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Supplement for "A Unified Complete Active Space Model of Diarylmethane Dyes and their Azomethine Analogues"

by Seth Olsen

"A mathematician is a person who can find analogies between theorems; a better mathematician is one who can see analogies between proofs and the best mathematician can notice analogies between theories. One can imagine that the ultimate mathematician is one who can see analogies between analogies."

--Stefan Banach

"The price of metaphor is eternal vigilance."

--Norbert Wiener

Table S1. Cartesian coordinates (Å), SA2-CAS(4,3)/cc-pvdz state energies (a.u.), MS-MRPT2 state energies (a.u.) and mixing coefficients, state-averaged natural orbital graphics and occupation numbers for Michler's Hydrol Blue (HB).

ATOMIC COORDINATES (Ångstrom)

C	1.52725	0.00002	0.00000
H	2.62639	0.00004	0.00000
C	0.92958	-0.04732	1.28148
C	-0.43209	-0.40627	1.53280
C	-0.94844	-0.40827	2.81614
C	-0.14364	-0.03587	3.94687
C	1.23740	0.26291	3.70405
C	1.75029	0.23526	2.42094
H	-1.05870	-0.76450	0.71244
H	-1.97807	-0.73454	2.96311
H	1.90187	0.50925	4.53329
H	2.80695	0.47177	2.26378
N	-0.65968	-0.00325	5.19465
C	-2.06694	-0.32302	5.42242
H	-2.29868	-0.15214	6.48080
H	-2.71662	0.32632	4.81433
H	-2.28339	-1.37796	5.18042
C	0.19457	0.30657	6.34127
H	-0.41599	0.28767	7.25150
H	1.00179	-0.43652	6.44571
H	0.63926	1.31032	6.23993
C	0.92958	0.04734	-1.28148
C	-0.43209	0.40628	-1.53280
C	-0.94844	0.40827	-2.81615
C	-0.14364	0.03586	-3.94686
C	1.23739	-0.26292	-3.70404
C	1.75028	-0.23527	-2.42093
H	-1.05870	0.76452	-0.71245
H	-1.97808	0.73452	-2.96311
H	1.90186	-0.50930	-4.53328
H	2.80694	-0.47177	-2.26377
N	-0.65968	0.00325	-5.19465
C	-2.06693	0.32303	-5.42243
H	-2.28338	1.37796	-5.18042
H	-2.29866	0.15216	-6.48081
H	-2.71662	-0.32632	-4.81435
C	0.19458	-0.30658	-6.34126
H	1.00180	0.43650	-6.44571
H	-0.41598	-0.28767	-7.25150
H	0.63926	-1.31033	-6.23993

SA2-CAS(4,3)/cc-pvdz State Energies (a.u.)
S1 Energy = -764.729444 au
S2 Energy = -764.605940 au

MS-MRPT2 Results

STATE	ENERGY	MIXING COEFFICIENTS	
1	-766.1476616	1.0000	0.0000
2	-766.0700239	0.0000	1.0000

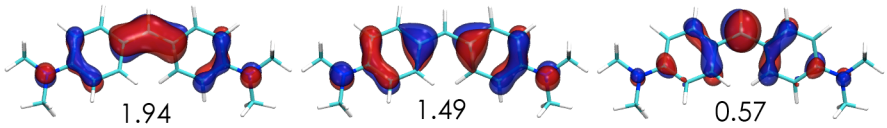


Table S2. Cartesian coordinates (Å), SA2-CAS(4,3)/cc-pvdz state energies (a.u.), MS-MRPT2 state energies (a.u.) and mixing coefficients, state-averaged natural orbital graphics and occupation numbers for Bis-Phenoxymethine (BP).

ATOMIC COORDINATES (Ångstrom)

C	-0.00002	-1.13835	-0.00000
C	0.03847	-0.56676	1.29314
C	0.32979	0.81233	1.59153
C	0.32049	1.29047	2.88628
C	0.00913	0.45399	4.05122
C	-0.22615	-0.95458	3.72139
C	-0.19520	-1.42619	2.42613
O	-0.01939	0.89836	5.22096
C	-0.03853	-0.56677	-1.29315
C	0.19518	-1.42620	-2.42613
C	0.22621	-0.95456	-3.72139
C	-0.00909	0.45400	-4.05121
C	-0.32049	1.29048	-2.88627
C	-0.32984	0.81231	-1.59154
O	0.01942	0.89836	-5.22095
H	-0.00000	-2.24242	0.00001
H	0.62965	1.47916	0.77686
H	0.57750	2.33682	3.09401
H	-0.42496	-1.63059	4.56234
H	-0.38328	-2.49154	2.22937
H	0.38331	-2.49154	-2.22937
H	0.42505	-1.63057	-4.56234
H	-0.57750	2.33682	-3.09400
H	-0.62972	1.47914	-0.77687

SA2-CAS(4,3)/cc-pvdz State Energies
S1 Energy = -647.315558 au
S2 Energy = -647.185850 au

MS-MRPT2 Results

STATE	ENERGY	MIXING COEFFICIENTS	
1	-649.0228084	1.0000	0.0000
2	-648.9397750	0.0000	1.0000

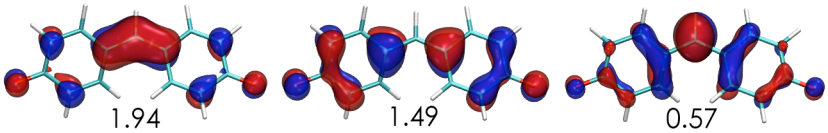


Table S3. Cartesian coordinates (Å), SA2-CAS(4,3)/cc-pvdz state energies (a.u.), MS-MRPT2 state energies (a.u.) and mixing coefficients, state-averaged natural orbital graphics and occupation numbers for Bindschedler's Green (BG).

ATOMIC COORDINATES (Ångstrom)

N	-0.00007	-1.68021	-0.00000
C	-0.05500	-1.02251	1.17866
C	-0.53297	0.31855	1.39157
C	-0.54564	0.87630	2.65680
C	-0.04759	0.15194	3.79647
C	0.36161	-1.21415	3.59380
C	0.31657	-1.78472	2.33922
H	-0.99453	0.86186	0.56086
H	-0.98700	1.86624	2.78903
H	0.69841	-1.81901	4.43778
H	0.62172	-2.82354	2.17927
N	-0.01503	0.71590	5.02139
C	-0.43234	2.10658	5.21246
H	-0.20184	2.40408	6.24267
H	-1.51482	2.22535	5.04433
H	0.11368	2.77242	4.52618
C	0.38873	-0.06962	6.19081
H	-0.28020	-0.93308	6.33673
H	0.33428	0.57113	7.07921
H	1.42271	-0.43089	6.08097
C	0.05480	-1.02246	-1.17865
C	-0.31656	-1.78471	-2.33925
C	-0.36152	-1.21416	-3.59383
C	0.04759	0.15196	-3.79647
C	0.54545	0.87637	-2.65675
C	0.53276	0.31860	-1.39153
H	-0.62165	-2.82356	-2.17933
H	-0.69815	-1.81906	-4.43785
H	0.98679	1.86633	-2.78894
H	0.99421	0.86195	-0.56078
N	0.01514	0.71591	-5.02141
C	-0.38844	-0.06966	-6.19086
H	-0.33392	0.57108	-7.07926
H	0.28057	-0.93307	-6.33669
H	-1.42241	-0.43099	-6.08114
C	0.43236	2.10662	-5.21244
H	0.20198	2.40408	-6.24268
H	1.51481	2.22547	-5.04416
H	-0.11381	2.77242	-4.52624

SA2-CAS(4,3)/cc-pvdz State Energies
S1 Energy = -780.704168 au
S2 Energy = -780.596830 au

MS-MRPT2 Results

STATE	ENERGY	MIXING COEFFICIENTS	
1	-782.1385755	1.0000	0.0000
2	-782.0723913	0.0000	1.0000

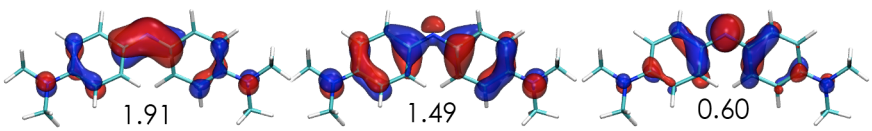
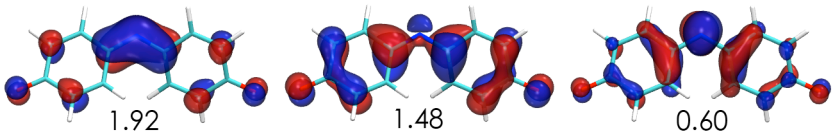


Table S4. Cartesian coordinates (Å), SA2-CAS(4,3)/cc-pvdz state energies (a.u.), MS-MRPT2 state energies (a.u.) and mixing coefficients, state-averaged natural orbital graphics and occupation numbers for Phenol-Indophenol (PI).

ATOMIC COORDINATES (Ångstrom)

N	0.00012	1.30197	-0.00001
C	0.04711	0.65149	1.18821
C	-0.29025	1.43451	2.35158
C	-0.34034	0.88856	3.61531
C	0.02305	-0.50771	3.88359
C	0.48365	-1.24346	2.70017
C	0.48159	-0.70538	1.42860
H	-0.56141	2.48142	2.16642
H	-0.64076	1.49186	4.48102
H	0.87202	-2.25427	2.87770
H	0.89948	-1.27867	0.59339
O	-0.00805	-1.01305	5.02841
C	-0.04695	0.65146	-1.18820
C	-0.48114	-0.70551	-1.42851
C	-0.48350	-1.24354	-2.70011
C	-0.02324	-0.50773	-3.88360
C	0.34002	0.88860	-3.61538
C	0.29026	1.43448	-2.35162
H	-0.89874	-1.27893	-0.59324
H	-0.87165	-2.25445	-2.87752
H	0.64048	1.49184	-4.48112
H	0.56150	2.48137	-2.16647
O	0.00764	-1.01302	-5.02846

SA2-CAS(4,3)/cc-pvdz State Energies
S1 Energy = -663.300531 au
S2 Energy = -663.186585 au

MS-MRPT2 Results

STATE	ENERGY	MIXING COEFFICIENTS	
1	-665.0329332	1.0000	0.0000
2	-664.9597812	0.0000	1.0000