

Supporting Information

Density Functional Theory Study on the Donating Strength of Donor Systems in Dye-sensitized Solar Cells.

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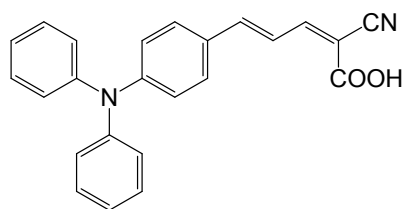
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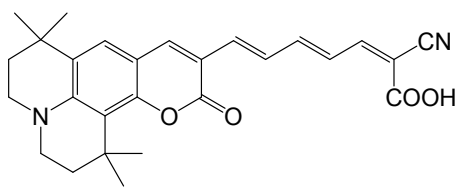
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1. Table S1. Benchmark time-dependent DFT calculations using DFT/SMD/cc-pVDZ method to obtain the absorption spectra. The absorption maxima λ_{max} (nm) and oscillator strength (f) are given along with experimentally known λ_{max} . All the geometries are optimized at B3LYP/cc-pVDZ level.

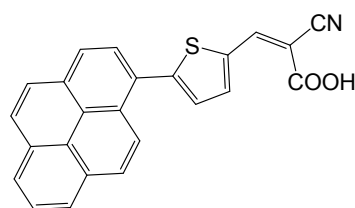
Systems	CAM-B3LYP		B3LYP		PBE1PBE		ω B97XD		Exp. λ_{max}	Deviation from exp. λ_{max} (CAM-B3LYP)
	λ_{max}	f	λ_{max}	f	λ_{max}	f	λ_{max}	f		
1	422	1.52	559	1.44	488	1.24	429	1.48	417 (EtOH) ¹	-5
2	499	1.99	577	1.71	560	1.80	488	2.01	506 (MeOH) ²	7
3	409	1.25	508	0.65	482	0.75	398	1.35	388 (THF) ³	-21
4	460	1.41	599	0.78	563	0.90	448	1.44	494 (DCM) ⁴	34
5	355	1.09	445	0.39	420	0.49	348	1.15	338 (DCM) ⁵	-17
6	388	1.60	462	0.64	436	0.93	382	1.67	388 (DCM) ⁶	0



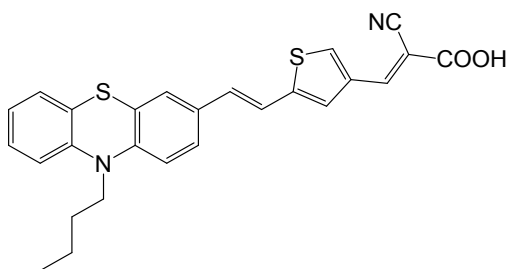
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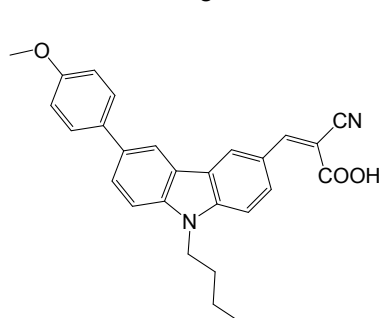
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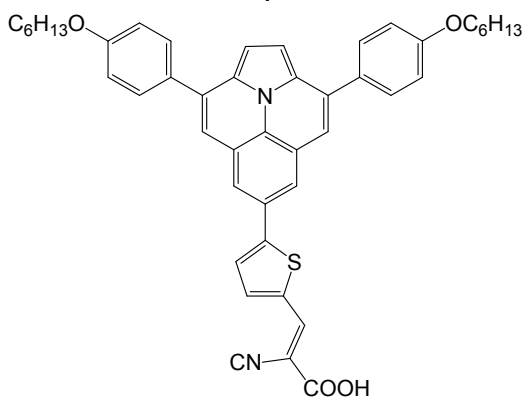
3



4



5



6

Fig. S1 Chemdraw representations of known systems (**1 – 6**).

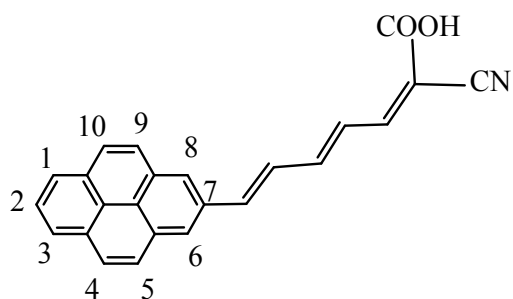
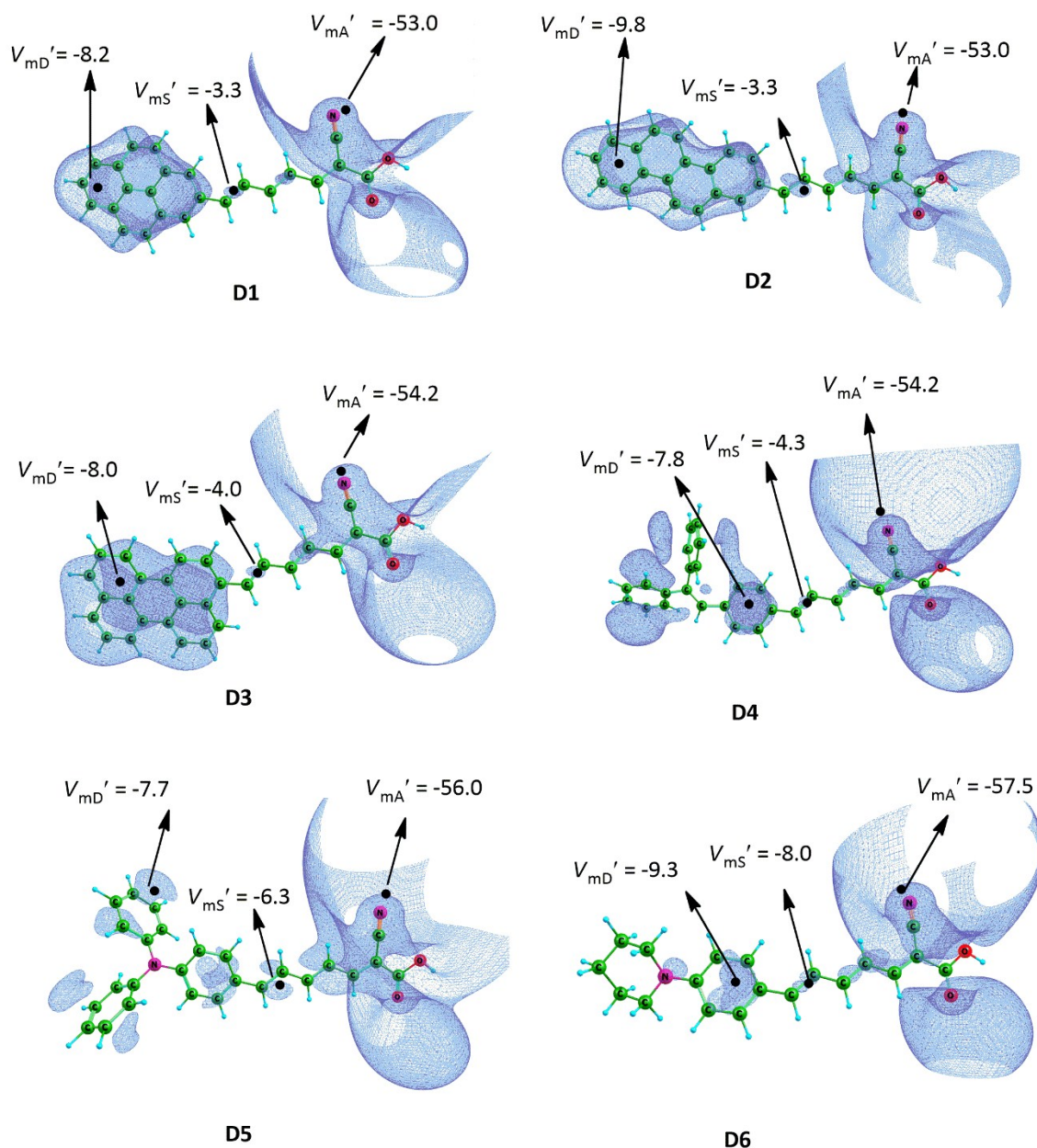


Fig. S2 ChemDraw of D1- π -A system.

Table S2. Absorption maxima of methyl substituted pyrene based D1- π -A systems at TD-CAM-B3LYP/SMD/cc-pVDZ//B3LYP/cc-pVDZ level. Here D1 represents unsubstituted pyrene based D- π -A system, while D1-1, D1-2, D1-3 etc represents the methyl substitution at 1, 2, 3, 4 and 5 positions of D1- π -A (see Fig. S2 for numbering).

D- π -A Systems	HOMO-1 (eV)	HOMO (eV)	LUMO (eV)	HLG (eV)	λ_{max} (nm)	f	MO contribution
D1	-6.02	-5.88	-2.99	2.89	S1 $\rightarrow$ 401	2.22	H-1 $\rightarrow$ L (94.17 %)
					S2 $\rightarrow$ 376	0.03	H $\rightarrow$ L (74.56 %)
D1-1	-5.73	-5.39	-2.81	2.58	430	2.21	H $\rightarrow$ L (72.12%)
D1-2	-5.95	-5.46	-2.92	2.54	404	1.05	H $\rightarrow$ L (45.84%)
D1-3	-5.94	-5.62	-2.92	2.70	405	1.95	H-1 $\rightarrow$ L (69.83%)
							H $\rightarrow$ L (21.06%)
D1-4	-5.93	-5.62	-2.94	2.69	407	2.07	H-1 $\rightarrow$ L (74.28%)
							H $\rightarrow$ L (17.43%)
D1-5	-5.93	-5.83	-2.91	2.92	S1 $\rightarrow$ 405	2.19	H-1 $\rightarrow$ L (94.84%)
					S2 $\rightarrow$ 381	0.03	H $\rightarrow$ L (75.33%)

The data in Table S2 clearly suggest that with a suitable substitution (CH_3 substitution) at one or two positions of D1- π -A system, the oscillator strength of HOMO $\rightarrow$ LUMO transition can be increased from 0.03 for the unsubstituted to 2.21 for the substituted.



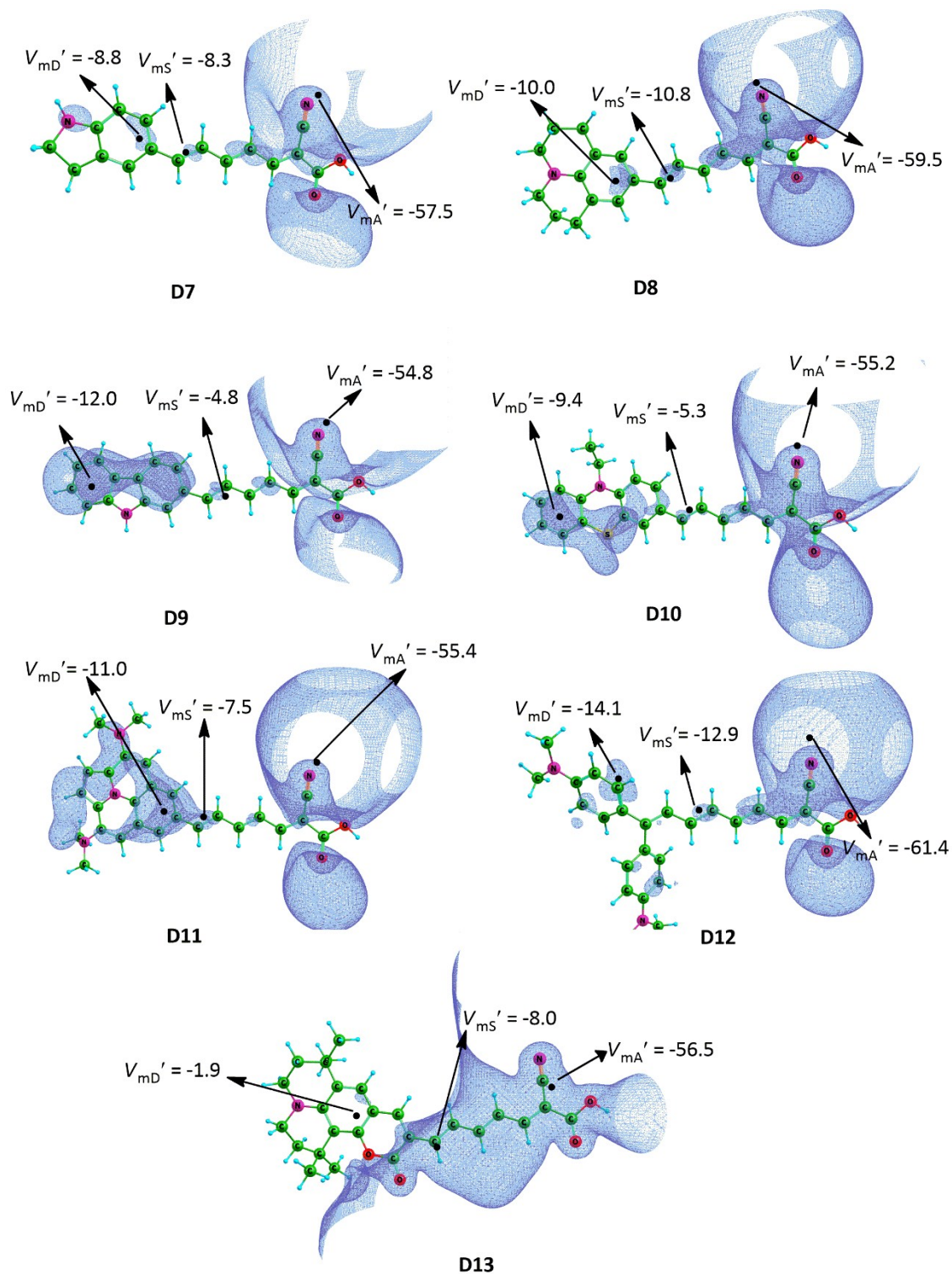


Fig. S3 MESP isosurface of D- π -A systems. The V_m values at various positions are given in kcal/mol.

Table S3. Cartesian coordinates (in Angstrom unit) of B3LYP/cc-pVDZ optimized geometries of donor (D1 - D13) systems.

D1 E(RB3LYP) = -615.809327961 a. u.				D2 E(RB3LYP) = -693.223060183 a. u.			
6	0.681962000	2.467295000	0.000017000	6	-1.873155000	-0.376823000	0.000000000
6	1.431218000	1.237859000	0.000006000	6	-2.406091000	0.949539000	-0.000001000
6	-0.681962000	2.467295000	0.000021000	6	-0.430578000	-0.564294000	-0.000001000
6	0.714468000	0.000000000	-0.000002000	6	-1.505429000	2.059004000	-0.000002000
6	-1.431218000	1.237859000	0.000013000	6	0.430579000	0.564293000	-0.000001000
6	-0.714468000	0.000000000	0.000002000	6	-0.151746000	1.873886000	-0.000002000
1	1.234144000	3.410598000	0.000023000	6	0.151746000	-1.873886000	-0.000002000
6	2.837506000	1.212488000	0.000002000	6	1.505430000	-2.059004000	-0.000002000
6	1.431216000	-1.237859000	-0.000013000	6	2.406091000	-0.949539000	-0.000001000
6	-1.431216000	-1.237858000	-0.000006000	6	1.873154000	0.376823000	0.000000000
6	2.837508000	-1.212488000	-0.000016000	6	3.810878000	-1.146489000	-0.000001000
6	3.529447000	-0.000002000	-0.000009000	6	4.679814000	-0.073310000	0.000001000
1	3.386562000	2.157418000	0.000008000	6	2.795834000	1.456776000	0.000002000
6	0.681963000	-2.467294000	-0.000021000	6	4.162203000	1.240057000	0.000003000
1	3.386560000	-2.157420000	-0.000025000	6	-2.795834000	-1.456775000	0.000002000
6	-2.837506000	1.212489000	0.000017000	6	-3.810877000	1.146489000	-0.000001000
6	-2.837508000	-1.212488000	-0.000002000	1	-1.920907000	3.069832000	-0.000004000
6	-3.529447000	-0.000002000	0.000009000	1	0.495122000	2.750197000	-0.000003000
1	-1.234143000	3.410598000	0.000030000	1	-0.495121000	-2.750197000	-0.000003000
6	-0.681963000	-2.467293000	-0.000018000	1	1.920907000	-3.069832000	-0.000004000
1	1.234143000	-3.410598000	-0.000030000	1	4.194520000	-2.170049000	-0.000002000
1	-3.386560000	-2.157420000	-0.000008000	1	2.433552000	2.484335000	0.000004000
1	-4.621823000	0.000001000	0.000012000	1	4.844221000	2.093254000	0.000005000
1	-1.234143000	-3.410597000	-0.000024000	6	-4.162204000	-1.240056000	0.000003000
1	-3.386564000	2.157417000	0.000025000	6	-4.679814000	0.073310000	0.000001000
1	4.621823000	0.000000000	-0.000011000	1	-2.433553000	-2.484335000	0.000004000
				1	-4.194520000	2.170049000	-0.000002000
				1	-4.844222000	-2.093253000	0.000004000
				1	-5.759758000	0.236374000	0.000002000
				1	5.759758000	-0.236373000	0.000002000
D3 E(RB3LYP) = -769.451069602 a. u.				D4 E(RB3LYP) = -771.803147464 a. u.			
6	2.889053000	2.426915000	0.000126000	6	-0.530861000	-0.324471000	0.022794000
6	1.480432000	2.431435000	0.000108000	6	-3.753294000	-2.254361000	-0.633878000
6	0.739119000	1.251132000	0.000029000	6	-4.693485000	-1.478940000	0.051447000
6	1.441707000	0.000000000	-0.000001000	6	-4.276158000	-0.316755000	0.707493000
6	2.878797000	0.000000000	-0.000002000	6	-2.409876000	-1.875629000	-0.656567000
6	3.580347000	1.234999000	0.000063000	6	-2.933682000	0.064364000	0.682051000
6	-0.739119000	1.251132000	-0.000029000	6	-1.969842000	-0.715525000	0.012025000

6	0.739119000	-1.251132000	-0.000031000	1	-4.069491000	-3.154238000	-1.166998000
6	-0.739119000	-1.251132000	0.000030000	1	-1.691623000	-2.472114000	-1.222570000
6	-1.441707000	0.000000000	0.000001000	1	-2.621026000	0.972527000	1.200440000
6	-1.480432000	-2.431435000	0.000112000	1	-5.001515000	0.299034000	1.244684000
6	1.480432000	-2.431435000	-0.000113000	6	-0.234602000	1.141168000	0.022745000
6	2.889052000	-2.426915000	-0.000132000	6	0.500855000	1.728025000	1.067498000
6	3.580346000	-1.234999000	-0.000067000	6	-0.717704000	1.971374000	-1.004934000
1	4.672806000	-1.220878000	-0.000071000	1	0.868996000	1.097222000	1.878938000
1	3.426877000	-3.377474000	-0.000196000	1	-1.303760000	1.533146000	-1.815907000
1	3.426878000	3.377474000	0.000188000	6	0.760049000	3.100619000	1.075949000
6	-1.480432000	2.431435000	-0.000107000	6	-0.448616000	3.342116000	-1.002825000
6	-2.889052000	2.426915000	-0.000125000	1	1.329879000	3.538448000	1.899002000
6	-3.580347000	1.234999000	-0.000062000	1	-0.822420000	3.968732000	-1.816160000
6	-2.878797000	0.000000000	0.000002000	6	0.291410000	3.912039000	0.038117000
1	-3.426878000	3.377474000	-0.000186000	6	0.426593000	-1.288291000	0.080660000
1	-4.672806000	1.220877000	-0.000065000	1	-5.745465000	-1.772854000	0.065607000
6	-2.889052000	-2.426915000	0.000131000	1	0.496387000	4.985075000	0.043423000
1	-3.426877000	-3.377474000	0.000194000	6	1.894008000	-1.191006000	-0.001376000
6	-3.580346000	-1.234999000	0.000067000	6	2.582176000	-0.176238000	-0.699261000
1	-4.672806000	-1.220878000	0.000070000	6	2.661603000	-2.209379000	0.601973000
1	-0.973285000	3.395670000	-0.000160000	1	2.020158000	0.606525000	-1.207974000
1	0.973285000	3.395670000	0.000161000	1	2.148431000	-3.017745000	1.129914000
1	-0.973284000	-3.395669000	0.000167000	6	3.975391000	-0.172780000	-0.765298000
1	0.973284000	-3.395669000	-0.000168000	6	4.055612000	-2.199670000	0.544342000
1	4.672806000	1.220877000	0.000065000	1	4.484618000	0.620357000	-1.318102000
				1	4.624083000	-2.997055000	1.028943000
				6	4.721022000	-1.177550000	-0.138650000
				1	5.812054000	-1.168924000	-0.192058000
				1	0.067097000	-2.312805000	0.222967000
D5 E(RB3LYP) = -749.742344106 a. u.				D6 E(RB3LYP) = -482.978101397 a. u.			
7	0.000059000	0.000065000	0.000063000	6	0.849893000	-0.001311000	-0.055338000
6	-2.211229000	0.693214000	0.815160000	6	1.577975000	-1.159648000	0.282822000
6	-1.086956000	0.916949000	-0.000073000	6	1.582823000	1.166099000	-0.365842000
6	-3.279585000	1.591346000	0.804814000	1	1.050003000	2.069988000	-0.666493000
1	-4.144511000	1.400740000	1.444717000	1	1.057595000	-2.079228000	0.549390000
6	-1.055965000	2.062726000	-0.815486000	6	2.974928000	1.171940000	-0.332802000
6	-3.241632000	2.734263000	-0.000291000	6	2.976969000	-1.148207000	0.299184000
1	-0.190739000	2.241839000	-1.455710000	1	3.510251000	2.090746000	-0.585214000
1	-4.076292000	3.438242000	-0.000376000	1	3.511349000	-2.063877000	0.565043000
6	-2.121400000	2.964326000	-0.805311000	6	3.688183000	0.013261000	-0.001571000
1	-2.079341000	3.848926000	-1.445325000	1	4.779818000	0.018377000	0.015935000
1	-2.241958000	-0.189799000	1.455408000	7	-0.561308000	0.018468000	-0.129874000
6	3.988951000	1.439993000	0.000278000	6	-1.250940000	1.072769000	0.627342000
6	3.017895000	2.044873000	0.804685000	6	-2.673401000	1.291289000	0.108535000
6	3.628258000	0.354377000	-0.804233000	6	-3.468249000	-0.018423000	0.133505000

1	3.285144000	2.889555000	1.444212000	6	-2.697902000	-1.112941000	-0.611565000
1	4.373512000	-0.124825000	-1.443658000	6	-1.268198000	-1.258668000	-0.077534000
6	1.705864000	1.568850000	0.814836000	1	-0.674089000	2.003152000	0.556324000
6	2.314691000	-0.117409000	-0.814597000	1	-1.290510000	0.801895000	1.707534000
1	0.956349000	2.037485000	1.454516000	1	-3.168851000	2.062992000	0.721460000
1	2.037396000	-0.956725000	-1.454316000	1	-2.621095000	1.675446000	-0.925592000
6	1.337655000	0.482926000	0.000057000	1	-4.469100000	0.122052000	-0.307450000
6	-0.250588000	-1.399786000	0.000062000	1	-3.625661000	-0.329748000	1.183421000
6	-1.258365000	-1.945735000	-0.815387000	1	-3.214394000	-2.083704000	-0.526290000
6	0.505096000	-2.261568000	0.815479000	1	-2.647587000	-0.862746000	-1.685950000
1	-1.846026000	-1.285912000	-1.455612000	1	-0.720136000	-1.986229000	-0.693232000
1	1.285204000	-1.846711000	1.455721000	1	-1.300913000	-1.665355000	0.959809000
6	-1.506620000	-3.319201000	-0.805177000				
6	0.261313000	-3.635834000	0.805175000				
1	-2.293721000	-3.725034000	-1.445233000				
1	0.858687000	-4.289628000	1.445174000				
6	-0.747424000	-4.174342000	-0.000033000				
1	-0.939872000	-5.249149000	-0.000084000				
1	5.015987000	1.810724000	0.000367000				
D7 E(RB3LYP) = -365.040386239 a. u.				D8 E(RB3LYP) = -521.099548859 a. u.			
6	1.032717000	1.418871000	0.018249000	6	2.507425000	0.051903000	0.313492000
6	-0.167057000	0.721226000	-0.039842000	6	1.214672000	0.820017000	0.152907000
6	-0.170250000	-0.687581000	-0.069864000	6	2.436097000	-1.261791000	-0.469448000
6	1.026530000	-1.408467000	-0.031134000	6	-0.000005000	0.100533000	-0.000042000
6	2.230495000	-0.692725000	0.034647000	6	1.229758000	-2.074036000	-0.005337000
6	2.242699000	0.705351000	0.060020000	7	0.000059000	-1.292805000	-0.000128000
6	-1.603361000	1.195082000	-0.134174000	1	2.689958000	-0.174924000	1.381514000
6	-2.389686000	-0.085140000	0.232276000	6	1.193636000	2.216981000	0.134883000
7	-1.481015000	-1.172654000	-0.177783000	6	-1.214760000	0.819895000	-0.152960000
1	1.037287000	2.512104000	0.040698000	6	-1.229551000	-2.074191000	0.005475000
1	1.027091000	-2.501072000	-0.049927000	6	-1.193890000	2.216856000	-0.134842000
1	3.174537000	-1.242017000	0.071890000	6	-0.000166000	2.929817000	0.000047000
1	-1.843811000	2.039793000	0.528162000	1	2.141569000	2.753874000	0.238247000
1	-3.355737000	-0.161667000	-0.288772000	6	-2.507397000	0.051611000	-0.313607000
1	-1.657249000	-2.077200000	0.250882000	1	-2.141882000	2.753649000	-0.238179000
1	-2.583240000	-0.110125000	1.324099000	1	-0.000226000	4.021607000	0.000084000
1	-1.835945000	1.506539000	-1.168994000	1	3.349150000	-1.862387000	-0.330429000
1	3.191650000	1.242516000	0.115380000	6	-2.435957000	-1.261986000	0.469488000
				1	-3.357095000	0.665646000	0.024999000
				1	-2.343079000	-1.043338000	1.547182000
				1	1.425081000	-2.488932000	1.006627000
				1	-1.085556000	-2.942206000	0.674887000
				1	3.357005000	0.666014000	-0.025273000
				1	2.343193000	-1.043294000	-1.547171000
				1	-3.348956000	-1.862683000	0.330547000
				1	-2.689779000	-0.175365000	-1.381624000

				1	1.085944000	-2.942260000	-0.674510000
				1	-1.424922000	-2.489405000	-1.006344000
D9 E(RB3LYP) = -517.504742141 a. u.				D10 E(RB3LYP) = -994.310143043 a. u.			
6	2.484393000	1.223499000	0.000001000	6	-2.401400000	1.085150000	-0.112395000
6	1.133787000	0.856817000	-0.000003000	6	-1.236025000	0.329759000	0.124991000
6	0.726133000	-0.506712000	-0.000003000	7	-0.000043000	0.946705000	0.431125000
6	1.702434000	-1.513612000	-0.000003000	6	-1.358187000	-1.077639000	0.066228000
6	3.049786000	-1.154266000	0.000001000	16	0.000293000	-2.123508000	0.555709000
6	3.433533000	0.200786000	0.000004000	6	1.358544000	-1.077337000	0.066219000
7	0.000000000	1.655193000	-0.000014000	6	1.236086000	0.330040000	0.124981000
6	-0.726134000	-0.506711000	-0.000005000	6	-3.624678000	0.471472000	-0.398825000
1	2.787389000	2.273092000	0.000002000	6	-2.572961000	-1.683174000	-0.263780000
1	1.410772000	-2.566447000	-0.000006000	6	2.573456000	-1.682623000	-0.263740000
1	3.818214000	-1.929999000	0.000001000	6	2.401349000	1.085657000	-0.112247000
6	-2.484393000	1.223499000	0.000008000	6	3.624764000	0.472227000	-0.398623000
6	-3.433533000	0.200787000	0.000009000	6	3.718995000	-0.914761000	-0.488571000
6	-1.133786000	0.856818000	0.000001000	1	2.618750000	-2.772597000	-0.316663000
1	-4.495045000	0.458516000	0.000015000	1	2.367205000	2.171975000	-0.075952000
6	-3.049786000	-1.154266000	0.000001000	1	4.503871000	1.098389000	-0.565108000
1	-3.818215000	-1.929999000	0.000002000	1	4.667487000	-1.399301000	-0.726814000
6	-1.702434000	-1.513612000	-0.000007000	6	-3.718639000	-0.915541000	-0.488697000
1	-1.410770000	-2.566446000	-0.000011000	1	-2.367436000	2.171483000	-0.076214000
1	-2.787390000	2.273092000	0.000011000	1	-4.503888000	1.097459000	-0.565427000
1	0.000001000	2.665157000	0.000052000	1	-2.618034000	-2.773158000	-0.316694000
1	4.495045000	0.458516000	0.000007000	6	-0.000267000	2.358651000	0.827762000
D11 E(RB3LYP) = -861.656153170 a. u.				1	-0.878885000	2.512605000	1.472565000
6	1.245498000	-1.793777000	-0.088244000	1	0.878806000	2.513166000	1.471819000
6	2.447654000	-0.999685000	-0.134448000	6	-0.001188000	3.400229000	-0.302766000
6	2.423580000	0.378173000	-0.088965000	1	-0.885541000	3.311740000	-0.950055000
6	1.143079000	1.044394000	-0.034171000	1	0.882527000	3.312342000	-0.950996000
7	-0.000001000	0.250710000	0.000001000	1	-0.001302000	4.412700000	0.134094000
6	0.000000000	-1.124910000	-0.000004000	1	-4.667020000	-1.400272000	-0.726991000
6	-1.245496000	-1.793780000	0.088230000	D12 E(RB3LYP) = -808.674999064 a. u.			
6	-2.447654000	-0.999691000	0.134442000	6	0.000000000	1.798891000	0.000000000
6	-2.423582000	0.378167000	0.088972000	6	-3.603469000	0.794812000	0.756262000
				6	-3.776910000	-0.382393000	-0.010937000
				6	-2.665432000	-0.821416000	-0.770613000
				6	-2.387106000	1.472320000	0.768811000
				6	-1.455203000	-0.133964000	-0.739935000
				6	-1.279299000	1.036452000	0.020462000
				1	-4.419928000	1.183207000	1.363595000
				1	-2.288811000	2.362179000	1.394666000

6	-1.143083000	1.044391000	0.034180000	1	-0.625676000	-0.508338000	-1.343481000
1	3.398688000	-1.530155000	-0.172055000	1	-2.741007000	-1.709490000	-1.396598000
1	-3.398686000	-1.530163000	0.172045000	6	1.279298000	1.036451000	-0.020463000
6	-0.703748000	2.375704000	0.029830000	6	2.387106000	1.472319000	-0.768811000
6	0.703740000	2.375706000	-0.029819000	6	1.455201000	-0.133966000	0.739932000
6	-1.215708000	-3.203289000	0.089448000	1	2.288813000	2.362179000	-1.394664000
6	1.215713000	-3.203286000	-0.089474000	1	0.625674000	-0.508340000	1.343478000
6	0.000003000	-3.886051000	-0.000016000	6	3.603468000	0.794809000	-0.756263000
1	-2.155500000	-3.755879000	0.155199000	6	2.665430000	-0.821420000	0.770609000
1	2.155505000	-3.755873000	-0.155229000	1	4.419928000	1.183205000	-1.363594000
1	-1.344139000	3.250945000	0.080230000	1	2.741003000	-1.709494000	1.396594000
1	1.344128000	3.250949000	-0.080219000	6	3.776908000	-0.382398000	0.010933000
7	-3.581502000	1.182104000	0.146385000	7	-4.977665000	-1.083944000	-0.004988000
7	3.581501000	1.182109000	-0.146374000	7	4.977662000	-1.083953000	0.004978000
6	-3.828325000	2.051787000	-1.004589000	6	-6.151624000	-0.475781000	0.593156000
1	-2.893354000	2.497375000	-1.362582000	1	-6.994697000	-1.175721000	0.522071000
1	-4.287582000	1.496156000	-1.849958000	1	-5.989740000	-0.262752000	1.662971000
1	-4.515640000	2.863107000	-0.714835000	1	-6.447801000	0.473953000	0.102687000
6	-4.801451000	0.544591000	0.610290000	6	-5.180204000	-2.153076000	-0.964890000
1	-5.552811000	1.324667000	0.809267000	1	-5.139482000	-1.807385000	-2.018149000
1	-5.241540000	-0.162325000	-0.126462000	1	-4.423059000	-2.945488000	-0.843956000
1	-4.611747000	-0.001230000	1.545572000	1	-6.163801000	-2.609701000	-0.792071000
6	4.801445000	0.544599000	-0.610293000	6	5.180209000	-2.153073000	0.964892000
1	4.611734000	-0.001209000	-1.545581000	1	5.139509000	-1.807370000	2.018147000
1	5.552807000	1.324674000	-0.809264000	1	4.423055000	-2.945479000	0.843980000
1	5.241535000	-0.162329000	0.126447000	1	6.163798000	-2.609711000	0.792059000
6	3.828334000	2.051774000	1.004613000	6	6.151626000	-0.475773000	-0.593143000
1	4.515650000	2.863095000	0.714866000	1	6.447802000	0.473946000	-0.102646000
1	2.893368000	2.497360000	1.362620000	1	6.994697000	-1.175717000	-0.522075000
1	4.287596000	1.496128000	1.849969000	1	5.989746000	-0.262715000	-1.662953000
1	0.000004000	-4.978665000	-0.000020000	6	0.000001000	3.150120000	0.000001000
				1	-0.930286000	3.718413000	-0.058099000
				1	0.930288000	3.718412000	0.058102000
D13 E(RB3LYP) = -943.146937737 a. u.							
8	2.712446000	-0.119853000	-0.064285000				
8	4.867713000	-0.683541000	-0.133730000				
6	2.061519000	2.313764000	1.241511000				
6	1.567263000	2.590279000	-1.215826000				
6	3.285972000	-2.471921000	-0.087617000				
6	1.961302000	-2.776594000	-0.045907000				
6	1.376676000	-0.407529000	-0.003801000				
6	0.987605000	2.127968000	0.140660000				
6	3.730682000	-1.090936000	-0.097715000				
6	0.958913000	-1.754337000	-0.008359000				
6	0.480292000	0.673331000	0.040456000				

6	-0.194463000	3.029277000	0.553041000
6	-0.423020000	-2.014389000	0.031075000
6	-0.914621000	0.364690000	-0.031532000
6	-1.449172000	2.765954000	-0.252015000
6	-1.364046000	-1.002943000	0.024896000
6	-2.865424000	-1.296685000	0.091359000
6	-3.255322000	1.139600000	-0.482458000
6	-3.219997000	-2.723041000	-0.360156000
6	-3.366935000	-1.097950000	1.541945000
6	-3.548726000	-0.301239000	-0.866254000
7	-1.854141000	1.373555000	-0.140094000
1	2.220293000	3.392637000	1.407796000
1	2.411833000	1.953098000	-1.513679000
1	1.726573000	1.874505000	2.195201000
1	0.097570000	4.086254000	0.446355000
1	0.814863000	2.550436000	-2.019430000
1	1.933488000	3.628649000	-1.140771000
1	3.023434000	1.864983000	0.973419000
1	1.637088000	-3.821591000	-0.039589000
1	-0.422093000	2.861162000	1.619663000
1	-1.307180000	3.042606000	-1.317149000
1	-2.277488000	3.388556000	0.125177000
1	-2.843333000	-2.933476000	-1.373583000
1	-3.520439000	1.805157000	-1.324153000
1	-3.100012000	-0.107828000	1.940848000
1	-2.817177000	-3.487681000	0.321444000
1	-2.915786000	-1.850714000	2.207195000
1	-3.892445000	1.451076000	0.367582000
1	-3.188516000	-0.497758000	-1.890156000
1	-4.640853000	-0.451799000	-0.871227000
1	-4.314977000	-2.847040000	-0.372253000
1	-4.464002000	-1.207143000	1.596749000
1	-0.742874000	-3.056462000	0.060383000
1	4.068767000	-3.229161000	-0.114873000

Table S4. Cartesian coordinates (in Angstrom unit) of B3LYP/cc-pVDZ optimized geometries of D- π -A (**D1-D13**) systems.

D1 E(RB3LYP) = -1128.88061603 a. u.				D2 E(RB3LYP) = -1206.29563524 a. u.			
6	5.631431000	-0.482809000	0.000042000	6	6.657372000	-0.431253000	-0.000030000
6	6.794548000	0.241238000	0.000050000	6	7.838562000	0.263025000	-0.000014000
6	6.792874000	1.671097000	0.000047000	6	7.873418000	1.692393000	0.000040000
7	6.753355000	2.835964000	0.000067000	7	7.863693000	2.857903000	0.000077000

6	8.086100000	-0.496085000	0.000066000	6	9.110977000	-0.506906000	-0.000065000
8	8.188399000	-1.705762000	-0.000094000	8	9.182589000	-1.718758000	0.000306000
8	9.150128000	0.335591000	-0.000116000	8	10.195825000	0.297512000	0.000448000
1	9.938765000	-0.236697000	-0.000238000	1	10.969670000	-0.294683000	0.000750000
6	1.846208000	-0.278144000	0.000027000	6	2.878883000	-0.132628000	-0.000016000
1	1.707212000	0.807262000	0.000026000	1	6.758327000	-1.521025000	-0.000069000
1	5.759735000	-1.569731000	0.000042000	6	4.219024000	-0.644200000	-0.000037000
6	3.199068000	-0.756705000	0.000034000	6	5.344735000	0.131092000	-0.000013000
6	4.304796000	0.046504000	0.000039000	1	4.336262000	-1.734655000	-0.000073000
1	3.343169000	-1.843955000	0.000034000	1	5.249343000	1.221555000	0.000023000
1	4.182140000	1.134273000	0.000039000	6	-6.191165000	-0.224833000	-0.000091000
6	0.769783000	-1.109983000	0.000022000	6	-6.598131000	1.145451000	-0.000002000
1	0.967885000	-2.188064000	0.000021000	6	-4.772872000	-0.544737000	-0.000094000
6	-2.922325000	2.275872000	0.000047000	6	-5.598711000	2.167498000	0.000081000
6	-2.451847000	0.912872000	0.000027000	6	-3.810424000	0.501063000	-0.000009000
6	-4.254262000	2.564971000	0.000038000	6	-4.268204000	1.859791000	0.000078000
6	-3.419803000	-0.142496000	-0.000002000	6	-4.313877000	-1.902002000	-0.000182000
6	-5.249521000	1.523235000	0.000009000	6	-2.983489000	-2.212950000	-0.000187000
6	-4.813329000	0.160848000	-0.000011000	6	-1.986195000	-1.189009000	-0.000102000
1	-2.182371000	3.079899000	0.000069000	6	-2.396676000	0.179465000	-0.000011000
6	-1.088668000	0.595172000	0.000035000	6	-0.610068000	-1.510943000	-0.000105000
6	-2.979875000	-1.502426000	-0.000021000	6	0.383034000	-0.532256000	-0.000025000
6	-5.775770000	-0.897442000	-0.000039000	6	-1.370758000	1.166727000	0.000075000
6	-1.603917000	-1.772518000	-0.000011000	6	-0.035666000	0.830592000	0.000068000
6	-0.642877000	-0.742768000	0.000016000	6	-7.209406000	-1.214970000	-0.000172000
1	-0.365969000	1.413183000	0.000059000	6	-7.978021000	1.472005000	0.000002000
6	-3.971107000	-2.547360000	-0.000049000	1	-5.919434000	3.212005000	0.000148000
1	-1.269659000	-2.813474000	-0.000025000	1	-3.543557000	2.672725000	0.000142000
6	-6.627889000	1.796990000	-0.000001000	1	-5.039030000	-2.714405000	-0.000249000
6	-7.144523000	-0.573580000	-0.000048000	1	-2.663397000	-3.257512000	-0.000256000
6	-7.561917000	0.758235000	-0.000029000	1	-0.323944000	-2.566426000	-0.000175000
1	-4.592404000	3.604141000	0.000053000	1	-1.633610000	2.223748000	0.000151000
6	-5.303864000	-2.257474000	-0.000058000	1	0.708526000	1.628079000	0.000142000
1	-3.631385000	-3.585930000	-0.000064000	6	-8.549487000	-0.872018000	-0.000166000
1	-7.882280000	-1.379564000	-0.000070000	6	-8.942455000	0.483654000	-0.000078000
1	-8.629054000	0.990739000	-0.000036000	1	-6.944497000	-2.271681000	-0.000241000
1	-6.042950000	-3.062449000	-0.000080000	1	-8.265456000	2.526376000	0.000071000
1	-6.964432000	2.836519000	0.000014000	1	-9.307787000	-1.657862000	-0.000229000
				1	-10.002379000	0.746285000	-0.000074000
				6	1.781389000	-0.937844000	-0.000040000
				1	1.950864000	-2.020858000	-0.000079000
				1	2.766212000	0.955722000	0.000017000
D3 E(RB3LYP) = -1282.51961031 a. u.				D4 E(RB3LYP) = -1284.87655539 a. u.			
6	-6.352882000	-0.322303000	-0.106071000	6	2.175715000	-1.684803000	0.411130000
6	-7.562528000	0.302104000	0.059915000	6	3.142591000	-0.788259000	0.067276000

6	-7.655144000	1.685648000	0.407438000	6	4.541626000	-1.054968000	0.226446000
7	-7.691305000	2.815825000	0.690608000	6	7.987725000	0.306849000	-0.225184000
6	-8.801493000	-0.496077000	-0.131008000	6	7.812559000	1.613882000	-0.777353000
8	-8.824461000	-1.673772000	-0.426246000	7	7.631177000	2.674155000	-1.226373000
8	-9.919140000	0.238084000	0.061568000	1	2.506120000	-2.644132000	0.826801000
1	-10.667058000	-0.368899000	-0.085058000	1	4.818770000	-2.030442000	0.644524000
6	-2.591086000	0.119516000	-0.026486000	1	2.869436000	0.186100000	-0.349411000
1	-2.522185000	1.175067000	0.253920000	6	5.541296000	-0.182029000	-0.104986000
1	-6.409935000	-1.382407000	-0.372388000	6	6.920871000	-0.500016000	0.075447000
6	-3.907577000	-0.429484000	-0.155399000	1	5.286267000	0.796776000	-0.523651000
6	-5.065178000	0.275484000	0.034478000	1	7.180646000	-1.477734000	0.493269000
1	-3.982192000	-1.490139000	-0.424926000	6	9.357763000	-0.206672000	0.036618000
1	-5.013201000	1.335666000	0.302285000	8	9.607027000	-1.299990000	0.502441000
6	-1.460554000	-0.620542000	-0.218074000	8	10.313293000	0.685598000	-0.303744000
1	-1.611991000	-1.675422000	-0.460282000	1	11.164411000	0.259143000	-0.096288000
6	0.206769000	1.211996000	-0.215969000	6	-4.449710000	-0.243317000	-0.010606000
6	1.515883000	1.691524000	-0.186209000	6	-7.689924000	-1.814966000	-1.257312000
6	2.617150000	0.836411000	-0.094721000	6	-8.651230000	-1.031864000	-0.610715000
6	2.375125000	-0.575359000	-0.018923000	6	-8.239066000	0.019692000	0.213549000
6	1.021911000	-1.074589000	-0.033433000	6	-6.331104000	-1.554313000	-1.075029000
6	-0.085155000	-0.151470000	-0.147425000	6	-6.880536000	0.284431000	0.392480000
6	3.997048000	1.350753000	-0.077880000	6	-5.898229000	-0.506900000	-0.236509000
6	3.474277000	-1.496597000	0.079403000	1	-7.999876000	-2.626737000	-1.919602000
6	4.860871000	-0.984926000	0.080436000	1	-5.591877000	-2.152147000	-1.611743000
6	5.089980000	0.426743000	0.005193000	1	-6.572121000	1.106266000	1.040872000
6	5.965104000	-1.833986000	0.152683000	1	-8.980976000	0.639619000	0.722323000
6	3.200386000	-2.858971000	0.175716000	6	-4.051387000	1.180831000	0.203465000
6	1.882928000	-3.342673000	0.183889000	6	-3.419721000	1.580056000	1.394661000
6	0.816049000	-2.473931000	0.085014000	6	-4.332210000	2.158554000	-0.768285000
1	-0.194763000	-2.876973000	0.115174000	1	-3.212042000	0.833600000	2.163904000
1	1.705200000	-4.416214000	0.274357000	1	-4.836382000	1.866528000	-1.692163000
1	-0.605040000	1.931807000	-0.328695000	6	-3.063124000	2.914781000	1.600859000
6	4.280953000	2.715886000	-0.142240000	6	-3.963299000	3.490719000	-0.567483000
6	5.601812000	3.201984000	-0.130441000	1	-2.577751000	3.207155000	2.534932000
6	6.664200000	2.326355000	-0.055283000	1	-4.177411000	4.234126000	-1.338900000
6	6.436551000	0.926388000	0.013699000	6	-3.327579000	3.873613000	0.618066000
1	5.776041000	4.278619000	-0.182470000	6	-3.576231000	-1.287536000	0.042329000
1	7.692697000	2.694540000	-0.047270000	1	-9.714775000	-1.233692000	-0.756365000
6	7.284542000	-1.342050000	0.157693000	1	-3.045438000	4.916710000	0.777867000
1	8.117139000	-2.046175000	0.215515000	6	-2.112141000	-1.307939000	0.131069000
6	7.521732000	0.014077000	0.091080000	6	-1.266070000	-0.263408000	-0.313272000
1	8.541628000	0.405374000	0.096183000	6	-1.490457000	-2.472307000	0.631960000
1	3.471785000	3.442305000	-0.204121000	1	-1.701512000	0.637007000	-0.744129000
1	1.662139000	2.768349000	-0.254016000	1	-2.114077000	-3.306762000	0.962579000
1	5.824713000	-2.912781000	0.206383000	6	0.114016000	-0.371229000	-0.233751000
1	4.012922000	-3.579446000	0.256124000	6	-0.107650000	-2.575765000	0.722450000
				1	0.725266000	0.455878000	-0.599194000
				1	0.339604000	-3.487742000	1.126500000

				6	0.734735000	-1.526528000	0.296982000
				1	-4.022452000	-2.287016000	0.027097000
D5				D6			
E(RB3LYP) = -1262.81666934 a. u.				E(RB3LYP) = -996.053614721 a. u.			
6	6.566075000	-0.477895000	-0.168300000	6	3.815482000	-0.208996000	-0.025768000
6	7.729039000	0.177953000	0.148553000	6	3.327686000	-1.532485000	-0.133141000
6	7.722488000	1.471860000	0.755940000	6	2.846568000	0.826761000	0.061644000
7	7.677758000	2.526518000	1.250651000	1	3.168570000	1.861361000	0.180583000
6	9.020757000	-0.488692000	-0.154579000	1	4.017635000	-2.368792000	-0.233523000
8	9.129674000	-1.584287000	-0.667821000	6	1.490488000	0.554012000	0.046052000
8	10.084376000	0.263335000	0.206745000	6	1.962039000	-1.794746000	-0.141937000
1	10.872355000	-0.257650000	-0.031640000	1	0.792685000	1.389078000	0.131643000
6	2.782018000	-0.310637000	-0.119437000	1	1.626419000	-2.831298000	-0.234259000
1	2.629733000	0.671546000	0.338759000	6	0.998454000	-0.769535000	-0.057340000
1	6.699732000	-1.461653000	-0.629186000	7	5.178184000	0.084868000	0.035635000
6	4.136184000	-0.733810000	-0.307473000	6	5.693962000	1.247201000	-0.702330000
6	5.239112000	-0.002719000	0.044590000	6	6.986699000	1.781872000	-0.083927000
1	4.290789000	-1.717272000	-0.768252000	6	8.040446000	0.674734000	0.012624000
1	5.109025000	0.981395000	0.505978000	6	7.461033000	-0.529487000	0.759594000
6	1.711573000	-1.073124000	-0.485363000	6	6.144430000	-1.008894000	0.136193000
1	1.925572000	-2.046446000	-0.942992000	1	4.931881000	2.033931000	-0.724975000
7	-3.871877000	0.027046000	-0.015130000	1	5.884708000	0.956235000	-1.758956000
6	-5.966600000	-1.092449000	-0.636807000	1	7.354274000	2.623786000	-0.693735000
6	-4.806017000	-1.039988000	0.152284000	1	6.766668000	2.177464000	0.923347000
6	-6.889921000	-2.124458000	-0.458827000	1	8.949655000	1.042297000	0.515700000
1	-7.788542000	-2.153050000	-1.079162000	1	8.343652000	0.367571000	-1.005873000
6	-4.585157000	-2.037186000	1.117252000	1	8.175222000	-1.369421000	0.767739000
6	-6.663424000	-3.122524000	0.493974000	1	7.271439000	-0.253741000	1.811955000
1	-3.689969000	-1.993467000	1.739835000	1	5.716621000	-1.798020000	0.768563000
1	-7.384838000	-3.931202000	0.626840000	1	6.342228000	-1.456755000	-0.862926000
6	-5.505647000	-3.074278000	1.277322000	6	-0.411048000	-1.107965000	-0.077333000
1	-5.321990000	-3.842701000	2.031645000	6	-1.479658000	-0.261007000	-0.017239000
1	-6.140658000	-0.319312000	-1.386881000	6	-2.834270000	-0.719847000	-0.044047000
6	0.302071000	-0.757505000	-0.346416000	6	-3.937059000	0.090765000	0.013521000
6	-0.663060000	-1.679284000	-0.808959000	6	-5.263653000	-0.428050000	-0.017445000
6	-0.181662000	0.437891000	0.235192000	6	-6.427507000	0.298307000	0.033979000
1	-0.327465000	-2.610552000	-1.272817000	6	-6.421096000	1.724466000	0.128482000
1	0.520176000	1.177590000	0.624455000	7	-6.376220000	2.886927000	0.205257000
6	-2.025701000	-1.430994000	-0.710066000	6	-7.718267000	-0.432618000	-0.011005000
6	-1.539129000	0.693937000	0.346645000	8	-7.827863000	-1.640068000	-0.090843000
1	-2.739322000	-2.161601000	-1.091436000	8	-8.782965000	0.399019000	0.047059000
1	-1.876950000	1.619294000	0.813781000	1	-9.569872000	-0.174133000	0.011233000
6	-2.495022000	-0.235071000	-0.127074000	1	-0.628874000	-2.180430000	-0.150521000
6	-4.366966000	1.365014000	-0.077112000	1	-1.324128000	0.820045000	0.054181000
6	-5.300125000	1.816170000	0.870679000	1	-2.990848000	-1.803354000	-0.116340000
6	-3.941268000	2.238108000	-1.092386000	1	-3.806007000	1.175189000	0.085909000
1	-5.632255000	1.140294000	1.660330000	1	-5.397423000	-1.512114000	-0.089179000

1	-3.224925000	1.887632000	-1.837312000				
6	-5.798768000	3.118157000	0.799385000				
6	-4.432757000	3.543606000	-1.146293000				
1	-6.523889000	3.456248000	1.543041000				
1	-4.093261000	4.212077000	-1.940681000				
6	-5.365427000	3.989922000	-0.204497000				
1	-5.752882000	5.009468000	-0.253704000				
D7				D8			
E(RB3LYP) = -878.115992511 a. u.				E(RB3LYP) = -1034.17795001 a. u.			
6	3.858251000	-0.501190000	0.002920000	6	3.505307000	2.492622000	0.210469000
6	5.096803000	0.091856000	0.011604000	6	3.059057000	1.053307000	0.084992000
6	5.250531000	1.512796000	0.011052000	6	4.822656000	2.700170000	-0.538801000
7	5.336423000	2.675523000	0.010489000	6	4.049923000	0.028850000	-0.003955000
6	6.296921000	-0.780301000	0.022032000	6	5.872420000	1.728526000	-0.010921000
8	6.270652000	-1.995206000	0.023724000	7	5.392634000	0.349102000	0.019008000
8	7.448685000	-0.071409000	0.029747000	1	3.651006000	2.752134000	1.276296000
1	8.165796000	-0.730706000	0.036113000	6	1.715800000	0.714631000	0.045554000
6	0.116881000	0.086029000	-0.025090000	6	3.629258000	-1.327066000	-0.115670000
1	0.083222000	1.179976000	-0.028535000	6	6.438933000	-0.668934000	0.068355000
1	3.869540000	-1.595791000	0.004616000	6	2.272319000	-1.620112000	-0.121193000
6	1.411462000	-0.521036000	-0.014920000	6	1.273269000	-0.624844000	-0.049992000
6	2.598556000	0.163426000	-0.007686000	1	0.983439000	1.523421000	0.100926000
1	1.446337000	-1.617681000	-0.012499000	6	4.674654000	-2.415212000	-0.212391000
1	2.589687000	1.258094000	-0.009830000	1	1.967014000	-2.668526000	-0.193291000
6	-3.467832000	-1.100243000	-0.049618000	1	5.193863000	3.729876000	-0.419595000
6	-4.782977000	-0.677792000	-0.049817000	6	5.923329000	-2.011982000	0.574162000
6	-5.087068000	0.701241000	-0.048755000	1	4.264953000	-3.367749000	0.158010000
6	-4.061683000	1.659322000	-0.043160000	1	5.676401000	-1.933786000	1.646755000
6	-2.741115000	1.219376000	-0.039302000	1	6.195913000	2.035350000	1.005174000
6	-2.406244000	-0.155781000	-0.040718000	1	7.242273000	-0.299322000	0.729645000
6	-6.088869000	-1.445826000	-0.099052000	1	2.722458000	3.166157000	-0.170915000
6	-7.124346000	-0.363983000	0.293704000	1	4.666844000	2.528080000	-1.617545000
7	-6.458039000	0.895450000	-0.084808000	1	6.721339000	-2.763948000	0.473530000
1	-3.231074000	-2.168085000	-0.048721000	1	4.952139000	-2.583276000	-1.270387000
1	-4.289720000	2.727367000	-0.038954000	1	6.773147000	1.761746000	-0.648875000
1	-1.945132000	1.965902000	-0.028430000	1	6.891596000	-0.791037000	-0.937393000
1	-6.279120000	-1.807119000	-1.125365000	6	-0.119900000	-1.011045000	-0.076556000
1	-7.323024000	-0.396175000	1.383030000	6	-1.222739000	-0.204891000	-0.014309000
1	-6.829348000	1.759782000	0.296453000	6	-2.556025000	-0.714111000	-0.050425000
1	-8.083081000	-0.474828000	-0.233329000	6	-3.692986000	0.051402000	0.009172000
1	-6.120744000	-2.317457000	0.570430000	6	-4.995326000	-0.519347000	-0.031526000
6	-1.039244000	-0.640352000	-0.030632000	6	-6.190688000	0.157523000	0.021388000
1	-0.936882000	-1.732425000	-0.027877000	6	-6.243679000	1.581458000	0.128487000
				7	-6.246083000	2.744237000	0.216030000
				6	-7.447825000	-0.625289000	-0.035308000
				8	-7.508867000	-1.836051000	-0.126138000

				8	-8.548409000	0.159949000	0.025598000
				1	-9.308386000	-0.447722000	-0.018717000
				1	-2.670323000	-1.802405000	-0.132196000
				1	-3.605491000	1.139558000	0.090956000
				1	-5.084440000	-1.607363000	-0.113162000
				1	-0.299603000	-2.090255000	-0.156521000
				1	-1.108336000	0.880587000	0.067163000
D9				D10			
E(RB3LYP) = -1030.57760506 a. u.				E(RB3LYP) = -1507.38398515 a. u.			
6	-5.150890000	-0.476250000	0.000073000	6	-5.150890000	-0.476250000	0.000073000
6	-6.364139000	0.162248000	0.000082000	6	-6.364139000	0.162248000	0.000082000
6	-6.465597000	1.588293000	0.000079000	6	-6.465597000	1.588293000	0.000079000
7	-6.510395000	2.753065000	0.000064000	7	-6.510395000	2.753065000	0.000064000
6	-7.598148000	-0.665882000	0.000100000	6	-7.598148000	-0.665882000	0.000100000
8	-7.614119000	-1.880162000	-0.000040000	8	-7.614119000	-1.880162000	-0.000040000
8	-8.720420000	0.086325000	-0.000064000	8	-8.720420000	0.086325000	-0.000064000
1	-9.464481000	-0.542732000	-0.000170000	1	-9.464481000	-0.542732000	-0.000170000
6	-1.389875000	-0.012716000	0.000050000	6	-1.389875000	-0.012716000	0.000050000
1	-1.322073000	1.079252000	0.000042000	1	-1.322073000	1.079252000	0.000042000
1	-5.201575000	-1.569604000	0.000078000	1	-5.201575000	-1.569604000	0.000078000
6	-2.706010000	-0.580125000	0.000061000	6	-2.706010000	-0.580125000	0.000061000
6	-3.866016000	0.144728000	0.000065000	6	-3.866016000	0.144728000	0.000065000
1	-2.776500000	-1.674789000	0.000066000	1	-2.776500000	-1.674789000	0.000066000
1	-3.819306000	1.238379000	0.000060000	1	-3.819306000	1.238379000	0.000060000
6	2.141065000	-1.296694000	-0.000029000	6	2.141065000	-1.296694000	-0.000029000
6	3.471949000	-0.882467000	-0.000046000	6	3.471949000	-0.882467000	-0.000046000
6	3.830269000	0.495580000	0.000004000	6	3.830269000	0.495580000	0.000004000
6	2.809130000	1.461474000	0.000073000	6	2.809130000	1.461474000	0.000073000
6	1.482493000	1.056426000	0.000088000	6	1.482493000	1.056426000	0.000088000
6	1.123915000	-0.321011000	0.000036000	6	1.123915000	-0.321011000	0.000036000
7	4.633398000	-1.637992000	-0.000106000	7	4.633398000	-1.637992000	-0.000106000
6	5.276441000	0.551186000	-0.000029000	6	5.276441000	0.551186000	-0.000029000
1	1.880932000	-2.358040000	-0.000067000	1	1.880932000	-2.358040000	-0.000067000
1	3.055605000	2.525319000	0.000117000	1	3.055605000	2.525319000	0.000117000
1	0.698833000	1.814528000	0.000148000	1	0.698833000	1.814528000	0.000148000
6	-0.259826000	-0.773559000	0.000046000	6	-0.259826000	-0.773559000	0.000046000
1	-0.391869000	-1.862077000	0.000047000	1	-0.391869000	-1.862077000	0.000047000
6	7.098987000	-1.112258000	-0.000146000	6	7.098987000	-1.112258000	-0.000146000
6	8.006610000	-0.053540000	-0.000124000	6	8.006610000	-0.053540000	-0.000124000
6	5.735427000	-0.797089000	-0.000098000	6	5.735427000	-0.797089000	-0.000098000
1	9.077112000	-0.269904000	-0.000160000	1	9.077112000	-0.269904000	-0.000160000
6	7.572001000	1.287401000	-0.000056000	6	7.572001000	1.287401000	-0.000056000
1	8.311340000	2.090556000	-0.000040000	1	8.311340000	2.090556000	-0.000040000
6	6.213990000	1.596523000	-0.000008000	6	6.213990000	1.596523000	-0.000008000
1	5.882461000	2.637194000	0.000045000	1	5.882461000	2.637194000	0.000045000
1	7.442272000	-2.149058000	-0.000199000	1	7.442272000	-2.149058000	-0.000199000
1	4.671876000	-2.647449000	-0.000154000	1	4.671876000	-2.647449000	-0.000154000

D11				D12			
E(RB3LYP) = -1374.72894027 a. u.				E(RB3LYP) = -1321.75730925 a. u.			
6	1.426491000	0.911924000	0.052172000	6	-4.619649000	-1.222007000	-0.077868000
6	1.919649000	2.265903000	0.096509000	6	-7.117522000	-1.148036000	0.018450000
6	3.266429000	2.562513000	0.065414000	6	-7.288144000	-2.525696000	-0.319059000
6	4.212444000	1.469517000	0.030051000	7	-7.388113000	-3.653912000	-0.596735000
7	3.704519000	0.172688000	-0.000699000	6	-8.304389000	-0.297718000	0.266811000
6	2.370416000	-0.144955000	-0.016636000	8	-8.266491000	0.882450000	0.557931000
6	2.007107000	-1.510612000	-0.100976000	8	-9.466494000	-0.979694000	0.134565000
6	3.054618000	-2.499409000	-0.126566000	1	-10.172114000	-0.333602000	0.317159000
6	4.390323000	-2.158911000	-0.062914000	6	-0.966462000	-0.434761000	0.003326000
6	4.742353000	-0.758168000	-0.012337000	1	-1.034903000	0.625532000	0.266399000
1	1.182554000	3.067600000	0.118618000	1	-4.618390000	-2.284039000	-0.343430000
1	2.756812000	-3.546624000	-0.161221000	6	-2.137921000	-1.138490000	-0.135773000
6	5.933967000	-0.022642000	0.002896000	6	-3.424204000	-0.556934000	0.051491000
6	5.607507000	1.348045000	0.047343000	1	-2.094060000	-2.200233000	-0.404384000
6	0.632388000	-1.803090000	-0.119097000	1	-3.453774000	0.506922000	0.319025000
6	0.067379000	0.562875000	0.037311000	6	1.541070000	-0.337336000	-0.069290000
6	-0.341188000	-0.785268000	-0.049541000	6	4.060461000	-3.117351000	0.578589000
1	0.313742000	-2.846162000	-0.183231000	6	5.251656000	-2.605781000	0.000460000
1	-0.674309000	1.361036000	0.088261000	6	5.181831000	-1.313158000	-0.579655000
1	6.934971000	-0.441222000	-0.030025000	6	2.882945000	-2.382554000	0.561555000
1	6.312318000	2.171891000	0.101170000	6	3.996456000	-0.589231000	-0.578208000
7	5.434789000	-3.101373000	-0.101532000	6	2.803655000	-1.098615000	-0.020884000
7	3.774374000	3.873236000	0.124216000	1	4.057451000	-4.093595000	1.061198000
6	6.348785000	-3.124233000	1.041924000	1	2.000859000	-2.806314000	1.045653000
1	6.555276000	-2.108520000	1.396700000	1	3.986136000	0.395959000	-1.047392000
1	5.927920000	-3.703059000	1.891015000	1	6.061179000	-0.869609000	-1.044456000
1	7.300711000	-3.593606000	0.745861000	6	1.617003000	1.142858000	-0.054451000
6	5.099010000	-4.441546000	-0.551546000	6	0.899657000	1.937400000	-0.970417000
1	6.032919000	-4.993449000	-0.739144000	6	2.422575000	1.825791000	0.879445000
1	4.509973000	-5.023327000	0.189942000	1	0.295914000	1.450219000	-1.738795000
1	4.529527000	-4.394831000	-1.490698000	1	2.999556000	1.250178000	1.606338000
6	2.861578000	4.917246000	0.558772000	6	0.963918000	3.326888000	-0.952960000
1	2.351004000	4.613937000	1.483833000	6	2.486385000	3.213111000	0.924105000
1	3.443523000	5.828375000	0.766365000	1	0.400700000	3.882982000	-1.700975000
1	2.092474000	5.177169000	-0.200057000	1	3.110178000	3.681233000	1.684235000
6	4.609414000	4.311804000	-0.995510000	6	1.754501000	4.009834000	0.005565000
1	5.242541000	5.155587000	-0.677232000	7	6.425114000	-3.330296000	0.009941000
1	5.257659000	3.498996000	-1.340851000	7	1.816246000	5.388236000	0.039064000
1	3.994865000	4.647342000	-1.857320000	6	6.455182000	-4.663499000	0.583200000
6	-6.619488000	-0.685228000	-0.025139000	1	7.464612000	-5.079714000	0.476117000
6	-7.806284000	0.000436000	0.023388000	1	6.203545000	-4.658395000	1.659800000
6	-7.849453000	1.426168000	0.119607000	1	5.749989000	-5.348474000	0.077461000
7	-7.845664000	2.589224000	0.197997000	6	7.628284000	-2.776773000	-0.583467000
6	-9.072438000	-0.774708000	-0.026605000	1	7.507452000	-2.579357000	-1.664986000

8	-9.139020000	-1.984716000	-0.108042000	1	7.927277000	-1.828128000	-0.101384000
8	-10.163824000	0.020540000	0.028955000	1	8.452558000	-3.490373000	-0.460933000
1	-10.932010000	-0.577411000	-0.009979000	6	2.644474000	6.057481000	1.024633000
6	-1.744964000	-1.180916000	-0.071514000	1	2.330009000	5.826381000	2.059430000
6	-2.842322000	-0.376874000	-0.013441000	1	3.710298000	5.779211000	0.928907000
1	-1.919967000	-2.260760000	-0.143965000	1	2.566893000	7.142849000	0.884147000
1	-2.729383000	0.709000000	0.060091000	6	1.043278000	6.174857000	-0.904017000
1	-6.714674000	-1.773192000	-0.098385000	1	-0.041194000	5.978165000	-0.816958000
6	-4.180919000	-0.888486000	-0.044457000	1	1.208775000	7.241221000	-0.705968000
6	-5.310585000	-0.118790000	0.010419000	1	1.336425000	5.975331000	-1.951555000
1	-4.296054000	-1.976932000	-0.117966000	6	0.334883000	-1.005145000	-0.140252000
1	-5.219057000	0.969576000	0.083880000	1	0.365722000	-2.087781000	-0.296315000
				6	-5.869860000	-0.577116000	0.121855000
				1	-5.870313000	0.485090000	0.386702000
D13							
E(RB3LYP) = -1456.22331650 a. u.							
8	1.546085000	-2.144786000	-0.026382000				
8	-0.208643000	-3.501374000	-0.065841000				
6	3.892967000	-3.134343000	1.228148000				
6	4.374720000	-2.900020000	-1.237126000				
6	-0.686928000	-1.154253000	-0.012422000				
6	-0.076860000	0.083164000	0.018539000				
6	2.144827000	-0.917126000	0.022412000				
6	4.385103000	-2.166476000	0.123549000				
6	-2.113981000	-1.392550000	-0.024662000				
6	0.163924000	-2.351880000	-0.036124000				
6	1.331314000	0.239214000	0.030560000				
6	3.543871000	-0.874745000	0.042623000				
6	5.826552000	-1.782037000	0.514776000				
6	-3.110826000	-0.460319000	-0.008039000				
6	1.977086000	1.494895000	0.059765000				
6	4.154626000	0.420254000	-0.044350000				
6	6.374603000	-0.631869000	-0.302437000				
6	-4.496881000	-0.812038000	-0.023352000				
6	3.348809000	1.618243000	0.029440000				
6	-7.990358000	0.511723000	-0.011484000				
6	4.035843000	2.985811000	0.089452000				
6	6.193850000	1.799767000	-0.498599000				
6	-7.857507000	1.934496000	0.021740000				
6	3.121088000	4.137281000	-0.359631000				
6	4.504389000	3.261846000	1.538500000				
6	5.237238000	2.918112000	-0.872946000				
7	5.516454000	0.540226000	-0.194560000				
7	-7.708323000	3.090472000	0.048912000				
1	4.653023000	-3.918922000	1.379581000				
1	3.350258000	-3.181191000	-1.519044000				
1	3.763516000	-2.605547000	2.186299000				

1	-2.389962000	-2.450575000	-0.050779000
1	6.482716000	-2.659324000	0.400591000
1	4.786772000	-2.275590000	-2.045656000
1	4.976215000	-3.823026000	-1.177079000
1	2.947323000	-3.623081000	0.972250000
1	-0.688642000	0.989210000	0.035818000
1	5.848497000	-1.497016000	1.580570000
1	-4.737637000	-1.881687000	-0.049298000
1	6.497130000	-0.916611000	-1.366628000
1	7.374713000	-0.349231000	0.064577000
1	-2.873799000	0.608759000	0.017936000
1	2.717517000	3.965240000	-1.369832000
1	6.893545000	1.615442000	-1.332814000
1	5.127641000	2.447593000	1.938030000
1	2.275101000	4.290055000	0.327484000
1	3.635344000	3.364994000	2.206747000
1	6.816798000	2.093048000	0.367739000
1	4.859783000	2.760830000	-1.897432000
1	5.789426000	3.871934000	-0.872833000
1	3.693293000	5.078642000	-0.378560000
1	5.087172000	4.197564000	1.589606000
1	1.349606000	2.385336000	0.101909000
6	-5.528789000	0.089063000	-0.007997000
6	-6.894846000	-0.315636000	-0.024562000
1	-5.307298000	1.160903000	0.017854000
1	-7.121619000	-1.386146000	-0.050319000
6	-9.341156000	-0.103175000	-0.032804000
8	-9.557068000	-1.298225000	-0.061271000
8	-10.327499000	0.821770000	-0.016795000
1	-11.162398000	0.320022000	-0.032678000

Table S5. Cartesian coordinates (in Angstrom unit) of B3LYP/cc-pVDZ optimized geometries of methyl substituted pyrene based D- π -A systems (D1 - D1-5).

D1 E(RB3LYP) = -1128.88061604 a. u.				D1-1 E(RB3LYP) = -1262.85188298 a. u.			
6	-5.631681000	-0.482865000	-0.000105000	6	-6.762189000	-0.383642000	0.006482000
6	-6.794734000	0.241399000	-0.000129000	6	-7.905268000	0.374028000	0.006218000
6	-6.793117000	1.671269000	-0.000135000	6	-7.862434000	1.803000000	0.001159000
7	-6.752212000	2.836088000	-0.000124000	7	-7.788867000	2.966352000	-0.003119000
6	-8.086342000	-0.495871000	-0.000157000	6	-9.216092000	-0.325192000	0.011387000
8	-8.188653000	-1.705544000	0.000225000	8	-9.355166000	-1.531692000	0.015919000
8	-9.150346000	0.335805000	0.000269000	8	-10.257291000	0.536284000	0.010520000
1	-9.938994000	-0.236398000	0.000559000	1	-11.060393000	-0.015285000	0.014116000
				6	-2.973608000	-0.301479000	-0.001536000

6	-1.846280000	-0.278424000	-0.000063000	1	-2.796856000	0.778444000	-0.005701000
1	-1.707236000	0.807036000	-0.000065000	1	-6.922837000	-1.466340000	0.010597000
1	-5.760029000	-1.569833000	-0.000103000	6	-4.340083000	-0.733616000	0.002723000
6	-3.199221000	-0.756964000	-0.000078000	6	-5.421498000	0.104351000	0.002009000
6	-4.304933000	0.046358000	-0.000095000	1	-4.520012000	-1.815691000	0.006862000
1	-3.343370000	-1.844256000	-0.000074000	1	-5.264780000	1.187756000	-0.002093000
1	-4.182212000	1.134176000	-0.000099000	6	-1.925177000	-1.170957000	-0.000601000
6	-0.769845000	-1.110347000	-0.000045000	1	-2.162778000	-2.241249000	0.003469000
1	-0.967903000	-2.188482000	-0.000041000	6	2.763542000	-2.778194000	-0.004272000
6	2.922143000	2.275858000	-0.000039000	6	1.805555000	-1.701921000	-0.006948000
6	2.451741000	0.912775000	-0.000026000	6	4.105544000	-2.534432000	-0.007215000
6	4.254119000	2.565074000	-0.000022000	6	2.295583000	-0.358609000	-0.012555000
6	3.419827000	-0.142561000	0.000006000	6	4.626893000	-1.189758000	-0.014949000
6	5.249504000	1.523385000	0.000010000	6	3.694713000	-0.107240000	-0.017060000
6	4.813388000	0.160905000	0.000023000	1	2.390481000	-3.805507000	0.000533000
1	2.182095000	3.079863000	-0.000063000	6	0.421911000	-1.921464000	-0.003305000
6	1.088528000	0.594958000	-0.000043000	6	1.366290000	0.731759000	-0.012461000
6	2.979979000	-1.502588000	0.000019000	6	4.192215000	1.231877000	-0.020240000
6	5.775958000	-0.897353000	0.000055000	6	-0.006479000	0.464797000	-0.008735000
6	1.603981000	-1.772801000	0.000001000	6	-0.502512000	-0.856864000	-0.004442000
6	0.642841000	-0.743068000	-0.000029000	1	0.049358000	-2.949589000	0.000814000
1	0.365697000	1.412926000	-0.000067000	6	1.892827000	2.074776000	-0.015182000
6	3.971334000	-2.547476000	0.000051000	1	-0.699211000	1.308621000	-0.008759000
1	1.269779000	-2.813825000	0.000011000	6	6.002756000	-0.925906000	-0.017576000
6	6.627908000	1.797261000	0.000027000	6	5.572681000	1.463069000	-0.022757000
6	7.144748000	-0.573375000	0.000072000	6	6.506073000	0.397172000	-0.030927000
6	7.562059000	0.758529000	0.000058000	1	4.814735000	-3.366162000	-0.004787000
1	4.592199000	3.604314000	-0.000033000	6	3.234966000	2.312124000	-0.017958000
6	5.304132000	-2.257467000	0.000068000	1	1.186150000	2.908494000	-0.014619000
1	3.631680000	-3.586116000	0.000061000	1	5.916387000	2.496489000	-0.020323000
1	7.882603000	-1.379336000	0.000095000	1	3.610980000	3.338441000	-0.019648000
1	8.629227000	0.991128000	0.000072000	1	6.684405000	-1.775265000	-0.010924000
1	6.043315000	-3.062419000	0.000091000	7	7.868009000	0.642801000	-0.053674000
1	6.964397000	2.836860000	0.000017000	6	8.804523000	-0.459315000	0.067798000
				1	8.698737000	-1.006526000	1.024855000
				1	8.679609000	-1.188842000	-0.751100000
				1	9.828541000	-0.069406000	0.010278000
				6	8.361528000	2.002548000	0.066480000
				1	9.457336000	1.993604000	0.011063000
				1	7.992140000	2.641715000	-0.754114000
				1	8.070119000	2.480024000	1.022286000
D1-2 E(RB3LYP) = -1262.84625813 a. u.				D1-3 E(RB3LYP) = -1262.84706555 a. u.			
6	6.622273000	-0.608625000	-0.010164000	6	-6.347221000	-0.632968000	-0.013979000
6	7.822156000	0.051297000	0.042710000	6	-7.576897000	-0.029392000	0.027632000
6	7.896009000	1.476644000	0.128106000	6	-7.717592000	1.391564000	0.101180000
7	7.917683000	2.639950000	0.197420000	7	-7.793803000	2.553106000	0.160993000

6	9.072638000	-0.752278000	0.009205000	6	-8.788271000	-0.890712000	-0.005427000
8	9.111696000	-1.963688000	-0.062048000	8	-8.770432000	-2.103174000	-0.067097000
8	10.179359000	0.019926000	0.067355000	8	-9.930148000	-0.170646000	0.041170000
1	10.936162000	-0.593115000	0.039513000	1	-10.657315000	-0.818618000	0.014659000
6	2.852935000	-0.207933000	-0.031832000	6	-2.600395000	-0.058499000	-0.017999000
1	2.768260000	0.881198000	0.031975000	1	-2.566006000	1.033850000	0.037177000
1	6.693416000	-1.698962000	-0.073995000	1	-6.367155000	-1.725907000	-0.069371000
6	4.179444000	-0.754319000	-0.047735000	6	-3.900189000	-0.665379000	-0.037323000
6	5.325374000	-0.011249000	0.010130000	6	-5.079687000	0.024220000	0.008162000
1	4.267853000	-1.845730000	-0.111430000	1	-3.937804000	-1.760191000	-0.092584000
1	5.259142000	1.079564000	0.073993000	1	-5.064483000	1.117398000	0.063534000
6	1.736087000	-0.982843000	-0.091963000	6	-1.448884000	-0.782032000	-0.064448000
1	1.880356000	-2.067805000	-0.153276000	1	-1.543588000	-1.872865000	-0.118094000
6	-1.776088000	2.583628000	0.033239000	6	1.909799000	2.930813000	0.062679000
6	-1.380471000	1.198165000	-0.017435000	6	1.567528000	1.531518000	0.016956000
6	-3.091286000	2.940241000	0.024098000	6	3.209641000	3.338880000	0.040677000
6	-2.402200000	0.194055000	-0.070663000	6	2.628414000	0.572435000	-0.027636000
6	-4.136599000	1.952383000	-0.021430000	6	4.295563000	2.394126000	-0.022621000
6	-3.781463000	0.566708000	-0.057178000	6	3.990838000	0.994948000	-0.033520000
1	-0.994623000	3.346178000	0.073362000	1	1.100051000	3.663272000	0.105587000
6	-0.035257000	0.811387000	-0.021648000	6	0.238556000	1.090070000	0.007595000
6	-2.027889000	-1.183054000	-0.145365000	6	2.321393000	-0.819852000	-0.087702000
6	-4.795522000	-0.440926000	-0.096044000	6	5.049648000	0.033436000	-0.085886000
6	-0.666664000	-1.523561000	-0.149618000	6	0.975756000	-1.216578000	-0.100428000
6	0.343806000	-0.545833000	-0.084796000	6	-0.077870000	-0.282399000	-0.051047000
1	0.727265000	1.591293000	0.021027000	1	-0.557034000	1.836468000	0.042177000
6	-3.069339000	-2.169680000	-0.241935000	6	3.398401000	-1.770888000	-0.096458000
1	-0.386385000	-2.578741000	-0.207853000	1	0.739172000	-2.283113000	-0.145325000
6	-5.496920000	2.293049000	-0.038979000	6	5.637368000	2.804523000	-0.093405000
6	-6.165522000	-0.056461000	-0.045944000	6	6.372578000	0.495466000	-0.203852000
6	-6.486800000	1.310732000	-0.044538000	6	6.659802000	1.862222000	-0.201596000
1	-3.377400000	3.994664000	0.054654000	1	3.453467000	4.403955000	0.063140000
6	-4.387143000	-1.814454000	-0.223704000	6	4.716232000	-1.387426000	-0.066154000
1	-2.784039000	-3.219007000	-0.350855000	1	3.135343000	-2.829417000	-0.095234000
1	-7.532829000	1.617597000	-0.023438000	1	7.696265000	2.194365000	-0.293887000
1	-5.163146000	-2.571005000	-0.338296000	1	5.869826000	3.872172000	-0.085187000
1	-5.783297000	3.347658000	-0.024981000	1	7.175203000	-0.231326000	-0.324211000
7	-7.164579000	-1.068296000	-0.015443000	7	5.788612000	-2.318940000	-0.057540000
6	-8.464864000	-0.719594000	-0.568681000	6	6.505992000	-2.413949000	1.217589000
1	-8.341048000	-0.232802000	-1.546551000	1	5.926258000	-2.980519000	1.977204000
1	-9.046331000	-1.643863000	-0.714920000	1	7.466735000	-2.930991000	1.062468000
1	-9.067164000	-0.051594000	0.084842000	1	6.711343000	-1.415078000	1.622561000
6	-7.295821000	-1.764161000	1.267333000	6	5.510350000	-3.637510000	-0.606231000
1	-7.806136000	-1.139445000	2.031715000	1	5.017586000	-3.542243000	-1.584263000
1	-7.886224000	-2.684366000	1.127976000	1	6.464460000	-4.169503000	-0.747353000
1	-6.309253000	-2.043125000	1.659210000	1	4.873525000	-4.270135000	0.049710000
D1-4				D1-5			

E(RB3LYP) = -1262.84720296 a. u.				E(RB3LYP) = -1262.83864351 a. u.			
6	6.041051000	0.398660000	-0.081922000	6	-5.764501000	0.159237000	-0.000008000
6	7.257360000	-0.230825000	-0.031682000	6	-6.938315000	-0.548614000	0.000111000
6	7.367129000	-1.650035000	0.102845000	6	-6.956666000	-1.978263000	0.000433000
7	7.417947000	-2.809261000	0.213210000	7	-6.932934000	-3.143630000	0.000511000
6	8.487126000	0.599930000	-0.120680000	6	-8.218708000	0.206329000	-0.000093000
8	8.495529000	1.808621000	-0.235524000	8	-8.305236000	1.417517000	-0.000312000
8	9.613092000	-0.143684000	-0.059563000	8	-9.295062000	-0.610105000	0.000043000
1	10.354177000	0.485427000	-0.125576000	1	-10.074690000	-0.025744000	-0.000089000
6	2.282774000	-0.088938000	-0.004420000	6	-1.981791000	-0.089343000	-0.000021000
1	2.225151000	-1.176844000	0.099082000	1	-1.857870000	-1.176835000	0.000285000
1	6.084677000	1.487345000	-0.186040000	1	-5.878052000	1.247858000	-0.000217000
6	3.595209000	0.486464000	-0.070055000	6	-3.329368000	0.403198000	-0.000086000
6	4.759640000	-0.227443000	-0.011851000	6	-4.445425000	-0.386789000	0.000127000
1	3.656259000	1.576641000	-0.174265000	1	-3.460034000	1.492108000	-0.000338000
1	4.720878000	-1.316502000	0.092036000	1	-4.336207000	-1.476042000	0.000393000
6	1.146815000	0.658089000	-0.064201000	6	-0.902294000	0.739857000	-0.000281000
1	1.263580000	1.743267000	-0.165962000	1	-1.077134000	1.818215000	-0.000453000
6	-2.287811000	-2.972570000	0.159700000	6	2.651229000	-2.753012000	-0.000433000
6	-1.919857000	-1.579464000	0.102732000	6	2.249804000	-1.368752000	-0.000345000
6	-3.592251000	-3.364366000	0.118826000	6	3.966460000	-3.107042000	-0.000295000
6	-2.961800000	-0.597313000	0.031596000	6	3.257779000	-0.353998000	-0.000170000
6	-4.659101000	-2.402902000	0.011784000	6	5.007077000	-2.111526000	-0.000066000
6	-4.324352000	-1.013555000	-0.027392000	6	4.636616000	-0.728754000	-0.000023000
1	-1.489292000	-3.715339000	0.228715000	1	1.871028000	-3.518068000	-0.000610000
6	-0.581905000	-1.169922000	0.097506000	6	0.906476000	-0.988365000	-0.000399000
6	-2.620378000	0.790753000	-0.013019000	6	2.876964000	1.027139000	-0.000108000
6	-5.354343000	-0.031282000	-0.145653000	6	5.653855000	0.275207000	0.000188000
6	-1.266306000	1.148740000	-0.064680000	6	1.503925000	1.381665000	-0.000165000
6	-0.234161000	0.190845000	-0.006150000	6	0.508409000	0.362295000	-0.000281000
1	0.195342000	-1.934396000	0.153234000	1	0.149127000	-1.774312000	-0.000615000
6	-3.690998000	1.781848000	-0.054500000	6	3.931874000	2.011660000	0.000093000
1	-1.009986000	2.202158000	-0.180883000	6	6.370203000	-2.453641000	0.000118000
6	-6.010790000	-2.781712000	-0.062256000	6	7.005490000	-0.114457000	0.000369000
6	-6.693275000	-0.458186000	-0.221555000	6	7.356593000	-1.464644000	0.000335000
6	-7.013288000	-1.816233000	-0.178044000	1	4.255880000	-4.160781000	-0.000344000
1	-3.851389000	-4.425321000	0.157511000	6	5.247997000	1.653294000	0.000225000
6	-4.993425000	1.359084000	-0.146289000	1	8.410564000	-1.751054000	0.000489000
1	-8.058927000	-2.126731000	-0.236370000	1	6.652730000	-3.509174000	0.000090000
1	-6.270073000	-3.842647000	-0.032217000	1	7.781008000	0.655295000	0.000533000
1	-7.486135000	0.288448000	-0.311010000	1	6.023723000	2.423158000	0.000357000
1	-5.803243000	2.088623000	-0.191684000	1	3.667675000	3.066780000	0.000125000
7	-3.321935000	3.154802000	-0.035701000	7	1.059087000	2.746059000	-0.000067000
6	-4.254045000	4.085781000	-0.654545000	6	1.226211000	3.506433000	1.230839000
1	-5.175959000	4.259044000	-0.058069000	1	2.249735000	3.906331000	1.394424000
1	-3.753599000	5.059792000	-0.773629000	1	0.533612000	4.365712000	1.222633000
1	-4.545692000	3.720674000	-1.649551000	1	0.970398000	2.874039000	2.093989000

6	-2.871010000	3.643445000	1.271194000	6	1.226965000	3.507120000	-1.230420000
1	-2.164605000	2.937292000	1.726168000	1	0.971855000	2.875228000	-2.094162000
1	-2.362374000	4.613116000	1.146756000	1	0.534271000	4.366324000	-1.222173000
1	-3.717893000	3.784295000	1.976140000	1	2.250532000	3.907262000	-1.393117000

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