	4.09	4.46	4.50	5.00	5.20
	f	0.65	0.00	0.03	0.12	0.07	0.64	0.00	0.04	0.00	0.13
BHLYP	E	4.46	4.98	5.34	5.99	6.32	4.42	4.94	5.32	5.59	5.94
	f	0.69	0.04	0.00	0.22	0.24	0.67	0.04	0.00	0.00	0.25
CAM-B3LYP	E	4.39	4.83	4.99	5.89	6.25	4.34	4.79	4.97	5.49	5.83
	f	0.67	0.05	0.00	0.21	0.19	0.66	0.06	0.00	0.00	0.23
CAMh-B3LYP	E	4.31	4.74	4.84	5.70	6.15	4.26	4.71	4.82	5.33	5.64
	f	0.67	0.05	0.00	0.18	0.15	0.65	0.05	0.00	0.00	0.20
BP86	E	3.69	3.84	4.15	4.64	4.69	3.68	3.81	4.13	4.63	4.66
	f	0.00	0.57	0.02	0.00	0.07	0.00	0.57	0.02	0.00	0.07
PBE	E	3.66	3.84	4.16	4.61	4.69	3.66	3.80	4.13	4.60	4.65
	f	0.00	0.57	0.02	0.00	0.07	0.00	0.57	0.02	0.00	0.07
PBE0	E	4.22	4.60	4.65	5.42	5.86	4.18	4.58	4.62	5.30	5.37
	f	0.67	0.00	0.03	0.14	0.07	0.65	0.00	0.04	0.00	0.15
PBE50	E	4.50	5.01	5.30	6.03	6.39	4.46	4.98	5.28	5.85	5.97
	f	0.71	0.04	0.00	0.22	0.22	0.69	0.04	0.00	0.00	0.23
ωPBE	E	4.47	4.84	4.87	6.07	6.33	4.43	4.81	4.84	5.84	6.01
	f	0.67	0.07	0.00	0.23	0.15	0.66	0.08	0.00	0.00	0.26
ωhPBE0	E	4.31	4.74	4.75	5.62	6.11	4.27	4.71	4.73	5.46	5.58
	f	0.68	0.04	0.00	0.17	0.10	0.67	0.04	0.00	0.00	0.17
ωPBEh	E	4.42	4.83	4.89	5.90	6.28	4.38	4.80	4.86	5.66	5.85
	f	0.68	0.06	0.00	0.20	0.16	0.67	0.06	0.00	0.00	0.23
BNL	E	4.62	5.06	5.33	6.46	6.48	4.57	5.02	5.29	5.85	6.31
	f	0.66	0.08	0.00	0.13	0.41	0.64	0.09	0.00	0.00	0.00
ωB97X	E	4.52	4.94	5.15	6.20	6.34	4.48	4.91	5.12	6.10	6.13
	f	0.67	0.07	0.00	0.25	0.21	0.66	0.07	0.00	0.00	0.27
ωB97X-D	E	4.43	4.85	4.95	5.92	6.28	4.38	4.82	4.93	5.80	5.87
	f	0.68	0.05	0.00	0.21	0.17	0.67	0.06	0.00	0.00	0.22
M06-2X	E	4.43	4.89	4.97	5.92	6.36	4.39	4.86	4.95	5.43	5.86
	f	0.68	0.05	0.00	0.21	0.15	0.66	0.06	0.00	0.00	0.20
M11	E	4.53	5.00	5.01	6.17	6.40	4.47	4.96	4.99	5.21	5.62
	f	0.70	0.05	0.00	0.25	0.16	0.66	0.06	0.00	0.00	0.00
M11-L	E	4.02	4.20	4.37	4.90	5.18	3.75	3.99	4.16	4.19	4.34
	f	0.58	0.00	0.02	0.09	0.00	0.00	0.56	0.00	0.00	0.03
CC2	E	4.52	4.77	4.96	6.02	6.43	4.44	4.72	4.90	5.45	5.88
	f	0.54	0.27	0.00	0.22	0.16	0.54	0.27	0.00	0.22	0.16

Table S4: TDDFT and CC2 excitation energies (E, in eV) and oscillator strengths (f) for pCA$'^{-}$ with the def2-TZVP and aug-def2-TZVP basis sets.

molecule		def2-TZVP					aug-def2-TZVP				
		1a	2a	3a	4a	5a	1a	2a	3a	4a	5a
RPA	E	3.93	4.94	5.61	6.47	6.51	3.68	3.84	3.87	4.08	4.36
	f	1.07	0.09	0.00	0.00	0.14	0.01	1.01	0.00	0.00	0.00
B3LYP	E	3.40	3.43	4.19	4.69	4.69	3.05	3.36	3.38	3.41	3.45
	f	0.00	0.86	0.09	0.04	0.00	0.00	0.87	0.00	0.00	0.00
BHLYP	E	3.62	4.41	4.55	5.45	5.66	3.54	3.58	3.77	3.85	4.24
	f	0.96	0.00	0.09	0.07	0.00	0.94	0.00	0.00	0.00	0.00
CAM-B3LYP	E	3.51	4.12	4.40	5.30	5.47	3.42	3.57	3.76	3.83	4.12
	f	0.91	0.00	0.09	0.06	0.00	0.91	0.00	0.00	0.00	0.00
CAMh-B3LYP	E	3.48	3.91	4.34	5.10	5.24	3.40	3.40	3.59	3.67	3.91
	f	0.89	0.00	0.09	0.05	0.00	0.01	0.88	0.00	0.00	0.00
BP86	E	2.56	3.29	3.86	3.92	4.18	2.57	2.88	3.24	3.26	3.35
	f	0.00	0.73	0.00	0.09	0.02	0.00	0.00	0.71	0.07	0.00
PBE	E	2.54	3.30	3.84	3.92	4.18	2.55	2.75	3.11	3.22	3.28
	f	0.00	0.73	0.00	0.09	0.00	0.00	0.00	0.00	0.00	0.83
PBE0	E	3.48	3.54	4.29	4.85	4.95	3.29	3.42	3.54	3.57	3.64
	f	0.87	0.00	0.09	0.04	0.00	0.00	0.88	0.00	0.00	0.00
PBE50	E	3.64	4.36	4.59	5.48	5.78	3.57	3.79	3.97	4.04	4.35
	f	0.97	0.00	0.09	0.07	0.00	0.95	0.00	0.00	0.00	0.00
ωPBE	E	3.48	4.13	4.40	5.31	5.34	3.41	3.83	4.02	4.13	4.16
	f	0.92	0.00	0.08	0.00	0.00	0.93	0.00	0.00	0.00	0.00
ωhPBE0	E	3.50	3.78	4.35	5.02	5.13	3.43	3.49	3.68	3.74	3.78
	f	0.89	0.00	0.09	0.05	0.00	0.89	0.00	0.00	0.00	0.00
ωPBEh	E	3.51	4.08	4.40	5.28	5.30	3.44	3.65	3.82	3.96	4.08
	f	0.91	0.00	0.09	0.06	0.00	0.91	0.00	0.00	0.00	0.00
BNL	E	3.58	4.55	4.57	5.80	6.14	3.49	3.85	4.09	4.26	4.49
	f	0.99	0.00	0.10	0.00	0.00	0.97	0.01	0.00	0.00	0.11
ωB97X	E	3.54	4.41	4.48	5.63	5.75	3.47	4.08	4.30	4.41	4.46
	f	0.94	0.00	0.09	0.00	0.00	0.94	0.01	0.00	0.00	0.00
ωB97X-D	E	3.51	4.15	4.40	5.30	5.38	3.44	3.76	3.93	4.08	4.15
	f	0.91	0.00	0.09	0.06	0.00	0.91	0.00	0.00	0.00	0.00
M06-2X	E	3.47	4.05	4.45	5.36	5.43	3.37	3.40	3.57	3.62	4.01
	f	0.92	0.00	0.09	0.06	0.00	0.00	0.90	0.00	0.00	0.00
M11	E	3.51	4.23	4.51	5.48	5.62	3.06	3.24	3.39	3.43	3.71
	f	0.94	0.00	0.08	0.00	0.08	0.00	0.00	0.00	0.89	0.00
M11-L	E	3.12	3.44	4.03	4.09	4.39	1.60	2.10	2.14	2.31	2.50
	f	0.00	0.73	0.00	0.09	0.03	0.00	0.00	0.00	0.00	0.00
CC2	E	3.24	3.54	4.23	4.50	5.27	3.25	3.43	3.53	3.88	4.01
	f	1.01	0.00	0.10	0.00	0.05	1.01	0.00	0.10	0.00	0.05

Table S5: TDDFT and CC2 excitation energies (E, in eV) and oscillator strengths (f) for pCA$''^{-}$ with the def2-TZVP and aug-def2-TZVP basis sets.

molecule		def2-TZVP					aug-def2-TZVP				
		1a	2a	3a	4a	5a	1a	2a	3a	4a	5a
RPA	E	4.83	5.17	5.65	6.22	6.37	4.51	4.70	5.01	5.07	5.11
	f	0.34	0.19	0.00	0.00	0.00	0.00	0.30	0.00	0.16	0.00
B3LYP	E	2.66	2.81	3.07	3.22	3.27	2.65	2.73	2.81	2.87	3.06
	f	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
BHLYP	E	4.09	4.23	4.47	4.74	4.86	4.11	4.13	4.28	4.38	4.55
	f	0.00	0.00	0.12	0.03	0.49	0.00	0.00	0.00	0.13	0.00
CAM-B3LYP	E	3.71	3.71	4.35	4.43	4.79	3.77	3.78	4.10	4.21	4.31
	f	0.00	0.00	0.09	0.00	0.58	0.00	0.00	0.00	0.00	0.09
CAMh-B3LYP	E	3.38	3.44	4.06	4.24	4.27	3.45	3.50	3.70	3.83	3.87
	f	0.00	0.00	0.01	0.07	0.00	0.00	0.00	0.00	0.00	0.00
BP86	E	1.46	1.66	1.74	1.95	2.18	1.55	1.57	1.76	1.81	1.82
	f	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PBE	E	1.43	1.62	1.70	1.91	2.16	1.39	1.52	1.64	1.73	1.78
	f	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PBE0	E	2.89	2.99	3.40	3.50	3.51	2.95	3.04	3.07	3.19	3.44
	f	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PBE50	E	4.03	4.19	4.51	4.73	4.89	4.06	4.23	4.35	4.45	4.68
	f	0.00	0.00	0.12	0.01	0.54	0.00	0.00	0.00	0.13	0.00
ωPBE	E	3.66	3.71	4.44	4.58	4.86	3.72	3.78	4.39	4.48	4.54
	f	0.00	0.00	0.09	0.00	0.59	0.00	0.00	0.10	0.01	0.01
ωhPBE0	E	3.23	3.28	3.90	4.02	4.08	3.29	3.33	3.64	3.75	3.94
	f	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ωPBEh	E	3.59	3.62	4.36	4.41	4.82	3.65	3.69	4.29	4.32	4.35
	f	0.00	0.00	0.07	0.02	0.63	0.00	0.00	0.00	0.10	0.00
BNL	E	4.43	4.63	4.66	5.03	5.56	4.47	4.57	4.67	4.67	4.94
	f	0.00	0.00	0.13	0.49	0.05	0.00	0.14	0.00	0.00	0.42
ωB97X	E	4.06	4.13	4.53	4.87	5.00	4.12	4.19	4.47	4.82	4.84
	f	0.00	0.00	0.11	0.35	0.20	0.00	0.00	0.13	0.41	0.00
ωB97X-D	E	3.70	3.72	4.38	4.49	4.80	3.75	3.78	4.33	4.43	4.53
	f	0.00	0.00	0.09	0.00	0.57	0.00	0.00	0.11	0.00	0.01
M06-2X	E	3.79	3.98	4.42	4.55	4.86	3.83	3.99	4.03	4.26	4.34
	f	0.00	0.00	0.09	0.00	0.61	0.00	0.00	0.00	0.00	0.00
M11	E	4.03	4.26	4.59	4.92	5.15	3.84	4.05	4.27	4.29	4.30
	f	0.00	0.00	0.13	0.47	0.09	0.00	0.00	0.00	0.00	0.01
M11-L	E	2.09	2.28	2.30	2.48	2.50	0.65	0.83	1.17	1.38	1.53
	f	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CC2	E	3.28	3.43	4.17	4.34	4.41	3.27	3.33	3.41	3.50	3.60
	f	0.00	0.00	0.02	0.02	0.05	0.00	0.00	0.02	0.02	0.05

Table S6: TDDFT and CC2 excitation energies (E, in eV) and oscillator strengths (f) for $TMpCA^-$ with the def2-TZVP and aug-def2-TZVP basis sets.

molecule		def2-TZVP					aug-def2-TZVP				
		1a	2a	3a	4a	5a	1a	2a	3a	4a	5a
RPA	E	3.76	4.96	5.53	5.64	5.85	3.68	3.76	3.95	4.17	4.38
	f	1.30	0.08	0.00	0.00	0.00	1.26	0.00	0.00	0.00	0.00
B3LYP	E	3.28	3.29	4.04	4.19	4.22	2.97	3.22	3.30	3.41	3.49
	f	1.10	0.00	0.00	0.08	0.00	0.00	1.10	0.00	0.00	0.00
BHLYP	E	3.45	4.31	4.57	4.83	4.93	3.38	3.64	3.77	3.88	4.23
	f	1.17	0.00	0.08	0.00	0.00	1.15	0.00	0.00	0.00	0.00
CAM-B3LYP	E	3.34	4.02	4.43	4.59	4.89	3.27	3.67	3.79	3.86	4.03
	f	1.11	0.00	0.09	0.00	0.00	1.11	0.00	0.00	0.00	0.00
CAMh-B3LYP	E	3.32	3.80	4.36	4.48	4.63	3.25	3.45	3.59	3.71	3.81
	f	1.09	0.00	0.09	0.00	0.00	1.10	0.00	0.00	0.00	0.00
BP86	E	2.43	3.14	3.53	3.70	3.87	2.45	2.74	3.12	3.13	3.38
	f	0.00	0.95	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00
PBE	E	2.41	3.15	3.47	3.68	3.79	2.43	2.62	2.98	3.12	3.24
	f	0.00	0.95	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00
PBE0	E	3.31	3.42	4.29	4.30	4.31	3.24	3.26	3.43	3.61	3.69
	f	1.07	0.00	0.08	0.00	0.00	0.00	1.10	0.00	0.00	0.00
PBE50	E	3.46	4.25	4.61	4.80	5.06	3.40	3.85	3.98	4.08	4.25
	f	1.18	0.00	0.08	0.00	0.00	1.17	0.00	0.00	0.00	0.00
ωPBE	E	3.30	4.03	4.42	4.51	5.27	3.24	3.94	4.04	4.11	4.26
	f	1.12	0.00	0.07	0.00	0.00	1.12	0.00	0.00	0.00	0.00
ωhPBE0	E	3.33	3.67	4.36	4.43	4.64	3.27	3.53	3.68	3.70	3.79
	f	1.09	0.00	0.08	0.00	0.00	1.10	0.00	0.00	0.00	0.00
ωPBEh	E	3.33	3.98	4.42	4.54	5.10	3.27	3.76	3.91	3.98	4.03
	f	1.11	0.00	0.08	0.00	0.00	1.11	0.00	0.00	0.00	0.00
BNL	E	3.41	4.46	4.60	4.78	5.43	3.33	3.93	4.16	4.34	4.45
	f	1.19	0.00	0.09	0.00	0.00	1.17	0.00	0.00	0.00	0.00
ωB97X	E	3.37	4.31	4.50	4.72	5.34	3.31	4.18	4.32	4.38	4.53
	f	1.14	0.00	0.08	0.00	0.00	1.14	0.00	0.00	0.00	0.00
ωB97X-D	E	3.34	4.05	4.43	4.59	5.12	3.28	3.87	4.02	4.06	4.15
	f	1.11	0.00	0.08	0.00	0.00	1.11	0.00	0.00	0.00	0.00
M06-2X	E	3.30	3.95	4.45	4.46	4.83	3.24	3.43	3.56	3.65	3.95
	f	1.12	0.00	0.00	0.09	0.00	1.11	0.00	0.00	0.00	0.00
M11	E	3.32	4.13	4.47	4.53	5.21	3.15	3.26	3.32	3.48	3.74
	f	1.13	0.00	0.00	0.08	0.00	0.00	1.10	0.00	0.00	0.00
M11-L	E	2.97	3.26	3.41	4.06	4.13	1.49	2.10	2.17	2.22	2.25
	f	0.00	0.97	0.00	0.06	0.00	0.00	0.00	0.00	0.00	0.00
CC2	E	3.04	3.40	4.23	4.44	4.92	2.96	3.30	3.45	3.47	3.84
	f	1.21	0.00	0.09	0.00	0.00	1.21	0.00	0.09	0.00	0.00

Table S7: TDDFT and CC2 excitation energies (E, in eV) and oscillator strengths (f) for pCT$^-$ with the def2-TZVP and aug-def2-TZVP basis sets.

molecule		def2-TZVP					aug-def2-TZVP				
		1a	2a	3a	4a	5a	1a	2a	3a	4a	5a
RPA	E	3.73	4.98	5.41	5.47	5.62	3.68	3.83	4.04	4.30	4.45
	f	1.47	0.07	0.08	0.00	0.00	1.41	0.01	0.00	0.00	0.00
B3LYP	E	2.95	3.18	3.24	3.28	4.19	2.92	2.98	3.14	3.23	3.26
	f	0.19	0.05	0.00	0.94	0.00	0.18	0.00	0.05	0.96	0.00
BHLYP	E	3.42	4.12	4.26	4.48	4.60	3.38	3.72	3.84	3.98	4.03
	f	1.34	0.00	0.00	0.00	0.07	1.32	0.00	0.00	0.00	0.00
CAM-B3LYP	E	3.31	3.97	4.15	4.46	4.54	3.26	3.77	3.91	3.96	3.98
	f	1.28	0.00	0.01	0.06	0.00	1.26	0.00	0.00	0.00	0.00
CAMh-B3LYP	E	3.28	3.75	3.78	4.09	4.39	3.23	3.55	3.67	3.72	3.77
	f	1.25	0.00	0.00	0.00	0.07	1.25	0.00	0.00	0.00	0.00
BP86	E	2.26	2.36	2.38	2.60	2.68	2.26	2.37	2.38	2.62	2.70
	f	0.05	0.00	0.00	0.00	0.00	0.05	0.00	0.00	0.00	0.00
PBE	E	2.25	2.33	2.37	2.56	2.65	2.24	2.35	2.36	2.59	2.59
	f	0.05	0.00	0.00	0.00	0.00	0.05	0.00	0.00	0.00	0.00
PBE0	E	3.12	3.34	3.37	3.42	4.28	3.10	3.26	3.29	3.38	3.39
	f	0.41	0.75	0.00	0.06	0.00	0.41	0.02	0.76	0.03	0.00
PBE50	E	3.43	4.14	4.20	4.51	4.65	3.40	3.94	4.04	4.08	4.19
	f	1.34	0.00	0.00	0.00	0.07	1.34	0.00	0.00	0.00	0.00
ωPBE	E	3.27	3.97	4.46	4.55	4.65	3.23	3.98	4.04	4.23	4.41
	f	1.27	0.00	0.07	0.00	0.02	1.26	0.00	0.00	0.00	0.06
ωhPBE0	E	3.29	3.62	3.67	3.95	4.40	3.25	3.61	3.64	3.64	3.78
	f	1.23	0.00	0.02	0.00	0.07	1.23	0.01	0.00	0.00	0.00
ωPBEh	E	3.31	3.92	4.38	4.48	4.56	3.26	3.86	3.93	4.04	4.23
	f	1.27	0.00	0.04	0.04	0.00	1.26	0.00	0.00	0.00	0.01
BNL	E	3.39	4.40	4.63	4.80	5.09	3.34	4.03	4.27	4.41	4.50
	f	1.35	0.00	0.08	0.00	0.07	1.34	0.00	0.00	0.00	0.02
ωB97X	E	3.34	4.26	4.53	4.75	4.83	3.29	4.26	4.27	4.45	4.50
	f	1.30	0.00	0.07	0.00	0.03	1.29	0.00	0.00	0.08	0.00
ωB97X-D	E	3.31	3.99	4.42	4.50	4.61	3.27	3.96	4.00	4.14	4.32
	f	1.28	0.00	0.05	0.03	0.00	1.26	0.00	0.00	0.00	0.03
M06-2X	E	3.27	3.89	4.02	4.39	4.43	3.23	3.54	3.65	3.76	3.88
	f	1.28	0.00	0.00	0.00	0.00	1.26	0.00	0.00	0.00	0.00
M11	E	3.29	4.07	4.47	4.56	4.77	3.25	3.26	3.43	3.68	3.85
	f	1.29	0.00	0.00	0.07	0.04	1.20	0.05	0.01	0.00	0.00
M11-L	E	2.45	2.56	2.90	3.16	3.24	1.47	1.86	2.11	2.18	2.35
	f	0.05	0.00	0.00	0.01	1.01	0.00	0.00	0.00	0.00	0.01
CC2	E	3.04	3.36	3.89	4.26	4.40	2.98	3.33	3.37	3.55	3.57
	f	1.37	0.00	0.00	0.08	0.00	1.37	0.00	0.00	0.08	0.00

Table S8: TDDFT and CC2 excitation energies (E, in eV) and oscillator strengths (f) for p-HBDI$^-$ with the def2-TZVP and aug-def2-TZVP basis sets.

molecule		def2-TZVP					aug-def2-TZVP				
		1a	2a	3a	4a	5a	1a	2a	3a	4a	5a
RPA	E	3.56	5.01	5.46	5.63	5.90	3.35	3.48	3.59	3.73	3.85
	f	1.34	0.05	0.00	0.00	0.07	0.00	1.25	0.00	0.00	0.01
B3LYP	E	3.10	3.20	3.73	4.16	4.18	2.46	3.00	3.01	3.19	3.28
	f	1.00	0.00	0.00	0.00	0.05	0.00	0.00	0.87	0.10	0.00
BHLYP	E	3.25	4.22	4.54	4.60	5.03	3.03	3.20	3.53	3.62	3.67
	f	1.10	0.00	0.00	0.06	0.01	0.00	1.09	0.00	0.00	0.01
CAM-B3LYP	E	3.15	3.92	4.47	4.62	4.71	3.09	3.12	3.60	3.60	3.74
	f	1.05	0.00	0.05	0.00	0.00	1.05	0.00	0.00	0.00	0.00
CAMh-B3LYP	E	3.13	3.70	4.32	4.39	4.53	2.88	3.07	3.38	3.49	3.53
	f	1.02	0.00	0.00	0.05	0.00	0.00	1.02	0.00	0.00	0.01
BP86	E	2.37	2.97	3.43	3.50	3.70	2.33	2.39	2.82	2.86	2.94
	f	0.00	0.85	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.73
PBE	E	2.34	2.97	3.29	3.41	3.71	2.17	2.37	2.63	2.76	2.91
	f	0.00	0.85	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.27
PBE0	E	3.13	3.33	4.06	4.28	4.29	2.71	3.07	3.24	3.41	3.47
	f	1.00	0.00	0.00	0.00	0.05	0.00	0.97	0.00	0.02	0.00
PBE50	E	3.27	4.15	4.63	4.84	5.03	3.22	3.25	3.73	3.81	3.87
	f	1.11	0.00	0.05	0.00	0.01	1.10	0.00	0.00	0.00	0.00
ωPBE	E	3.10	3.92	4.49	4.57	4.94	3.05	3.59	3.87	3.97	4.12
	f	1.06	0.00	0.05	0.00	0.01	1.06	0.00	0.00	0.00	0.00
ωhPBE0	E	3.14	3.57	4.39	4.43	4.45	2.96	3.09	3.45	3.56	3.60
	f	1.02	0.00	0.05	0.00	0.00	0.00	1.01	0.00	0.00	0.01
ωPBEh	E	3.14	3.87	4.47	4.59	4.84	3.09	3.36	3.68	3.75	3.90
	f	1.05	0.00	0.05	0.00	0.01	1.04	0.00	0.00	0.00	0.00
BNL	E	3.21	4.36	4.69	5.16	5.36	3.15	3.59	3.88	4.03	4.15
	f	1.15	0.00	0.06	0.00	0.00	1.14	0.00	0.00	0.00	0.00
ωB97X	E	3.16	4.21	4.57	4.92	5.12	3.11	3.85	4.10	4.24	4.40
	f	1.09	0.00	0.05	0.00	0.02	1.09	0.00	0.00	0.00	0.00
ωB97X-D	E	3.14	3.94	4.47	4.67	4.88	3.09	3.48	3.78	3.86	4.02
	f	1.05	0.00	0.05	0.00	0.01	1.05	0.00	0.00	0.00	0.00
M06-2X	E	3.12	3.84	4.51	4.69	4.71	2.86	3.07	3.34	3.42	3.45
	f	1.04	0.00	0.06	0.00	0.00	0.00	1.03	0.00	0.00	0.01
M11	E	3.12	4.01	4.61	4.79	5.06	2.78	3.06	3.10	3.17	3.23
	f	1.07	0.00	0.05	0.00	0.01	0.00	1.02	0.00	0.00	0.03
M11-L	E	2.88	3.06	3.10	3.93	3.96	1.02	1.49	1.61	1.84	1.96
	f	0.00	0.90	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00
CC2	E	2.92	3.30	4.30	4.54	4.57	2.77	2.85	3.24	3.25	3.35
	f	1.17	0.00	0.07	0.00	0.00	1.17	0.00	0.07	0.00	0.00

Table S9: TDDFT and CC2 excitation energies (E, in eV) and oscillator strengths (f) for p-HBDI with the def2-TZVP and aug-def2-TZVP basis sets.

molecule		def2-TZVP					aug-def2-TZVP				
		1a	2a	3a	4a	5a	1a	2a	3a	4a	5a
RPA	E	4.13	5.33	5.63	5.80	6.63	4.10	5.26	5.42	5.63	5.74
	f	0.93	0.02	0.00	0.05	0.12	0.90	0.02	0.00	0.00	0.00
B3LYP	E	3.44	3.66	4.16	4.27	4.77	3.42	3.65	4.15	4.24	4.61
	f	0.69	0.00	0.07	0.00	0.08	0.68	0.00	0.07	0.00	0.00
BHLYP	E	3.77	4.50	4.81	4.96	5.62	3.74	4.49	4.77	4.95	5.21
	f	0.82	0.00	0.02	0.03	0.15	0.80	0.00	0.02	0.03	0.00
CAM-B3LYP	E	3.67	4.11	4.67	4.74	5.54	3.64	4.10	4.64	4.71	5.18
	f	0.76	0.00	0.03	0.04	0.16	0.75	0.00	0.03	0.05	0.00
CAMh-B3LYP	E	3.60	3.97	4.53	4.59	5.30	3.57	3.96	4.51	4.56	4.99
	f	0.74	0.00	0.06	0.02	0.13	0.73	0.00	0.06	0.03	0.00
BP86	E	3.00	3.18	3.63	3.78	4.11	3.00	3.16	3.62	3.76	4.09
	f	0.00	0.55	0.11	0.00	0.04	0.00	0.55	0.11	0.00	0.04
PBE	E	2.98	3.18	3.62	3.78	4.11	2.98	3.16	3.61	3.75	4.09
	f	0.00	0.55	0.12	0.00	0.04	0.00	0.55	0.12	0.00	0.04
PBE0	E	3.51	3.76	4.30	4.40	4.95	3.49	3.75	4.28	4.37	4.90
	f	0.71	0.00	0.08	0.00	0.09	0.70	0.00	0.08	0.00	0.09
PBE50	E	3.78	4.44	4.84	4.96	5.65	3.76	4.43	4.80	4.95	5.45
	f	0.82	0.00	0.02	0.04	0.15	0.81	0.00	0.02	0.04	0.00
ωPBE	E	3.70	3.95	4.73	4.77	5.39	3.67	3.94	4.70	4.74	5.37
	f	0.74	0.00	0.04	0.08	0.00	0.73	0.00	0.03	0.08	0.00
ωhPBE0	E	3.58	3.88	4.48	4.55	5.21	3.55	3.87	4.47	4.53	5.10
	f	0.73	0.00	0.08	0.01	0.11	0.72	0.00	0.08	0.01	0.00
ωPBEh	E	3.67	3.98	4.69	4.73	5.46	3.64	3.97	4.66	4.70	5.35
	f	0.74	0.00	0.06	0.04	0.00	0.73	0.00	0.05	0.05	0.00
BNL	E	3.90	4.46	4.98	5.23	5.89	3.87	4.44	4.93	5.20	5.53
	f	0.82	0.00	0.03	0.05	0.00	0.81	0.00	0.03	0.05	0.00
ωB97X	E	3.78	4.27	4.84	4.98	5.73	3.76	4.26	4.81	4.96	5.72
	f	0.78	0.00	0.02	0.06	0.00	0.77	0.00	0.02	0.06	0.00
ωB97X-D	E	3.68	4.06	4.71	4.76	5.53	3.66	4.05	4.68	4.74	5.47
	f	0.75	0.00	0.04	0.05	0.00	0.74	0.00	0.04	0.06	0.00
M06-2X	E	3.67	4.08	4.71	4.75	5.55	3.65	4.07	4.68	4.73	5.06
	f	0.75	0.00	0.05	0.03	0.15	0.74	0.00	0.04	0.05	0.00
M11	E	3.74	4.12	4.89	4.92	5.59	3.71	4.11	4.84	4.86	4.90
	f	0.76	0.00	0.05	0.05	0.00	0.75	0.00	0.03	0.00	0.07
M11-L	E	3.34	3.55	3.92	4.01	4.33	3.22	3.28	3.35	3.55	3.89
	f	0.65	0.00	0.05	0.01	0.05	0.00	0.00	0.66	0.00	0.02
CC2	E	3.71	3.90	4.53	4.56	5.57	3.66	3.87	4.49	4.51	5.01
	f	0.77	0.00	0.15	0.00	0.16	0.77	0.00	0.15	0.00	0.16

Table S10: TDDFT and CC2 excitation energies (E, in eV) and oscillator strengths (f) for p-HBDI$^+$ with the def2-TZVP and aug-def2-TZVP basis sets.

molecule		def2-TZVP					aug-def2-TZVP				
		1a	2a	3a	4a	5a	1a	2a	3a	4a	5a
RPA	E	3.76	5.03	5.82	6.44	6.62	3.74	5.01	5.79	6.17	6.36
	f	1.13	0.02	0.03	0.20	0.01	1.12	0.02	0.03	0.00	0.18
B3LYP	E	3.25	3.67	4.01	4.14	5.03	3.24	3.66	4.00	4.13	4.98
	f	0.93	0.03	0.00	0.02	0.06	0.92	0.03	0.00	0.02	0.04
BHLYP	E	3.45	4.26	4.87	5.09	5.62	3.44	4.25	4.86	5.08	5.57
	f	1.02	0.02	0.01	0.00	0.09	1.02	0.02	0.01	0.00	0.08
CAM-B3LYP	E	3.34	4.17	4.56	4.68	5.45	3.32	4.16	4.55	4.66	5.41
	f	0.99	0.02	0.00	0.01	0.09	0.98	0.02	0.00	0.02	0.08
CAMh-B3LYP	E	3.31	4.01	4.38	4.51	5.32	3.30	4.00	4.37	4.50	5.28
	f	0.97	0.02	0.00	0.02	0.08	0.96	0.02	0.00	0.02	0.07
BP86	E	3.09	3.26	3.28	3.63	4.34	3.08	3.25	3.27	3.62	4.33
	f	0.77	0.00	0.06	0.04	0.02	0.78	0.00	0.06	0.04	0.02
PBE	E	3.09	3.24	3.28	3.62	4.33	3.08	3.23	3.27	3.61	4.31
	f	0.77	0.00	0.07	0.04	0.02	0.77	0.00	0.06	0.04	0.02
PBE0	E	3.30	3.80	4.15	4.27	5.16	3.29	3.79	4.14	4.26	5.12
	f	0.96	0.02	0.00	0.02	0.06	0.95	0.02	0.00	0.02	0.06
PBE50	E	3.47	4.29	4.87	5.03	5.65	3.45	4.28	4.86	5.02	5.61
	f	1.03	0.02	0.01	0.00	0.09	1.02	0.02	0.01	0.00	0.09
ωPBE	E	3.31	4.30	4.36	4.74	5.52	3.29	4.29	4.35	4.73	5.48
	f	1.00	0.01	0.00	0.02	0.10	0.99	0.01	0.00	0.02	0.10
ωhPBE0	E	3.32	3.96	4.29	4.45	5.30	3.31	3.95	4.28	4.44	5.26
	f	0.97	0.02	0.00	0.03	0.07	0.96	0.02	0.00	0.02	0.07
ωPBEh	E	3.34	4.18	4.40	4.66	5.46	3.32	4.17	4.39	4.65	5.42
	f	0.99	0.02	0.00	0.02	0.09	0.99	0.02	0.00	0.02	0.08
BNL	E	3.43	4.68	5.04	5.25	5.89	3.41	4.66	5.02	5.22	5.83
	f	1.07	0.01	0.00	0.01	0.16	1.07	0.01	0.00	0.01	0.15
ωB97X	E	3.38	4.43	4.78	4.95	5.67	3.36	4.42	4.77	4.93	5.63
	f	1.02	0.01	0.00	0.01	0.12	1.02	0.01	0.00	0.01	0.11
ωB97X-D	E	3.35	4.20	4.50	4.70	5.48	3.33	4.19	4.49	4.69	5.45
	f	0.99	0.02	0.00	0.02	0.09	0.99	0.02	0.00	0.02	0.09
M06-2X	E	3.33	4.19	4.62	4.71	5.50	3.31	4.18	4.61	4.69	5.44
	f	0.99	0.02	0.00	0.01	0.09	0.98	0.02	0.00	0.01	0.08
M11	E	3.35	4.43	4.68	4.91	5.69	3.33	4.42	4.67	4.89	5.63
	f	1.01	0.02	0.00	0.01	0.11	1.00	0.02	0.00	0.01	0.07
M11-L	E	3.22	3.46	3.85	3.93	4.60	3.20	3.45	3.73	3.84	3.93
	f	0.81	0.06	0.02	0.01	0.00	0.81	0.06	0.00	0.02	0.01
CC2	E	3.15	4.03	4.36	4.44	5.32	3.12	4.00	4.33	4.41	5.25
	f	1.09	0.02	0.00	0.00	0.10	1.09	0.02	0.00	0.00	0.10

Table S11: TDDFT and CC2 excitation energies (E, in eV) and oscillator strengths (f) for $PSBT^+$ with the def2-TZVP and aug-def2-TZVP basis sets.

molecule		def2-TZVP					aug-def2-TZVP				
		1a	2a	3a	4a	5a	1a	2a	3a	4a	5a
RPA	E	2.78	4.51	5.68	5.73	6.68	2.77	4.49	5.44	5.66	5.73
	f	2.38	0.23	0.01	0.05	0.15	2.38	0.23	0.00	0.01	0.05
B3LYP	E	2.29	3.12	3.83	3.88	4.15	2.28	3.11	3.83	3.88	4.15
	f	1.66	0.64	0.01	0.01	0.02	1.66	0.63	0.01	0.01	0.02
BHLYP	E	2.49	3.72	4.52	4.90	5.20	2.48	3.71	4.50	4.89	5.20
	f	2.05	0.35	0.03	0.05	0.01	2.04	0.34	0.03	0.05	0.01
CAM-B3LYP	E	2.42	3.67	4.49	4.81	4.97	2.41	3.67	4.48	4.80	4.97
	f	2.00	0.32	0.03	0.03	0.01	2.00	0.32	0.03	0.03	0.01
CAMh-B3LYP	E	2.38	3.50	4.29	4.56	4.69	2.37	3.49	4.27	4.56	4.68
	f	1.91	0.39	0.02	0.01	0.05	1.91	0.38	0.02	0.02	0.04
BP86	E	2.10	2.73	2.97	3.18	3.29	2.10	2.73	2.97	3.18	3.29
	f	1.12	1.03	0.00	0.00	0.00	1.12	1.03	0.00	0.00	0.00
PBE	E	2.10	2.73	2.95	3.17	3.28	2.09	2.72	2.94	3.17	3.27
	f	1.11	1.02	0.00	0.00	0.00	1.12	1.01	0.00	0.00	0.00
PBE0	E	2.32	3.22	3.96	4.01	4.29	2.31	3.21	3.95	4.00	4.28
	f	1.75	0.57	0.01	0.01	0.02	1.74	0.56	0.01	0.01	0.03
PBE50	E	2.49	3.71	4.54	4.90	5.11	2.48	3.71	4.52	4.89	5.11
	f	2.05	0.36	0.03	0.05	0.01	2.04	0.35	0.03	0.04	0.01
ωPBE	E	2.42	3.83	4.81	4.94	5.15	2.41	3.82	4.79	4.93	5.14
	f	2.04	0.26	0.03	0.02	0.01	2.04	0.25	0.03	0.02	0.00
ωhPBE0	E	2.37	3.44	4.22	4.39	4.59	2.37	3.43	4.21	4.38	4.58
	f	1.88	0.42	0.02	0.00	0.06	1.88	0.41	0.02	0.00	0.06
ωPBEh	E	2.42	3.75	4.62	4.85	5.00	2.42	3.75	4.61	4.84	5.00
	f	2.03	0.29	0.03	0.03	0.01	2.03	0.28	0.03	0.03	0.01
BNL	E	2.54	4.11	5.23	5.29	5.80	2.53	4.10	5.20	5.27	5.56
	f	2.22	0.22	0.00	0.07	0.00	2.20	0.22	0.00	0.07	0.00
ωB97X	E	2.48	3.95	4.94	5.08	5.49	2.47	3.94	4.93	5.06	5.48
	f	2.10	0.24	0.03	0.03	0.01	2.10	0.24	0.03	0.03	0.01
ωB97X-D	E	2.44	3.78	4.65	4.89	5.10	2.43	3.77	4.63	4.88	5.09
	f	2.04	0.28	0.03	0.03	0.01	2.04	0.28	0.03	0.03	0.01
M06-2X	E	2.37	3.60	4.45	4.66	4.80	2.37	3.59	4.44	4.66	4.79
	f	1.94	0.34	0.03	0.01	0.04	1.94	0.34	0.03	0.01	0.03
M11	E	2.44	3.89	4.90	5.02	5.27	2.44	3.88	4.86	4.87	5.01
	f	2.07	0.25	0.03	0.03	0.00	2.07	0.24	0.00	0.03	0.03
M11-L	E	2.20	2.83	3.34	3.46	3.64	2.19	2.82	3.34	3.45	3.58
	f	1.20	1.00	0.00	0.02	0.00	1.19	0.99	0.00	0.02	0.00
CC2	E	2.17	3.35	4.22	4.54	4.73	2.16	3.34	4.20	4.52	4.70
	f	1.92	0.50	0.10	0.01	0.05	1.92	0.50	0.10	0.01	0.05

Table S12: TDDFT and CC2 excitation energies (E, in eV) and oscillator strengths (f) for $PSB11Me_2^+$ with the def2-TZVP and aug-def2-TZVP basis sets.

molecule		def2-TZVP					aug-def2-TZVP				
		1a	2a	3a	4a	5a	1a	2a	3a	4a	5a
RPA	E	2.77	4.46	5.60	5.66	6.60	2.76	4.44	5.47	5.55	5.68
	f	2.01	0.36	0.07	0.04	0.17	2.00	0.36	0.00	0.08	0.03
B3LYP	E	2.27	3.09	3.80	3.88	4.15	2.26	3.08	3.79	3.88	4.14
	f	1.35	0.53	0.06	0.01	0.06	1.36	0.53	0.07	0.01	0.07
BHLYP	E	2.47	3.69	4.44	4.86	5.20	2.46	3.69	4.41	4.85	5.19
	f	1.69	0.35	0.15	0.03	0.00	1.68	0.35	0.16	0.03	0.00
CAM-B3LYP	E	2.40	3.65	4.41	4.78	4.97	2.39	3.64	4.39	4.77	4.96
	f	1.65	0.34	0.13	0.02	0.01	1.65	0.33	0.13	0.02	0.01
CAMh-B3LYP	E	2.36	3.48	4.21	4.55	4.66	2.35	3.47	4.20	4.55	4.66
	f	1.57	0.37	0.13	0.03	0.03	1.56	0.36	0.13	0.02	0.03
BP86	E	2.09	2.71	2.97	3.17	3.29	2.08	2.70	2.97	3.17	3.28
	f	0.90	0.85	0.00	0.00	0.01	0.90	0.83	0.00	0.00	0.01
PBE	E	2.08	2.70	2.95	3.16	3.27	2.08	2.70	2.95	3.16	3.27
	f	0.90	0.85	0.00	0.00	0.00	0.90	0.85	0.00	0.00	0.01
PBE0	E	2.30	3.19	3.92	4.01	4.28	2.29	3.18	3.91	4.01	4.26
	f	1.43	0.49	0.08	0.01	0.07	1.42	0.49	0.08	0.01	0.08
PBE50	E	2.46	3.69	4.45	4.86	5.11	2.46	3.68	4.43	4.85	5.11
	f	1.69	0.36	0.15	0.03	0.00	1.68	0.36	0.15	0.03	0.00
ωPBE	E	2.39	3.79	4.72	4.90	5.13	2.38	3.78	4.70	4.89	5.13
	f	1.69	0.31	0.12	0.01	0.00	1.69	0.30	0.12	0.01	0.00
ωhPBE0	E	2.35	3.41	4.15	4.39	4.55	2.34	3.41	4.13	4.38	4.54
	f	1.54	0.39	0.12	0.01	0.07	1.54	0.39	0.12	0.01	0.06
ωPBEh	E	2.40	3.72	4.54	4.82	4.99	2.39	3.71	4.52	4.81	4.99
	f	1.67	0.32	0.12	0.02	0.01	1.67	0.32	0.12	0.01	0.00
BNL	E	2.52	4.07	5.16	5.23	5.76	2.51	4.06	5.13	5.21	5.55
	f	1.86	0.31	0.11	0.03	0.00	1.83	0.31	0.11	0.03	0.00
ωB97X	E	2.45	3.91	4.85	5.04	5.47	2.45	3.90	4.83	5.03	5.47
	f	1.75	0.31	0.12	0.01	0.00	1.74	0.31	0.12	0.01	0.00
ωB97X-D	E	2.41	3.75	4.56	4.85	5.08	2.40	3.74	4.54	4.84	5.08
	f	1.68	0.32	0.12	0.02	0.00	1.68	0.32	0.12	0.01	0.00
M06-2X	E	2.36	3.58	4.38	4.66	4.78	2.35	3.57	4.35	4.66	4.77
	f	1.60	0.34	0.13	0.01	0.02	1.60	0.34	0.13	0.01	0.02
M11	E	2.42	3.85	4.81	4.97	5.24	2.41	3.84	4.77	4.90	4.97
	f	1.72	0.31	0.11	0.01	0.00	1.71	0.30	0.11	0.00	0.01
M11-L	E	2.19	2.79	3.35	3.44	3.63	2.18	2.78	3.35	3.43	3.52
	f	0.98	0.82	0.00	0.03	0.00	0.97	0.81	0.00	0.04	0.00
CC2	E	2.17	3.34	4.16	4.53	4.70	2.16	3.32	4.14	4.51	4.68
	f	1.56	0.47	0.15	0.06	0.07	1.56	0.47	0.15	0.06	0.07

Table S13: TDA and CC2 excitation energies (E, in eV) and oscillator strengths (f) for pVP with the def2-TZVP and aug-def2-TZVP basis sets.

molecule		def2-TZVP					aug-def2-TZVP				
		1a	2a	3a	4a	5a	1a	2a	3a	4a	5a
CIS	E	5.31	5.62	7.01	7.14	7.51	5.18	5.53	5.56	5.88	6.06
	f	0.35	0.13	0.71	0.00	0.78	0.33	0.11	0.01	0.00	0.00
B3LYP	E	4.58	5.02	5.60	5.98	6.21	4.51	4.76	4.90	5.16	5.37
	f	0.07	0.52	0.00	0.18	0.07	0.09	0.00	0.46	0.01	0.00
BHLYP	E	4.97	5.30	6.30	6.69	6.90	4.88	5.20	5.32	5.64	5.87
	f	0.14	0.45	0.00	0.22	0.85	0.17	0.37	0.00	0.01	0.00
CAM-B3LYP	E	4.84	5.25	6.19	6.59	6.85	4.77	5.14	5.26	5.61	5.85
	f	0.09	0.52	0.00	0.25	0.74	0.11	0.45	0.00	0.01	0.00
CAMh-B3LYP	E	4.76	5.18	6.00	6.41	6.77	4.69	5.07	5.09	5.45	5.67
	f	0.08	0.53	0.00	0.25	0.00	0.10	0.46	0.00	0.01	0.00
BP86	E	4.26	4.75	5.39	5.40	5.59	4.22	4.62	4.66	5.06	5.34
	f	0.05	0.46	0.06	0.00	0.22	0.05	0.00	0.44	0.01	0.06
PBE	E	4.26	4.75	5.39	5.59	5.89	4.21	4.45	4.65	4.91	5.32
	f	0.05	0.46	0.05	0.23	0.03	0.06	0.00	0.43	0.00	0.05
PBE0	E	4.69	5.12	5.95	6.16	6.43	4.62	5.01	5.05	5.42	5.62
	f	0.08	0.53	0.00	0.20	0.06	0.09	0.47	0.00	0.01	0.00
PBE50	E	5.01	5.35	6.62	6.74	6.96	4.94	5.27	5.58	5.89	6.11
	f	0.13	0.47	0.00	0.23	0.82	0.16	0.41	0.00	0.01	0.00
ωPBE	E	4.87	5.34	6.69	6.75	6.97	4.82	5.25	5.63	5.99	6.22
	f	0.06	0.57	0.00	0.25	0.76	0.07	0.52	0.00	0.01	0.00
ωhPBE0	E	4.77	5.19	6.19	6.35	6.71	4.70	5.09	5.22	5.56	5.76
	f	0.08	0.54	0.00	0.24	0.06	0.10	0.48	0.00	0.01	0.00
ωPBEh	E	4.85	5.28	6.51	6.61	6.90	4.79	5.19	5.42	5.75	5.95
	f	0.07	0.55	0.00	0.26	0.70	0.09	0.49	0.00	0.01	0.00
BNL	E	5.09	5.46	6.67	7.01	7.18	5.00	5.36	5.64	6.02	6.29
	f	0.12	0.49	0.00	0.35	0.89	0.14	0.41	0.00	0.01	0.00
ωB97X	E	4.96	5.35	6.84	6.88	6.98	4.91	5.28	5.87	6.21	6.49
	f	0.09	0.51	0.21	0.00	0.91	0.10	0.47	0.00	0.01	0.00
ωB97X-D	E	4.86	5.27	6.62	6.70	6.87	4.80	5.19	5.55	5.86	6.07
	f	0.08	0.53	0.25	0.00	0.74	0.09	0.48	0.00	0.01	0.00
M06-2X	E	4.91	5.34	6.29	6.65	6.98	4.83	5.19	5.23	5.54	5.73
	f	0.09	0.56	0.00	0.29	0.67	0.10	0.00	0.48	0.01	0.00
M11	E	5.02	5.41	6.52	6.86	7.03	4.93	4.97	5.28	5.31	5.46
	f	0.10	0.55	0.00	0.24	0.82	0.12	0.00	0.43	0.00	0.00
M11-L	E	4.44	4.80	5.02	5.55	5.79	3.51	3.94	4.03	4.34	4.35
	f	0.09	0.42	0.00	0.10	0.00	0.00	0.00	0.00	0.11	0.00
CC2	E	4.66	5.25	6.42	6.44	6.84	4.58	5.11	5.22	5.60	5.80
	f	0.05	0.52	0.00	0.28	0.45	0.05	0.52	0.00	0.28	0.45

Table S14: TDA and CC2 excitation energies (E, in eV) and oscillator strengths (f) for pCA with the def2-TZVP and aug-def2-TZVP basis sets.

molecule		def2-TZVP					aug-def2-TZVP				
		1a	2a	3a	4a	5a	1a	2a	3a	4a	5a
CIS	E	5.00	5.60	6.52	6.74	7.25	4.94	5.54	5.90	6.29	6.50
	f	0.76	0.03	0.00	0.52	0.59	0.72	0.04	0.00	0.00	0.00
B3LYP	E	4.37	4.49	4.58	5.44	5.77	4.31	4.47	4.54	5.00	5.38
	f	0.77	0.00	0.13	0.14	0.15	0.77	0.00	0.12	0.00	0.15
BHLYP	E	4.69	5.05	5.38	6.27	6.49	4.64	5.01	5.36	5.59	6.02
	f	0.86	0.08	0.00	0.27	0.00	0.83	0.08	0.00	0.00	0.00
CAM-B3LYP	E	4.62	4.90	5.01	6.18	6.35	4.56	4.87	4.98	5.49	5.95
	f	0.81	0.13	0.00	0.27	0.00	0.79	0.13	0.00	0.00	0.00
CAMh-B3LYP	E	4.54	4.81	4.86	5.94	6.17	4.48	4.77	4.83	5.33	5.80
	f	0.81	0.13	0.00	0.22	0.00	0.79	0.13	0.00	0.00	0.00
BP86	E	3.69	4.08	4.19	4.83	5.10	3.68	4.04	4.17	4.79	5.05
	f	0.00	0.59	0.17	0.06	0.20	0.00	0.63	0.14	0.06	0.20
PBE	E	3.67	4.08	4.19	4.83	5.09	3.66	4.03	4.16	4.78	5.04
	f	0.00	0.59	0.17	0.06	0.19	0.00	0.62	0.14	0.06	0.20
PBE0	E	4.46	4.61	4.70	5.62	5.97	4.41	4.59	4.66	5.30	5.56
	f	0.81	0.00	0.12	0.16	0.14	0.80	0.00	0.12	0.00	0.17
PBE50	E	4.73	5.08	5.34	6.31	6.62	4.68	5.05	5.32	5.85	6.24
	f	0.88	0.08	0.00	0.27	0.36	0.85	0.08	0.00	0.00	0.29
ωPBE	E	4.70	4.89	4.94	6.41	6.58	4.64	4.86	4.91	5.84	6.30
	f	0.76	0.00	0.20	0.30	0.25	0.75	0.00	0.19	0.00	0.00
ωhPBE0	E	4.55	4.77	4.80	5.86	6.25	4.49	4.75	4.77	5.46	5.80
	f	0.82	0.00	0.13	0.20	0.13	0.81	0.00	0.12	0.00	0.21
ωPBEh	E	4.65	4.90	4.91	6.21	6.52	4.60	4.88	4.88	5.66	6.08
	f	0.80	0.03	0.12	0.26	0.27	0.79	0.12	0.03	0.00	0.00
BNL	E	4.85	5.21	5.37	6.73	6.82	4.79	5.16	5.33	5.86	6.32
	f	0.80	0.13	0.00	0.29	0.00	0.76	0.14	0.00	0.00	0.00
ωB97X	E	4.74	5.04	5.18	6.55	6.60	4.70	5.02	5.15	6.10	6.47
	f	0.79	0.13	0.00	0.29	0.38	0.78	0.13	0.00	0.00	0.40
ωB97X-D	E	4.65	4.92	4.97	6.23	6.51	4.60	4.89	4.95	5.80	6.16
	f	0.81	0.14	0.00	0.27	0.29	0.79	0.14	0.00	0.00	0.29
M06-2X	E	4.67	4.97	5.02	6.22	6.45	4.62	4.93	5.00	5.44	5.86
	f	0.84	0.13	0.00	0.26	0.00	0.80	0.13	0.00	0.00	0.00
M11	E	4.77	5.07	5.10	6.54	6.67	4.71	5.04	5.06	5.22	5.62
	f	0.85	0.00	0.11	0.33	0.29	0.81	0.00	0.12	0.00	0.00
M11-L	E	4.21	4.25	4.41	5.05	5.34	3.75	4.16	4.19	4.20	4.38
	f	0.00	0.66	0.11	0.09	0.17	0.00	0.00	0.51	0.13	0.12
CC2	E	4.52	4.77	4.96	6.02	6.43	4.44	4.72	4.90	5.45	5.88
	f	0.54	0.27	0.00	0.22	0.16	0.54	0.27	0.00	0.22	0.16

Table S15: TDA and CC2 excitation energies (E, in eV) and oscillator strengths (f) for pCA$'^{-}$ with the def2-TZVP and aug-def2-TZVP basis sets.

molecule		def2-TZVP					aug-def2-TZVP				
		1a	2a	3a	4a	5a	1a	2a	3a	4a	5a
CIS	E	4.17	5.14	5.74	6.49	6.56	3.68	3.87	4.05	4.08	4.36
	f	1.27	0.12	0.00	0.00	0.00	0.01	0.00	1.16	0.00	0.00
B3LYP	E	3.41	3.80	4.33	4.69	4.76	3.05	3.38	3.41	3.45	3.68
	f	0.00	1.28	0.18	0.00	0.08	0.00	0.00	0.00	0.00	1.23
BHLYP	E	3.90	4.44	4.69	5.56	5.66	3.58	3.77	3.79	3.85	4.24
	f	1.33	0.00	0.13	0.11	0.00	0.00	0.00	1.26	0.00	0.00
CAM-B3LYP	E	3.79	4.14	4.54	5.42	5.48	3.57	3.67	3.76	3.83	4.14
	f	1.29	0.00	0.13	0.10	0.00	0.00	1.24	0.00	0.00	0.00
CAMh-B3LYP	E	3.79	3.92	4.48	5.20	5.25	3.40	3.59	3.67	3.67	3.92
	f	1.30	0.00	0.14	0.09	0.00	0.00	0.00	0.00	1.25	0.00
BP86	E	2.57	3.73	3.87	4.07	4.22	2.58	2.88	3.26	3.35	3.62
	f	0.00	1.01	0.00	0.25	0.00	0.00	0.00	0.00	0.00	1.02
PBE	E	2.55	3.73	3.85	4.07	4.18	2.56	2.75	3.11	3.22	3.57
	f	0.00	1.00	0.00	0.25	0.00	0.00	0.00	0.00	0.00	0.17
PBE0	E	3.55	3.84	4.43	4.93	4.96	3.29	3.55	3.57	3.64	3.73
	f	0.00	1.32	0.16	0.08	0.00	0.00	0.00	0.00	0.00	1.27
PBE50	E	3.92	4.39	4.73	5.59	5.82	3.79	3.83	3.97	4.04	4.39
	f	1.35	0.00	0.13	0.11	0.00	0.00	1.30	0.00	0.00	0.00
ωPBE	E	3.74	4.15	4.56	5.33	5.36	3.64	3.83	4.02	4.15	4.16
	f	1.25	0.00	0.12	0.00	0.00	1.23	0.00	0.00	0.00	0.00
ωhPBE0	E	3.80	3.83	4.49	5.11	5.14	3.49	3.68	3.72	3.74	3.80
	f	0.00	1.32	0.14	0.08	0.00	0.00	0.00	1.27	0.00	0.00
ωPBEh	E	3.78	4.10	4.55	5.31	5.39	3.65	3.68	3.82	3.96	4.10
	f	1.27	0.00	0.12	0.00	0.02	0.00	1.23	0.00	0.00	0.00
BNL	E	3.81	4.59	4.75	5.84	6.16	3.70	3.85	4.09	4.26	4.57
	f	1.25	0.00	0.13	0.00	0.00	1.20	0.01	0.00	0.00	0.00
ωB97X	E	3.78	4.44	4.64	5.65	5.77	3.70	4.09	4.30	4.43	4.46
	f	1.25	0.00	0.12	0.00	0.00	1.21	0.01	0.00	0.00	0.00
ωB97X-D	E	3.78	4.17	4.55	5.40	5.42	3.69	3.76	3.93	4.08	4.17
	f	1.27	0.00	0.12	0.00	0.10	1.23	0.00	0.00	0.00	0.00
M06-2X	E	3.77	4.10	4.59	5.47	5.48	3.37	3.57	3.62	3.67	4.01
	f	1.31	0.00	0.13	0.00	0.09	0.00	0.00	0.00	1.24	0.00
M11	E	3.77	4.28	4.69	5.53	5.78	3.06	3.24	3.39	3.66	3.71
	f	1.26	0.00	0.11	0.00	0.12	0.00	0.00	0.00	1.16	0.00
M11-L	E	3.12	3.82	4.03	4.22	4.46	1.60	2.10	2.14	2.31	2.50
	f	0.00	1.04	0.00	0.19	0.10	0.00	0.00	0.00	0.00	0.00
CC2	E	3.24	3.54	4.23	4.50	5.27	3.25	3.43	3.53	3.88	4.01
	f	1.01	0.00	0.10	0.00	0.05	1.01	0.00	0.10	0.00	0.05

Table S16: TDA and CC2 excitation energies (E, in eV) and oscillator strengths (f) for pCA$''^{-}$ with the def2-TZVP and aug-def2-TZVP basis sets.

molecule		def2-TZVP					aug-def2-TZVP				
		1a	2a	3a	4a	5a	1a	2a	3a	4a	5a
CIS	E	5.09	5.42	5.76	6.33	6.39	4.51	4.94	5.01	5.11	5.29
	f	0.36	0.29	0.00	0.00	0.00	0.00	0.31	0.00	0.00	0.20
B3LYP	E	2.67	2.82	3.07	3.22	3.31	2.65	2.73	2.81	2.88	3.06
	f	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
BHLYP	E	4.12	4.25	4.60	4.81	5.07	4.11	4.16	4.29	4.51	4.55
	f	0.00	0.00	0.10	0.01	0.71	0.00	0.00	0.00	0.11	0.00
CAM-B3LYP	E	3.72	3.74	4.47	4.51	4.87	3.78	3.79	4.11	4.23	4.35
	f	0.00	0.00	0.06	0.02	0.00	0.00	0.00	0.00	0.00	0.00
CAMh-B3LYP	E	3.39	3.46	4.12	4.27	4.34	3.46	3.51	3.70	3.83	3.87
	f	0.00	0.00	0.01	0.00	0.02	0.00	0.00	0.00	0.00	0.00
BP86	E	1.46	1.66	1.74	1.95	2.19	1.55	1.57	1.76	1.81	1.82
	f	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PBE	E	1.43	1.63	1.70	1.92	2.16	1.39	1.52	1.64	1.73	1.78
	f	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PBE0	E	2.90	3.01	3.40	3.50	3.56	2.96	3.05	3.07	3.19	3.44
	f	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
PBE50	E	4.06	4.21	4.64	4.81	5.11	4.10	4.25	4.35	4.56	4.68
	f	0.00	0.00	0.10	0.00	0.73	0.00	0.00	0.00	0.11	0.00
ωPBE	E	3.66	3.74	4.59	4.67	5.10	3.73	3.80	4.48	4.53	4.54
	f	0.00	0.00	0.07	0.00	0.77	0.00	0.00	0.01	0.05	0.04
ωhPBE0	E	3.23	3.30	3.96	4.02	4.08	3.29	3.35	3.64	3.75	3.94
	f	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ωPBEh	E	3.60	3.65	4.46	4.52	4.96	3.66	3.71	4.29	4.35	4.39
	f	0.00	0.00	0.03	0.04	0.00	0.00	0.00	0.00	0.00	0.00
BNL	E	4.47	4.65	4.85	5.27	5.66	4.51	4.67	4.69	4.75	5.14
	f	0.00	0.00	0.12	0.63	0.07	0.00	0.00	0.00	0.14	0.50
ωB97X	E	4.09	4.14	4.68	5.03	5.16	4.14	4.20	4.62	4.84	5.00
	f	0.00	0.00	0.10	0.11	0.62	0.00	0.00	0.11	0.00	0.39
ωB97X-D	E	3.71	3.74	4.51	4.57	5.03	3.77	3.80	4.43	4.46	4.55
	f	0.00	0.00	0.08	0.00	0.76	0.00	0.00	0.00	0.09	0.00
M06-2X	E	3.83	4.00	4.55	4.63	5.04	3.87	3.99	4.05	4.26	4.34
	f	0.00	0.00	0.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00
M11	E	4.09	4.28	4.75	5.15	5.27	3.84	4.10	4.29	4.30	4.31
	f	0.00	0.00	0.10	0.45	0.33	0.00	0.00	0.00	0.00	0.01
M11-L	E	2.09	2.28	2.30	2.48	2.50	0.66	0.83	1.17	1.38	1.54
	f	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CC2	E	3.28	3.43	4.17	4.34	4.41	3.27	3.33	3.41	3.50	3.60
	f	0.00	0.00	0.02	0.02	0.05	0.00	0.00	0.02	0.02	0.05

Table S17: TDA and CC2 excitation energies (E, in eV) and oscillator strengths (f) for $TMpCA^-$ with the def2-TZVP and aug-def2-TZVP basis sets.

molecule		def2-TZVP					aug-def2-TZVP				
		1a	2a	3a	4a	5a	1a	2a	3a	4a	5a
CIS	E	3.98	5.16	5.66	5.79	5.91	3.76	3.89	3.95	4.17	4.38
	f	1.51	0.10	0.00	0.00	0.00	0.00	1.43	0.00	0.00	0.00
B3LYP	E	3.30	3.63	4.05	4.23	4.31	2.97	3.30	3.41	3.49	3.53
	f	0.00	1.66	0.00	0.00	0.13	0.00	0.00	0.00	0.01	1.58
BHLYP	E	3.72	4.34	4.69	4.87	4.93	3.63	3.64	3.77	3.88	4.23
	f	1.63	0.00	0.11	0.00	0.00	1.56	0.01	0.00	0.00	0.00
CAM-B3LYP	E	3.61	4.04	4.55	4.61	4.89	3.51	3.67	3.78	3.86	4.04
	f	1.57	0.00	0.11	0.00	0.00	1.52	0.00	0.00	0.00	0.00
CAMh-B3LYP	E	3.61	3.82	4.48	4.50	4.63	3.45	3.52	3.59	3.71	3.82
	f	1.61	0.00	0.12	0.00	0.00	0.00	1.56	0.00	0.00	0.00
BP86	E	2.44	3.53	3.57	3.70	3.88	2.45	2.74	3.12	3.38	3.42
	f	0.00	0.00	1.49	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PBE	E	2.42	3.48	3.57	3.69	3.79	2.43	2.62	2.98	3.24	3.30
	f	0.00	0.00	1.48	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PBE0	E	3.43	3.67	4.30	4.33	4.41	3.24	3.44	3.57	3.61	3.69
	f	0.00	1.68	0.00	0.00	0.12	0.00	0.00	1.63	0.00	0.00
PBE50	E	3.74	4.29	4.73	4.84	5.07	3.66	3.85	3.98	4.08	4.29
	f	1.65	0.00	0.11	0.00	0.00	1.60	0.00	0.00	0.00	0.00
ωPBE	E	3.55	4.05	4.53	4.58	5.28	3.47	3.94	4.05	4.11	4.26
	f	1.49	0.00	0.00	0.10	0.00	1.47	0.00	0.00	0.00	0.00
ωhPBE0	E	3.64	3.68	4.44	4.49	4.64	3.53	3.55	3.69	3.70	3.79
	f	1.64	0.00	0.00	0.11	0.00	0.00	1.59	0.00	0.00	0.00
ωPBEh	E	3.59	4.00	4.56	4.56	5.11	3.51	3.76	3.91	4.00	4.03
	f	1.54	0.00	0.02	0.08	0.00	1.50	0.00	0.00	0.00	0.00
BNL	E	3.63	4.50	4.77	4.83	5.46	3.54	3.93	4.16	4.34	4.49
	f	1.48	0.00	0.12	0.00	0.00	1.43	0.00	0.00	0.00	0.00
ωB97X	E	3.60	4.34	4.66	4.75	5.35	3.52	4.18	4.34	4.38	4.53
	f	1.49	0.00	0.11	0.00	0.00	1.45	0.00	0.00	0.00	0.00
ωB97X-D	E	3.60	4.07	4.56	4.61	5.13	3.52	3.87	4.02	4.07	4.15
	f	1.53	0.00	0.10	0.00	0.00	1.50	0.00	0.00	0.00	0.00
M06-2X	E	3.59	4.00	4.50	4.60	4.85	3.43	3.50	3.56	3.65	4.00
	f	1.60	0.00	0.00	0.11	0.00	0.00	1.54	0.00	0.00	0.00
M11	E	3.57	4.18	4.53	4.70	5.24	3.15	3.32	3.49	3.49	3.74
	f	1.50	0.00	0.00	0.10	0.00	0.00	0.00	0.03	1.40	0.00
M11-L	E	2.97	3.41	3.65	4.18	4.20	1.49	2.10	2.17	2.22	2.25
	f	0.00	0.00	1.50	0.09	0.00	0.00	0.00	0.00	0.00	0.00
CC2	E	3.04	3.40	4.23	4.44	4.92	2.96	3.30	3.45	3.47	3.84
	f	1.21	0.00	0.09	0.00	0.00	1.21	0.00	0.09	0.00	0.00

Table S18: TDA and CC2 excitation energies (E, in eV) and oscillator strengths (f) for pCT$^-$ with the def2-TZVP and aug-def2-TZVP basis sets.

molecule		def2-TZVP					aug-def2-TZVP				
		1a	2a	3a	4a	5a	1a	2a	3a	4a	5a
CIS	E	3.96	5.17	5.60	5.61	5.79	3.84	3.89	4.04	4.30	4.45
	f	1.69	0.09	0.00	0.07	0.01	0.02	1.57	0.01	0.00	0.00
B3LYP	E	2.97	3.18	3.25	3.60	4.19	2.94	2.98	3.15	3.26	3.37
	f	0.11	0.01	0.00	1.71	0.00	0.10	0.00	0.01	0.00	0.01
BHLYP	E	3.68	4.14	4.29	4.49	4.71	3.62	3.72	3.84	3.98	4.04
	f	1.82	0.01	0.00	0.00	0.09	1.76	0.00	0.00	0.01	0.00
CAM-B3LYP	E	3.57	3.99	4.17	4.54	4.58	3.50	3.77	3.91	3.97	4.00
	f	1.76	0.00	0.00	0.01	0.09	1.71	0.00	0.00	0.00	0.00
CAMh-B3LYP	E	3.54	3.76	3.81	4.09	4.50	3.48	3.56	3.67	3.74	3.83
	f	1.66	0.00	0.15	0.00	0.09	1.63	0.02	0.01	0.08	0.00
BP86	E	2.27	2.36	2.38	2.60	2.68	2.27	2.37	2.39	2.62	2.71
	f	0.05	0.00	0.00	0.00	0.00	0.05	0.00	0.00	0.00	0.00
PBE	E	2.26	2.34	2.37	2.57	2.65	2.25	2.36	2.37	2.59	2.59
	f	0.05	0.00	0.00	0.00	0.00	0.05	0.00	0.00	0.00	0.00
PBE0	E	3.16	3.38	3.41	3.65	4.29	3.13	3.26	3.38	3.40	3.57
	f	0.16	0.00	0.02	1.68	0.00	0.16	0.00	0.02	0.00	1.45
PBE50	E	3.70	4.16	4.23	4.51	4.76	3.64	3.94	4.04	4.09	4.19
	f	1.83	0.02	0.00	0.00	0.09	1.79	0.00	0.00	0.01	0.00
ωPBE	E	3.51	3.99	4.57	4.59	4.70	3.45	4.00	4.04	4.23	4.44
	f	1.68	0.00	0.01	0.07	0.02	1.64	0.00	0.00	0.00	0.01
ωhPBE0	E	3.53	3.63	3.73	3.96	4.43	3.48	3.63	3.67	3.78	3.90
	f	1.26	0.00	0.57	0.01	0.00	1.33	0.07	0.36	0.01	0.01
ωPBEh	E	3.56	3.94	4.42	4.58	4.60	3.50	3.86	3.95	4.04	4.23
	f	1.73	0.00	0.01	0.01	0.07	1.68	0.00	0.00	0.00	0.00
BNL	E	3.61	4.44	4.79	4.85	5.16	3.54	4.03	4.27	4.44	4.51
	f	1.66	0.00	0.10	0.00	0.05	1.59	0.00	0.00	0.00	0.01
ωB97X	E	3.57	4.28	4.67	4.78	4.87	3.51	4.27	4.29	4.49	4.58
	f	1.67	0.00	0.09	0.00	0.02	1.62	0.00	0.00	0.00	0.10
ωB97X-D	E	3.56	4.01	4.46	4.60	4.63	3.50	3.96	4.02	4.14	4.33
	f	1.73	0.00	0.01	0.07	0.00	1.68	0.00	0.00	0.00	0.01
M06-2X	E	3.54	3.94	4.04	4.40	4.48	3.48	3.54	3.65	3.76	3.89
	f	1.78	0.00	0.01	0.00	0.00	1.72	0.00	0.00	0.01	0.00
M11	E	3.53	4.12	4.53	4.71	4.82	3.26	3.43	3.48	3.68	3.85
	f	1.69	0.00	0.00	0.08	0.02	0.00	0.09	1.52	0.00	0.00
M11-L	E	2.46	2.56	2.90	3.16	3.55	1.47	1.86	2.11	2.18	2.35
	f	0.05	0.00	0.00	0.00	1.33	0.00	0.00	0.00	0.00	0.01
CC2	E	3.04	3.36	3.89	4.26	4.40	2.98	3.33	3.37	3.55	3.57
	f	1.37	0.00	0.00	0.08	0.00	1.37	0.00	0.00	0.08	0.00

Table S19: TDA and CC2 excitation energies (E, in eV) and oscillator strengths (f) for p-HBDI$^-$ with the def2-TZVP and aug-def2-TZVP basis sets.

molecule		def2-TZVP					aug-def2-TZVP				
		1a	2a	3a	4a	5a	1a	2a	3a	4a	5a
CIS	E	3.78	5.19	5.59	5.63	6.18	3.35	3.59	3.70	3.73	3.85
	f	1.53	0.07	0.00	0.00	0.09	0.00	0.00	1.39	0.00	0.08
B3LYP	E	3.21	3.49	3.73	4.16	4.29	2.46	3.00	3.15	3.28	3.40
	f	0.00	1.57	0.00	0.00	0.09	0.00	0.00	0.10	0.00	1.34
BHLYP	E	3.55	4.25	4.54	4.71	5.17	3.03	3.47	3.53	3.62	3.68
	f	1.60	0.00	0.00	0.07	0.01	0.00	1.47	0.00	0.00	0.08
CAM-B3LYP	E	3.44	3.94	4.59	4.62	4.73	3.12	3.36	3.60	3.60	3.74
	f	1.54	0.00	0.08	0.00	0.00	0.00	1.48	0.00	0.00	0.02
CAMh-B3LYP	E	3.45	3.72	4.32	4.50	4.55	2.88	3.36	3.38	3.49	3.54
	f	1.57	0.00	0.00	0.08	0.00	0.00	1.40	0.00	0.00	0.12
BP86	E	2.37	3.43	3.44	3.50	3.81	2.33	2.39	2.82	2.86	3.34
	f	0.00	0.00	1.30	0.00	0.01	0.00	0.00	0.00	0.00	0.66
PBE	E	2.35	3.29	3.41	3.44	3.81	2.17	2.37	2.63	2.76	3.32
	f	0.00	0.00	0.00	1.30	0.01	0.00	0.00	0.00	0.00	1.05
PBE0	E	3.34	3.51	4.06	4.40	4.51	2.71	3.24	3.36	3.47	3.47
	f	0.00	1.61	0.00	0.08	0.00	0.00	0.00	0.56	0.00	0.98
PBE50	E	3.57	4.19	4.75	4.84	5.09	3.25	3.50	3.73	3.81	3.87
	f	1.62	0.00	0.07	0.00	0.00	0.00	1.55	0.00	0.00	0.02
ωPBE	E	3.37	3.94	4.59	4.63	5.12	3.31	3.59	3.87	3.97	4.12
	f	1.47	0.00	0.00	0.07	0.01	1.44	0.00	0.00	0.00	0.00
ωhPBE0	E	3.49	3.59	4.44	4.45	4.49	2.96	3.40	3.45	3.56	3.61
	f	1.59	0.00	0.00	0.00	0.08	0.00	1.46	0.00	0.00	0.08
ωPBEh	E	3.42	3.89	4.60	4.60	5.00	3.35	3.36	3.68	3.75	3.90
	f	1.51	0.00	0.07	0.00	0.01	1.47	0.00	0.00	0.00	0.00
BNL	E	3.45	4.40	4.84	5.20	5.36	3.37	3.59	3.88	4.03	4.15
	f	1.48	0.00	0.08	0.00	0.00	1.44	0.00	0.00	0.00	0.00
ωB97X	E	3.41	4.23	4.71	4.94	5.32	3.36	3.85	4.10	4.24	4.40
	f	1.47	0.00	0.07	0.00	0.01	1.44	0.00	0.00	0.00	0.00
ωB97X-D	E	3.42	3.96	4.60	4.68	5.04	3.36	3.48	3.78	3.86	4.02
	f	1.50	0.00	0.07	0.00	0.01	1.47	0.00	0.00	0.00	0.00
M06-2X	E	3.44	3.89	4.62	4.69	4.74	2.86	3.34	3.35	3.42	3.46
	f	1.57	0.00	0.08	0.00	0.00	0.00	0.00	1.27	0.00	0.24
M11	E	3.39	4.06	4.76	4.83	5.27	2.78	3.10	3.17	3.22	3.33
	f	1.48	0.00	0.06	0.00	0.01	0.00	0.00	0.00	0.11	1.28
M11-L	E	2.88	3.10	3.47	4.03	4.08	1.02	1.49	1.61	1.84	1.96
	f	0.00	0.00	1.41	0.00	0.05	0.00	0.00	0.01	0.00	0.00
CC2	E	2.92	3.30	4.30	4.54	4.57	2.77	2.85	3.24	3.25	3.35
	f	1.17	0.00	0.07	0.00	0.00	1.17	0.00	0.07	0.00	0.00

Table S20: TDA and CC2 excitation energies (E, in eV) and oscillator strengths (f) for p-HBDI with the def2-TZVP and aug-def2-TZVP basis sets.

molecule		def2-TZVP					aug-def2-TZVP				
		1a	2a	3a	4a	5a	1a	2a	3a	4a	5a
CIS	E	4.38	5.51	5.76	6.05	6.87	4.35	5.42	5.44	5.75	5.76
	f	1.10	0.02	0.00	0.04	0.20	1.07	0.00	0.03	0.00	0.00
B3LYP	E	3.67	3.74	4.22	4.30	4.89	3.66	3.71	4.20	4.27	4.61
	f	0.00	0.98	0.11	0.02	0.09	0.00	0.97	0.11	0.02	0.00
BHLYP	E	4.03	4.53	4.86	5.06	5.83	3.99	4.52	4.82	5.03	5.21
	f	1.11	0.00	0.02	0.04	0.18	1.09	0.00	0.02	0.04	0.00
CAM-B3LYP	E	3.93	4.13	4.73	4.83	5.58	3.90	4.12	4.69	4.80	5.18
	f	1.05	0.00	0.03	0.07	0.00	1.02	0.00	0.03	0.08	0.00
CAMh-B3LYP	E	3.87	3.99	4.59	4.66	5.43	3.84	3.97	4.56	4.63	4.99
	f	1.04	0.00	0.05	0.06	0.00	1.01	0.00	0.05	0.06	0.00
BP86	E	3.01	3.48	3.71	3.80	4.19	3.00	3.46	3.70	3.77	4.17
	f	0.00	0.58	0.38	0.02	0.06	0.00	0.60	0.36	0.01	0.06
PBE	E	2.99	3.48	3.71	3.79	4.19	2.98	3.45	3.69	3.77	4.16
	f	0.00	0.57	0.40	0.02	0.05	0.00	0.59	0.37	0.01	0.06
PBE0	E	3.77	3.80	4.36	4.44	5.08	3.76	3.77	4.34	4.41	5.04
	f	0.00	1.01	0.12	0.02	0.10	0.00	0.99	0.11	0.02	0.11
PBE50	E	4.04	4.48	4.89	5.05	5.86	4.01	4.47	4.86	5.03	5.45
	f	1.11	0.00	0.02	0.05	0.18	1.09	0.00	0.02	0.05	0.00
ωPBE	E	3.96	3.97	4.80	4.88	5.40	3.93	3.96	4.77	4.86	5.39
	f	1.00	0.00	0.03	0.12	0.00	0.98	0.00	0.03	0.12	0.00
ωhPBE0	E	3.86	3.89	4.54	4.60	5.38	3.83	3.88	4.52	4.58	5.10
	f	1.03	0.00	0.09	0.04	0.13	1.01	0.00	0.08	0.05	0.00
ωPBEh	E	3.93	4.00	4.74	4.82	5.47	3.90	3.99	4.71	4.80	5.35
	f	1.01	0.00	0.04	0.10	0.00	0.99	0.00	0.04	0.10	0.00
BNL	E	4.14	4.50	5.10	5.36	5.93	4.11	4.48	5.05	5.31	5.53
	f	1.06	0.00	0.03	0.05	0.00	1.03	0.00	0.03	0.06	0.00
ωB97X	E	4.03	4.30	4.92	5.10	5.75	4.01	4.28	4.89	5.07	5.74
	f	1.03	0.00	0.02	0.08	0.00	1.01	0.00	0.03	0.08	0.00
ωB97X-D	E	3.94	4.08	4.76	4.86	5.55	3.91	4.07	4.73	4.84	5.47
	f	1.02	0.00	0.03	0.09	0.00	1.00	0.00	0.03	0.09	0.00
M06-2X	E	3.95	4.13	4.77	4.85	5.64	3.92	4.12	4.73	4.82	5.06
	f	1.05	0.00	0.04	0.08	0.00	1.02	0.00	0.04	0.08	0.00
M11	E	4.00	4.17	4.97	5.05	5.64	3.97	4.16	4.86	4.92	5.02
	f	1.03	0.00	0.03	0.10	0.00	1.01	0.00	0.00	0.03	0.10
M11-L	E	3.56	3.63	3.96	4.04	4.41	3.22	3.28	3.55	3.59	3.91
	f	0.00	0.90	0.10	0.03	0.07	0.00	0.00	0.00	0.87	0.00
CC2	E	3.71	3.90	4.53	4.56	5.57	3.66	3.87	4.49	4.51	5.01
	f	0.77	0.00	0.15	0.00	0.16	0.77	0.00	0.15	0.00	0.16

Table S21: TDA and CC2 excitation energies (E, in eV) and oscillator strengths (f) for p-HBDI$^+$ with the def2-TZVP and aug-def2-TZVP basis sets.

molecule		def2-TZVP					aug-def2-TZVP				
		1a	2a	3a	4a	5a	1a	2a	3a	4a	5a
CIS	E	4.00	5.20	6.08	6.71	6.72	3.98	5.18	6.05	6.17	6.61
	f	1.32	0.02	0.04	0.21	0.06	1.31	0.02	0.03	0.00	0.21
B3LYP	E	3.61	3.76	4.02	4.25	5.12	3.59	3.74	4.01	4.23	5.03
	f	1.26	0.24	0.00	0.03	0.09	1.28	0.20	0.00	0.03	0.02
BHLYP	E	3.74	4.35	5.01	5.11	5.77	3.72	4.34	4.99	5.10	5.71
	f	1.44	0.03	0.01	0.00	0.12	1.42	0.03	0.01	0.00	0.10
CAM-B3LYP	E	3.63	4.26	4.58	4.82	5.61	3.60	4.25	4.56	4.80	5.56
	f	1.41	0.02	0.00	0.01	0.12	1.39	0.02	0.00	0.01	0.11
CAMh-B3LYP	E	3.62	4.10	4.39	4.63	5.45	3.60	4.08	4.38	4.62	5.40
	f	1.43	0.03	0.00	0.01	0.10	1.41	0.03	0.00	0.01	0.09
BP86	E	3.27	3.32	3.56	3.73	4.37	3.26	3.31	3.53	3.72	4.35
	f	0.00	0.05	1.17	0.24	0.03	0.00	0.05	1.18	0.22	0.03
PBE	E	3.24	3.32	3.55	3.73	4.36	3.23	3.31	3.53	3.71	4.33
	f	0.00	0.05	1.16	0.25	0.03	0.00	0.05	1.17	0.22	0.03
PBE0	E	3.65	3.88	4.16	4.38	5.26	3.63	3.87	4.15	4.36	5.22
	f	1.42	0.10	0.00	0.02	0.09	1.41	0.09	0.00	0.02	0.08
PBE50	E	3.75	4.38	5.01	5.06	5.80	3.73	4.37	4.99	5.05	5.75
	f	1.45	0.03	0.01	0.00	0.12	1.44	0.03	0.01	0.00	0.11
ωPBE	E	3.57	4.38	4.41	4.90	5.71	3.55	4.37	4.40	4.88	5.67
	f	1.35	0.00	0.02	0.01	0.13	1.34	0.00	0.02	0.01	0.13
ωhPBE0	E	3.65	4.04	4.30	4.56	5.42	3.62	4.03	4.29	4.54	5.38
	f	1.44	0.04	0.00	0.02	0.10	1.43	0.04	0.00	0.02	0.09
ωPBEh	E	3.62	4.27	4.42	4.80	5.62	3.60	4.26	4.41	4.78	5.58
	f	1.39	0.02	0.00	0.01	0.11	1.37	0.02	0.00	0.01	0.11
BNL	E	3.66	4.81	5.08	5.42	6.14	3.64	4.79	5.06	5.39	6.07
	f	1.34	0.01	0.00	0.00	0.20	1.32	0.01	0.00	0.00	0.18
ωB97X	E	3.63	4.54	4.80	5.11	5.87	3.61	4.53	4.79	5.09	5.83
	f	1.34	0.02	0.00	0.00	0.15	1.33	0.02	0.00	0.01	0.14
ωB97X-D	E	3.62	4.29	4.51	4.84	5.65	3.60	4.29	4.50	4.82	5.61
	f	1.38	0.02	0.00	0.01	0.12	1.36	0.02	0.00	0.01	0.11
M06-2X	E	3.63	4.28	4.65	4.84	5.65	3.61	4.27	4.64	4.82	5.59
	f	1.43	0.03	0.00	0.01	0.11	1.41	0.02	0.00	0.01	0.10
M11	E	3.61	4.54	4.72	5.08	5.90	3.60	4.53	4.71	5.06	5.66
	f	1.35	0.02	0.00	0.01	0.15	1.34	0.02	0.00	0.01	0.00
M11-L	E	3.49	3.64	3.89	4.00	4.61	3.48	3.62	3.74	3.88	3.99
	f	0.15	1.23	0.02	0.04	0.00	0.18	1.15	0.03	0.02	0.03
CC2	E	3.15	4.03	4.36	4.44	5.32	3.12	4.00	4.33	4.41	5.25
	f	1.09	0.02	0.00	0.00	0.10	1.09	0.02	0.00	0.00	0.10

Table S22: TDA and CC2 excitation energies (E, in eV) and oscillator strengths (f) for PSBT$^+$ with the def2-TZVP and aug-def2-TZVP basis sets.

molecule		def2-TZVP					aug-def2-TZVP				
		1a	2a	3a	4a	5a	1a	2a	3a	4a	5a
CIS	E	3.00	4.79	5.88	6.03	6.90	2.99	4.77	5.44	5.83	5.88
	f	2.46	0.30	0.02	0.02	0.12	2.44	0.30	0.00	0.02	0.00
B3LYP	E	2.59	3.34	3.86	3.95	4.19	2.58	3.33	3.86	3.95	4.19
	f	2.17	1.77	0.00	0.03	0.01	2.18	1.74	0.00	0.03	0.01
BHLYP	E	2.72	3.91	4.71	5.11	5.25	2.72	3.90	4.69	5.10	5.24
	f	2.74	0.61	0.03	0.08	0.06	2.73	0.60	0.03	0.08	0.05
CAM-B3LYP	E	2.65	3.89	4.67	4.93	5.12	2.64	3.88	4.65	4.92	5.10
	f	2.65	0.58	0.02	0.01	0.10	2.63	0.57	0.03	0.01	0.09
CAMh-B3LYP	E	2.63	3.70	4.45	4.60	4.89	2.63	3.69	4.43	4.59	4.87
	f	2.66	0.78	0.02	0.01	0.08	2.66	0.76	0.02	0.01	0.09
BP86	E	2.37	2.97	3.11	3.20	3.31	2.37	2.96	3.10	3.20	3.31
	f	0.93	0.03	3.10	0.11	0.06	2.37	2.96	3.10	3.20	3.31
PBE	E	2.37	2.95	3.11	3.19	3.29	2.36	2.94	3.10	3.18	3.29
	f	0.92	0.02	3.00	0.22	0.05	0.93	0.02	3.04	0.16	0.05
PBE0	E	2.62	3.42	4.00	4.09	4.34	2.61	3.41	3.99	4.08	4.33
	f	2.39	1.48	0.00	0.02	0.01	2.39	1.46	0.00	0.02	0.01
PBE50	E	2.72	3.91	4.72	5.06	5.20	2.72	3.90	4.70	5.05	5.19
	f	2.75	0.64	0.03	0.03	0.11	2.74	0.63	0.03	0.04	0.10
ωPBE	E	2.61	4.08	4.97	5.11	5.28	2.61	4.08	4.96	5.10	5.26
	f	2.48	0.43	0.03	0.01	0.05	2.48	0.42	0.03	0.01	0.04
ωhPBE0	E	2.64	3.63	4.36	4.41	4.72	2.63	3.62	4.35	4.40	4.72
	f	2.65	0.91	0.01	0.01	0.02	2.66	0.89	0.01	0.01	0.02
ωPBEh	E	2.63	3.99	4.79	4.96	5.18	2.62	3.98	4.78	4.95	5.16
	f	2.60	0.51	0.02	0.01	0.07	2.59	0.50	0.02	0.01	0.07
BNL	E	2.72	4.37	5.42	5.57	5.83	2.71	4.36	5.39	5.54	5.56
	f	2.44	0.33	0.04	0.02	0.00	2.43	0.32	0.04	0.02	0.00
ωB97X	E	2.67	4.21	5.11	5.35	5.52	2.66	4.20	5.09	5.34	5.52
	f	2.49	0.39	0.03	0.03	0.01	2.48	0.38	0.03	0.03	0.01
ωB97X-D	E	2.64	4.02	4.82	5.05	5.22	2.63	4.01	4.80	5.04	5.21
	f	2.59	0.49	0.02	0.01	0.07	2.58	0.48	0.02	0.01	0.06
M06-2X	E	2.62	3.81	4.62	4.70	5.01	2.61	3.80	4.60	4.70	4.99
	f	2.67	0.66	0.02	0.01	0.08	2.67	0.65	0.02	0.01	0.08
M11	E	2.64	4.16	5.07	5.23	5.37	2.64	4.15	4.86	5.04	5.19
	f	2.52	0.40	0.04	0.01	0.04	2.50	0.39	0.00	0.04	0.00
M11-L	E	2.45	3.14	3.35	3.52	3.65	2.44	3.12	3.35	3.51	3.58
	f	1.10	2.94	0.01	0.08	0.03	1.11	2.88	0.01	0.08	0.00
CC2	E	2.17	3.35	4.22	4.54	4.73	2.16	3.34	4.20	4.52	4.70
	f	1.92	0.50	0.10	0.01	0.05	1.92	0.50	0.10	0.01	0.05

Table S23: TDA and CC2 excitation energies (E, in eV) and oscillator strengths (f) for $PSB11Me_2^+$ with the def2-TZVP and aug-def2-TZVP basis sets.

molecule		def2-TZVP					aug-def2-TZVP				
		1a	2a	3a	4a	5a	1a	2a	3a	4a	5a
CIS	E	2.98	4.73	5.77	5.98	6.85	2.97	4.71	5.47	5.70	5.87
	f	2.09	0.48	0.11	0.01	0.18	2.08	0.47	0.00	0.11	0.00
B3LYP	E	2.56	3.30	3.87	3.92	4.19	2.55	3.29	3.86	3.92	4.18
	f	1.82	1.46	0.01	0.05	0.02	1.82	1.43	0.01	0.05	0.02
BHLYP	E	2.69	3.89	4.63	5.08	5.23	2.69	3.88	4.60	5.06	5.21
	f	2.28	0.58	0.20	0.12	0.03	2.27	0.58	0.20	0.11	0.00
CAM-B3LYP	E	2.62	3.87	4.59	4.92	5.08	2.60	3.85	4.56	4.91	5.06
	f	2.21	0.57	0.17	0.03	0.10	2.19	0.56	0.17	0.02	0.08
CAMh-B3LYP	E	2.60	3.67	4.38	4.60	4.86	2.59	3.66	4.36	4.60	4.84
	f	2.21	0.70	0.14	0.01	0.17	2.20	0.69	0.15	0.01	0.17
BP86	E	2.35	2.97	3.07	3.19	3.30	2.34	2.97	3.06	3.19	3.30
	f	0.78	0.04	2.64	0.02	0.04	0.78	0.04	2.62	0.02	0.04
PBE	E	2.34	2.95	3.07	3.18	3.28	2.34	2.95	3.06	3.18	3.28
	f	0.78	0.03	2.63	0.05	0.04	0.78	0.03	2.61	0.04	0.03
PBE0	E	2.59	3.39	4.00	4.06	4.33	2.58	3.38	4.00	4.05	4.33
	f	1.99	1.23	0.01	0.06	0.03	1.98	1.21	0.01	0.06	0.03
PBE50	E	2.69	3.88	4.64	5.04	5.17	2.69	3.88	4.62	5.03	5.16
	f	2.28	0.60	0.19	0.07	0.08	2.27	0.59	0.20	0.07	0.07
ωPBE	E	2.58	4.05	4.88	5.09	5.24	2.58	4.04	4.85	5.08	5.22
	f	2.08	0.49	0.15	0.01	0.05	2.08	0.48	0.16	0.01	0.04
ωhPBE0	E	2.61	3.60	4.30	4.40	4.71	2.60	3.59	4.29	4.40	4.70
	f	2.20	0.80	0.10	0.01	0.08	2.19	0.78	0.11	0.01	0.09
ωPBEh	E	2.60	3.96	4.70	4.95	5.13	2.59	3.95	4.68	4.94	5.11
	f	2.17	0.54	0.15	0.01	0.09	2.16	0.53	0.15	0.01	0.08
BNL	E	2.70	4.34	5.31	5.53	5.80	2.69	4.32	5.27	5.51	5.55
	f	2.07	0.45	0.17	0.01	0.00	2.06	0.44	0.17	0.00	0.00
ωB97X	E	2.64	4.17	5.01	5.32	5.50	2.63	4.16	4.99	5.30	5.49
	f	2.09	0.47	0.16	0.02	0.01	2.08	0.47	0.16	0.02	0.01
ωB97X-D	E	2.61	3.99	4.72	5.03	5.18	2.60	3.98	4.70	5.03	5.17
	f	2.17	0.52	0.15	0.02	0.07	2.16	0.52	0.16	0.02	0.06
M06-2X	E	2.59	3.79	4.55	4.71	4.98	2.59	3.78	4.52	4.70	4.96
	f	2.23	0.62	0.15	0.01	0.13	2.21	0.61	0.16	0.01	0.12
M11	E	2.61	4.12	4.97	5.21	5.34	2.61	4.12	4.90	4.93	5.20
	f	2.12	0.48	0.16	0.01	0.03	2.10	0.47	0.00	0.16	0.01
M11-L	E	2.43	3.08	3.35	3.50	3.64	2.42	3.07	3.35	3.49	3.52
	f	0.91	2.43	0.00	0.08	0.02	0.93	2.38	0.00	0.08	0.00
CC2	E	2.17	3.34	4.16	4.53	4.70	2.16	3.32	4.14	4.51	4.68
	f	1.56	0.47	0.15	0.06	0.07	1.56	0.47	0.15	0.06	0.07

Table S24: TDDFT excitation energies (in eV) for pVP using mixed basis sets: aug-def2-TZVP on hydrogens and def2-TZVP on other atoms (C, N, O, S).

Functional	1a	2a	3a	4a	5a
B3LYP	4.44	4.76	4.78	5.21	5.43
CAM-B3LYP	4.67	5.00	5.28	5.65	5.90
CAMh-B3LYP	4.60	4.93	5.11	5.49	5.73
PBE0	4.54	4.87	5.07	5.47	5.70
ωhPBE0	4.62	4.94	5.25	5.61	5.84
ωPBEh	4.70	5.03	5.46	5.80	6.03
ωB97X-D	4.71	5.02	5.60	5.92	6.17
M06-2X	4.74	5.08	5.22	5.58	5.79

Table S25: TDDFT excitation energies (in eV) for pCA using mixed basis sets: aug-def2-TZVP on hydrogens and def2-TZVP on other atoms (C, N, O, S).

Functional	1a	2a	3a	4a	5a
B3LYP	4.11	4.46	4.52	5.01	5.23
CAM-B3LYP	4.36	4.81	4.97	5.50	5.86
CAMh-B3LYP	4.28	4.73	4.83	5.34	5.67
PBE0	4.20	4.59	4.63	5.31	5.39
ωhPBE0	4.29	4.73	4.74	5.48	5.60
ωPBEh	4.40	4.82	4.87	5.69	5.89
ωB97X-D	4.40	4.83	4.94	5.84	5.90
M06-2X	4.41	4.88	4.95	5.46	5.90

Table S26: TDDFT excitation energies (in eV) for pCA'^{-} using mixed basis sets: aug-def2-TZVP on hydrogens and def2-TZVP on other atoms (C, N, O, S).

Functional	1a	2a	3a	4a	5a
B3LYP	3.17	3.41	3.41	3.60	3.70
CAM-B3LYP	3.47	3.73	3.97	4.04	4.13
CAMh-B3LYP	3.45	3.55	3.81	3.90	3.92
PBE0	3.44	3.46	3.55	3.80	3.90
ωhPBE0	3.47	3.67	3.79	3.92	4.00
ωPBEh	3.48	3.88	4.09	4.11	4.24
ωB97X-D	3.48	4.00	4.16	4.25	4.41
M06-2X	3.44	3.52	3.76	3.82	4.05

Table S27: TDDFT excitation energies (in eV) for pCA$''^{-}$ using mixed basis sets: aug-def2-TZVP on hydrogens and def2-TZVP on other atoms (C, N, O, S).

Functional	1a	2a	3a	4a	5a
B3LYP	2.64	2.67	2.80	2.81	3.05
CAM-B3LYP	3.72	3.73	4.16	4.31	4.33
CAMh-B3LYP	3.40	3.45	3.75	3.88	3.92
PBE0	2.90	2.99	3.09	3.22	3.40
ωhPBE0	3.24	3.29	3.73	3.84	3.90
ωPBEh	3.61	3.64	4.33	4.38	4.41
ωB97X-D	3.71	3.74	4.35	4.50	4.54
M06-2X	3.80	3.99	4.05	4.34	4.38

Table S28: TDDFT excitation energies (in eV) for TMpCA^{-} at a mixed basis sets: aug-def2-TZVP on hydrogens and def2-TZVP on other atoms (C, N, O, S).

Functional	1a	2a	3a	4a	5a
B3LYP	3.06	3.26	3.30	3.61	3.71
CAM-B3LYP	3.30	3.82	3.95	4.04	4.07
CAMh-B3LYP	3.29	3.59	3.79	3.81	3.93
PBE0	3.29	3.35	3.43	3.81	3.92
ωhPBE0	3.30	3.68	3.68	3.91	4.04
ωPBEh	3.31	3.98	3.99	4.17	4.29
ωB97X-D	3.31	4.06	4.09	4.30	4.43
M06-2X	3.27	3.58	3.74	3.85	3.96

Table S29: TDDFT excitation energies (in eV) for pCT^{-} using mixed basis sets: aug-def2-TZVP on hydrogens and def2-TZVP on other atoms (C, N, O, S).

Functional	1a	2a	3a	4a	5a
B3LYP	2.94	3.11	3.18	3.25	3.26
CAM-B3LYP	3.29	3.92	3.98	4.10	4.15
CAMh-B3LYP	3.26	3.72	3.77	3.77	3.88
PBE0	3.11	3.31	3.38	3.38	3.45
ωhPBE0	3.27	3.63	3.64	3.84	3.94
ωPBEh	3.29	3.93	4.07	4.28	4.38
ωB97X-D	3.29	4.01	4.18	4.36	4.44
M06-2X	3.25	3.72	3.84	3.90	3.93

Table S30: TDDFT excitation energies (in eV) for p-HBDI$^-$ at a mixed basis sets: aug-def2-TZVP on hydrogens and def2-TZVP on other atoms (C, N, O, S).

Functional	1a	2a	3a	4a	5a
B3LYP	2.57	3.04	3.19	3.21	3.33
CAM-B3LYP	3.12	3.25	3.80	3.84	3.87
CAMh-B3LYP	3.01	3.10	3.59	3.67	3.72
PBE0	2.82	3.09	3.34	3.44	3.55
ωhPBE0	3.10	3.11	3.68	3.75	3.83
ωPBEh	3.11	3.55	3.88	3.96	4.04
ωB97X-D	3.12	3.70	3.96	4.09	4.20
M06-2X	2.97	3.09	3.50	3.54	3.63

Table S31: TDDFT excitation energies (in eV) for p-HBDI using mixed basis sets: aug-def2-TZVP on hydrogens and def2-TZVP on other atoms (C, N, O, S).

Functional	1a	2a	3a	4a	5a
B3LYP	3.43	3.66	4.16	4.26	4.64
CAM-B3LYP	3.66	4.11	4.66	4.72	5.22
CAMh-B3LYP	3.58	3.96	4.52	4.57	5.03
PBE0	3.50	3.75	4.29	4.39	4.92
ωhPBE0	3.57	3.87	4.48	4.54	5.15
ωPBEh	3.66	3.98	4.67	4.71	5.43
ωB97X-D	3.67	4.05	4.69	4.75	5.52
M06-2X	3.66	4.08	4.70	4.74	5.11

Table S32: Experimental excitation energies are compared to VEEs obtained at the TDDFT level with aug-def2-TZVP basis sets. The VEEs that deviate by less than 0.25 eV from the experimental absorption maxima are marked in bold font. [a] Measured in solvent,[b]extrapolated to vacuum from solvent measurements, [c] absorption maxima in protein environment. CC2 *ext.* refers to CC2 values obtained at extrapolated QZVP + aug level.

Method/Molecule	pVP	pCA	pCA^-	$pCA'^{-,a}$	$TMpCA^{-,c}$	pCT^-	$pHBDI^-$	$pHBDI^b$	$pHBDI^+$	$PSBT^+$	$PSB11Me_2^+$
Exp.	4.12/4.75	4.04/4.37	2.88	4.36	2.78	2.70	2.59,2.76	3.51	2.84,2.99	2.00/3.22	2.03/3.18
CC2 ext.	4.53/**4.76**	**4.39**/4.68	3.19	3.28	**2.91**	**2.94**	**2.73**	**3.63**	**3.10**	**2.14/3.32**	**2.15/3.30**
CC2 aug-TZVP	**4.58**/5.11	4.44/4.72	3.25	3.27	**2.96**	**2.98**	**2.77**	**3.66**	**3.12**	**2.16/3.34**	**2.16/3.32**
RPA	4.93/5.30	4.68/5.34	3.68	**4.51**	3.68	3.68	3.35	4.10	3.74	2.77/4.49	2.76/4.44
B3LYP	4.41/**4.72**	**4.09/4.46**	**3.05**	2.65	**2.97**	**2.92**	**2.46**	**3.42**	**3.24**	2.28/**3.11**	**2.26/3.08**
BHLYP	4.74/5.04	4.42/4.94	3.54	**4.11**	3.38	3.38	3.03	**3.74**	3.44	2.48/3.71	2.46/3.69
CAM-B3LYP	4.64/**4.95**	4.34/4.79	3.42	3.77	3.27	3.26	3.09	**3.64**	3.32	2.41/3.67	2.39/3.64
CAMh-B3LYP	4.57/**4.88**	**4.26**/4.71	3.40	3.45	3.25	3.23	**2.88**	**3.57**	3.30	2.37/3.49	2.35/3.47
BP86	**4.13**/4.46	3.68/3.81	2.57	1.55	2.45	2.26	2.33	3.00	**3.08**	**2.10**/2.73	**2.08**/2.70
PBE	**4.11**/4.45	3.66/3.80	2.55	1.39	2.43	2.24	2.17	2.98	**3.08**	**2.09**/2.72	**2.08** /2.70
PBE0	4.51/**4.82**	**4.18/4.58**	3.29	2.95	3.24	3.10	**2.71**	**3.49**	3.29	2.31/**3.21**	2.29/**3.18**
PBE50	4.79/5.10	4.46/4.98	3.57	4.06	3.40	3.40	3.22	**3.76**	3.45	2.48/3.71	2.46/3.68
ωPBE	4.69/5.03	4.43/4.81	3.41	3.72	3.24	3.23	3.05	**3.67**	3.29	2.41/3.82	2.38/3.78
ωhPBE0	4.59/**4.90**	**4.27**/4.71	3.43	3.29	3.27	3.25	**2.96**	**3.55**	3.31	2.37/**3.43**	2.34/**3.41**
ωPBEh	4.67/**4.98**	4.38/4.80	3.44	3.65	3.27	3.26	3.09	**3.64**	3.32	2.42/3.75	2.39/3.71
BNL	4.82/5.15	4.57/5.02	3.49	**4.47**	3.33	3.34	3.15	3.87	3.41	2.53/4.10	2.51/4.06
ωB97X	4.76/5.08	4.48/4.91	3.47	**4.12**	3.31	3.29	3.11	**3.76**	3.36	2.47/3.94	2.45/3.90
ωB97X-D	4.68/**4.99**	4.38/4.82	3.44	3.75	3.28	3.27	3.09	**3.66**	3.33	2.43/3.77	2.40/3.74
M06-2X	4.70/5.03	4.39/4.86	3.37	3.83	3.24	3.23	**2.86**	**3.65**	3.31	2.37/3.59	2.35/3.57
M11	4.77/**4.96**	4.47/4.96	**3.06**	3.84	3.15	3.25	**2.78**	**3.71**	3.33	2.44/3.88	2.41/3.84
M11-L	3.50/3.93	3.75/3.99	1.60	0.65	1.49	1.47	1.02	3.22	**3.20**	**2.19**/2.82	**2.18**/2.78

Table S33: The root mean square (RMS) and mean signed average (MSA) values (in eV) of the TDDFT and TDA excitation energies calculated with the def2-TZVP basis set relative to the CC2 values. "Five States" compares the excitation energies of all five states. "First State" compares the excitation energies of only the lowest excited states. "Relative VEEs" compares the gaps, VEE(n)-VEE(0), between different excited states.

Functional	Five States				First State				Relative VEEs			
	TDDFT		TDA		TDDFT		TDA		TDDFT		TDA	
	RMS	MSA	RMS	MSA	RMS	MSA	RMS	MSA	RMS	MSA	RMS	MSA
CIS/RPA	1.24	1.13	1.41	1.33	0.72	0.65	0.94	0.89	0.72	0.60	0.68	0.56
B3LYP	0.51	-0.39	0.47	-0.29	0.27	-0.06	0.32	0.09	0.48	-0.41	0.56	-0.48
BHLYP	0.44	0.34	0.53	0.47	0.37	0.31	0.57	0.54	0.28	0.04	0.25	-0.08
CAM-B3LYP	0.28	0.18	0.38	0.31	0.24	0.19	0.44	0.41	0.20	-0.00	0.22	-0.13
CAMh-B3LYP	0.21	0.01	0.27	0.13	0.19	0.12	0.41	0.36	0.23	-0.13	0.35	-0.28
BP86	1.14	-1.01	1.09	-0.91	0.77	-0.61	0.77	-0.53	0.69	-0.50	0.76	-0.47
PBE	1.17	-1.03	1.10	-0.92	0.79	-0.62	0.78	-0.55	0.70	-0.51	0.75	-0.46
PBE0	0.38	-0.25	0.36	-0.14	0.22	0.03	0.33	0.21	0.41	-0.34	0.50	-0.43
PBE50	0.43	0.36	0.53	0.49	0.37	0.32	0.58	0.55	0.25	0.05	0.21	-0.07
ωPBE	0.33	0.25	0.44	0.38	0.21	0.18	0.40	0.38	0.22	0.09	0.21	-0.00
ωhPBE0	0.21	-0.04	0.26	0.07	0.20	0.11	0.42	0.35	0.26	-0.19	0.41	-0.35
ωPBEh	0.29	0.19	0.38	0.32	0.22	0.18	0.42	0.39	0.18	0.02	0.20	-0.09
BNL	0.68	0.59	0.80	0.74	0.45	0.37	0.60	0.57	0.44	0.28	0.36	0.22
ωB97X	0.50	0.42	0.61	0.56	0.33	0.27	0.50	0.47	0.32	0.18	0.25	0.10
ωB97X-D	0.31	0.23	0.42	0.36	0.24	0.19	0.43	0.41	0.19	0.05	0.19	-0.06
M06-2X	0.27	0.18	0.37	0.31	0.23	0.18	0.44	0.42	0.20	-0.00	0.23	-0.14
M11	0.44	0.36	0.56	0.52	0.31	0.25	0.49	0.47	0.27	0.14	0.21	0.06
M11-L	0.87	-0.73	0.81	-0.63	0.46	-0.28	0.45	-0.16	0.66	-0.56	0.71	-0.58

Table S34: Root mean square (RMS) and mean signed average (MSA) values (in eV) in TDDFT and TDA excitation energies with aug-def2-TZVP basis relative to the CC2 values. "Five States" compares the excitation energies of all five states. "First State" compares the excitation energies of only the lowest excited states. "Relative VEEs" compares the gaps, VEE(n)-VEE(0), between different excited states.

Functional	Five States				First State				Relative VEEs			
	TDDFT		TDA		TDDFT		TDA		TDDFT		TDA	
	RMS	MSA	RMS	MSA	RMS	MSA	RMS	MSA	RMS	MSA	RMS	MSA
CIS/RPA	0.89	0.79	0.99	0.89	0.64	0.59	0.78	0.75	0.43	0.24	0.39	0.18
B3LYP	0.37	-0.31	0.34	-0.23	0.26	-0.15	0.32	-0.01	0.33	-0.20	0.45	-0.28
BHLYP	0.42	0.35	0.49	0.44	0.37	0.31	0.52	0.48	0.17	0.06	0.18	-0.05
CAM-B3LYP	0.31	0.25	0.38	0.33	0.26	0.20	0.41	0.38	0.12	0.06	0.14	-0.06
CAMh-B3LYP	0.16	0.07	0.23	0.16	0.18	0.12	0.34	0.29	0.15	-0.06	0.24	-0.16
BP86	0.91	-0.80	0.86	-0.72	0.71	-0.56	0.71	-0.48	0.56	-0.31	0.64	-0.29
PBE	0.95	-0.85	0.90	-0.77	0.77	-0.60	0.77	-0.52	0.57	-0.32	0.64	-0.31
PBE0	0.23	-0.14	0.22	-0.05	0.18	0.00	0.28	0.14	0.29	-0.17	0.39	-0.25
PBE50	0.48	0.43	0.56	0.52	0.39	0.34	0.56	0.53	0.18	0.12	0.14	-0.01
ωPBE	0.48	0.40	0.55	0.49	0.23	0.20	0.41	0.40	0.31	0.25	0.23	0.12
ωhPBE0	0.17	0.06	0.24	0.15	0.19	0.12	0.36	0.30	0.19	-0.07	0.30	-0.19
ωPBEh	0.37	0.30	0.44	0.39	0.24	0.20	0.42	0.40	0.20	0.12	0.18	-0.02
BNL	0.70	0.63	0.78	0.73	0.46	0.38	0.61	0.57	0.36	0.32	0.27	0.20
ωB97X	0.68	0.60	0.75	0.70	0.36	0.29	0.51	0.49	0.43	0.39	0.31	0.27
ωB97X-D	0.43	0.36	0.50	0.46	0.26	0.22	0.44	0.42	0.24	0.19	0.18	0.04
M06-2X	0.26	0.17	0.33	0.26	0.23	0.18	0.39	0.35	0.13	-0.00	0.20	-0.11
M11	0.36	0.16	0.42	0.25	0.25	0.17	0.36	0.29	0.24	-0.01	0.25	-0.06
M11-L	1.32	-1.19	1.30	-1.15	1.31	-1.01	1.32	-0.94	0.58	-0.23	0.65	-0.27

Table S35: Deviation of TDDFT excitation energies (in eV) obtained with def2-TZVP basis sets and mixed basis sets from values obtained using aug-def2-TZVP basis sets. In the mixed basis sets, aug-def2-TZVP basis functions were employed on hydrogen atoms, and def2-TZVP basis functions on non-hydrogen atoms (C, N, O, S).

Functional	def2-TVZP			Mixed		
	RMS	MSA	MAX	RMS	MSA	MAX
B3LYP	0.54	0.38	1.28	0.11	0.05	0.34
CAM-B3LYP	0.57	0.42	1.48	0.10	0.07	0.24
CAMh-B3LYP	0.58	0.42	1.44	0.10	0.07	0.23
PBE0	0.52	0.35	1.30	0.09	0.05	0.26
ωhPBE0	0.53	0.36	1.34	0.11	0.08	0.25
ωPBEh	0.52	0.36	1.32	0.12	0.09	0.27
ωB97X-D	0.47	0.32	1.23	0.13	0.09	0.28
M06-2X	0.69	0.51	1.74	0.10	0.07	0.20

Table S36: Overlap integrals and VEEs (in eV) for the pVP molecule obtained using TDA and the B3LYP and CAM-B3LYP functionals. The overlap integrals are defined in Eqs. 11 and 12 and are computed between the detachment or attachment densities from a smaller basis set calculation (def2-TZVP or mixed basis sets) with densities obtained from the larger aug-def2-TZVP basis set calculation.

Functional	state	def2-TZVP			mixed			aug-def2-TZVP
		VEE	detach	attach	VEE	detach	attach	VEE
B3LYP	1	4.58	0.9994	0.9908	4.54	0.9999	0.9962	4.51
	2	5.02	0.9687	0.2361	4.78	0.9999	0.9951	4.76
	3	5.60	0.9676	0.2399	4.97	0.9997	0.9865	4.90
	4	5.98	0.8247	0.3664	5.21	0.9999	0.9908	5.16
	5	6.21	0.9369	0.2799	5.43	0.9999	0.9847	5.37
CAM-B3LYP	1	4.84	0.9993	0.9907	4.80	0.9998	0.9961	4.77
	2	5.25	0.9996	0.9816	5.21	0.9999	0.9885	5.14
	3	6.19	0.9896	0.7591	5.28	0.9998	0.9962	5.26
	4	6.59	0.8356	0.3705	5.65	0.9999	0.9928	5.61
	5	6.85	0.8285	0.3242	5.90	0.9999	0.9866	5.85

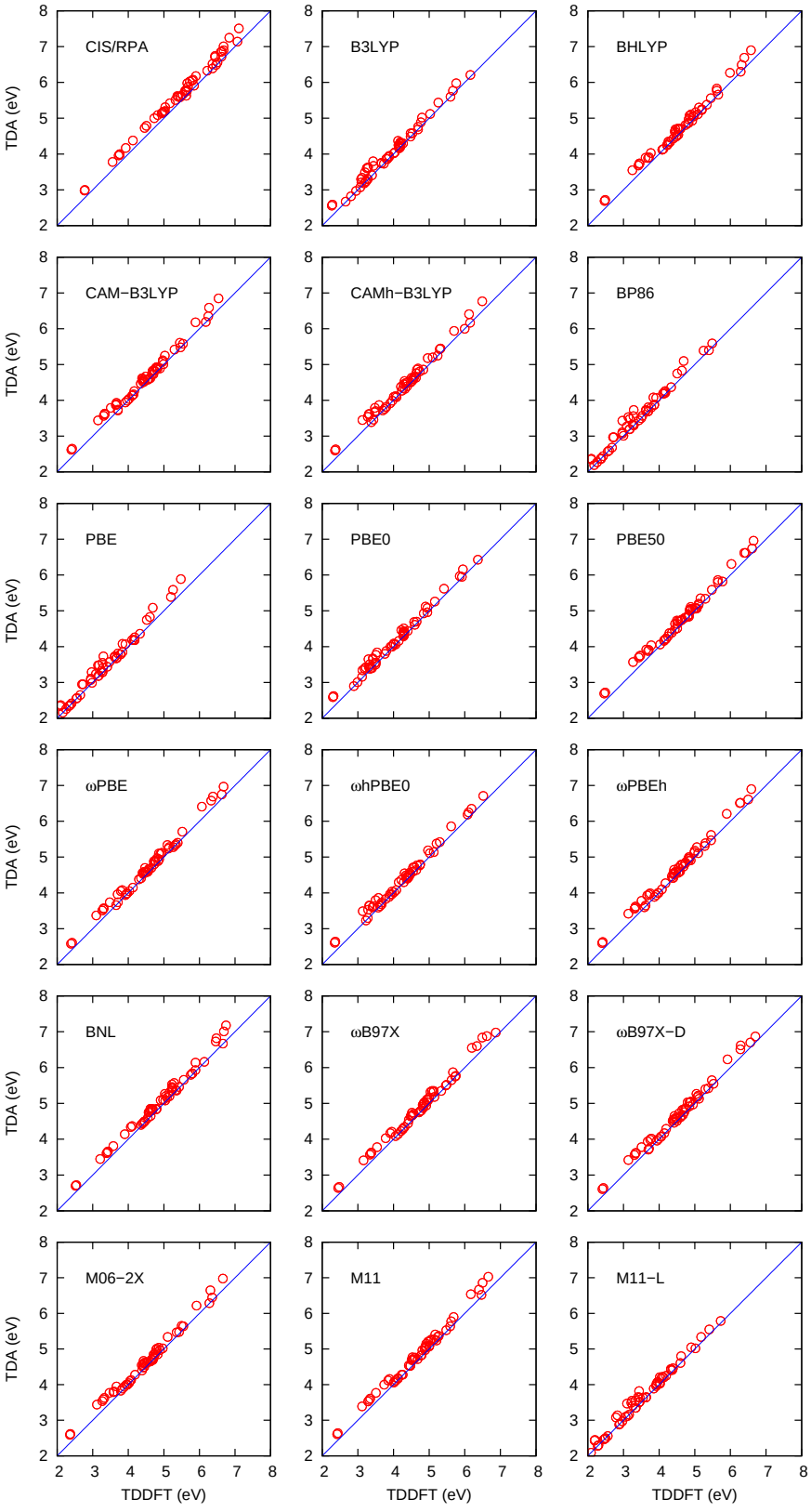

Figure S1: The VEEs calculated using the TDA method are compared with the VEEs calculated with TDDFT using def2-TZVP basis sets.

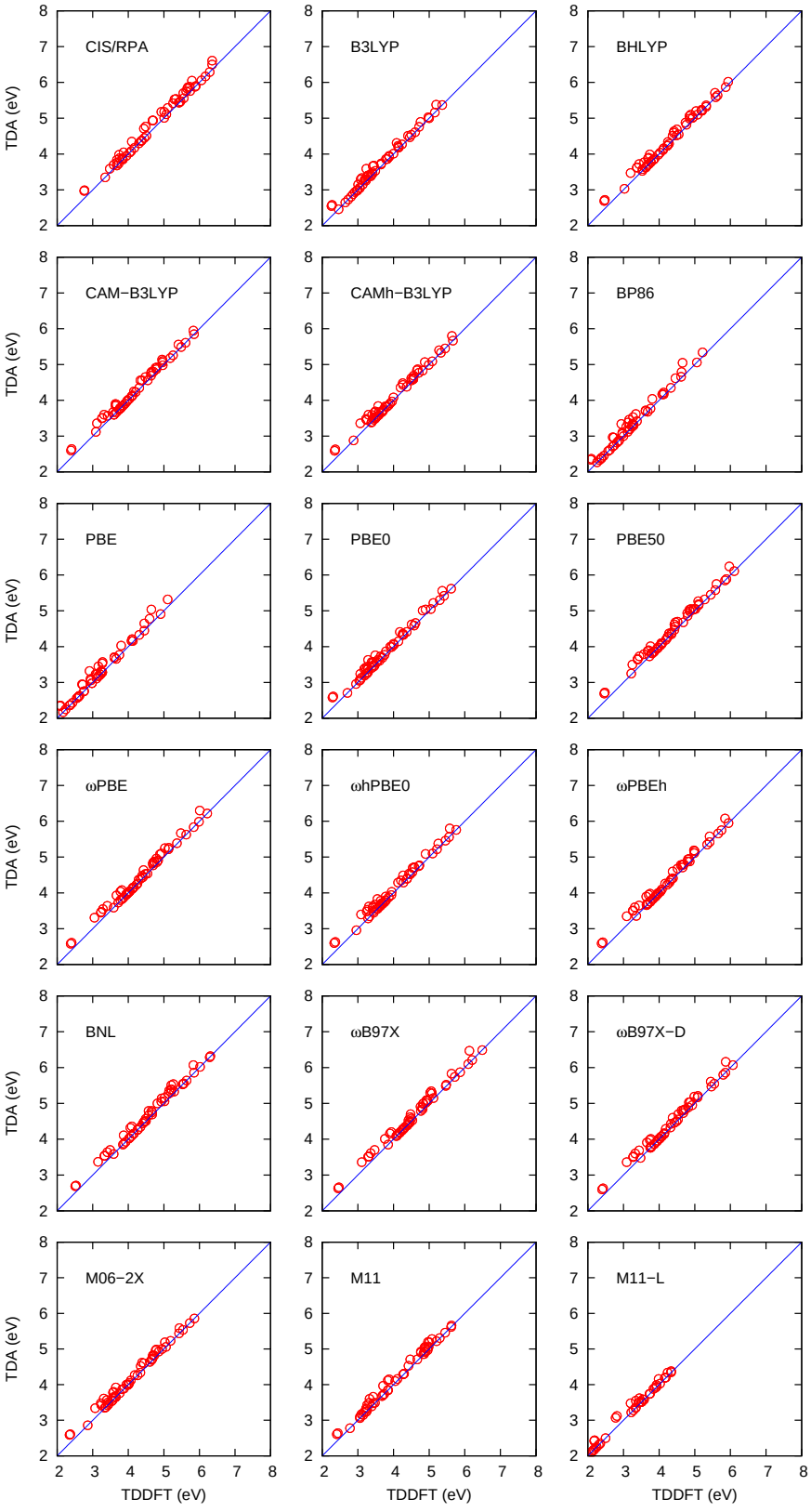

Figure S2: The VEEs calculated using the TDA method are compared with the VEEs calculated with TDDFT using aug-def2-TZVP basis sets.

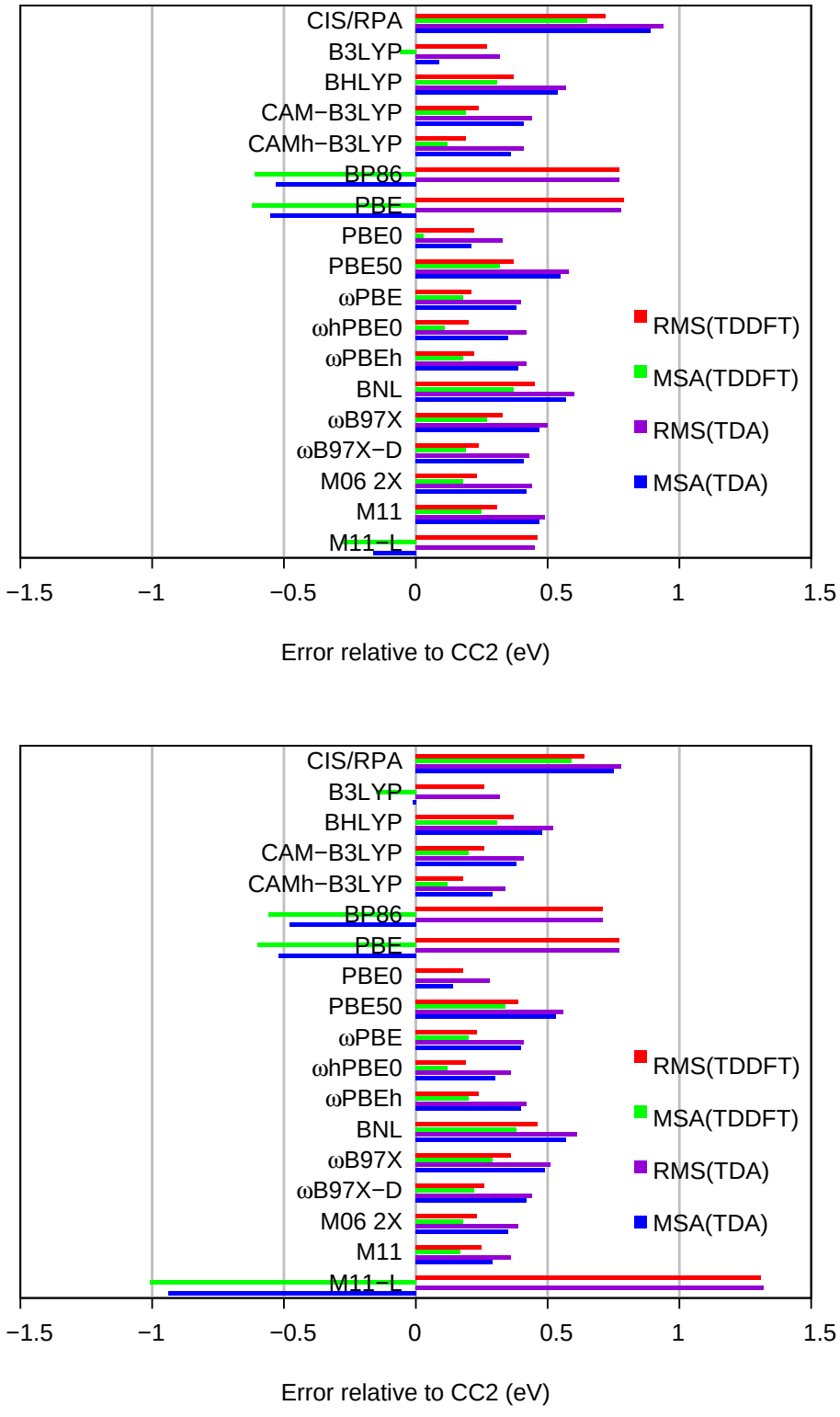

Figure S3: Root-mean-square (RMS) and mean signed average (MSA) values (in eV) of the lowest VEEs of the 11 chromophores calculated at the TDDFT and TDA levels as compared with the VEEs calculated at the CC2 level using def2-TZVP basis set sets (top panel) and aug-def2-TZVP basis set sets (bottom panel).

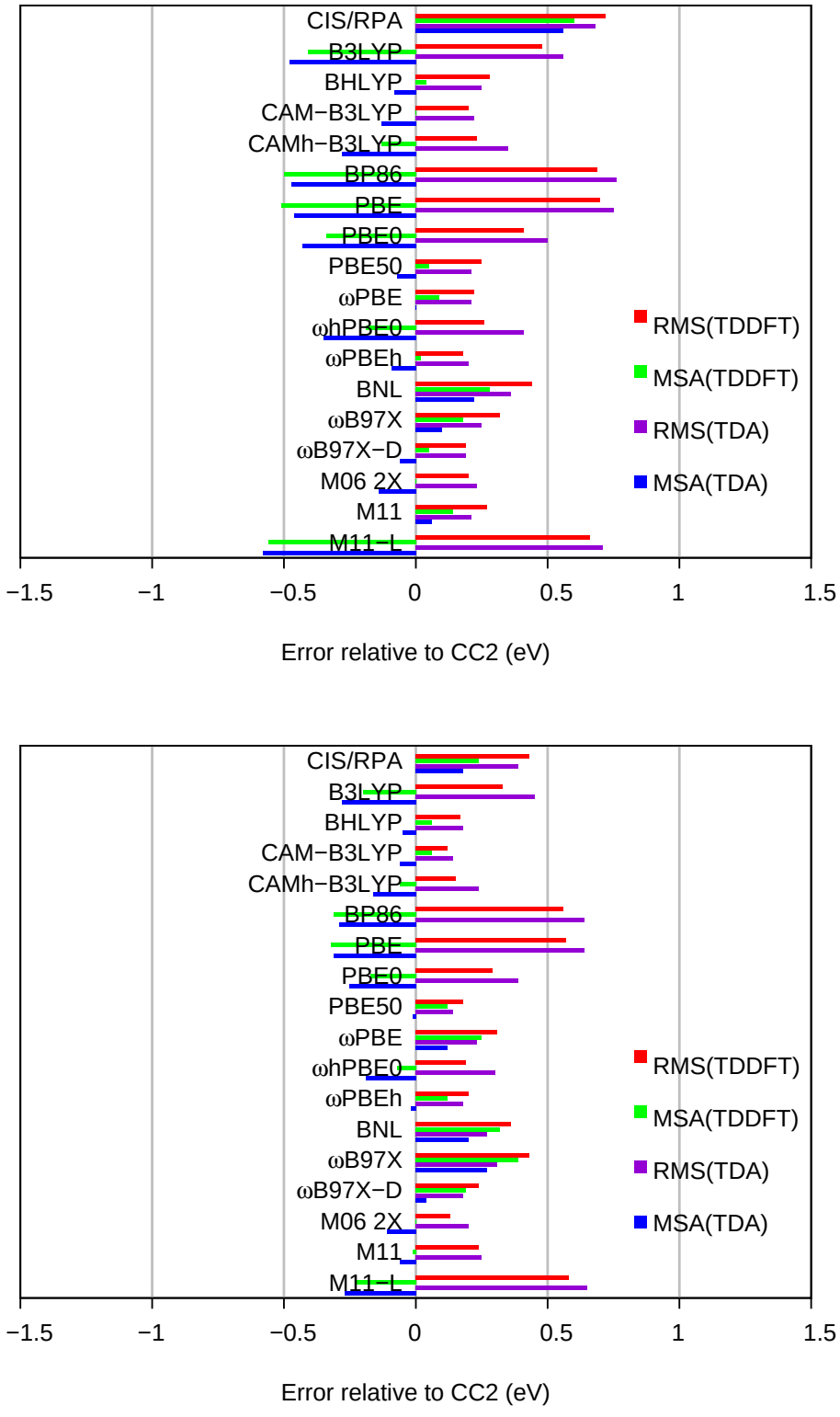

Figure S4: Root-mean-square (RMS) and mean signed average (MSA) values (in eV) of the 5 lowest VEEs calculated at the TDDFT and TDA levels as compared with the VEEs calculated at the CC2 level using def2-TZVP basis set sets (top panel) and aug-def2-TZVP basis set sets (bottom panel).