

## Supporting Information

### Tuning the donating strength of dye sensitizers using molecular electrostatic potential analysis

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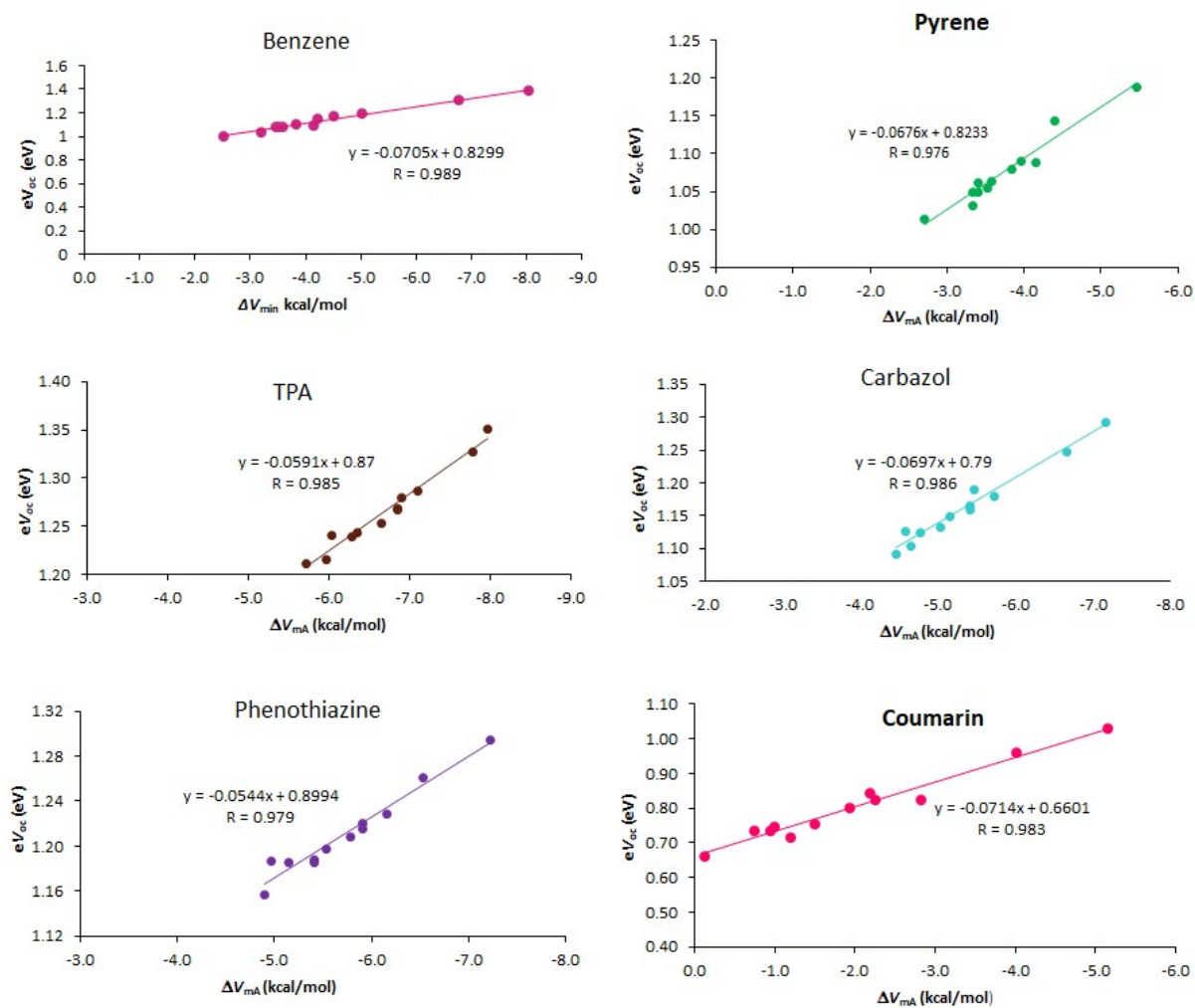
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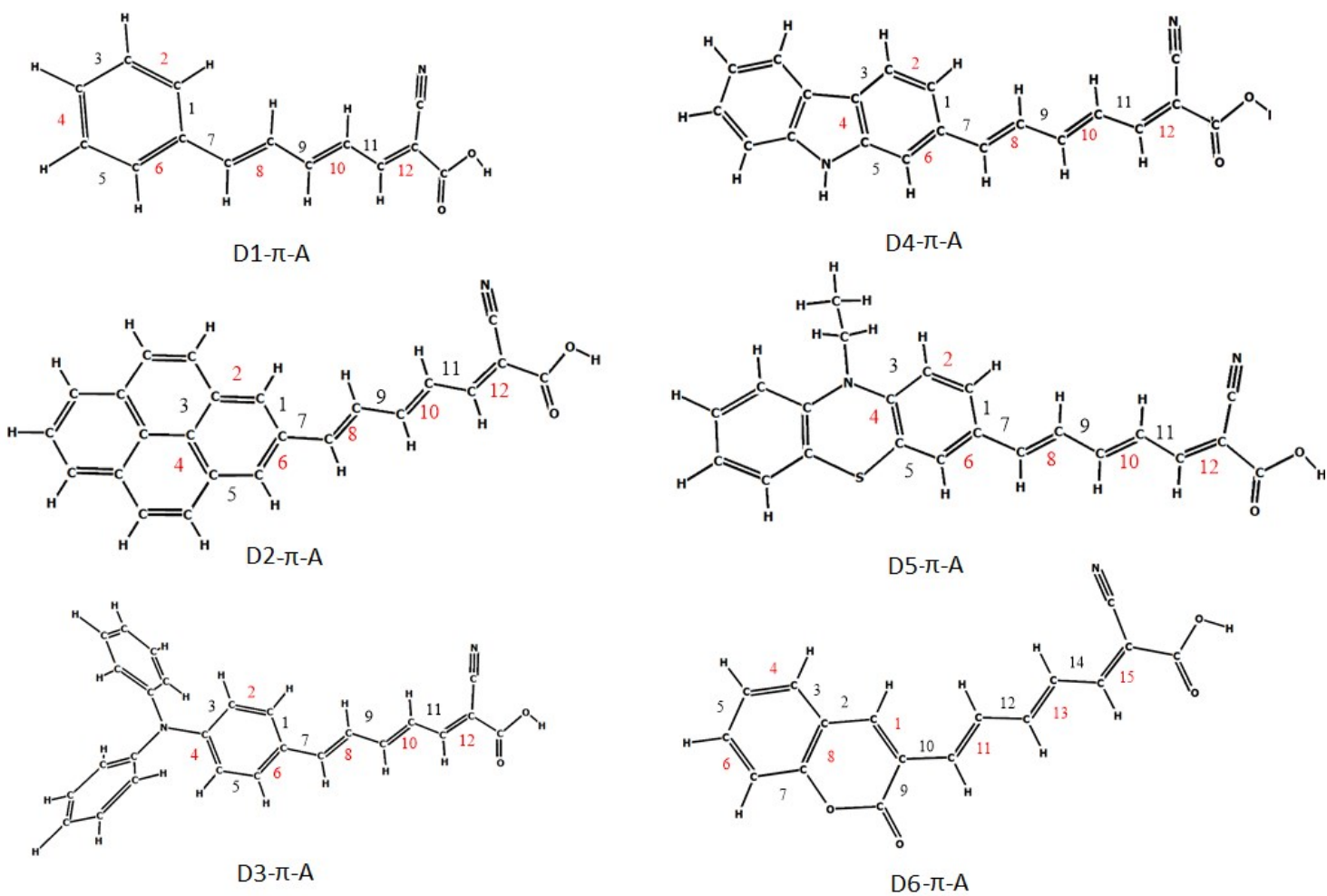
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**Fig. S1** Correlation between donating strength  $\Delta V_{mA}$  and open-circuit voltage  $eV_{OC}$  of six different D- $\pi$ -A systems.



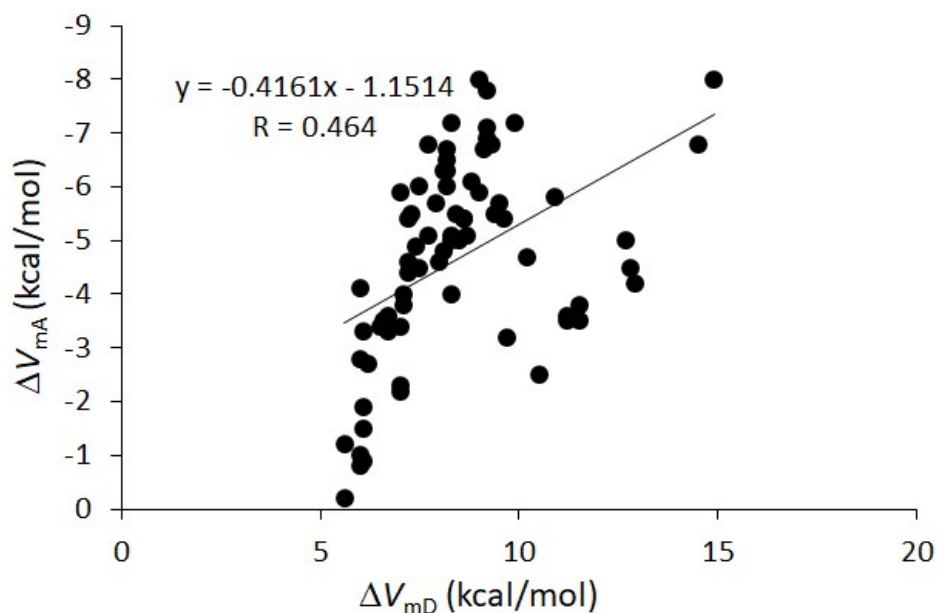
**Fig. S2** Labeled bonds employed to calculate the BLA index.

**Table S1.** BLA index for the unsubstituted D1 – D6- $\pi$ -A systems in ground state with B3LYP and CAM-B3LYP functional.

Bond	D1- $\pi$ -A		D2- $\pi$ -A		D3- $\pi$ -A		D4- $\pi$ -A		D5- $\pi$ -A		D6- $\pi$ -A	
	S0	S0	S0	S0	S0	S0	S0	S0	S0	S0	S0	S0
	B3LYP	CAM-B3LYP	B3LYP	CAM-B3LYP	B3LYP	CAM-B3LYP	B3LYP	CAM-B3LYP	B3LYP	CAM-B3LYP	B3LYP	CAM-B3LYP
BLA	0.039	0.046	0.039	0.043	0.035	0.046	0.036	0.048	0.034	0.045	0.035	0.039
1	1.413	1.404	1.410	1.400	1.415	1.405	1.423	1.415	1.409	1.399	1.37	1.357
2	1.392	1.388	1.400	1.397	1.386	1.383	1.387	1.383	1.389	1.386	1.432	1.436
3	1.401	1.395	1.432	1.420	1.415	1.406	1.406	1.399	1.414	1.406	1.413	1.405
4	1.398	1.391	1.429	1.423	1.411	1.402	1.424	1.413	1.417	1.408	1.388	1.383
5	1.395	1.39	1.402	1.394	1.389	1.386	1.394	1.392	1.391	1.387	1.406	1.401
6	1.411	1.402	1.409	1.402	1.412	1.402	1.409	1.399	1.412	1.402	1.393	1.387
7	1.460	1.464	1.460	1.464	1.451	1.457	1.456	1.461	1.452	1.458	1.397	1.392
8	1.360	1.347	1.360	1.348	1.364	1.35	1.362	1.349	1.363	1.349	1.411	1.400
9	1.435	1.422	1.435	1.422	1.431	1.439	1.433	1.441	1.432	1.440	1.482	1.479
10	1.366	1.353	1.367	1.353	1.369	1.355	1.368	1.354	1.369	1.354	1.454	1.459
11	1.429	1.435	1.428	1.435	1.425	1.432	1.427	1.434	1.426	1.433	1.361	1.347
12	1.370	1.356	1.370	1.356	1.372	1.358	1.371	1.357	1.372	1.357	1.435	1.422
13											1.367	1.352
14											1.429	1.436
15											1.369	1.356

**Table S2.** BLA index for the TPA (D3) based  $\pi$ -A systems in S0 and S1 states at CAM-B3LYP/cc-pVDZ level.

S0 equilibrium at CAM-B3LYP/cc-pVDZ			S1 equilibrium at CAM-B3LYP/cc-pVDZ		
Bond	BLA	D3	D3	D3-CH <sub>3</sub>	D3-OH
		0.046	0.010	0.011	0.011
1		1.405	1.428	1.426	1.428
2		1.383	1.373	1.372	1.373
3		1.406	1.415	1.418	1.414
4		1.402	1.418	1.415	1.417
5		1.386	1.372	1.373	1.373
6		1.402	1.426	1.428	1.425
7		1.457	1.421	1.421	1.423
8		1.35	1.39	1.389	1.388
9		1.439	1.404	1.404	1.405
10		1.355	1.390	1.390	1.389
11		1.432	1.403	1.404	1.404
12		1.358	1.388	1.388	1.388



**Fig S3.** Correlation between  $\Delta V_{mD}$  and  $\Delta V_{mA}$ .

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

D1				D1-CH <sub>3</sub>			
E(RB3LYP) = -232.262948971 a. u.				E(RB3LYP) = -271.580562370 a. u.			
6	-0.530780000	-1.293839000	0.000014000	6	-0.916742000	0.007349000	-0.000006000
6	-1.386158000	-0.187219000	-0.000006000	6	-0.190663000	1.206740000	-0.000017000
6	-0.855460000	1.106873000	-0.000003000	6	-0.199310000	-1.201254000	-0.000001000
6	0.530914000	1.293807000	0.000002000	1	-0.745235000	-2.149315000	0.000000000
6	1.386120000	0.187230000	0.000006000	1	-0.728108000	2.159197000	-0.000029000
6	0.855251000	-1.106740000	-0.000015000	6	1.196510000	-1.210145000	-0.000003000
1	-0.945685000	-2.304838000	0.000018000	6	1.208456000	1.203473000	-0.000018000
1	0.946155000	2.304609000	0.000005000	1	1.732849000	-2.162493000	-0.000003000
1	2.469058000	0.334029000	0.000010000	1	1.752142000	2.151559000	-0.000031000
1	-1.523211000	1.971707000	0.000000000	6	1.907847000	-0.005154000	-0.000011000
1	-2.468940000	-0.334619000	-0.000004000	6	-2.426946000	0.002909000	0.000039000
1	1.523301000	-1.971562000	-0.000011000	1	-2.826321000	-0.518121000	0.886613000
				1	-2.834159000	1.024917000	-0.000390000
				1	-2.826379000	-0.518906000	-0.886041000
				1	3.000309000	-0.010341000	-0.000016000

D1-C <sub>5</sub> H <sub>11</sub> E(RB3LYP) = -428.836629482 a. u.				D1-isopropyl E(RB3LYP) = -350.208210006 a. u.			
6	1.285641000	-0.338889000	-0.000128000	6	0.139830000	-0.195257000	-0.000164000
6	2.340282000	-1.269683000	0.000144000	6	-0.751023000	-1.278788000	-0.000476000
6	1.614293000	1.024190000	-0.000403000	6	-0.401689000	1.102144000	0.000288000
1	0.824895000	1.777331000	-0.000616000	1	0.264143000	1.969041000	0.000542000
1	2.107439000	-2.338828000	0.000367000	1	-0.353256000	-2.297804000	-0.000833000
6	2.950490000	1.443755000	-0.000407000	6	-1.783130000	1.306908000	0.000423000
6	3.672698000	-0.856831000	0.000140000	6	-2.135543000	-1.080036000	-0.000337000
1	3.179273000	2.512388000	-0.000621000	1	-2.179491000	2.325524000	0.000777000
1	4.471986000	-1.602106000	0.000358000	1	-2.807125000	-1.942294000	-0.000590000
6	3.985021000	0.507534000	-0.000136000	6	-2.657677000	0.215292000	0.000105000
6	-0.146225000	-0.849388000	-0.000153000	6	1.645512000	-0.427712000	-0.000247000
1	-0.278067000	-1.509590000	0.877389000	1	1.798557000	-1.521410000	-0.000906000
1	-0.278128000	-1.509352000	-0.877870000	6	2.312684000	0.130600000	1.269473000
6	-1.259948000	0.200625000	0.000023000	6	2.312871000	0.132145000	-1.269179000
1	-1.153905000	0.856134000	0.883564000	1	1.861395000	-0.293219000	-2.179449000
1	-1.154090000	0.856248000	-0.883455000	1	2.211048000	1.228948000	-1.326062000
6	-2.661313000	-0.419802000	0.000116000	1	3.390252000	-0.102642000	-1.278661000
1	-2.770126000	-1.078512000	0.882626000	1	2.210754000	1.227323000	1.327702000
1	-2.770286000	-1.078419000	-0.882444000	1	3.390082000	-0.104121000	1.278805000
6	-3.791206000	0.615261000	0.000273000	1	1.861117000	-0.295930000	2.179152000
1	-3.681424000	1.272763000	0.882510000	1	-3.738487000	0.374806000	0.000208000
1	-3.681589000	1.272852000	-0.881918000				
6	-5.187261000	-0.011659000	0.000372000				
1	-5.340699000	-0.647116000	0.889382000				
1	-5.340864000	-0.647028000	-0.888672000				
1	-5.976421000	0.757411000	0.000484000				
1	5.027165000	0.835157000	-0.000137000				
D1-t-but E(RB3LYP) = -389.518822278 a. u.				D1-OH E(RB3LYP) = -307.489739970 a. u.			
6	-0.076095000	0.028954000	0.000007000	6	0.945425000	-0.024733000	0.000000000
6	-0.820075000	1.219485000	0.000038000	6	0.221272000	-1.225162000	0.000000000
6	-0.796417000	-1.181238000	-0.000103000	6	0.264691000	1.200216000	0.000000000
1	-0.259585000	-2.132489000	-0.000143000	1	0.830032000	2.137678000	0.000001000
1	-0.312591000	2.184028000	0.000104000	1	0.770033000	-2.168672000	-0.000001000
6	-2.191816000	-1.202203000	-0.000158000	6	-1.133113000	1.220772000	0.000000000
6	-2.220225000	1.204744000	-0.000017000	6	-1.173262000	-1.191804000	-0.000002000

1	-2.717592000	-2.160251000	-0.000239000	1	-1.653618000	2.181382000	-0.000001000
1	-2.766957000	2.150984000	0.000012000	1	-1.729697000	-2.132166000	-0.000002000
6	-2.914549000	-0.004985000	-0.000111000	6	-1.860301000	0.027983000	0.000002000
6	1.465111000	0.005896000	0.000059000	8	2.308812000	-0.111667000	0.000003000
6	1.968530000	-0.733282000	1.261660000	1	2.676307000	0.784388000	-0.000019000
1	1.628684000	-0.224936000	2.178402000	1	-2.951814000	0.047091000	0.000004000
1	1.606225000	-1.772088000	1.300825000				
1	3.070986000	-0.762957000	1.275746000				
6	1.968626000	-0.733098000	-1.261610000				
1	1.606348000	-1.771908000	-1.300943000				
1	1.628831000	-0.224633000	-2.178304000				
1	3.071083000	-0.762748000	-1.275626000				
6	2.071716000	1.420811000	0.000182000				
1	3.171339000	1.353437000	0.000132000				
1	1.775609000	1.995390000	-0.891733000				
1	1.775684000	1.995208000	0.892238000				
1	-4.006904000	-0.017544000	-0.000157000				
D1-OCH <sub>3</sub> E(RB3LYP) = -346.790964285 a. u.				D1-OC <sub>2</sub> H <sub>5</sub> E(RB3LYP) = -386.111017911 a. u.			
6	0.457750000	-0.271036000	-0.000040000	6	0.051046000	-0.213966000	0.000000000
6	-0.494825000	-1.304471000	-0.000001000	6	0.945085000	-1.298730000	0.000000000
6	0.032220000	1.065107000	-0.000044000	6	0.552309000	1.096189000	0.000002000
1	0.751542000	1.883747000	-0.000077000	1	-0.119094000	1.954436000	0.000004000
1	-0.138384000	-2.336228000	0.000005000	1	0.531437000	-2.308932000	0.000000000
6	-1.339151000	1.352780000	-0.000008000	6	1.937662000	1.305933000	0.000000000
6	-1.853802000	-1.002549000	0.000029000	6	2.319004000	-1.074228000	0.000001000
1	-1.660596000	2.397162000	-0.000012000	1	2.317316000	2.330616000	0.000001000
1	-2.583167000	-1.816126000	0.000059000	1	3.001116000	-1.927838000	0.000000000
6	-2.287240000	0.330247000	0.000028000	6	2.826991000	0.231853000	-0.000003000
8	1.762996000	-0.671966000	-0.000078000	8	-1.273849000	-0.540436000	0.000003000
6	2.771628000	0.324473000	0.000077000	6	-2.242050000	0.507913000	-0.000001000
1	2.716057000	0.964360000	-0.899125000	1	-2.106095000	1.146139000	-0.893369000
1	2.715859000	0.964277000	0.899325000	1	-2.106098000	1.146143000	0.893365000
1	3.728821000	-0.213543000	0.000154000	6	-3.613961000	-0.140130000	-0.000002000
1	-3.353583000	0.564777000	0.000055000	1	-3.744820000	-0.771962000	0.892104000
				1	-3.744822000	-0.771957000	-0.892111000
				1	-4.399522000	0.631773000	0.000001000
				1	3.904855000	0.406070000	-0.000005000

D1-NH <sub>2</sub> E(RB3LYP) = -287.622688193 a. u.				D1-N(CH <sub>3</sub> ) <sub>2</sub> E(RB3LYP) = -366.232737443 a. u.			
6	-0.942414000	0.000293000	-0.008946000	6	-0.184406000	0.000002000	-0.066206000
6	-0.221983000	-1.209687000	-0.004296000	6	0.551070000	1.209849000	-0.028813000
6	-0.221962000	1.210028000	-0.004341000	6	0.551067000	-1.209847000	-0.028808000
1	-0.765745000	2.159059000	-0.010530000	1	0.035057000	-2.168867000	-0.035899000
1	-0.766328000	-2.158444000	-0.010435000	1	0.035062000	2.168870000	-0.035910000
6	1.173640000	1.204265000	0.003316000	6	1.945259000	-1.200039000	0.015180000
6	1.173458000	-1.204596000	0.003306000	6	1.945262000	1.200038000	0.015174000
1	1.710595000	2.156117000	0.008510000	1	2.477645000	-2.154445000	0.039361000
1	1.709442000	-2.156946000	0.008510000	1	2.477650000	2.154443000	0.039351000
6	1.884019000	-0.000098000	0.007426000	6	2.660715000	-0.000001000	0.035386000
7	-2.339367000	-0.000038000	-0.082184000	7	-1.574584000	0.000001000	-0.144971000
1	-2.778701000	0.835535000	0.293292000	6	-2.295842000	1.242665000	0.056462000
1	-2.778124000	-0.836288000	0.292438000	1	-2.007671000	1.997366000	-0.694148000
1	2.975883000	0.000002000	0.014707000	1	-3.371608000	1.056953000	-0.062189000
				1	-2.130064000	1.686374000	1.059719000
				6	-2.295836000	-1.242667000	0.056451000
				1	-3.371602000	-1.056965000	-0.062228000
				1	-2.007639000	-1.997369000	-0.694146000
				1	-2.130080000	-1.686370000	1.059717000
				1	3.751615000	-0.000002000	0.072216000
D1-PhCH <sub>3</sub> E(RB3LYP) = -502.651273213 a. u.				D2-PhNH <sub>2</sub> E(RB3LYP) = -518.693666665 a. u.			
6	-1.218600000	0.000709000	-0.000106000	6	-1.203062000	0.000216000	-0.000679000
6	-1.942540000	-1.140945000	-0.392788000	6	-1.932330000	-1.142205000	-0.384220000
6	-1.945065000	1.140555000	0.393081000	6	-1.929878000	1.143272000	0.385599000
1	-1.407575000	2.030558000	0.727359000	1	-1.391825000	2.035050000	0.714474000
1	-1.403198000	-2.029877000	-0.726968000	1	-1.396210000	-2.034169000	-0.715664000
6	-3.341421000	1.139481000	0.392786000	6	-3.326087000	1.145140000	0.386005000
6	-3.338903000	-1.143137000	-0.392258000	6	-3.328536000	-1.142817000	-0.379152000
1	-3.882321000	2.034274000	0.709982000	1	-3.864466000	2.043907000	0.696810000
1	-3.877654000	-2.039317000	-0.709183000	1	-3.868923000	-2.040998000	-0.688144000
6	-4.045722000	-0.002628000	0.000322000	6	-4.034188000	0.001439000	0.004840000
6	2.393527000	-1.130766000	0.392994000	6	2.409832000	-1.147535000	0.371566000
6	3.120598000	0.004505000	-0.001176000	6	3.136166000	-0.002149000	-0.005627000
6	2.393440000	1.136315000	-0.394007000	6	2.410302000	1.144088000	-0.381418000
6	0.999832000	-1.134099000	0.393508000	6	1.017313000	-1.141555000	0.369259000



6	0.996719000	1.137954000	-0.394519000	6	1.017830000	1.139348000	-0.377319000
6	0.268214000	0.002578000	-0.000810000	6	0.281914000	-0.000792000	-0.003530000
1	2.930112000	-2.028073000	0.714586000	1	2.947536000	-2.049670000	0.676789000
1	0.464030000	2.029932000	-0.731552000	1	0.488475000	2.039765000	-0.696844000
1	2.929072000	2.034017000	-0.714777000	1	2.948579000	2.043755000	-0.692712000
1	0.467271000	-2.026158000	0.730646000	1	0.487565000	-2.039943000	0.693822000
6	4.630191000	-0.004544000	0.001117000	7	4.530790000	-0.022414000	-0.067810000
1	5.028353000	-0.222284000	1.006617000	1	4.971837000	-0.708435000	0.537712000
1	5.027893000	-0.779402000	-0.676135000	1	4.972720000	0.887012000	0.029620000
1	5.040457000	0.964339000	-0.320009000	1	-5.126482000	0.001932000	0.006860000
1	-5.138061000	-0.003880000	0.000557000				

**Table S4.** Cartesian coordinates (in Angstrom unit) of B3LYP/cc-pVDZ geometries of D2 based donor systems.

D2 E(RB3LYP) = -615.809327961 a. u.				D2-CH <sub>3</sub> E(RB3LYP) = -655.126909590 a. u.			
6	0.681962000	2.467295000	0.000017000	6	-1.054586000	2.465873000	-0.000001000
6	1.431218000	1.237859000	0.000006000	6	-1.804527000	1.237042000	-0.000096000
6	-0.681962000	2.467295000	0.000021000	6	0.310050000	2.465623000	0.000033000
6	0.714468000	0.000000000	-0.000002000	6	-1.086739000	-0.000144000	-0.000156000
6	-1.431218000	1.237859000	0.000013000	6	1.058766000	1.236226000	0.000074000
6	-0.714468000	0.000000000	0.000002000	6	0.340943000	0.001953000	-0.000034000
1	1.234144000	3.410598000	0.000023000	1	-1.605778000	3.409768000	0.000025000
6	2.837506000	1.212488000	0.000002000	6	-3.211130000	1.209377000	-0.000166000
6	1.431216000	-1.237859000	-0.000013000	6	-1.801468000	-1.239296000	-0.000346000
6	-1.431216000	-1.237858000	-0.000006000	6	1.063724000	-1.231813000	-0.000173000
6	2.837508000	-1.212488000	-0.000016000	6	-3.207046000	-1.216090000	-0.000428000
6	3.529447000	-0.000002000	-0.000009000	6	-3.900970000	-0.003938000	-0.000311000
1	3.386562000	2.157418000	0.000008000	1	-3.761863000	2.153501000	-0.000111000
6	0.681963000	-2.467294000	-0.000021000	6	-1.047330000	-2.466847000	-0.000491000
1	3.386560000	-2.157420000	-0.000025000	1	-3.754949000	-2.161873000	-0.000567000
6	-2.837506000	1.212489000	0.000017000	6	2.465590000	1.209824000	0.000085000
6	-2.837508000	-1.212488000	-0.000002000	6	2.467085000	-1.201354000	-0.000164000
6	-3.529447000	-0.000002000	0.000009000	6	3.180370000	0.006838000	0.000098000
1	-1.234143000	3.410598000	0.000030000	1	0.861635000	3.409339000	0.000078000
6	-0.681963000	-2.467293000	-0.000018000	6	0.316430000	-2.463730000	-0.000459000
1	1.234143000	-3.410598000	-0.000030000	1	-1.596611000	-3.411914000	-0.000663000
1	-3.386560000	-2.157420000	-0.000008000	1	3.013882000	-2.149023000	-0.000447000
1	-4.621823000	0.000001000	0.000012000	1	0.870194000	-3.406161000	-0.000608000

1	-1.234143000	-3.410597000	-0.000024000	1	3.009228000	2.158835000	0.000002000
1	-3.386564000	2.157417000	0.000025000	6	4.691054000	-0.002979000	0.001723000
1	4.621823000	0.000000000	-0.000011000	1	5.085909000	-0.512618000	0.896786000
				1	5.087967000	-0.540521000	-0.875758000
				1	5.102508000	1.016876000	-0.013519000
				1	-4.993399000	-0.005606000	-0.000357000
D2-C <sub>5</sub> H <sub>11</sub> E(RB3LYP) = -812.382956643 a. u.				D2-isopropyl E(RB3LYP) = -733.754519717 a. u.			
6	2.257796000	-2.537613000	0.000118000	6	-1.872248000	2.438810000	-0.000038000
6	3.228051000	-1.474374000	-0.000054000	6	-2.543828000	1.165237000	-0.000012000
6	0.917995000	-2.277017000	0.000187000	6	-0.510347000	2.524178000	-0.000055000
6	2.758633000	-0.123423000	-0.000151000	6	-1.749985000	-0.024548000	-0.000001000
6	0.416778000	-0.927754000	0.000092000	6	0.313916000	1.343913000	-0.000046000
6	1.356666000	0.145522000	-0.000078000	6	-0.325271000	0.067179000	-0.000017000
1	2.618793000	-3.569322000	0.000192000	1	-2.481596000	3.346249000	-0.000048000
6	4.614568000	-1.714361000	-0.000129000	6	-3.945810000	1.049317000	0.000003000
6	3.695417000	0.957669000	-0.000324000	6	-2.385219000	-1.306169000	0.000024000
6	0.880561000	1.493744000	-0.000176000	6	0.473988000	-1.117820000	-0.000010000
6	5.070792000	0.668024000	-0.000393000	6	-3.789604000	-1.371276000	0.000039000
6	5.521956000	-0.654132000	-0.000295000	6	-4.558082000	-0.205079000	0.000033000
1	4.976064000	-2.745873000	-0.000055000	1	-4.554834000	1.956929000	-0.000005000
6	3.187445000	2.306255000	-0.000420000	6	-1.555167000	-2.483644000	0.000031000
1	5.788458000	1.492456000	-0.000525000	1	-4.277117000	-2.349554000	0.000057000
6	-0.961516000	-0.637515000	0.000162000	6	1.719310000	1.404191000	-0.000061000
6	-0.502296000	1.727454000	-0.000100000	6	1.873500000	-1.000308000	-0.000028000
6	-1.436712000	0.678545000	0.000070000	6	2.511463000	0.249647000	-0.000051000
1	0.196904000	-3.098601000	0.000317000	1	-0.018997000	3.500612000	-0.000077000
6	1.848001000	2.562002000	-0.000350000	6	-0.194230000	-2.394292000	0.000015000
1	3.906086000	3.129937000	-0.000552000	1	-2.043606000	-3.461529000	0.000049000
1	-0.859872000	2.761775000	-0.000176000	1	2.469648000	-1.916620000	-0.000022000
1	1.483032000	3.592376000	-0.000425000	1	0.417782000	-3.300015000	0.000020000
1	-1.662000000	-1.474385000	0.000292000	1	2.202257000	2.385801000	-0.000085000
6	-2.917900000	1.021979000	0.000151000	6	4.032113000	0.358274000	-0.000045000
1	-3.122572000	1.662844000	-0.877544000	1	4.273837000	1.435471000	-0.000207000
1	-3.122467000	1.662884000	0.877842000	6	4.651108000	-0.253226000	-1.269529000
6	-3.904826000	-0.147901000	0.000237000	6	4.651020000	-0.252822000	1.269685000
1	-3.725165000	-0.786966000	-0.883365000	1	4.234734000	0.207985000	2.179419000
1	-3.725089000	-0.786903000	0.883870000	1	4.461977000	-1.337891000	1.327230000
6	-5.367563000	0.309457000	0.000287000	1	5.743672000	-0.105053000	1.279448000

1	-5.550566000	0.951337000	-0.882304000	1	4.462112000	-1.338322000	-1.326733000
1	-5.550485000	0.951403000	0.882847000	1	5.743756000	-0.105429000	-1.279276000
6	-6.372118000	-0.847645000	0.000377000	1	4.234868000	0.207265000	-2.179445000
1	-6.188257000	-1.488388000	-0.881855000	1	-5.648261000	-0.275271000	0.000046000
1	-6.188177000	-1.488323000	0.882639000				
6	-7.830431000	-0.383708000	0.000426000				
1	-8.055353000	0.229982000	-0.888641000				
1	-8.055271000	0.230049000	0.889467000				
1	-8.526703000	-1.237740000	0.000490000				
1	6.594871000	-0.859783000	-0.000351000				
D2-t-but E(RB3LYP) = -773.065040310 a. u.				D2-OH E(RB3LYP) = -691.035993767 a. u			
6	-1.999076000	2.465886000	0.000147000	6	1.038168000	2.464046000	-0.000154000
6	-2.744163000	1.234069000	-0.000069000	6	1.785721000	1.233145000	-0.000033000
6	-0.634186000	2.471441000	0.000262000	6	-0.325589000	2.469377000	-0.000201000
6	-2.020990000	0.000601000	-0.000163000	6	1.063900000	-0.001898000	0.000037000
6	0.119981000	1.244997000	0.000172000	6	-1.080236000	1.241668000	-0.000133000
6	-0.593614000	0.010814000	-0.000041000	6	-0.363049000	0.003139000	-0.000013000
1	-2.554207000	3.407490000	0.000218000	1	1.591866000	3.406533000	-0.000206000
6	-4.150849000	1.198675000	-0.000193000	6	3.191202000	1.202865000	0.000019000
6	-2.727016000	-1.242961000	-0.000381000	6	1.777560000	-1.241561000	0.000157000
6	0.138243000	-1.215622000	-0.000135000	6	-1.087008000	-1.229001000	0.000057000
6	-4.132911000	-1.227523000	-0.000498000	6	3.183956000	-1.221325000	0.000205000
6	-4.833355000	-0.018885000	-0.000404000	6	3.880557000	-0.011786000	0.000135000
1	-4.707026000	2.139450000	-0.000122000	1	3.743256000	2.146282000	-0.000034000
6	-1.964265000	-2.465354000	-0.000472000	6	1.021837000	-2.466400000	0.000226000
1	-4.676051000	-2.175890000	-0.000665000	1	3.729201000	-2.168710000	0.000297000
6	1.527971000	1.228514000	0.000288000	6	-2.482485000	1.228591000	-0.000181000
6	1.541057000	-1.175405000	-0.000009000	6	-2.491965000	-1.200960000	0.000006000
6	2.259689000	0.033314000	0.000209000	6	-3.181668000	0.016282000	-0.000112000
1	-0.087102000	3.417820000	0.000426000	1	-0.873987000	3.414650000	-0.000293000
6	-0.600335000	-2.453118000	-0.000356000	6	-0.342557000	-2.461520000	0.000178000
1	-2.506996000	-3.414175000	-0.000640000	1	1.568451000	-3.413040000	0.000318000
1	2.076422000	-2.127650000	-0.000094000	1	-3.048104000	-2.143883000	0.000059000
1	-0.040576000	-3.392047000	-0.000429000	1	-0.896623000	-3.403766000	0.000231000
1	2.042315000	2.189705000	0.000448000	1	-3.049122000	2.161645000	-0.000272000
6	3.801494000	0.003629000	0.000310000	8	-4.545622000	0.085262000	-0.000165000
6	4.300869000	-0.737576000	-1.261660000	1	-4.902909000	-0.814803000	-0.000105000
1	3.934719000	-1.774995000	-1.301256000	1	4.972889000	-0.014985000	0.000173000

1	3.963211000	-0.227586000	-2.178237000				
1	5.403091000	-0.771688000	-1.275556000				
6	4.414318000	1.415890000	0.000260000				
1	4.121410000	1.991566000	-0.891917000				
1	4.121130000	1.991748000	0.892228000				
1	5.513381000	1.343030000	0.000437000				
6	4.300724000	-0.737419000	1.262430000				
1	5.402946000	-0.771459000	1.276496000				
1	3.962896000	-0.227357000	2.178904000				
1	3.934639000	-1.774858000	1.302077000				
1	-5.925714000	-0.026902000	-0.000498000				
D2-OCH <sub>3</sub> E(RB3LYP) = -730.337081432 a. u.				D2-OC <sub>2</sub> H <sub>5</sub> E(RB3LYP) = -769.657147314 a. u.			
6	1.583264000	2.428596000	0.000132000	6	1.992892000	2.427935000	0.000184000
6	2.236781000	1.144287000	0.000013000	6	2.646559000	1.143697000	0.000025000
6	0.224267000	2.536586000	0.000187000	6	0.633848000	2.535756000	0.000235000
6	1.424415000	-0.033312000	-0.000048000	6	1.834237000	-0.033950000	-0.000076000
6	-0.620536000	1.368068000	0.000127000	6	-0.210852000	1.367163000	0.000136000
6	0.001880000	0.078643000	0.000009000	6	0.411740000	0.077970000	-0.000016000
1	2.206556000	3.326601000	0.000178000	1	2.616091000	3.326016000	0.000259000
6	3.635413000	1.008630000	-0.000045000	6	4.045217000	1.008074000	-0.000035000
6	2.042388000	-1.323121000	-0.000167000	6	2.452227000	-1.323765000	-0.000242000
6	-0.813588000	-1.092314000	-0.000053000	6	-0.403970000	-1.092791000	-0.000130000
6	3.446975000	-1.408577000	-0.000220000	6	3.856802000	-1.409166000	-0.000296000
6	4.231778000	-0.255014000	-0.000160000	6	4.641588000	-0.255557000	-0.000191000
1	4.257036000	1.907746000	0.000002000	1	4.666824000	1.907211000	0.000042000
6	1.196117000	-2.486598000	-0.000227000	6	1.605831000	-2.487205000	-0.000349000
1	3.919560000	-2.394231000	-0.000311000	1	4.329431000	-2.394809000	-0.000422000
6	-2.017123000	1.456107000	0.000181000	6	-1.607457000	1.454708000	0.000198000
6	-2.216567000	-0.966548000	0.000005000	6	-1.806907000	-0.967380000	-0.000064000
6	-2.812710000	0.299944000	0.000121000	6	-2.404335000	0.299100000	0.000118000
1	-0.251956000	3.520225000	0.000277000	1	0.157538000	3.519373000	0.000352000
6	-0.164412000	-2.377233000	-0.000172000	6	0.245311000	-2.377751000	-0.000297000
1	1.668846000	-3.472215000	-0.000318000	1	2.078508000	-3.472854000	-0.000478000
1	-2.821248000	-1.873242000	-0.000042000	1	-2.410820000	-1.874486000	-0.000182000
1	-0.788492000	-3.274709000	-0.000219000	1	-0.378803000	-3.275216000	-0.000383000
1	-2.515739000	2.427327000	0.000271000	1	-2.105773000	2.426106000	0.000314000
8	-4.159676000	0.520376000	0.000186000	8	-3.750260000	0.519281000	0.000113000
6	-5.027640000	-0.601614000	0.000095000	6	-4.636018000	-0.600747000	0.000169000

1	-4.887535000	-1.227630000	-0.899387000	1	-4.451476000	-1.225970000	-0.893423000
1	-4.887519000	-1.227789000	0.899463000	1	-4.451257000	-1.226042000	0.893663000
1	-6.047171000	-0.194351000	0.000141000	6	-6.053071000	-0.058839000	0.000360000
1	5.320852000	-0.339913000	-0.000204000	1	-6.231837000	0.560979000	-0.891775000
				1	-6.231619000	0.560912000	0.892586000
				1	-6.777265000	-0.888522000	0.000415000
				1	5.730673000	-0.340442000	-0.000236000
D2-NH <sub>2</sub> E(RB3LYP) = -671.169185852 a. u.				D2-N(CH <sub>3</sub> ) <sub>2</sub> E(RB3LYP) = -749.779097286 a. u.			
6	-1.038548000	2.464479000	0.000045000	6	1.706599000	2.463709000	0.000973000
6	-1.791618000	1.237561000	0.001236000	6	2.462036000	1.237720000	0.007045000
6	0.325754000	2.463640000	-0.002349000	6	0.342372000	2.460688000	-0.013785000
6	-1.074327000	-0.000021000	-0.000409000	6	1.745425000	-0.000003000	-0.002426000
6	1.075665000	1.232992000	-0.004376000	6	-0.406825000	1.228751000	-0.026679000
6	0.352049000	0.000012000	-0.003491000	6	0.319820000	-0.000008000	-0.020036000
1	-1.587941000	3.409620000	0.000786000	1	2.254310000	3.409833000	0.008962000
6	-3.197818000	1.212341000	0.003948000	6	3.867976000	1.212506000	0.023230000
6	-1.791546000	-1.237620000	0.001235000	6	2.462051000	-1.237715000	0.007216000
6	1.075616000	-1.232995000	-0.004371000	6	-0.406828000	-1.228764000	-0.026534000
6	-3.197797000	-1.212257000	0.003949000	6	3.867982000	-1.212514000	0.023397000
6	-3.890824000	0.000000000	0.005232000	6	4.561002000	-0.000002000	0.030897000
1	-3.746326000	2.157723000	0.004982000	1	4.416849000	2.157767000	0.030229000
6	-1.038586000	-2.464520000	0.000043000	6	1.706609000	-2.463710000	0.001319000
1	-3.746588000	-2.157484000	0.004982000	1	4.416857000	-2.157774000	0.030525000
6	2.477937000	1.211500000	-0.004827000	6	-1.808804000	1.211723000	-0.041462000
6	2.477943000	-1.211517000	-0.004860000	6	-1.808797000	-1.211743000	-0.041303000
6	3.191316000	-0.000037000	-0.005336000	6	-2.538047000	-0.000005000	-0.062905000
1	0.876884000	3.407651000	-0.003663000	1	-0.209655000	3.404322000	-0.017724000
6	0.325761000	-2.463616000	-0.002348000	6	0.342391000	-2.460702000	-0.013453000
1	-1.587917000	-3.409686000	0.000783000	1	2.254343000	-3.409823000	0.009447000
1	3.025310000	-2.158577000	-0.009240000	1	-2.328430000	-2.168962000	-0.039313000
1	0.876892000	-3.407628000	-0.003659000	1	-0.209633000	-3.404338000	-0.017263000
1	3.025352000	2.158536000	-0.009139000	1	-2.328440000	2.168945000	-0.039751000
7	4.586669000	-0.000006000	-0.070203000	7	-3.927481000	0.000059000	-0.109844000
1	5.027536000	-0.836912000	0.299559000	6	-4.648425000	1.245030000	0.080399000
1	5.027439000	0.837227000	0.298930000	1	-4.460769000	1.708974000	1.069831000
1	-4.983188000	-0.000089000	0.007174000	1	-4.380552000	1.985021000	-0.692328000
				1	-5.725657000	1.053333000	-0.008495000
				6	-4.648616000	-1.245017000	0.078851000

	1	-5.725723000	-1.053383000	-0.011748000
	1	-4.379426000	-1.984618000	-0.693761000
	1	-4.462541000	-1.709394000	1.068399000
	1	5.653297000	0.000010000	0.043431000
D2-PhCH <sub>3</sub> E(RB3LYP) = -886.197377334 a. u.				
6	-2.889569000	2.456562000	0.216834000	
6	-3.640939000	1.232639000	0.108586000	
6	-1.525500000	2.455840000	0.215199000	
6	-2.924277000	-0.000549000	0.000111000	
6	-0.777073000	1.230132000	0.103625000	
6	-1.497064000	0.000286000	-0.000098000	
1	-3.440193000	3.396989000	0.301005000	
6	-5.046974000	1.206258000	0.106588000	
6	-3.639700000	-1.234544000	-0.108156000	
6	-0.775452000	-1.228637000	-0.103932000	
6	-5.045583000	-1.210181000	-0.105858000	
6	-5.738021000	-0.002298000	0.000426000	
1	-5.597122000	2.147053000	0.189323000	
6	-2.886628000	-2.457597000	-0.216552000	
1	-5.594317000	-2.151821000	-0.188481000	
6	0.626917000	1.205303000	0.100906000	
6	0.628287000	-1.202030000	-0.101445000	
6	1.345792000	0.002225000	-0.000526000	
1	-0.973005000	3.395249000	0.298351000	
6	-1.522710000	-2.455333000	-0.215230000	
1	-3.436336000	-3.398618000	-0.300554000	
1	1.170478000	-2.144384000	-0.207903000	
1	-0.969125000	-3.394084000	-0.298467000	
1	1.167894000	2.148347000	0.207483000	
6	4.957117000	-0.995586000	0.666111000	
6	5.684728000	0.003117000	-0.001790000	
6	4.958413000	0.999769000	-0.667583000	
6	3.563459000	-0.998123000	0.667096000	
6	3.561739000	1.002284000	-0.668543000	
6	2.833142000	0.003030000	-0.001337000	
1	5.493249000	-1.782791000	1.203970000	
1	3.029298000	1.780603000	-1.219581000	
1	5.494660000	1.787043000	-1.204444000	
1	3.030096000	-1.775786000	1.218242000	
D2-PhNH <sub>2</sub> E(RB3LYP) = -902.239892147 a. u.				
6	-2.881866000	-2.456104000	-0.215550000	
6	-3.633846000	-1.232757000	-0.106627000	
6	-1.517700000	-2.454929000	-0.215268000	
6	-2.917558000	0.000631000	0.000853000	
6	-0.769148000	-1.228955000	-0.104512000	
6	-1.490304000	0.000042000	-0.000482000	
1	-3.432340000	-3.396755000	-0.299220000	
6	-5.040080000	-1.206846000	-0.103146000	
6	-3.632651000	1.234585000	0.109613000	
6	-0.767994000	1.228497000	0.102111000	
6	-5.038922000	1.209720000	0.108756000	
6	-5.731300000	0.001719000	0.003462000	
1	-5.589811000	-2.147826000	-0.185126000	
6	-2.879547000	2.457355000	0.216915000	
1	-5.587919000	2.151053000	0.191632000	
6	0.634620000	-1.203538000	-0.105356000	
6	0.635757000	1.201889000	0.100447000	
6	1.356452000	-0.001106000	-0.003013000	
1	-0.965137000	-3.394266000	-0.299126000	
6	-1.515365000	2.455058000	0.214012000	
1	-3.429105000	3.398474000	0.301315000	
1	1.176027000	2.145072000	0.209909000	
1	-0.961919000	3.394023000	0.296417000	
1	1.174073000	-2.146998000	-0.216264000	
6	4.969729000	1.018915000	-0.644852000	
6	5.695459000	-0.002588000	-0.002706000	
6	4.968848000	-1.023591000	0.639093000	
6	3.577422000	1.014803000	-0.641073000	
6	3.576512000	-1.019136000	0.633775000	
6	2.841751000	-0.002082000	-0.004021000	
1	5.508097000	1.817010000	-1.163630000	
1	3.046554000	-1.812792000	1.165071000	
1	5.506272000	-1.825010000	1.153791000	
1	3.048255000	1.811137000	-1.169130000	

6	7.194278000	-0.006410000	0.002391000	7	7.089250000	-0.036452000	-0.056296000
1	7.592528000	0.030234000	1.030456000	1	7.531563000	-0.557736000	0.694779000
1	7.590792000	-0.924908000	-0.462778000	1	7.532721000	0.868092000	-0.185378000
1	7.605241000	0.852754000	-0.548117000	1	-6.823702000	0.002192000	0.004445000
1	-6.830432000	-0.002825000	0.000553000				

**Table S5.** Cartesian coordinates (in Angstrom unit) of B3LYP/cc-pVDZ geometries of D3 based donor systems.

D3 E(RB3LYP) = -749.742344106 a. u.				D3-CH <sub>3</sub> E(RB3LYP) = -789.059692283 a. u			
7	0.000059000	0.000065000	0.000063000	7	-0.354567000	-0.000174000	0.002985000
6	-2.211229000	0.693214000	0.815160000	6	1.791735000	0.859473000	0.841945000
6	-1.086956000	0.916949000	-0.000073000	6	1.069095000	-0.004002000	-0.000988000
6	-3.279585000	1.591346000	0.804814000	6	3.185130000	0.857373000	0.828584000
1	-4.144511000	1.400740000	1.444717000	1	3.722115000	1.539555000	1.493995000
6	-1.055965000	2.062726000	-0.815486000	6	1.784468000	-0.869010000	-0.843667000
6	-3.241632000	2.734263000	-0.000291000	6	3.911678000	-0.010637000	-0.003749000
1	-0.190739000	2.241839000	-1.455710000	1	1.241570000	-1.543340000	-1.508145000
1	-4.076292000	3.438242000	-0.000376000	6	3.181012000	-0.873400000	-0.832451000
6	-2.121400000	2.964326000	-0.805311000	1	3.713884000	-1.558353000	-1.497703000
1	-2.079341000	3.848926000	-1.445325000	1	1.251986000	1.535355000	1.507494000
1	-2.241958000	-0.189799000	1.455408000	6	-2.471527000	-3.675039000	0.000614000
6	3.988951000	1.439993000	0.000278000	6	-1.328745000	-3.515836000	0.791104000
6	3.017895000	2.044873000	0.804685000	6	-2.907634000	-2.606343000	-0.789147000
6	3.628258000	0.354377000	-0.804233000	1	-0.978320000	-4.338637000	1.418952000
1	3.285144000	2.889555000	1.444212000	1	-3.794185000	-2.716517000	-1.418324000
1	4.373512000	-0.124825000	-1.443658000	6	-0.634422000	-2.305214000	0.802171000
6	1.705864000	1.568850000	0.814836000	6	-2.210075000	-1.397458000	-0.798518000
6	2.314691000	-0.117409000	-0.814597000	1	0.249282000	-2.184333000	1.430613000
1	0.956349000	2.037485000	1.454516000	1	-2.549102000	-0.572921000	-1.427554000
1	2.037396000	-0.956725000	-1.454316000	6	-1.065701000	-1.230816000	0.002760000
6	1.337655000	0.482926000	0.000057000	6	-1.058471000	1.234166000	-0.000289000
6	-0.250588000	-1.399786000	0.000062000	6	-0.619961000	2.305247000	-0.800242000
6	-1.258365000	-1.945735000	-0.815387000	6	-2.203018000	1.408799000	0.799387000
6	0.505096000	-2.261568000	0.815479000	1	0.263638000	2.178542000	-1.427719000
1	-1.846026000	-1.285912000	-1.455612000	1	-2.547648000	0.586909000	1.428896000
1	1.285204000	-1.846711000	1.455721000	6	-1.307023000	3.520162000	-0.791228000
6	-1.506620000	-3.319201000	-0.805177000	6	-2.893277000	2.621681000	0.787845000
6	0.261313000	-3.635834000	0.805175000	1	-0.950838000	4.340171000	-1.419493000

1	-2.293721000	-3.725034000	-1.445233000	1	-3.779953000	2.737877000	1.415779000
1	0.858687000	-4.289628000	1.445174000	6	-2.449718000	3.686985000	-0.002485000
6	-0.747424000	-4.174342000	-0.000033000	6	5.421498000	-0.007490000	0.002296000
1	-0.939872000	-5.249149000	-0.000084000	1	5.821022000	-0.251147000	1.001598000
1	5.015987000	1.810724000	0.000367000	1	5.828843000	-0.741851000	-0.708472000
				1	5.823877000	0.982808000	-0.270992000
				1	-2.988498000	4.636701000	-0.003272000
				1	-3.015974000	-4.621448000	-0.000197000
D3-C <sub>5</sub> H <sub>11</sub> E(RB3LYP) = -946.315790717 a. u.				D3-isopropyl E(RB3LYP) = -867.687421670 a. u.			
7	1.935394000	0.023064000	0.035630000	7	-0.989798000	0.002184000	-0.017269000
6	-0.385300000	0.570249000	-0.567002000	6	-1.156628000	2.337629000	-0.758487000
6	0.533672000	-0.186407000	0.174040000	6	-1.625129000	1.272445000	0.032178000
6	-1.760591000	0.368121000	-0.417459000	6	-1.776293000	3.586840000	-0.698134000
1	-2.441076000	0.979998000	-1.011607000	1	-1.397755000	4.401770000	-1.319894000
6	0.036648000	-1.157878000	1.062031000	6	-2.730869000	1.488162000	0.875121000
6	-2.267793000	-0.603615000	0.456277000	6	-2.880992000	3.795006000	0.133750000
1	0.734937000	-1.753583000	1.652522000	1	-3.097920000	0.670654000	1.497628000
6	-1.334985000	-1.361301000	1.187156000	6	-3.354636000	2.735989000	0.914986000
1	-1.695022000	-2.123107000	1.885087000	1	-4.212073000	2.883947000	1.575963000
1	-0.020071000	1.326617000	-1.263888000	1	-0.302842000	2.179296000	-1.419174000
6	4.535196000	-3.310918000	-0.298715000	6	-3.308428000	-3.548810000	-0.040311000
6	3.302756000	-3.304033000	-0.959607000	6	-3.706130000	-2.438641000	-0.792322000
6	4.899797000	-2.203200000	0.473535000	6	-2.136651000	-3.472565000	0.719367000
1	3.005323000	-4.158548000	-1.572289000	1	-4.615013000	-2.484099000	-1.397170000
1	5.855770000	-2.195523000	1.002768000	1	-1.815433000	-4.328556000	1.317758000
6	2.448344000	-2.204818000	-0.860599000	6	-2.942248000	-1.270579000	-0.794907000
6	4.044844000	-1.106696000	0.593253000	6	-1.375358000	-2.302872000	0.737434000
1	1.493896000	-2.201660000	-1.389247000	1	-3.251939000	-0.413265000	-1.394586000
1	4.330863000	-0.252310000	1.208661000	1	-0.468957000	-2.246637000	1.342215000
6	2.808254000	-1.092232000	-0.078175000	6	-1.768038000	-1.187258000	-0.024340000
6	2.453301000	1.345930000	0.002917000	6	0.430368000	-0.078792000	-0.065753000
6	1.952149000	2.331174000	0.873380000	6	1.224914000	0.729886000	0.766134000
6	3.472613000	1.695247000	-0.901935000	6	1.071962000	-0.967168000	-0.943339000
1	1.164511000	2.069601000	1.581677000	1	0.743629000	1.422747000	1.458534000
1	3.863631000	0.940893000	-1.586460000	1	0.473734000	-1.600440000	-1.600669000
6	2.455371000	3.632256000	0.831067000	6	2.615713000	0.653912000	0.709305000
6	3.981406000	2.994716000	-0.924278000	6	2.465584000	-1.045240000	-0.975217000
1	2.053211000	4.383271000	1.515368000	1	3.200487000	1.298449000	1.370494000



1	4.772981000	3.246420000	-1.634257000	1	2.940008000	-1.746731000	-1.667411000
6	3.475367000	3.973429000	-0.062910000	6	3.269953000	-0.237497000	-0.158257000
1	3.871188000	4.990748000	-0.088342000	1	-3.367341000	4.771817000	0.173155000
6	-3.751754000	-0.870100000	0.643491000	6	4.789096000	-0.330304000	-0.216379000
1	-3.987361000	-0.783416000	1.720781000	1	5.031947000	-1.097589000	-0.972606000
1	-3.950533000	-1.928637000	0.390898000	6	5.389037000	-0.796949000	1.122168000
6	-4.719384000	0.014782000	-0.146393000	6	5.429067000	0.991123000	-0.678512000
1	-4.541214000	1.076548000	0.103910000	1	5.029823000	1.308795000	-1.654771000
1	-4.516002000	-0.083922000	-1.228274000	1	5.236639000	1.803709000	0.042200000
6	-6.189567000	-0.325668000	0.120577000	1	6.522453000	0.883442000	-0.773655000
1	-6.397092000	-0.228621000	1.203191000	1	5.194065000	-0.066882000	1.925746000
1	-6.369827000	-1.389187000	-0.126384000	1	6.482270000	-0.915977000	1.039841000
6	-7.174533000	0.548562000	-0.662722000	1	4.961991000	-1.762356000	1.436780000
1	-6.993558000	1.610963000	-0.415249000	1	-3.904943000	-4.463287000	-0.046399000
1	-6.966417000	0.450796000	-1.744313000				
6	-8.640277000	0.202682000	-0.390796000				
1	-8.889102000	0.325391000	0.677246000				
1	-8.861653000	-0.843783000	-0.662065000				
1	-9.322212000	0.847770000	-0.967899000				
1	5.203865000	-4.169856000	-0.384055000				
D3-t-but E(RB3LYP) = -906.998148614 a. u.				D3-OH E(RB3LYP) = -824.967896125 a. u			
7	-1.256360000	-0.001309000	-0.000911000	7	0.351758000	-0.000020000	0.004654000
6	-1.546812000	-2.304161000	0.801216000	6	0.567461000	2.319725000	0.774944000
6	-1.972424000	-1.229177000	-0.000326000	6	1.043129000	1.239522000	0.008190000
6	-2.246681000	-3.511636000	0.791586000	6	1.237347000	3.544097000	0.762965000
1	-1.900703000	-4.335023000	1.421131000	1	0.851509000	4.369499000	1.366258000
6	-3.116903000	-1.391857000	-0.802180000	6	2.206630000	1.418824000	-0.764019000
6	-3.389531000	-3.666722000	0.000476000	6	2.398858000	3.714787000	0.003218000
1	-3.451559000	-0.566580000	-1.432625000	1	2.580598000	0.592693000	-1.370662000
6	-3.820165000	-2.597431000	-0.791398000	6	2.878201000	2.642018000	-0.755578000
1	-4.706795000	-2.704565000	-1.420994000	1	3.779383000	2.760097000	-1.362258000
1	-0.663065000	-2.186285000	1.430202000	1	-0.331806000	2.192491000	1.379536000
6	-3.341336000	3.691582000	0.005142000	6	2.442513000	-3.690388000	-0.011259000
6	-3.783553000	2.627496000	0.797764000	6	2.917733000	-2.610254000	0.739915000
6	-2.203344000	3.521864000	-0.789721000	6	1.270389000	-3.535106000	-0.757728000
1	-4.666626000	2.745974000	1.430324000	1	3.826968000	-2.716347000	1.336686000
1	-1.848457000	4.340961000	-1.419914000	1	0.886902000	-4.366541000	-1.354136000
				6	2.231877000	-1.395213000	0.753720000

6	-3.096378000	1.412786000	0.805605000	6	0.585782000	-2.318726000	-0.764535000
6	-1.519566000	2.305119000	-0.802419000	1	2.602481000	-0.563705000	1.354984000
1	-3.439889000	0.591747000	1.436837000	1	-0.322152000	-2.204158000	-1.358484000
1	-0.639780000	2.175953000	-1.434740000	6	1.057565000	-1.231581000	-0.005549000
6	-1.956547000	1.235270000	-0.000029000	6	-1.075663000	-0.008113000	0.003721000
6	0.166577000	-0.010216000	-0.009757000	6	-1.796379000	0.761347000	-0.921483000
6	0.879341000	-0.884456000	-0.842523000	6	-1.790132000	-0.786344000	0.931321000
6	0.898115000	0.857634000	0.819790000	1	-1.257316000	1.368976000	-1.650293000
1	0.335232000	-1.565460000	-1.499239000	1	-1.242139000	-1.387922000	1.658672000
1	0.367117000	1.544437000	1.481181000	6	-3.192348000	0.764450000	-0.912975000
6	2.276877000	-0.895200000	-0.837174000	6	-3.182669000	-0.804632000	0.928409000
6	2.290779000	0.847637000	0.801112000	1	-3.737987000	1.374705000	-1.639409000
1	2.781865000	-1.595173000	-1.502857000	1	-3.739134000	-1.410333000	1.645717000
1	2.817024000	1.539266000	1.462733000	6	-3.894917000	-0.023033000	0.008158000
6	3.022728000	-0.029497000	-0.022149000	8	-5.259734000	-0.070182000	0.058897000
1	-3.938404000	-4.610651000	0.000909000	1	-5.616072000	0.513121000	-0.627106000
6	4.562422000	-0.010231000	0.000392000	1	2.923708000	4.672236000	0.001461000
6	5.066899000	1.394074000	-0.405807000	1	2.978365000	-4.641628000	-0.013331000
1	4.733261000	1.653669000	-1.423482000				
1	4.698677000	2.175433000	0.276898000				
1	6.169248000	1.427613000	-0.388329000				
6	5.060820000	-0.339321000	1.426980000				
1	4.691916000	0.386644000	2.168017000				
1	4.723271000	-1.340117000	1.741293000				
1	6.163093000	-0.323019000	1.463560000				
6	5.172195000	-1.038182000	-0.969905000				
1	6.271673000	-0.989263000	-0.920874000				
1	4.875406000	-2.068498000	-0.717384000				
1	4.878591000	-0.842882000	-2.013494000				
1	-3.877660000	4.642733000	0.007185000				
D3-OCH <sub>3</sub> E(RB3LYP) = -864.269310659 a. u.				D3-OC <sub>2</sub> H <sub>5</sub> E(RB3LYP) = -903.589386919 a. u.			
7	0.691920000	0.004195000	0.027806000	7	1.076397000	0.002703000	0.028799000
6	0.788465000	2.329044000	0.806966000	6	1.196471000	2.327277000	0.805196000
6	1.300658000	1.286418000	0.012310000	6	1.696792000	1.279156000	0.010140000
6	1.376936000	3.594220000	0.777909000	6	1.796176000	3.587078000	0.772929000
1	0.964062000	4.389454000	1.403426000	1	1.392348000	4.386647000	1.398837000
6	2.416969000	1.545098000	-0.805515000	6	2.812768000	1.527096000	-0.811534000

6	2.492588000	3.844126000	-0.027389000	6	2.911472000	3.826197000	-0.036132000
1	2.817825000	0.748312000	-1.433857000	1	3.204465000	0.726192000	-1.440410000
6	3.008182000	2.809163000	-0.814309000	6	3.415212000	2.785811000	-0.823580000
1	3.873926000	2.988897000	-1.456432000	1	4.280428000	2.957094000	-1.468728000
1	-0.075149000	2.140261000	1.446434000	1	0.333103000	2.146960000	1.447420000
6	3.019297000	-3.539650000	-0.091818000	6	3.368369000	-3.563859000	-0.100327000
6	3.451377000	-2.432977000	0.646749000	6	3.815852000	-2.460431000	0.633912000
6	1.811051000	-3.459635000	-0.791021000	6	2.156568000	-3.472902000	-0.792011000
1	4.388452000	-2.480685000	1.206872000	1	4.755890000	-2.516541000	1.188276000
1	1.460120000	-4.312531000	-1.377108000	1	1.793557000	-4.323126000	-1.374627000
6	2.687964000	-1.266056000	0.694620000	6	3.064268000	-1.285995000	0.684865000
6	1.047939000	-2.291184000	-0.763821000	6	1.405114000	-2.297010000	-0.761691000
1	3.026329000	-0.413887000	1.285884000	1	3.414719000	-0.436445000	1.272837000
1	0.111931000	-2.234673000	-1.321432000	1	0.466153000	-2.232132000	-1.313376000
6	1.476389000	-1.177770000	-0.017242000	6	1.849129000	-1.186697000	-0.019528000
6	-0.730819000	-0.098117000	0.078807000	6	-0.347215000	-0.086172000	0.086876000
6	-1.535807000	0.628539000	-0.806851000	6	-1.149658000	0.644158000	-0.798018000
6	-1.357340000	-0.930645000	1.025254000	6	-0.977118000	-0.908793000	1.039443000
1	-1.065888000	1.276851000	-1.548568000	1	-0.677140000	1.285094000	-1.544525000
1	-0.745109000	-1.502062000	1.725176000	1	-0.367192000	-1.483130000	1.739024000
6	-2.931439000	0.545895000	-0.751137000	6	-2.545676000	0.574816000	-0.735917000
6	-2.742296000	-1.035618000	1.072248000	6	-2.362831000	-1.000508000	1.092802000
1	-3.523270000	1.131469000	-1.454139000	1	-3.134530000	1.163215000	-1.438876000
1	-3.234120000	-1.680746000	1.802445000	1	-2.857015000	-1.638211000	1.827929000
6	-3.544816000	-0.294414000	0.188172000	6	-3.163638000	-0.255937000	0.209642000
8	-4.893097000	-0.461668000	0.326869000	8	-4.511801000	-0.410006000	0.354895000
6	-5.749800000	0.260976000	-0.541128000	6	-5.383328000	0.315242000	-0.511286000
1	-5.625701000	1.352907000	-0.424231000	1	-5.178263000	0.045015000	-1.564427000
1	-5.581908000	-0.007233000	-1.599987000	1	-5.204421000	1.401660000	-0.402093000
1	-6.773539000	-0.017060000	-0.257813000	6	-6.807349000	-0.041163000	-0.127544000
1	2.954108000	4.833558000	-0.042523000	1	-7.007047000	0.232229000	0.920088000
1	3.616271000	-4.453330000	-0.120563000	1	-6.980908000	-1.122456000	-0.240825000
				1	-7.520709000	0.496803000	-0.771387000
				1	3.381756000	4.811453000	-0.053813000
				1	3.956164000	-4.483393000	-0.131482000
D3-NH <sub>2</sub> E(RB3LYP) = -805.101132202 a. u.				D3-N(CH <sub>3</sub> ) <sub>2</sub> E(RB3LYP) = -883.711453255 a. u.			
7	0.366808000	0.000406000	0.000880000	7	-1.007178000	0.001184000	0.006603000
6	-1.783571000	0.719452000	-0.963545000	6	1.139399000	-0.781817000	-0.918634000

6	-1.062748000	-0.004519000	-0.001254000	6	0.422309000	-0.025578000	0.019298000
6	-3.176901000	0.725346000	-0.959666000	6	2.531729000	-0.818656000	-0.906305000
1	-3.716129000	1.297775000	-1.719515000	1	3.038351000	-1.420691000	-1.659073000
6	-1.781163000	-0.732337000	0.960044000	6	1.151351000	0.709336000	0.964660000
6	-3.900748000	-0.013283000	-0.004270000	6	3.277872000	-0.084698000	0.047797000
1	-1.237227000	-1.298020000	1.718947000	1	0.616933000	1.313107000	1.700857000
6	-3.174367000	-0.746752000	0.953220000	6	2.544356000	0.697446000	0.972780000
1	-3.711772000	-1.327611000	1.707990000	1	3.060693000	1.296448000	1.721311000
1	-1.241643000	1.292007000	-1.718717000	1	0.595231000	-1.354797000	-1.672092000
6	2.431160000	-3.705487000	-0.007152000	6	-2.987526000	3.750648000	-0.117579000
6	1.250812000	-3.546940000	-0.740116000	6	-1.803932000	3.546847000	-0.833747000
6	2.923539000	-2.622307000	0.728296000	6	-3.511357000	2.697988000	0.640104000
1	0.852794000	-4.380523000	-1.324004000	1	-1.381470000	4.356043000	-1.434622000
1	3.838957000	-2.730142000	1.315344000	1	-4.429757000	2.841362000	1.214825000
6	0.575591000	-2.325567000	-0.749259000	6	-1.156408000	2.310853000	-0.804508000
6	2.247937000	-1.401450000	0.739240000	6	-2.863722000	1.463070000	0.689168000
1	-0.339647000	-2.209333000	-1.331411000	1	-0.238077000	2.159220000	-1.373517000
1	2.633171000	-0.568574000	1.329216000	1	-3.273427000	0.654530000	1.296288000
6	1.065545000	-1.234092000	-0.007311000	6	-1.677919000	1.249468000	-0.040459000
6	1.057532000	1.238717000	0.008733000	6	-1.724251000	-1.221473000	0.040008000
6	0.561174000	2.327521000	0.750569000	6	-1.254186000	-2.302942000	0.809315000
6	2.239018000	1.414037000	-0.737768000	6	-2.905704000	-1.389658000	-0.708349000
1	-0.353127000	2.205316000	1.333054000	1	-0.339860000	-2.186588000	1.392874000
1	2.629427000	0.583488000	-1.327655000	1	-3.275879000	-0.565400000	-1.319696000
6	1.228589000	3.553202000	0.741454000	6	-1.947306000	-3.514169000	0.825315000
6	2.906855000	2.639060000	-0.726918000	6	-3.599141000	-2.599904000	-0.672457000
1	0.825636000	4.384297000	1.325595000	1	-1.564334000	-4.339625000	1.430524000
1	3.821505000	2.752703000	-1.314092000	1	-4.513178000	-2.708053000	-1.261676000
6	2.407772000	3.719190000	0.008489000	6	-3.126378000	-3.672742000	0.090469000
7	-5.297565000	-0.070998000	-0.046797000	7	4.668187000	-0.136786000	0.080231000
1	-5.737397000	0.737986000	-0.476377000	6	5.379661000	-0.747064000	-1.027508000
1	-5.735131000	-0.285030000	0.845023000	1	5.200702000	-0.236316000	-1.995955000
1	2.930188000	4.677981000	0.008505000	1	6.457630000	-0.720460000	-0.820302000
1	2.959520000	-4.660928000	-0.007189000	1	5.094380000	-1.805162000	-1.149729000
				6	5.392317000	0.802775000	0.916016000
				1	6.468514000	0.600963000	0.834064000
				1	5.216445000	1.861789000	0.636012000
				1	5.115964000	0.687246000	1.977180000
				1	-3.668735000	-4.620209000	0.110119000
				1	-3.494172000	4.717432000	-0.147532000

D3-PhCH <sub>3</sub> E(RB3LYP) = -1020.13104195 a. u.				D3-PhNH <sub>2</sub> E(RB3LYP) = -1036.17330739 a. u.			
7	2.101887000	0.000242000	-0.000514000	7	2.100787000	0.000127000	0.000515000
6	-0.040052000	0.914142000	-0.787386000	6	-0.041896000	0.886238000	-0.819759000
6	0.682160000	-0.000706000	-0.000313000	6	0.678600000	-0.000035000	-0.000445000
6	-1.432959000	0.914309000	-0.777068000	6	-1.435078000	0.886198000	-0.812376000
1	-1.963486000	1.619469000	-1.420524000	1	-1.964222000	1.566621000	-1.483070000
6	-0.038712000	-0.916366000	0.787098000	6	-0.042696000	-0.886684000	0.817769000
6	-2.166406000	-0.002430000	0.000149000	6	-2.171310000	-0.000779000	-0.002662000
1	0.501217000	-1.624519000	1.417596000	1	0.497224000	-1.572720000	1.472602000
6	-1.431591000	-0.918091000	0.777364000	6	-1.435863000	-0.887371000	0.808153000
1	-1.961258000	-1.623581000	1.421158000	1	-1.965571000	-1.568549000	1.477665000
1	0.498822000	1.623069000	-1.417919000	1	0.498648000	1.572332000	-1.474012000
6	4.229672000	-3.667821000	-0.022327000	6	4.211302000	-3.677889000	-0.043359000
6	3.102900000	-3.498515000	-0.833377000	6	3.072354000	-3.505056000	-0.836352000
6	4.646046000	-2.612810000	0.795913000	6	4.645844000	-2.622015000	0.764325000
1	2.769300000	-4.310703000	-1.483723000	1	2.723514000	-4.317666000	-1.478194000
1	5.520372000	-2.731740000	1.440340000	1	5.529533000	-2.743203000	1.395520000
6	2.404306000	-2.290195000	-0.836234000	6	2.379970000	-2.293210000	-0.832232000
6	3.943556000	-1.406825000	0.813249000	6	3.950199000	-1.412316000	0.788765000
1	1.533725000	-2.159944000	-1.481021000	1	1.499334000	-2.161308000	-1.462794000
1	4.266208000	-0.591976000	1.463271000	1	4.287634000	-0.597625000	1.431400000
6	2.815193000	-1.230475000	-0.007653000	6	2.809497000	-1.231787000	-0.014824000
6	2.813546000	1.231875000	0.007200000	6	2.809197000	1.232256000	0.016486000
6	2.401258000	2.290751000	0.836142000	6	2.378463000	2.293645000	0.833284000
6	3.941734000	1.409991000	-0.813586000	6	3.950740000	1.412928000	-0.785842000
1	1.530804000	2.159157000	1.480836000	1	1.497109000	2.161538000	1.462792000
1	4.265428000	0.595772000	-1.463889000	1	4.289051000	0.598281000	-1.428055000
6	3.098310000	3.499985000	0.833792000	6	3.070529000	3.505668000	0.838040000
6	4.642682000	2.616857000	-0.795763000	6	4.646030000	2.622819000	-0.760778000
1	2.763598000	4.311475000	1.484431000	1	2.720745000	4.318318000	1.479323000
1	5.516896000	2.737157000	-1.440080000	1	5.530338000	2.744178000	-1.391061000
6	4.224889000	3.671009000	0.022868000	6	4.210332000	3.678700000	0.046294000
6	-3.650681000	-0.003685000	0.000076000	6	-3.654212000	-0.000974000	-0.004127000
6	-4.383344000	1.196351000	-0.089340000	6	-4.390914000	1.189464000	-0.155057000
6	-4.381593000	-1.201478000	0.089388000	6	-4.391250000	-1.191208000	0.147070000
1	-3.851421000	2.149334000	-0.132607000	1	-3.862245000	2.140942000	-0.245891000
1	-3.850628000	-2.154957000	0.132552000	1	-3.862871000	-2.142405000	0.242374000
6	-5.776892000	1.193677000	-0.089930000	6	-5.783381000	1.195609000	-0.155475000
6	-5.778167000	-1.198765000	0.090512000	6	-5.783664000	-1.196900000	0.147874000

1	-6.312735000	2.145320000	-0.152006000	1	-6.320940000	2.141601000	-0.266423000
1	-6.314161000	-2.149835000	0.153326000	1	-6.321683000	-2.143223000	0.253188000
6	-6.505156000	-0.003987000	0.000376000	6	-6.509907000	-0.000532000	-0.003968000
6	-8.014752000	0.006132000	-0.000465000	7	-7.904964000	-0.008973000	-0.067969000
1	-8.412997000	0.454778000	-0.926420000	1	-8.345065000	0.870789000	0.185546000
1	-8.425477000	-1.011017000	0.083022000	1	-8.345864000	-0.787551000	0.413087000
1	-8.412564000	0.599571000	0.840216000	1	4.752999000	4.626147000	0.057838000
1	4.771746000	4.616086000	0.028952000	1	4.754262000	-4.625192000	-0.054482000
1	4.777726000	-4.612196000	-0.028032000				

**Table S6.** Cartesian coordinates (in Angstrom unit) of B3LYP/cc-pVDZ geometries of D4 based donor systems.

D4 E(RB3LYP) = -517.504742141 a. u.				D4-CH <sub>3</sub> E(RB3LYP) = -556.822087110 a. u.			
6	2.484393000	1.223499000	0.000001000	6	-2.859856000	-1.295608000	-0.000203000
6	1.133787000	0.856817000	-0.000003000	6	-1.527008000	-0.869668000	-0.000184000
6	0.726133000	-0.506712000	-0.000003000	6	-1.178850000	0.510851000	-0.000181000
6	1.702434000	-1.513612000	-0.000003000	6	-2.199199000	1.473185000	-0.000256000
6	3.049786000	-1.154266000	0.000001000	6	-3.529582000	1.054499000	-0.000270000
6	3.433533000	0.200786000	0.000004000	6	-3.853602000	-0.315850000	-0.000225000
7	0.000000000	1.655193000	-0.000014000	7	-0.358484000	-1.617079000	-0.000335000
6	-0.726134000	-0.506711000	-0.000005000	6	0.271487000	0.572432000	-0.000065000
1	2.787389000	2.273092000	0.000002000	1	-3.115830000	-2.357665000	-0.000197000
1	1.410772000	-2.566447000	-0.000006000	1	-1.954756000	2.538006000	-0.000284000
1	3.818214000	-1.929999000	0.000001000	1	-4.331264000	1.795846000	-0.000314000
6	-2.484393000	1.223499000	0.000008000	6	2.103798000	-1.080047000	0.000197000
6	-3.433533000	0.200787000	0.000009000	6	3.030800000	-0.033558000	0.000328000
6	-1.133786000	0.856818000	0.000001000	6	0.738452000	-0.769184000	0.000001000
1	-4.495045000	0.458516000	0.000015000	6	2.569900000	1.304998000	0.000211000
6	-3.049786000	-1.154266000	0.000001000	1	3.304096000	2.114752000	0.000282000
1	-3.818215000	-1.929999000	0.000002000	6	1.212690000	1.613085000	0.000010000
6	-1.702434000	-1.513612000	-0.000007000	1	0.885643000	2.655576000	-0.000070000
1	-1.410770000	-2.566446000	-0.000011000	1	2.442223000	-2.119557000	0.000246000
1	-2.787390000	2.273092000	0.000011000	1	-0.313838000	-2.626040000	0.000971000
1	0.000001000	2.665157000	0.000052000	6	4.514699000	-0.316270000	0.000611000
1	4.495045000	0.458516000	0.000007000	1	5.005214000	0.120763000	0.886994000
				1	4.722609000	-1.396625000	0.000265000
				1	5.005683000	0.121433000	-0.885177000
				1	-4.902762000	-0.620131000	-0.000223000

D4-C <sub>5</sub> H <sub>11</sub> E(RB3LYP) = -714.078236957 a. u.				D4-isopropyl E(RB3LYP) = -635.449498257 a. u.			
6	4.248453000	-1.841306000	-0.000079000	6	-3.461066000	-1.452126000	-0.000103000
6	3.080337000	-1.070876000	-0.000055000	6	-2.173006000	-0.905612000	-0.000087000
6	3.118446000	0.352583000	-0.000098000	6	-1.953806000	0.500966000	-0.000053000
6	4.361145000	1.003049000	-0.000165000	6	-3.057906000	1.365502000	-0.000049000
6	5.528704000	0.240152000	-0.000189000	6	-4.344401000	0.826467000	-0.000063000
6	5.470116000	-1.166823000	-0.000149000	6	-4.540740000	-0.567734000	-0.000085000
7	1.753405000	-1.474087000	0.000009000	7	-0.940946000	-1.542952000	-0.000148000
6	1.738819000	0.803318000	-0.000047000	6	-0.514906000	0.696196000	-0.000017000
1	4.207707000	-2.933032000	-0.000047000	1	-3.618466000	-2.533180000	-0.000129000
1	4.413809000	2.094304000	-0.000193000	1	-2.912106000	2.448240000	-0.000028000
1	6.501019000	0.737067000	-0.000237000	1	-5.210820000	1.490962000	-0.000055000
6	-0.473137000	-0.296667000	0.000038000	6	1.460038000	-0.783822000	0.000010000
6	-1.086862000	0.959444000	0.000033000	6	2.291592000	0.344451000	0.000077000
6	0.926639000	-0.360627000	-0.000004000	6	0.074755000	-0.598300000	-0.000037000
6	-0.278384000	2.123751000	-0.000007000	6	1.707914000	1.631498000	0.000083000
1	-0.768526000	3.101006000	-0.000010000	1	2.364458000	2.505157000	0.000129000
6	1.110677000	2.058593000	-0.000046000	6	0.325866000	1.816529000	0.000035000
1	1.704242000	2.975901000	-0.000084000	1	-0.093382000	2.825440000	0.000045000
1	-1.063823000	-1.213936000	0.000077000	1	1.882163000	-1.791797000	-0.000006000
1	1.437397000	-2.433324000	0.000020000	1	-0.804491000	-2.543619000	0.000166000
6	-2.597087000	1.131308000	0.000083000	6	3.809318000	0.195905000	0.000128000
1	-2.874775000	1.744731000	-0.877384000	1	4.227492000	1.217461000	0.000208000
1	-2.874721000	1.744698000	0.877590000	6	4.320295000	-0.509216000	-1.269020000
6	-3.445005000	-0.142815000	0.000086000	6	4.320205000	-0.509377000	1.269220000
1	-3.193819000	-0.757202000	-0.883793000	1	3.985099000	0.013276000	2.179033000
1	-3.193771000	-0.757230000	0.883932000	1	3.954451000	-1.548524000	1.326473000
6	-4.950560000	0.143996000	0.000132000	1	5.422432000	-0.544376000	1.279573000
1	-5.205670000	0.760845000	-0.882365000	1	3.954533000	-1.548351000	-1.326434000
1	-5.205621000	0.760815000	0.882665000	1	5.422522000	-0.544223000	-1.279296000
6	-5.816635000	-1.120102000	0.000135000	1	3.985259000	0.013559000	-2.178789000
1	-5.560926000	-1.735705000	-0.882191000	1	-5.557433000	-0.967332000	-0.000092000
1	-5.560874000	-1.735739000	0.882422000				
6	-7.318462000	-0.825927000	0.000185000				
1	-7.611924000	-0.241790000	-0.888792000				
1	-7.611871000	-0.241827000	0.889204000				
1	-7.912838000	-1.753814000	0.000183000				
1	6.397922000	-1.743470000	-0.000168000				

D4-t-but E(RB3LYP) = -674.759728612 a. u.				D4-OH E(RB3LYP) = -592.730528897 a. u			
6	3.830184000	-1.364250000	0.000023000	6	2.836453000	-1.290837000	-0.000028000
6	2.519077000	-0.875683000	-0.000023000	6	1.504599000	-0.866444000	-0.000011000
6	2.238384000	0.519998000	-0.000024000	6	1.152132000	0.512417000	-0.000018000
6	3.302707000	1.432766000	0.000005000	6	2.171046000	1.475835000	-0.000041000
6	4.611929000	0.951362000	0.000052000	6	3.502744000	1.058967000	-0.000057000
6	4.869697000	-0.432782000	0.000066000	6	3.830244000	-0.309663000	-0.000051000
7	1.316594000	-1.567057000	-0.000120000	7	0.335138000	-1.617606000	0.000016000
6	0.792089000	0.650901000	-0.000047000	6	-0.298510000	0.570186000	-0.000003000
1	4.035643000	-2.437220000	0.000025000	1	3.093563000	-2.352706000	-0.000023000
1	3.108651000	2.507886000	-0.000002000	1	1.925680000	2.540440000	-0.000047000
1	5.448124000	1.653510000	0.000080000	1	4.302493000	1.802500000	-0.000076000
6	-1.114210000	-0.913667000	-0.000063000	6	-2.125371000	-1.092332000	0.000039000
6	-2.007136000	0.170413000	-0.000053000	6	-3.037914000	-0.032831000	0.000045000
6	0.260068000	-0.667370000	-0.000060000	6	-0.761938000	-0.773639000	0.000022000
6	-1.476129000	1.481268000	-0.000032000	6	-2.600284000	1.309501000	0.000023000
1	-2.149614000	2.336845000	-0.000017000	1	-3.356018000	2.095922000	0.000032000
6	-0.102088000	1.726813000	-0.000040000	6	-1.242390000	1.608604000	-0.000004000
1	0.266503000	2.755347000	-0.000031000	1	-0.917189000	2.651407000	-0.000019000
1	-1.480985000	-1.942317000	-0.000059000	1	-2.469160000	-2.130820000	0.000033000
1	1.224758000	-2.572793000	0.000236000	1	0.293958000	-2.626643000	-0.000011000
6	-3.525528000	-0.104209000	0.000024000	8	-4.390044000	-0.234493000	0.000039000
6	-4.357175000	1.191674000	0.000476000	1	-4.563508000	-1.187094000	0.000249000
1	-4.159980000	1.806643000	0.892571000	1	4.879701000	-0.612404000	-0.000065000
1	-4.159856000	1.807334000	-0.891117000				
1	-5.430381000	0.942866000	0.000314000				
6	-3.903722000	-0.914616000	-1.261702000				
1	-3.648939000	-0.358346000	-2.178124000				
1	-3.379674000	-1.882135000	-1.301042000				
1	-4.987170000	-1.120915000	-1.276598000				
6	-3.903417000	-0.915320000	1.261389000				
1	-4.986838000	-1.121759000	1.276365000				
1	-3.379233000	-1.882793000	1.300125000				
1	-3.648541000	-0.359503000	2.178061000				
1	5.903000000	-0.787041000	0.000107000				



D4-OCH <sub>3</sub> E(RB3LYP) = -632.032131995 a. u.				D4-OC <sub>2</sub> H <sub>5</sub> E(RB3LYP) = -671.352181336a. u.			
6	3.107455000	-1.444362000	0.000004000	6	3.512989000	-1.512856000	-0.000008000
6	1.818181000	-0.903284000	0.000004000	6	2.242488000	-0.929069000	-0.000006000
6	1.589916000	0.501899000	-0.000042000	6	2.061276000	0.483012000	-0.000055000
6	2.690646000	1.370982000	-0.000090000	6	3.190459000	1.314775000	-0.000105000
6	3.979840000	0.837263000	-0.000090000	6	4.461168000	0.738309000	-0.000107000
6	4.184116000	-0.555304000	-0.000044000	6	4.618802000	-0.660279000	-0.000059000
7	0.586934000	-1.546250000	0.000046000	7	0.990500000	-1.530500000	0.000038000
6	0.150673000	0.687653000	-0.000027000	6	0.629027000	0.716670000	-0.000037000
1	3.269163000	-2.524872000	0.000040000	1	3.638501000	-2.598175000	0.000029000
1	2.540885000	2.453200000	-0.000126000	1	3.076936000	2.401400000	-0.000143000
1	4.842739000	1.506477000	-0.000127000	1	5.345932000	1.378349000	-0.000147000
6	-1.818014000	-0.814203000	0.000057000	6	-1.388683000	-0.719111000	0.000052000
6	-2.634732000	0.321840000	0.000029000	6	-2.168416000	0.443133000	0.000024000
6	-0.430845000	-0.606926000	0.000028000	6	0.004512000	-0.557672000	0.000021000
6	-2.075523000	1.622456000	-0.000025000	6	-1.565037000	1.724201000	-0.000033000
1	-2.762925000	2.469329000	-0.000045000	1	-2.223715000	2.593623000	-0.000053000
6	-0.699947000	1.805799000	-0.000053000	6	-0.184200000	1.862252000	-0.000064000
1	-0.286548000	2.816886000	-0.000096000	1	0.262230000	2.859218000	-0.000107000
1	-2.229556000	-1.822904000	0.000099000	1	-1.832657000	-1.713855000	0.000096000
1	0.455154000	-2.547507000	0.000084000	1	0.825292000	-2.526779000	0.000078000
8	-4.000220000	0.284476000	0.000051000	8	-3.533428000	0.451118000	0.000048000
6	-4.638303000	-0.980166000	0.000105000	6	-4.231127000	-0.792110000	0.000104000
1	-4.380948000	-1.568975000	-0.899200000	1	-3.950108000	-1.381373000	0.893614000
1	-4.380922000	-1.568912000	0.899443000	1	-3.950138000	-1.381436000	-0.893375000
1	-5.717243000	-0.776591000	0.000113000	6	-5.716511000	-0.482115000	0.000118000
1	5.202642000	-0.950065000	-0.000045000	1	-5.991006000	0.101739000	-0.891966000
				1	-5.990975000	0.101802000	0.892170000
				1	-6.300398000	-1.415915000	0.000160000
				1	5.623568000	-1.088879000	-0.000062000
D4-NH <sub>2</sub> E(RB3LYP) = -572.863738451 a. u.				D4-N(CH <sub>3</sub> ) <sub>2</sub> E(RB3LYP) = -651.473709094 a. u.			
6	2.847470000	-1.290184000	0.001626000	6	3.551241000	-1.342258000	0.019759000
6	1.515813000	-0.865972000	-0.000014000	6	2.235894000	-0.870513000	0.001448000
6	1.164274000	0.513765000	0.000468000	6	1.934369000	0.521522000	-0.002683000
6	2.183647000	1.476303000	0.003179000	6	2.987990000	1.446345000	0.012606000
6	3.515839000	1.058983000	0.005010000	6	4.304229000	0.981097000	0.031174000

6	3.842539000	-0.309393000	0.004100000	6	4.581246000	-0.398076000	0.034621000
7	0.346093000	-1.615975000	-0.001675000	7	1.040123000	-1.577437000	-0.015246000
6	-0.286166000	0.571565000	-0.002856000	6	0.487560000	0.629974000	-0.023508000
1	3.104192000	-2.352226000	0.000886000	1	3.769525000	-2.412916000	0.022575000
1	1.938675000	2.541076000	0.003338000	1	2.781712000	2.519314000	0.009731000
1	4.315899000	1.802292000	0.006888000	1	5.130566000	1.695063000	0.043091000
6	-2.112502000	-1.094098000	-0.004341000	6	-1.395688000	-0.975393000	-0.045303000
6	-3.043715000	-0.043313000	-0.005993000	6	-2.308318000	0.103009000	-0.066932000
6	-0.752566000	-0.771918000	-0.004785000	6	-0.027939000	-0.693293000	-0.031687000
6	-2.589884000	1.300941000	-0.005093000	6	-1.794922000	1.434411000	-0.045422000
1	-3.328620000	2.106425000	-0.011343000	1	-2.480432000	2.279366000	-0.044176000
6	-1.233119000	1.605538000	-0.002920000	6	-0.428522000	1.689880000	-0.028238000
1	-0.912837000	2.650087000	0.000491000	1	-0.078387000	2.724842000	-0.013820000
1	-2.449283000	-2.134125000	-0.008409000	1	-1.735873000	-2.009581000	-0.042290000
1	0.304094000	-2.624918000	-0.010002000	1	0.961750000	-2.584200000	-0.019461000
7	-4.415200000	-0.311767000	-0.073774000	7	-3.680840000	-0.125361000	-0.115675000
1	-5.002389000	0.422807000	0.311279000	6	-4.600734000	0.975455000	0.105458000
1	-4.685288000	-1.217463000	0.299477000	1	-4.469274000	1.766268000	-0.651626000
1	4.891758000	-0.613070000	0.005260000	1	-5.630344000	0.604715000	0.015760000
				1	-4.488058000	1.443503000	1.104338000
				6	-4.179581000	-1.474762000	0.062052000
				1	-5.273852000	-1.470496000	-0.026451000
				1	-3.788123000	-2.150312000	-0.717530000
				1	-3.913866000	-1.910771000	1.047121000
				1	5.618716000	-0.739587000	0.049110000
D4-PhCH <sub>3</sub> E (RB3LYP) = -787.892917043 a. u.				D4-PhNH <sub>2</sub> E (RB3LYP) = -803.935179188 a. u.			
6	-4.764384000	-1.453146000	-0.251722000	6	4.757539000	-1.450378000	0.251077000
6	-3.473073000	-0.922363000	-0.157998000	6	3.465821000	-0.920862000	0.157497000
6	-3.245664000	0.463924000	0.073962000	6	3.237400000	0.465839000	-0.072151000
6	-4.344887000	1.324253000	0.212642000	6	4.335877000	1.327141000	-0.208554000
6	-5.634001000	0.800657000	0.120120000	6	5.625803000	0.804588000	-0.116175000
6	-5.838421000	-0.573643000	-0.109651000	6	5.831372000	-0.569714000	0.111220000
7	-2.244969000	-1.558739000	-0.258867000	7	2.238111000	-1.558119000	0.256335000
6	-1.806861000	0.647203000	0.110139000	6	1.798276000	0.647975000	-0.109003000
1	-4.928208000	-2.518394000	-0.429867000	1	4.922164000	-2.515859000	0.427353000
1	-4.192716000	2.391251000	0.391047000	1	4.182688000	2.394318000	-0.385155000
1	-6.496680000	1.461419000	0.226611000	1	6.487904000	1.466423000	-0.220996000
6	0.158853000	-0.825013000	-0.129348000	6	-0.166515000	-0.826224000	0.129072000

6	0.998271000	0.285985000	0.051476000	6	-1.009691000	0.282645000	-0.052891000
6	-1.224614000	-0.633531000	-0.097959000	6	1.216638000	-0.633122000	0.096340000
6	0.420122000	1.564258000	0.260018000	6	-0.430333000	1.561440000	-0.260750000
1	1.077367000	2.418719000	0.429323000	1	-1.087374000	2.415545000	-0.432961000
6	-0.958997000	1.749290000	0.290840000	6	0.948405000	1.748840000	-0.288332000
1	-1.373582000	2.745198000	0.463158000	1	1.361255000	2.745837000	-0.459121000
1	0.581760000	-1.813394000	-0.320668000	1	-0.586792000	-1.815391000	0.322472000
1	-2.113635000	-2.546307000	-0.424787000	1	2.107403000	-2.546182000	0.419432000
6	4.693668000	0.931399000	-0.597868000	6	-4.708515000	0.944447000	0.573214000
6	5.311601000	-0.191546000	-0.031054000	6	-5.322770000	-0.197600000	0.025413000
6	4.483550000	-1.156076000	0.566272000	6	-4.493456000	-1.178491000	-0.550689000
6	3.306082000	1.088271000	-0.571590000	6	-3.324472000	1.094505000	0.542434000
6	3.098504000	-1.003842000	0.595179000	6	-3.110309000	-1.018540000	-0.574301000
6	2.475752000	0.123550000	0.025006000	6	-2.485371000	0.119239000	-0.029422000
1	5.308770000	1.697230000	-1.078390000	1	-5.327242000	1.719387000	1.034565000
1	2.487683000	-1.760114000	1.093298000	1	-2.500655000	-1.788352000	-1.052776000
1	4.933814000	-2.039902000	1.027540000	1	-4.944130000	-2.068803000	-0.998345000
1	2.858446000	1.964037000	-1.046212000	1	-2.881621000	1.981173000	1.001173000
6	6.811009000	-0.365797000	-0.053642000	7	-6.713121000	-0.322660000	-0.005235000
1	7.223787000	-0.420788000	0.968097000	1	-7.201477000	0.202637000	0.714012000
1	7.099563000	-1.298805000	-0.566756000	1	-7.051903000	-1.279148000	-0.051303000
1	7.306818000	0.469063000	-0.570753000	1	6.850660000	-0.956509000	0.179946000
1	-6.857476000	-0.961037000	-0.178500000				

**Table S7.** Cartesian coordinates (in Angstrom unit) of B3LYP/cc-pVDZ geometries of D5 based donor systems.

D5 E(RB3LYP) = -994.310143043 a. u.				D5-CH <sub>3</sub> E(RB3LYP) = -1033.62761228 a. u.			
6	-2.401400000	1.085150000	-0.112395000	6	-2.867230000	0.796336000	-0.190252000
6	-1.236025000	0.329759000	0.124991000	6	-1.616690000	0.218092000	0.106256000
7	-0.000043000	0.946705000	0.431125000	7	-0.494168000	1.008274000	0.443843000
6	-1.358187000	-1.077639000	0.066228000	6	-1.536895000	-1.193635000	0.074424000
16	0.000293000	-2.123508000	0.555709000	16	-0.066454000	-2.031016000	0.636373000
6	1.358544000	-1.077337000	0.066219000	6	1.152736000	-0.811007000	0.184033000
6	1.236086000	0.330040000	0.124981000	6	0.828945000	0.565056000	0.203073000
6	-3.624678000	0.471472000	-0.398825000	6	-3.979522000	0.010775000	-0.507277000
6	-2.572961000	-1.683174000	-0.263780000	6	-2.640705000	-1.970381000	-0.285787000
6	2.573456000	-1.682623000	-0.263740000	6	2.452304000	-1.244414000	-0.078053000
6	2.401349000	1.085657000	-0.112247000	6	1.889289000	1.464635000	-0.005678000
6	3.624764000	0.472227000	-0.398623000	6	3.197501000	1.018977000	-0.224438000

6	3.718995000	-0.914761000	-0.488571000	6	3.508081000	-0.341080000	-0.277424000
1	2.618750000	-2.772597000	-0.316663000	1	2.645992000	-2.320258000	-0.100075000
1	2.367205000	2.171975000	-0.075952000	1	1.709654000	2.537322000	-0.000698000
1	4.503871000	1.098389000	-0.565108000	1	3.985884000	1.761608000	-0.370867000
1	4.667487000	-1.399301000	-0.726814000	6	-3.873568000	-1.377009000	-0.569514000
6	-3.718639000	-0.915541000	-0.488697000	1	-2.987971000	1.877054000	-0.177373000
1	-2.367436000	2.171483000	-0.076214000	1	-4.930957000	0.502969000	-0.720007000
1	-4.503888000	1.097459000	-0.565427000	1	-2.529823000	-3.056578000	-0.315836000
1	-2.618034000	-2.773158000	-0.316694000	6	-0.706225000	2.413623000	0.803394000
6	-0.000267000	2.358651000	0.827762000	1	-1.624418000	2.458152000	1.408717000
1	-0.878885000	2.512605000	1.472565000	1	0.115361000	2.701847000	1.476762000
1	0.878806000	2.513166000	1.471819000	6	-0.801854000	3.421048000	-0.353905000
6	-0.001188000	3.400229000	-0.302766000	1	-1.637458000	3.197043000	-1.032603000
1	-0.885541000	3.311740000	-0.950055000	1	0.112596000	3.441653000	-0.964067000
1	0.882527000	3.312342000	-0.950996000	1	-0.959351000	4.433076000	0.054712000
1	-0.001302000	4.412700000	0.134094000	6	4.911166000	-0.835535000	-0.531886000
1	-4.667020000	-1.400272000	-0.726991000	1	5.288684000	-1.433452000	0.315198000
				1	4.955585000	-1.480654000	-1.425675000
				1	5.608651000	0.000947000	-0.687447000
				1	-4.733985000	-1.995266000	-0.831410000
D5-C <sub>5</sub> H <sub>11</sub> E(RB3LYP) = -1190.88380677 a. u.				D5-isopropyl E(RB3LYP) = -1112.25529707 a. u.			
6	4.469774000	0.802255000	0.391129000	6	3.525296000	0.723361000	0.263882000
6	3.254048000	0.220522000	-0.021133000	6	2.270682000	0.187591000	-0.089264000
7	2.167036000	1.007613000	-0.464771000	7	1.188521000	1.016021000	-0.465717000
6	3.174853000	-1.191480000	0.005887000	6	2.144724000	-1.221058000	-0.072918000
16	1.766559000	-2.034319000	-0.690818000	16	0.673141000	-2.006863000	-0.703286000
6	0.506907000	-0.815984000	-0.360885000	6	-0.523329000	-0.750505000	-0.291036000
6	0.827993000	0.561107000	-0.351626000	6	-0.156079000	0.611773000	-0.283716000
6	5.548902000	0.020120000	0.813590000	6	4.597914000	-0.099697000	0.620348000
6	4.241574000	-1.964654000	0.470528000	6	3.207105000	-2.035219000	0.326880000
6	-0.810392000	-1.249861000	-0.224769000	6	-1.848475000	-1.143293000	-0.085318000
6	-0.250457000	1.455616000	-0.248268000	6	-1.197007000	1.544198000	-0.108311000
6	-1.574744000	1.009066000	-0.155634000	6	-2.524494000	1.140876000	0.052903000
6	-1.886766000	-0.351564000	-0.129732000	6	-2.882283000	-0.212173000	0.080422000
1	-1.003446000	-2.326308000	-0.219590000	1	-2.077273000	-2.212366000	-0.080699000
1	-0.074983000	2.529016000	-0.238344000	1	-0.982073000	2.610409000	-0.096505000
1	-2.363863000	1.758939000	-0.088926000	1	-3.286954000	1.913822000	0.173725000
6	5.440716000	-1.367802000	0.868432000	6	4.445288000	-1.483686000	0.666695000

1	4.588717000	1.883243000	0.387480000	1	3.680667000	1.799731000	0.264932000
1	6.474778000	0.515116000	1.114396000	1	5.554821000	0.360187000	0.876403000
1	4.130806000	-3.051069000	0.492304000	1	3.060650000	-3.117483000	0.343195000
6	2.408222000	2.414159000	-0.800127000	6	1.459294000	2.416534000	-0.804218000
1	3.379920000	2.462915000	-1.314780000	1	2.402355000	2.436145000	-1.371446000
1	1.653748000	2.701355000	-1.548263000	1	0.675559000	2.736000000	-1.507917000
6	2.388961000	3.418654000	0.363455000	6	1.539528000	3.411879000	0.364636000
1	3.157725000	3.196368000	1.117546000	1	2.338765000	3.155947000	1.075079000
1	1.420599000	3.432339000	0.884038000	1	0.601788000	3.457668000	0.936945000
1	2.579174000	4.432778000	-0.025584000	1	1.746146000	4.421229000	-0.028427000
6	-3.299656000	-0.895209000	-0.009464000	6	-4.321691000	-0.668743000	0.277566000
1	-3.343829000	-1.559616000	0.873724000	1	-4.311318000	-1.772753000	0.257404000
1	-3.495859000	-1.554537000	-0.875682000	6	-5.236413000	-0.195062000	-0.866020000
6	-4.426425000	0.136019000	0.091333000	6	-4.878295000	-0.238053000	1.646394000
1	-4.254041000	0.790684000	0.965053000	1	-4.246288000	-0.607806000	2.469218000
1	-4.407431000	0.795526000	-0.795457000	1	-4.928988000	0.860652000	1.730774000
6	-5.812604000	-0.506542000	0.210177000	1	-5.898431000	-0.629999000	1.794111000
1	-5.834252000	-1.169250000	1.096061000	1	-5.303160000	0.905610000	-0.896191000
1	-5.987332000	-1.164293000	-0.662346000	1	-6.259183000	-0.586413000	-0.735864000
6	-6.954100000	0.510591000	0.312411000	1	-4.861476000	-0.534172000	-1.844636000
1	-6.778510000	1.167286000	1.184577000	1	5.273894000	-2.131093000	0.958972000
1	-6.931532000	1.172283000	-0.573272000				
6	-8.335022000	-0.138282000	0.430764000				
1	-8.401003000	-0.778475000	1.327118000				
1	-8.555092000	-0.773625000	-0.444202000				
1	-9.133041000	0.618227000	0.502249000				
1	6.273840000	-1.983475000	1.211968000				
D5-t-butyl E(RB3LYP) = -1151.56629947 a. u.				D5-OH E(RB3LYP) = -1069.53458714 a. u.			
6	3.811541000	0.565618000	0.278361000	6	-2.841958000	0.829327000	-0.182294000
6	2.521976000	0.129566000	-0.086187000	6	-1.596817000	0.234737000	0.106279000
7	1.507290000	1.041353000	-0.457510000	7	-0.463746000	1.005496000	0.443684000
6	2.290482000	-1.265783000	-0.086592000	6	-1.535693000	-1.178105000	0.070152000
16	0.767048000	-1.932193000	-0.730196000	16	-0.077037000	-2.038515000	0.630827000
6	-0.335012000	-0.593919000	-0.310443000	6	1.160118000	-0.838191000	0.180724000
6	0.135471000	0.738174000	-0.288441000	6	0.854593000	0.542093000	0.191113000
6	4.817735000	-0.339543000	0.629101000	6	-3.964644000	0.058377000	-0.498190000
6	3.287425000	-2.161823000	0.306854000	6	-2.649589000	-1.940127000	-0.289834000
6	-1.683823000	-0.888471000	-0.117718000	6	2.449807000	-1.299432000	-0.081010000

6	-0.835377000	1.738172000	-0.113321000	6	1.923459000	1.425807000	-0.033638000
6	-2.193503000	1.432244000	0.035852000	6	3.228478000	0.970393000	-0.253146000
6	-2.656996000	0.113409000	0.050515000	6	3.499840000	-0.397240000	-0.288179000
1	-1.975071000	-1.940790000	-0.127223000	1	2.657966000	-2.370292000	-0.100510000
1	-0.547041000	2.786744000	-0.089841000	1	1.757217000	2.500518000	-0.038137000
1	-2.885799000	2.264943000	0.156423000	1	4.029656000	1.698052000	-0.410888000
6	4.561799000	-1.708733000	0.657836000	6	-3.875955000	-1.330407000	-0.567606000
1	4.047125000	1.627230000	0.293305000	1	-2.949189000	1.911485000	-0.164010000
1	5.805048000	0.044368000	0.894721000	1	-4.910965000	0.562853000	-0.705108000
1	3.060227000	-3.230185000	0.309879000	1	-2.552489000	-3.027555000	-0.323730000
6	1.883653000	2.422806000	-0.772443000	6	-0.651127000	2.409326000	0.817641000
1	2.830074000	2.381340000	-1.332732000	1	-1.564021000	2.463123000	1.430625000
1	1.131139000	2.809729000	-1.476292000	1	0.180498000	2.678678000	1.487048000
6	2.026796000	3.390684000	0.413171000	6	-0.741639000	3.431277000	-0.327924000
1	2.799121000	3.065044000	1.124879000	1	-1.586013000	3.226706000	-1.001883000
1	1.089873000	3.495518000	0.978984000	1	0.167271000	3.446568000	-0.946650000
1	2.310101000	4.388412000	0.038697000	1	-0.881410000	4.440867000	0.093088000
6	-4.136735000	-0.268294000	0.234053000	8	4.744492000	-0.917203000	-0.513904000
6	-4.288396000	-1.155603000	1.491326000	1	5.365739000	-0.185758000	-0.642386000
1	-3.697974000	-2.081697000	1.413454000	1	-4.744613000	-1.936859000	-0.829775000
1	-3.953817000	-0.620198000	2.394438000				
1	-5.343427000	-1.443444000	1.634821000				
6	-5.035012000	0.969743000	0.407383000				
1	-4.754139000	1.559637000	1.294280000				
1	-4.995748000	1.632070000	-0.471950000				
1	-6.082419000	0.654273000	0.537544000				
6	-4.626764000	-1.050980000	-1.006376000				
1	-5.685562000	-1.336545000	-0.888293000				
1	-4.536966000	-0.440048000	-1.919046000				
1	-4.048304000	-1.974573000	-1.163395000				
1	5.338199000	-2.419793000	0.945468000				
D5-OCH <sub>3</sub> E(RB3LYP) = -1108.83620931 a. u.				D5-OC <sub>2</sub> H <sub>5</sub> E(RB3LYP) = -1148.15629098 a. u.			
6	-3.190244000	0.825154000	-0.236408000	6	-3.607917000	0.699869000	-0.299460000
6	-1.953356000	0.232479000	0.089622000	6	-2.351558000	0.174574000	0.065476000
7	-0.832777000	1.005852000	0.461422000	7	-1.281680000	1.007975000	0.455891000
6	-1.888949000	-1.180373000	0.054475000	6	-2.215002000	-1.233561000	0.049953000
16	-0.446790000	-2.039583000	0.657065000	16	-0.747782000	-2.011554000	0.700531000
6	0.801502000	-0.835704000	0.248061000	6	0.448701000	-0.750530000	0.308719000

6	0.493722000	0.545701000	0.252434000	6	0.071530000	0.613142000	0.287075000
6	-4.301769000	0.052846000	-0.586369000	6	-4.669521000	-0.131825000	-0.667804000
6	-2.990724000	-1.943667000	-0.338910000	6	-3.266210000	-2.056190000	-0.361761000
6	2.098275000	-1.289659000	0.027820000	6	1.772210000	-1.140348000	0.127958000
6	1.568303000	1.428282000	0.067027000	6	1.104894000	1.546638000	0.117484000
6	2.885619000	0.981471000	-0.111762000	6	2.447284000	1.165421000	-0.021608000
6	3.158950000	-0.386827000	-0.142862000	6	2.791148000	-0.187737000	-0.027547000
1	2.312835000	-2.359397000	0.012352000	1	2.040394000	-2.198031000	0.132072000
1	1.400632000	2.502867000	0.060520000	1	0.883525000	2.611206000	0.092490000
1	3.674291000	1.722044000	-0.237596000	1	3.199947000	1.944028000	-0.137040000
6	-4.209081000	-1.335815000	-0.653254000	6	-4.505117000	-1.514666000	-0.714766000
1	-3.299638000	1.907127000	-0.221263000	1	-3.772088000	1.775003000	-0.300833000
1	-5.242035000	0.556142000	-0.821817000	1	-5.627538000	0.320349000	-0.933507000
1	-2.890943000	-3.030934000	-0.370444000	1	-3.110887000	-3.137281000	-0.376917000
6	-1.034870000	2.410648000	0.824408000	6	-1.563682000	2.404773000	0.795495000
1	-1.967379000	2.464967000	1.406967000	1	-2.512732000	2.418578000	1.353200000
1	-0.225974000	2.683714000	1.519529000	1	-0.787992000	2.726461000	1.507466000
6	-1.088911000	3.427515000	-0.327827000	6	-1.638512000	3.404312000	-0.370651000
1	-1.911066000	3.219340000	-1.027692000	1	-2.430542000	3.146875000	-1.088642000
1	-0.160284000	3.439985000	-0.916549000	1	-0.696549000	3.456890000	-0.935483000
1	-1.242529000	4.438940000	0.083858000	1	-1.853465000	4.411354000	0.023993000
8	4.392193000	-0.946297000	-0.325907000	8	4.054567000	-0.685620000	-0.171411000
6	5.495090000	-0.074584000	-0.503769000	6	5.132711000	0.233282000	-0.335959000
1	5.376235000	0.558917000	-1.401689000	1	5.187416000	0.910296000	0.537703000
1	5.648859000	0.576857000	0.375848000	1	4.962153000	0.857022000	-1.233974000
1	6.374699000	-0.719131000	-0.632170000	6	6.407154000	-0.578490000	-0.473568000
1	-5.068512000	-1.943486000	-0.941722000	1	6.348559000	-1.247870000	-1.345712000
				1	6.573431000	-1.194827000	0.423450000
				1	7.272361000	0.090403000	-0.603568000
				1	-5.324933000	-2.168448000	-1.017359000
D5-NH <sub>2</sub> E(RB3LYP) = -1049.66783900 a. u.				D5-N(CH <sub>3</sub> ) <sub>2</sub> E(RB3LYP) = -1128.27832266 a. u.			
6	-2.857336000	0.808035000	-0.188140000	6	-3.548969000	0.619555000	-0.237549000
6	-1.606021000	0.227200000	0.103992000	6	-2.259236000	0.152899000	0.090458000
7	-0.482955000	1.008347000	0.443729000	7	-1.219136000	1.031377000	0.454010000
6	-1.530431000	-1.185751000	0.068856000	6	-2.057743000	-1.248115000	0.065756000
16	-0.067038000	-2.030116000	0.642515000	16	-0.540166000	-1.956733000	0.680731000
6	1.162021000	-0.819207000	0.194716000	6	0.588249000	-0.642958000	0.252379000
6	0.842091000	0.554689000	0.197834000	6	0.146253000	0.694955000	0.245297000

6	-3.970508000	0.025168000	-0.508151000	6	-4.579862000	-0.260063000	-0.580979000
6	-2.634906000	-1.959097000	-0.295749000	6	-3.079867000	-2.117436000	-0.322154000
6	2.457267000	-1.269199000	-0.064235000	6	1.922942000	-0.982903000	0.031962000
6	1.906025000	1.444238000	-0.033690000	6	1.139069000	1.669273000	0.050382000
6	3.212405000	0.999915000	-0.250405000	6	2.485085000	1.343477000	-0.128884000
6	3.514237000	-0.368392000	-0.279607000	6	2.915703000	0.002126000	-0.170374000
1	2.649239000	-2.345244000	-0.069704000	1	2.180803000	-2.040581000	0.039674000
1	1.730390000	2.517759000	-0.046624000	1	0.877659000	2.725461000	0.044799000
1	4.004444000	1.736030000	-0.409707000	1	3.193226000	2.160605000	-0.253942000
6	-3.866836000	-1.362614000	-0.578382000	6	-4.352022000	-1.633491000	-0.639631000
1	-2.976194000	1.889021000	-0.169459000	1	-3.763131000	1.685964000	-0.229270000
1	-4.921583000	0.519613000	-0.717814000	1	-5.565066000	0.147366000	-0.818420000
1	-2.526435000	-3.045557000	-0.328231000	1	-2.874673000	-3.190063000	-0.345782000
6	-0.682973000	2.410673000	0.814792000	6	-1.550833000	2.413828000	0.803734000
1	-1.596998000	2.458621000	1.426908000	1	-2.484615000	2.388066000	1.386517000
1	0.146101000	2.688630000	1.483797000	1	-0.770761000	2.768314000	1.495105000
6	-0.781032000	3.429762000	-0.332877000	6	-1.698382000	3.409222000	-0.359085000
1	-1.622853000	3.216666000	-1.007491000	1	-2.497065000	3.117535000	-1.056416000
1	0.128773000	3.451260000	-0.950072000	1	-0.773981000	3.500721000	-0.947526000
1	-0.929907000	4.439071000	0.085854000	1	-1.945644000	4.406683000	0.041163000
7	4.828400000	-0.827181000	-0.446237000	7	4.246754000	-0.341949000	-0.409138000
1	5.422911000	-0.186172000	-0.965040000	6	4.672550000	-1.707256000	-0.162416000
1	4.890632000	-1.760321000	-0.844872000	1	4.547439000	-2.022693000	0.894415000
1	-4.728041000	-1.978205000	-0.843962000	1	4.112298000	-2.416962000	-0.792644000
				1	5.734175000	-1.804780000	-0.426293000
				6	5.257457000	0.696006000	-0.330358000
				1	5.321257000	1.172139000	0.670411000
				1	6.237784000	0.261115000	-0.567073000
				1	5.065435000	1.492130000	-1.068207000
				1	-5.148177000	-2.324000000	-0.923533000
D5-PhCH <sub>3</sub> E(RB3LYP) = -1264.69880091 a. u.				D5-PhNH <sub>2</sub> E(RB3LYP) = -1280.74102337 a. u.			
6	4.682755000	0.337932000	0.414561000	6	4.676904000	0.343843000	0.413164000
6	3.384112000	0.023244000	-0.032222000	6	3.377869000	0.027631000	-0.032157000
7	2.445234000	1.031881000	-0.353248000	7	2.438165000	1.033774000	-0.354337000
6	3.063200000	-1.347275000	-0.166830000	6	3.058399000	-1.343761000	-0.165245000
16	1.526031000	-1.848940000	-0.918215000	16	1.522829000	-1.847976000	-0.918111000
6	0.499149000	-0.481800000	-0.410340000	6	0.492541000	-0.482183000	-0.411896000
6	1.052904000	0.810003000	-0.260726000	6	1.044671000	0.809455000	-0.260649000



6	5.613878000	-0.660484000	0.716296000	6	5.609119000	-0.653298000	0.715737000
6	3.983838000	-2.339920000	0.177626000	6	3.980212000	-2.334852000	0.180559000
6	-0.872368000	-0.700991000	-0.289740000	6	-0.878961000	-0.703863000	-0.294145000
6	0.144036000	1.862299000	-0.037374000	6	0.134085000	1.859051000	-0.034189000
6	-1.231967000	1.641038000	0.038546000	6	-1.241578000	1.635062000	0.043875000
6	-1.777197000	0.354071000	-0.072361000	6	-1.787194000	0.347996000	-0.071828000
1	-1.246147000	-1.718382000	-0.421173000	1	-1.250454000	-1.721423000	-0.430889000
1	0.503625000	2.880348000	0.093013000	1	0.491832000	2.877622000	0.098225000
1	-1.886233000	2.493247000	0.231364000	1	-1.895888000	2.486215000	0.241586000
6	5.269471000	-2.006339000	0.611594000	6	5.265840000	-1.999671000	0.613573000
1	4.984858000	1.375791000	0.533966000	1	4.978186000	1.382195000	0.530637000
1	6.612221000	-0.369170000	1.049577000	1	6.607488000	-0.360556000	1.047846000
1	3.688615000	-3.386578000	0.076201000	1	3.685938000	-3.381935000	0.080416000
6	2.925350000	2.405283000	-0.539006000	6	2.915265000	2.407448000	-0.541605000
1	3.888061000	2.342546000	-1.068521000	1	3.877592000	2.346796000	-1.072310000
1	2.229144000	2.899672000	-1.233359000	1	2.216856000	2.900171000	-1.235005000
6	3.086481000	3.260942000	0.727619000	6	3.076584000	3.264792000	0.724067000
1	3.806754000	2.825370000	1.435079000	1	3.799023000	2.831450000	1.430733000
1	2.137488000	3.385253000	1.268876000	1	2.128104000	3.387162000	1.266653000
1	3.450543000	4.263344000	0.447454000	1	3.437892000	4.267879000	0.442550000
6	-5.113950000	-1.277950000	0.747805000	6	-5.122116000	-1.304269000	0.732085000
6	-6.044844000	-0.358998000	0.236128000	6	-6.053604000	-0.372121000	0.237236000
6	-5.543725000	0.796397000	-0.378810000	6	-5.556322000	0.800629000	-0.362060000
6	-3.742438000	-1.050907000	0.650253000	6	-3.753502000	-1.068755000	0.629326000
6	-4.170227000	1.027375000	-0.481522000	6	-4.185637000	1.025591000	-0.460182000
6	-3.237346000	0.109521000	0.031844000	6	-3.245471000	0.100373000	0.031802000
1	-5.470868000	-2.186350000	1.241708000	1	-5.479515000	-2.220634000	1.210276000
1	-3.817333000	1.925261000	-0.993586000	1	-3.837028000	1.935040000	-0.954634000
1	-6.241163000	1.527796000	-0.796427000	1	-6.256678000	1.535725000	-0.768555000
1	-3.049228000	-1.774770000	1.084428000	1	-3.061938000	-1.801653000	1.050882000
6	-7.528212000	-0.614990000	0.350540000	7	-7.425110000	-0.632394000	0.279820000
1	-7.811287000	-1.562882000	-0.137667000	1	-8.013372000	0.195753000	0.271126000
1	-7.841825000	-0.691521000	1.405626000	1	-7.710976000	-1.273292000	1.014296000
1	-8.114250000	0.191000000	-0.115522000	1	5.983644000	-2.783161000	0.862757000
1	5.986491000	-2.790805000	0.859864000				

**Table S8.** Cartesian coordinates (in Angstrom unit) of B3LYP/cc-pVDZ geometries of D6 based donor systems.

D6 E(RB3LYP) = -497.056838502 a. u.				D6-CH <sub>3</sub> E(RB3LYP) = -536.375356562 a. u.			
6	-2.168928000	-0.271710000	-0.000006000	6	-2.479449000	-0.572951000	-0.000618000
6	-1.929250000	1.170351000	0.000002000	6	-2.534657000	0.886889000	-0.000063000
6	-0.676830000	1.684768000	0.000028000	6	-1.410105000	1.642655000	-0.000019000
6	0.475620000	0.815688000	0.000027000	6	-0.108600000	1.022225000	-0.000075000
6	0.237866000	-0.574527000	-0.000008000	6	-0.060392000	-0.385597000	-0.000082000
6	1.298182000	-1.487160000	-0.000018000	6	1.160608000	-1.068600000	-0.000002000
6	2.606428000	-1.009426000	0.000008000	6	2.364129000	-0.360392000	0.000062000
6	2.866733000	0.371569000	0.000042000	6	2.323094000	1.051943000	0.000054000
6	1.808859000	1.272901000	0.000051000	6	1.112158000	1.727869000	0.000003000
1	-0.520128000	2.767079000	0.000043000	1	-1.473823000	2.734384000	0.000165000
1	1.996592000	2.349447000	0.000076000	1	1.090013000	2.820531000	0.000028000
1	3.896160000	0.734026000	0.000062000	1	3.259009000	1.615642000	0.000103000
1	1.072940000	-2.554350000	-0.000045000	1	1.143829000	-2.159846000	-0.000023000
8	-1.027578000	-1.083614000	-0.000030000	8	-1.197056000	-1.139222000	-0.000214000
8	-3.243748000	-0.817067000	-0.000079000	8	-3.421975000	-1.324869000	0.000423000
1	-2.823385000	1.793820000	-0.000010000	6	3.689295000	-1.081276000	0.000232000
1	3.436350000	-1.719293000	0.000000000	1	4.287674000	-0.809072000	-0.885366000
				1	4.286631000	-0.810508000	0.886985000
				1	3.558360000	-2.172734000	-0.000704000
				1	-3.535940000	1.317737000	0.000189000
D6-C <sub>5</sub> H <sub>11</sub> E(RB3LYP) = -693.631324450 a. u.				D6-isopropyl E(RB3LYP) = -615.002952802 a. u.			
6	-4.360268000	-0.776307000	-0.000033000	6	2.977689000	-0.915677000	-0.000192000
6	-4.563311000	0.671165000	-0.000070000	6	3.350566000	0.497068000	-0.000118000
6	-3.521257000	1.536596000	-0.000086000	6	2.418940000	1.480340000	0.000052000
6	-2.163750000	1.050575000	-0.000063000	6	1.012961000	1.159530000	0.000106000
6	-1.972472000	-0.347596000	-0.000022000	6	0.657281000	-0.205482000	-0.000017000
6	-0.692157000	-0.899834000	0.000003000	6	-0.680045000	-0.606230000	0.000000000
6	0.440679000	-0.075081000	-0.000011000	6	-1.704539000	0.347756000	0.000149000
6	0.255718000	1.322403000	-0.000052000	6	-1.354087000	1.713822000	0.000274000
6	-1.022215000	1.871780000	-0.000077000	6	-0.022965000	2.112388000	0.000248000
1	-3.694503000	2.616448000	-0.000116000	1	2.719914000	2.531721000	0.000127000
1	-1.152300000	2.956930000	-0.000108000	1	0.234992000	3.174385000	0.000340000
1	1.118569000	1.988059000	-0.000063000	1	-2.144572000	2.467815000	0.000388000
1	-0.598042000	-1.987837000	0.000035000	1	-0.891508000	-1.676577000	-0.000102000

8	-3.029506000	-1.211855000	-0.000007000	8	1.604326000	-1.188710000	-0.000154000
8	-5.223779000	-1.618006000	-0.000010000	8	3.734643000	-1.854387000	-0.000523000
6	1.813128000	-0.725914000	0.000013000	6	-3.167892000	-0.074420000	0.000158000
1	1.873398000	-1.396209000	-0.877244000	1	-3.765861000	0.853313000	0.000345000
1	1.873365000	-1.396213000	0.877269000	6	-3.534834000	-0.862950000	1.270173000
6	3.027201000	0.206204000	0.000038000	6	-3.534957000	-0.862520000	-1.270091000
1	2.989185000	0.868475000	-0.883874000	1	-3.303334000	-0.287243000	-2.180315000
1	2.989142000	0.868483000	0.883942000	1	-2.983109000	-1.815582000	-1.325306000
6	4.356949000	-0.555854000	0.000072000	1	-4.611371000	-1.099882000	-1.279298000
1	4.396990000	-1.222002000	-0.882474000	1	-2.982997000	-1.816040000	1.325007000
1	4.396950000	-1.221993000	0.882628000	1	-4.611251000	-1.100301000	1.279409000
6	5.586896000	0.358029000	0.000095000	1	-3.303112000	-0.287988000	2.180571000
1	5.545282000	1.023172000	-0.882236000	1	4.421750000	0.699398000	-0.000207000
1	5.545242000	1.023182000	0.882418000				
6	6.910756000	-0.409549000	0.000130000				
1	6.998106000	-1.057161000	-0.888947000				
1	6.998065000	-1.057151000	0.889218000				
1	7.774450000	0.274538000	0.000146000				
1	-5.602997000	0.998450000	-0.000086000				
D6-t-butyl E(RB3LYP) = -654.313904858 a. u.				D6-OH E(RB3LYP) = -572.285516562 a. u.			
6	-3.347883000	-0.803411000	-0.000731000	6	-2.465986000	-0.534341000	-0.000636000
6	-3.632912000	0.629766000	0.000016000	6	-2.491621000	0.923372000	-0.000027000
6	-2.641677000	1.553414000	0.000062000	6	-1.349628000	1.655632000	0.000002000
6	-1.259346000	1.144132000	-0.000064000	6	-0.062100000	1.013596000	-0.000078000
6	-0.988816000	-0.236280000	-0.000110000	6	-0.040845000	-0.397455000	-0.000079000
6	0.322869000	-0.724050000	-0.000048000	6	1.162690000	-1.106568000	0.000004000
6	1.410686000	0.153932000	0.000041000	6	2.369557000	-0.402073000	0.000057000
6	1.139363000	1.543933000	0.000056000	6	2.375569000	1.008284000	0.000052000
6	-0.160363000	2.026350000	0.000022000	6	1.173335000	1.695427000	0.000001000
1	-2.876157000	2.621580000	0.000325000	1	-1.392576000	2.748434000	0.000206000
1	-0.346718000	3.103260000	0.000081000	1	1.171960000	2.788030000	0.000038000
1	1.964056000	2.257943000	0.000102000	1	3.334121000	1.527970000	0.000112000
1	0.449699000	-1.805078000	-0.000093000	1	1.131768000	-2.198366000	-0.000001000
8	-1.993182000	-1.160558000	-0.000259000	8	-1.189236000	-1.127178000	-0.000207000
8	-4.161000000	-1.693967000	0.000603000	8	-3.417467000	-1.274287000	0.000518000
6	2.868142000	-0.341787000	0.000032000	8	3.577847000	-1.022869000	0.000123000
6	2.962378000	-1.878060000	-0.000588000	1	3.442824000	-1.982506000	0.000121000
1	2.490331000	-2.319733000	0.891008000	1	-3.483073000	1.375874000	0.000277000

1	2.491019000	-2.318980000	-0.892918000				
1	4.020324000	-2.183864000	-0.000318000				
6	3.587016000	0.188992000	-1.262462000				
1	3.096885000	-0.176229000	-2.179173000				
1	3.595545000	1.289124000	-1.300729000				
1	4.634852000	-0.153650000	-1.275819000				
6	3.586720000	0.187943000	1.263139000				
1	4.634498000	-0.154874000	1.276551000				
1	3.595421000	1.288042000	1.302236000				
1	3.096260000	-0.177890000	2.179429000				
1	-4.689607000	0.897309000	0.000376000				
D6-OCH <sub>3</sub> E(RB3LYP) = -611.585898334 a. u.				D6-OC <sub>2</sub> H <sub>5</sub> E(RB3LYP) = -650.906112819 a. u.			
6	-2.875318000	-0.600689000	0.000071000	6	-3.265038000	-0.776539000	-0.000022000
6	-2.955342000	0.856423000	-0.000179000	6	-3.477974000	0.667318000	0.000047000
6	-1.842420000	1.630604000	-0.000176000	6	-2.440240000	1.539675000	0.000039000
6	-0.532195000	1.034725000	-0.000066000	6	-1.081234000	1.065454000	-0.000004000
6	-0.457558000	-0.378265000	0.000004000	6	-0.878096000	-0.334582000	-0.000030000
6	0.766254000	-1.039397000	0.000070000	6	0.400528000	-0.881798000	-0.000057000
6	1.953395000	-0.294118000	0.000072000	6	1.516423000	-0.032860000	-0.000065000
6	1.907121000	1.116188000	0.000003000	6	1.340921000	1.367872000	-0.000044000
6	0.673448000	1.757467000	-0.000068000	6	0.054132000	1.894330000	-0.000012000
1	-1.925251000	2.721180000	-0.000291000	1	-2.621881000	2.618230000	0.000074000
1	0.633719000	2.849437000	-0.000135000	1	-0.084332000	2.978238000	0.000007000
1	2.821130000	1.707615000	-0.000009000	1	2.196747000	2.040518000	-0.000057000
1	0.804129000	-2.128387000	0.000127000	1	0.536542000	-1.962919000	-0.000073000
8	-1.582786000	-1.147717000	0.000028000	8	-1.929125000	-1.203599000	-0.000026000
8	-3.803387000	-1.370424000	-0.000269000	8	-4.119846000	-1.627323000	0.000061000
8	3.098102000	-1.023565000	0.000121000	8	2.721549000	-0.654795000	-0.000110000
6	4.344537000	-0.339853000	0.000338000	6	3.917889000	0.132309000	0.000038000
1	4.464267000	0.287811000	-0.900023000	1	3.936057000	0.781777000	0.894343000
1	4.463922000	0.287866000	0.900704000	1	3.936236000	0.781845000	-0.894215000
1	5.114175000	-1.122149000	0.000505000	6	5.090922000	-0.828893000	0.000114000
1	-3.963054000	1.271769000	-0.000331000	1	5.065812000	-1.472867000	-0.892281000
				1	5.065660000	-1.472916000	0.892470000
				1	6.038688000	-0.268288000	0.000208000
				1	-4.519550000	0.988401000	0.000095000

D6-NH <sub>2</sub> E(RB3LYP) = -552.420154689 a. u.				D6-N(CH <sub>3</sub> ) <sub>2</sub> E(RB3LYP) = -631.031239869 a. u.			
6	-2.473926000	-0.545271000	0.001812000	6	3.087582000	-0.751215000	-0.000669000
6	-2.511118000	0.911617000	0.003594000	6	3.334570000	0.684280000	-0.000061000
6	-1.371934000	1.650787000	0.002742000	6	2.313759000	1.580823000	-0.000071000
6	-0.082873000	1.018335000	-0.000935000	6	0.948197000	1.140287000	-0.000153000
6	-0.047830000	-0.394353000	-0.004778000	6	0.707858000	-0.251377000	-0.000118000
6	1.155765000	-1.095885000	-0.006021000	6	-0.580219000	-0.778601000	-0.000022000
6	2.373928000	-0.396035000	-0.005403000	6	-1.702144000	0.081725000	-0.000005000
6	2.354075000	1.022354000	-0.001164000	6	-1.467390000	1.489151000	-0.000041000
6	1.149685000	1.703978000	0.001039000	6	-0.177223000	1.988740000	-0.000100000
1	-1.421459000	2.743597000	0.004796000	1	2.520825000	2.654980000	0.000113000
1	1.144686000	2.796819000	0.005998000	1	-0.020805000	3.070519000	-0.000095000
1	3.297872000	1.572510000	-0.004124000	1	-2.302715000	2.186396000	-0.000032000
1	1.127125000	-2.186961000	-0.010453000	1	-0.677664000	-1.861701000	0.000035000
8	-1.194334000	-1.130376000	-0.003112000	8	1.737961000	-1.145550000	-0.000214000
8	-3.420790000	-1.292510000	0.004325000	8	3.917544000	-1.627533000	0.000610000
7	3.577994000	-1.076421000	-0.065395000	7	-2.982793000	-0.424426000	0.000048000
1	3.563199000	-2.044868000	0.235326000	6	-4.126658000	0.470413000	0.000472000
1	4.394296000	-0.573606000	0.265046000	1	-4.143969000	1.121615000	0.893384000
1	-3.505325000	1.357393000	0.006165000	1	-4.144664000	1.121624000	-0.892427000
				1	-5.048087000	-0.124803000	0.000834000
				6	-3.195706000	-1.861233000	-0.000090000
				1	-4.273208000	-2.066635000	-0.000433000
				1	-2.756136000	-2.343162000	-0.892199000
				1	-2.756644000	-2.343329000	0.892192000
				1	4.382814000	0.982199000	0.000270000
D6-PhCH <sub>3</sub> E(RB3LYP) = -767.445767092 a. u.				D6-PhNH <sub>2</sub> E(RB3LYP) = -783.489103748 a. u.			
6	4.192978000	-1.109112000	-0.171516000	6	-4.186774000	-1.101584000	0.166698000
6	4.673718000	0.257464000	0.018934000	6	-4.664842000	0.266509000	-0.015938000
6	3.820289000	1.299155000	0.169517000	6	-3.807528000	1.306696000	-0.161160000
6	2.394725000	1.088256000	0.145689000	6	-2.383883000	1.092705000	-0.139316000
6	1.934658000	-0.232526000	-0.033763000	6	-1.925553000	-0.230031000	0.031486000
6	0.570840000	-0.526944000	-0.073093000	6	-0.563230000	-0.527898000	0.070015000
6	-0.379952000	0.494292000	0.069536000	6	0.393709000	0.490092000	-0.068558000
6	0.077426000	1.821619000	0.251804000	6	-0.064076000	1.820021000	-0.243372000
6	1.433763000	2.108757000	0.288341000	6	-1.419063000	2.111067000	-0.275795000

1	4.200965000	2.314574000	0.310363000	1	-4.185521000	2.324117000	-0.296047000
1	1.773321000	3.136406000	0.439355000	1	-1.755546000	3.140717000	-0.420760000
1	-0.647019000	2.624690000	0.393360000	1	0.660444000	2.623164000	-0.384046000
1	0.273081000	-1.561989000	-0.242411000	1	-0.270543000	-1.564803000	0.236586000
8	2.801908000	-1.275168000	-0.186249000	8	-2.796119000	-1.271526000	0.178977000
8	4.874876000	-2.093143000	-0.314491000	8	-4.870368000	-2.085653000	0.305121000
6	-4.619644000	-0.402666000	-0.042283000	6	4.630598000	-0.417997000	0.036855000
6	-3.703098000	-1.291293000	0.544242000	6	3.705394000	-1.330255000	-0.508360000
6	-4.114386000	0.784918000	-0.589052000	6	4.135519000	0.799005000	0.545440000
1	-4.065664000	-2.222353000	0.988739000	1	4.063098000	-2.276475000	-0.923237000
1	-4.800276000	1.493597000	-1.060722000	1	4.829435000	1.521635000	0.983445000
6	-2.340021000	-1.006343000	0.580224000	6	2.346681000	-1.034605000	-0.538146000
6	-2.749728000	1.077678000	-0.552387000	6	2.775089000	1.086984000	0.504488000
1	-1.660214000	-1.709377000	1.066092000	1	1.663363000	-1.757640000	-0.988274000
1	-2.390720000	2.001049000	-1.011727000	1	2.426847000	2.028819000	0.933579000
6	-1.832236000	0.187515000	0.032036000	6	1.841823000	0.180478000	-0.035125000
6	-6.093233000	-0.726054000	-0.079368000	7	5.995920000	-0.684147000	0.016077000
1	-6.492026000	-0.891848000	0.935486000	1	6.246422000	-1.667261000	-0.019790000
1	-6.674044000	0.085611000	-0.541576000	1	6.547178000	-0.180657000	0.703884000
1	-6.285567000	-1.647762000	-0.654319000	1	-5.747909000	0.387732000	-0.025926000
1	5.757301000	0.375598000	0.030109000				

**Table S9.** Cartesian coordinates (in Angstrom unit) of B3LYP/cc-pVDZ optimized geometries of benzene based D- $\pi$ -A systems.

D1 E(RB3LYP) = -749.742344106 a. u.				D1-CH <sub>3</sub> E(RB3LYP) = -784.652966670 a. u.			
6	6.357744000	0.474263000	-0.000036000	6	5.879651000	0.278923000	-0.000011000
6	6.024458000	-0.883126000	-0.000331000	6	5.491164000	-1.067794000	-0.000017000
6	5.340030000	1.437344000	0.000247000	6	4.864056000	1.255018000	-0.000002000
1	5.594396000	2.499522000	0.000491000	1	5.139039000	2.313274000	0.000009000
1	6.810777000	-1.641118000	-0.000591000	1	6.256206000	-1.848351000	-0.000032000
6	4.002990000	1.049874000	0.000329000	6	3.520504000	0.903004000	-0.000002000
6	4.685311000	-1.272498000	-0.000246000	6	4.143874000	-1.427760000	-0.000013000
1	3.226402000	1.816662000	0.000623000	1	2.766178000	1.691902000	-0.000005000
1	4.429107000	-2.335163000	-0.000423000	1	3.869024000	-2.485856000	-0.000019000
6	3.647030000	-0.317111000	0.000061000	6	3.125281000	-0.454166000	-0.000008000
6	2.264047000	-0.784335000	0.000099000	6	1.733239000	-0.886272000	-0.000009000
6	1.131312000	-0.031456000	0.000005000	6	0.618191000	-0.105869000	-0.000016000
6	-0.184398000	-0.605448000	0.000059000	6	-0.709954000	-0.647908000	-0.000008000

6	-1.344282000	0.116842000	-0.000028000	6	-1.853873000	0.100621000	-0.000010000
6	-2.630078000	-0.506022000	0.000036000	6	-3.152524000	-0.493063000	-0.000001000
6	-3.841555000	0.133352000	-0.000036000	6	-4.350585000	0.172341000	0.000000000
6	-3.942015000	1.559723000	-0.000198000	6	-4.420080000	1.600446000	-0.000010000
7	-3.985265000	2.724429000	-0.000252000	7	-4.437932000	2.765887000	-0.000011000
6	-5.077561000	-0.694270000	0.000052000	6	-5.603457000	-0.628131000	0.000015000
8	-5.093121000	-1.908081000	0.000188000	8	-5.646027000	-1.841529000	0.000019000
8	-6.197890000	0.059541000	-0.000017000	8	-6.707977000	0.149378000	0.000011000
1	-6.944066000	-0.567085000	0.000055000	1	-7.466640000	-0.461998000	0.000017000
1	2.143206000	-1.874036000	0.000198000	1	1.585425000	-1.972744000	0.000000000
1	1.192450000	1.061225000	-0.000132000	1	0.706214000	0.985001000	-0.000026000
1	-0.250525000	-1.700236000	0.000182000	1	-0.801796000	-1.740922000	0.000002000
1	-1.299745000	1.210638000	-0.000149000	1	-1.784530000	1.193120000	-0.000020000
1	-2.680426000	-1.599361000	0.000148000	1	-3.226949000	-1.585059000	0.000008000
1	7.405155000	0.783477000	-0.000071000	6	7.332292000	0.682939000	0.000040000
				1	7.575978000	1.293015000	0.886244000
				1	7.996893000	-0.193155000	-0.000387000
				1	7.575831000	1.293797000	-0.885658000
D1-C <sub>5</sub> H <sub>11</sub> E(RB3LYP) = -941.909101875 a. u.				D1-isopropyl E(RB3LYP) = -863.280577609 a. u.			
6	3.830108000	-1.001819000	0.000219000	6	5.002137000	-0.143311000	-0.000320000
6	3.217041000	-2.267629000	-0.000116000	6	4.543064000	-1.468362000	-0.001144000
6	2.991255000	0.125757000	0.000459000	6	4.035201000	0.881494000	0.000640000
1	3.423838000	1.126907000	0.000690000	1	4.353170000	1.926660000	0.001314000
1	3.842480000	-3.164760000	-0.000350000	1	5.268056000	-2.286651000	-0.001937000
6	1.603872000	-0.001793000	0.000415000	6	2.675164000	0.596205000	0.000783000
6	1.833202000	-2.401100000	-0.000152000	6	3.180124000	-1.762030000	-0.000977000
1	0.992766000	0.902680000	0.000627000	1	1.961555000	1.422177000	0.001620000
1	1.386740000	-3.399075000	-0.000401000	1	2.853019000	-2.805212000	-0.001618000
6	0.987990000	-1.269818000	0.000114000	6	2.211471000	-0.738537000	-0.000044000
6	-0.456277000	-1.465799000	0.000036000	6	0.799373000	-1.100078000	0.000024000
6	-1.427613000	-0.512290000	0.000076000	6	-0.274959000	-0.264554000	-0.000032000
6	-2.826614000	-0.828451000	-0.000008000	6	-1.628694000	-0.739152000	0.000046000
6	-3.832418000	0.097633000	0.000021000	6	-2.733585000	0.065857000	-0.000019000
6	-5.210585000	-0.275304000	-0.000068000	6	-4.060363000	-0.462007000	0.000065000
6	-6.283905000	0.577042000	-0.000049000	6	-5.223633000	0.262490000	0.000021000
6	-6.119013000	1.997272000	0.000065000	6	-5.221681000	1.692286000	-0.000109000
7	-5.946159000	3.149977000	0.000185000	7	-5.181243000	2.857161000	-0.000293000
6	-7.650589000	-0.007817000	-0.000153000	6	-6.514927000	-0.474413000	0.000112000

8	-7.891193000	-1.197945000	-0.000255000	8	-6.618016000	-1.684175000	0.000236000
8	-8.613363000	0.939735000	-0.000121000	8	-7.579253000	0.357264000	0.000060000
1	-9.461570000	0.460280000	-0.000195000	1	-8.367488000	-0.215481000	0.000133000
1	-0.781659000	-2.512939000	-0.000082000	1	0.597124000	-2.177742000	0.000057000
1	-1.160832000	0.549124000	0.000165000	1	-0.132099000	0.820490000	-0.000192000
1	-3.096798000	-1.891546000	-0.000102000	1	-1.775327000	-1.826173000	0.000167000
1	-3.584871000	1.163970000	0.000116000	1	-2.609521000	1.153500000	-0.000133000
1	-5.462683000	-1.340414000	-0.000163000	1	-4.189385000	-1.548903000	0.000176000
6	5.344929000	-0.912196000	0.000246000	6	6.491625000	0.168039000	-0.000348000
1	5.721634000	-1.470975000	-0.876845000	1	7.019564000	-0.801492000	-0.001649000
1	5.721579000	-1.470702000	0.877539000	6	6.917448000	0.925462000	1.270588000
6	5.960649000	0.489193000	0.000050000	6	6.916865000	0.928495000	-1.269661000
1	5.607751000	1.051143000	-0.883734000	1	6.644538000	0.372466000	-2.180565000
1	5.607928000	1.051320000	0.883792000	1	6.436833000	1.919821000	-1.324925000
6	7.492998000	0.462565000	-0.000083000	1	8.007768000	1.086795000	-1.278078000
1	7.849095000	-0.101873000	-0.882677000	1	6.437234000	1.916541000	1.328516000
1	7.849251000	-0.101733000	0.882537000	1	8.008331000	1.083915000	1.278763000
6	8.130332000	1.856059000	-0.000251000	1	6.645709000	0.367158000	2.180272000
1	7.773198000	2.418722000	-0.882541000				
1	7.773358000	2.418862000	0.882014000				
6	9.660202000	1.821422000	-0.000387000				
1	10.048779000	1.296050000	-0.889503000				
1	10.048941000	1.296193000	0.888742000				
1	10.087270000	2.837048000	-0.000508000				
D1-t-but E(RB3LYP) = -902.591347521 a. u.				D1-OH E(RB3LYP) = -820.563021181 a. u.			
6	-4.620590000	-0.036443000	-0.000065000	6	-5.880544000	0.285186000	0.000105000
6	-4.172749000	-1.366488000	0.000156000	6	-5.512938000	-1.068359000	0.000710000
6	-3.630879000	0.970291000	-0.000267000	6	-4.882300000	1.274636000	-0.000703000
1	-3.927548000	2.020934000	-0.000455000	1	-5.164217000	2.331814000	-0.001249000
1	-4.888461000	-2.187978000	0.000307000	1	-6.297154000	-1.826858000	0.001294000
6	-2.275260000	0.669947000	-0.000267000	6	-3.540319000	0.914862000	-0.000861000
6	-2.811804000	-1.675474000	0.000136000	6	-4.168018000	-1.415842000	0.000509000
1	-1.553390000	1.488735000	-0.000406000	1	-2.787401000	1.704709000	-0.001553000
1	-2.501903000	-2.723966000	0.000315000	1	-3.892287000	-2.473493000	0.000949000
6	-1.827290000	-0.669805000	-0.000053000	6	-3.144645000	-0.440895000	-0.000225000
6	-0.420742000	-1.051130000	-0.000056000	6	-1.755268000	-0.871744000	-0.000280000
6	0.664602000	-0.229950000	-0.000002000	6	-0.636818000	-0.093954000	-0.000060000
6	2.011975000	-0.722300000	-0.000031000	6	0.688441000	-0.639106000	-0.000165000



6	3.127421000	0.068047000	0.000021000	6	1.836290000	0.105114000	0.000036000
6	4.447087000	-0.477302000	-0.000020000	6	3.131638000	-0.493071000	-0.000082000
6	5.619879000	0.231714000	0.000019000	6	4.333475000	0.167201000	0.000079000
6	5.636910000	1.661406000	0.000107000	6	4.408482000	1.594867000	0.000394000
7	5.611986000	2.826719000	0.000182000	7	4.429775000	2.760350000	0.000626000
6	6.901279000	-0.522218000	-0.000032000	6	5.582080000	-0.638159000	-0.000084000
8	6.988385000	-1.733245000	-0.000104000	8	5.620460000	-1.851979000	-0.000359000
8	7.976558000	0.295277000	0.000012000	8	6.690732000	0.134316000	0.000086000
1	8.757100000	-0.287903000	-0.000025000	1	7.445821000	-0.481394000	-0.000047000
1	-0.233446000	-2.131505000	-0.000099000	1	-1.608121000	-1.958347000	-0.000463000
1	0.535797000	0.856867000	0.000081000	1	-0.721386000	0.997332000	0.000257000
1	2.144232000	-1.811167000	-0.000108000	1	0.777011000	-1.732477000	-0.000427000
1	3.017724000	1.157232000	0.000093000	1	1.771033000	1.197875000	0.000291000
1	4.561692000	-1.565814000	-0.000088000	1	3.201804000	-1.585388000	-0.000324000
6	-6.110358000	0.347807000	0.000040000	8	-7.207428000	0.577587000	0.000357000
6	-6.422416000	1.185432000	1.262532000	1	-7.320984000	1.539971000	-0.000027000
1	-6.213215000	0.611454000	2.179504000				
1	-5.826138000	2.109978000	1.301251000				
1	-7.486486000	1.473951000	1.275326000				
6	-6.422656000	1.185452000	-1.262404000				
1	-5.826439000	2.110029000	-1.301240000				
1	-6.213572000	0.611501000	-2.179423000				
1	-7.486744000	1.473920000	-1.275069000				
6	-7.031218000	-0.885768000	0.000063000				
1	-8.083907000	-0.562071000	0.000184000				
1	-6.878997000	-1.513330000	-0.892277000				
1	-6.878896000	-1.513435000	0.892317000				
D1-OCH <sub>3</sub> E(RB3LYP) = -859.864424848 a. u.				D1-OC <sub>2</sub> H <sub>5</sub> E(RB3LYP) = -899.184641823 a. u.			
6	5.422864000	-0.049373000	-0.000169000	6	4.912108000	-0.256222000	-0.000069000
6	4.993919000	-1.388844000	-0.000728000	6	4.446206000	-1.583696000	-0.000523000
6	4.464994000	0.980710000	0.000552000	6	3.980570000	0.798666000	0.000520000
1	4.768011000	2.027108000	0.001073000	1	4.310526000	1.836751000	0.000959000
1	5.749872000	-2.175663000	-0.001316000	1	5.180690000	-2.390600000	-0.000978000
6	3.108446000	0.666812000	0.000692000	6	2.616403000	0.520656000	0.000617000
6	3.639794000	-1.685500000	-0.000566000	6	3.084792000	-1.844685000	-0.000398000
1	2.387862000	1.486524000	0.001324000	1	1.917813000	1.359230000	0.001128000
1	3.322765000	-2.731570000	-0.000984000	1	2.740362000	-2.882088000	-0.000738000
6	2.655934000	-0.668571000	0.000115000	6	2.128164000	-0.802204000	0.000139000

6	1.250311000	-1.042245000	0.000207000	6	0.713292000	-1.138141000	0.000183000
6	0.164031000	-0.219756000	-0.000025000	6	-0.350920000	-0.287053000	0.000022000
6	-1.181839000	-0.711048000	0.000144000	6	-1.709160000	-0.742498000	0.000114000
6	-2.299298000	0.078447000	-0.000072000	6	-2.805631000	0.076112000	-0.000034000
6	-3.617152000	-0.467750000	0.000116000	6	-4.137194000	-0.435328000	0.000070000
6	-4.792280000	0.239335000	-0.000052000	6	-5.293657000	0.302114000	-0.000050000
6	-4.811179000	1.668808000	-0.000453000	6	-5.275376000	1.731575000	-0.000302000
7	-4.786845000	2.834254000	-0.000763000	7	-5.220776000	2.896009000	-0.000509000
6	-6.071343000	-0.516273000	0.000197000	6	-6.591799000	-0.419923000	0.000092000
8	-6.157651000	-1.727709000	0.000519000	8	-6.709769000	-1.628736000	0.000294000
8	-7.149056000	0.299041000	-0.000019000	8	-7.648099000	0.423085000	-0.000060000
1	-7.927449000	-0.286905000	0.000152000	1	-8.441298000	-0.142642000	0.000037000
1	1.058842000	-2.121983000	0.000442000	1	0.493075000	-2.212411000	0.000325000
1	0.292941000	0.867169000	-0.000396000	1	-0.193127000	0.796047000	-0.000220000
1	-1.314220000	-1.800009000	0.000473000	1	-1.870256000	-1.827599000	0.000320000
1	-2.190485000	1.167731000	-0.000391000	1	-2.668239000	1.162160000	-0.000235000
1	-3.730471000	-1.556444000	0.000427000	1	-4.278908000	-1.520697000	0.000265000
8	6.766375000	0.141547000	-0.000481000	8	6.258887000	-0.101001000	-0.000254000
6	7.266152000	1.472902000	0.000435000	6	6.811567000	1.220531000	0.000186000
1	6.946468000	2.027027000	-0.899389000	1	6.462803000	1.768549000	0.894598000
1	6.946500000	2.025749000	0.901068000	1	6.462494000	1.769282000	-0.893655000
1	8.359820000	1.382540000	0.000340000	6	8.321557000	1.080608000	-0.000136000
				1	8.661282000	0.533531000	-0.892912000
				1	8.661610000	0.532859000	0.892102000
				1	8.792926000	2.075710000	0.000151000
D1-NH <sub>2</sub> E(RB3LYP) = -800.698145256 a. u.				D1-N(CH <sub>3</sub> ) <sub>2</sub> E(RB3LYP) = -879.309419441 a. u.			
6	-5.892602000	0.286076000	-0.001512000	6	5.003777000	0.058963000	-0.000227000
6	-5.501881000	-1.069362000	0.000399000	6	4.562565000	-1.290235000	-0.000470000
6	-4.878896000	1.272298000	-0.004657000	6	4.001865000	1.069347000	0.000236000
1	-5.159831000	2.328768000	-0.008615000	1	4.283429000	2.121082000	0.000506000
1	-6.266452000	-1.850570000	0.000825000	1	5.282969000	-2.106518000	-0.000775000
6	-3.540230000	0.915994000	-0.005504000	6	2.655931000	0.744730000	0.000353000
6	-4.157456000	-1.414197000	-0.001036000	6	3.209342000	-1.594659000	-0.000323000
1	-2.789751000	1.708552000	-0.005426000	1	1.929025000	1.559177000	0.000735000
1	-3.881015000	-2.471906000	0.002527000	1	2.907740000	-2.645684000	-0.000511000
6	-3.134367000	-0.439612000	-0.003852000	6	2.209293000	-0.597312000	0.000054000
6	-1.747424000	-0.863999000	-0.002965000	6	0.813443000	-0.983475000	0.000152000
6	-0.628084000	-0.083507000	-0.004280000	6	-0.285375000	-0.172368000	-0.000039000

6	0.695271000	-0.627146000	-0.002687000	6	-1.621906000	-0.679272000	0.000119000
6	1.846523000	0.114908000	-0.002507000	6	-2.754087000	0.093199000	-0.000062000
6	3.138242000	-0.486638000	-0.000433000	6	-4.060257000	-0.473795000	0.000104000
6	4.344995000	0.167688000	0.000815000	6	-5.250755000	0.211272000	-0.000045000
6	4.427238000	1.594663000	0.000379000	6	-5.296442000	1.639725000	-0.000396000
7	4.454437000	2.760188000	0.000165000	7	-5.293635000	2.805656000	-0.000690000
6	5.587883000	-0.643369000	0.002935000	6	-6.513142000	-0.567439000	0.000169000
8	5.622002000	-1.857894000	0.003854000	8	-6.579228000	-1.780933000	0.000496000
8	6.702164000	0.122636000	0.003788000	8	-7.608371000	0.226415000	0.000023000
1	7.452058000	-0.499227000	0.005047000	1	-8.372900000	-0.377282000	0.000204000
1	-1.596011000	-1.950301000	-0.001064000	1	0.632229000	-2.065310000	0.000379000
1	-0.714875000	1.007571000	-0.006523000	1	-0.168174000	0.915877000	-0.000353000
1	0.783571000	-1.720727000	-0.001286000	1	-1.739865000	-1.770130000	0.000405000
1	1.783679000	1.207804000	-0.003809000	1	-2.662148000	1.184041000	-0.000340000
1	3.204075000	-1.579294000	0.000354000	1	-4.154515000	-1.564395000	0.000378000
7	-7.226929000	0.643964000	-0.056441000	7	6.342098000	0.378543000	-0.000452000
1	-7.459113000	1.582048000	0.250745000	6	7.343491000	-0.673714000	-0.000283000
1	-7.897484000	-0.052502000	0.249445000	1	7.263123000	-1.320431000	-0.892929000
				1	8.342521000	-0.220927000	-0.000448000
				1	7.263205000	-1.320211000	0.892557000
				6	6.763933000	1.768942000	0.000781000
				1	7.859911000	1.812571000	0.000689000
				1	6.402396000	2.311502000	-0.891498000
				1	6.402562000	2.309957000	0.894106000
D1-PhCH <sub>3</sub> E(RB3LYP) = -1015.72383802 a. u.				D1-PhNH <sub>2</sub> E(RB3LYP) = -1031.76723247 a. u.			
6	-3.549888000	-0.282080000	0.035942000	6	3.561835000	-0.279931000	-0.037216000
6	-3.060090000	-1.594675000	0.177110000	6	3.067049000	-1.593170000	-0.171453000
6	-2.601615000	0.757767000	-0.075954000	6	2.610709000	0.760309000	0.068256000
1	-2.946094000	1.784369000	-0.213877000	1	2.953393000	1.787938000	0.202594000
1	-3.762094000	-2.422475000	0.293381000	1	3.766305000	-2.423432000	-0.286118000
6	-1.237001000	0.501852000	-0.048322000	6	1.246615000	0.505775000	0.040471000
6	-1.693310000	-1.852850000	0.205253000	6	1.700772000	-1.850220000	-0.196724000
1	-0.542265000	1.337631000	-0.148353000	1	0.552868000	1.343146000	0.135036000
1	-1.343751000	-2.881566000	0.325871000	1	1.350801000	-2.879607000	-0.311395000
6	-0.744448000	-0.814606000	0.093696000	6	0.751207000	-0.811152000	-0.092587000
6	0.673430000	-1.144654000	0.129160000	6	-0.665238000	-1.139395000	-0.126058000
6	1.730213000	-0.291468000	0.033042000	6	-1.723120000	-0.285414000	-0.033874000
6	3.093415000	-0.734070000	0.080371000	6	-3.084897000	-0.728731000	-0.078415000

6	4.180579000	0.089859000	-0.013118000	6	-4.174596000	0.093676000	0.012059000
6	5.518572000	-0.405577000	0.040247000	6	-5.510413000	-0.404897000	-0.038379000
6	6.665455000	0.339987000	-0.044450000	6	-6.660698000	0.337197000	0.044028000
6	6.631554000	1.760569000	-0.202571000	6	-6.631556000	1.758334000	0.196616000
7	6.565099000	2.917117000	-0.331284000	7	-6.568921000	2.915683000	0.320825000
6	7.972914000	-0.363683000	0.032030000	6	-7.964843000	-0.370904000	-0.028893000
8	8.103018000	-1.563438000	0.165472000	8	-8.092110000	-1.571814000	-0.157478000
8	9.018337000	0.486202000	-0.064127000	8	-9.014138000	0.475433000	0.064389000
1	9.819221000	-0.065439000	-0.003860000	1	-9.812067000	-0.080624000	0.006552000
1	0.898499000	-2.211218000	0.247214000	1	-0.891443000	-2.206450000	-0.238533000
1	1.563928000	0.783616000	-0.086447000	1	-1.556725000	0.790236000	0.080256000
1	3.263785000	-1.810949000	0.200290000	1	-3.254233000	-1.806399000	-0.193472000
1	4.032470000	1.167827000	-0.133220000	1	-4.028538000	1.172438000	0.127415000
1	5.671759000	-1.482683000	0.160065000	1	-5.660583000	-1.482948000	-0.153769000
6	-7.276455000	-0.631112000	-0.627431000	6	7.295123000	-0.658804000	0.583411000
6	-7.805286000	0.536629000	-0.052444000	6	7.816629000	0.537636000	0.052263000
6	-6.907031000	1.428036000	0.550467000	6	6.911060000	1.460161000	-0.508703000
6	-5.909435000	-0.897176000	-0.598857000	6	5.928958000	-0.917211000	0.548842000
6	-5.535688000	1.168353000	0.578909000	6	5.546261000	1.193916000	-0.532126000
6	-5.005619000	-0.001147000	0.005646000	6	5.014036000	-0.000879000	-0.007241000
1	-7.948929000	-1.342466000	-1.115051000	1	7.973320000	-1.388280000	1.034444000
1	-4.870715000	1.874390000	1.080748000	1	4.879729000	1.923389000	-0.996829000
1	-7.287371000	2.341722000	1.014848000	1	7.289362000	2.390343000	-0.941230000
1	-5.532009000	-1.802292000	-1.079446000	1	5.560765000	-1.842939000	0.995933000
6	-9.288658000	0.811692000	-0.087689000	7	9.187150000	0.772838000	0.025971000
1	-9.664343000	0.846192000	-1.124196000	1	9.729153000	0.268037000	0.720105000
1	-9.854667000	0.020577000	0.432659000	1	9.460896000	1.748778000	-0.029518000
1	-9.533615000	1.770970000	0.391371000				

**Table S10.** Cartesian coordinates (in Angstrom unit) of B3LYP/cc-pVDZ optimized geometries of pyrene based D- $\pi$ -A systems.

D2 E(RB3LYP) = -1128.88061603 a. u.				D2-CH <sub>3</sub> E(RB3LYP) = -1168.19847043 a. u.			
6	5.631431000	-0.482809000	0.000042000	6	6.028999000	-0.442115000	0.000408000
6	6.794548000	0.241238000	0.000050000	6	7.182210000	0.298062000	0.000255000
6	6.792874000	1.671097000	0.000047000	6	7.160963000	1.727725000	0.000303000
7	6.753355000	2.835964000	0.000067000	7	7.104949000	2.891941000	0.000299000
6	8.086100000	-0.496085000	0.000066000	6	8.483597000	-0.421287000	-0.000064000

8	8.188399000	-1.705762000	-0.000094000	8	8.602905000	-1.629490000	-0.000203000
8	9.150128000	0.335591000	-0.000116000	8	9.536326000	0.424859000	-0.000322000
1	9.938765000	-0.236697000	-0.000238000	1	10.332479000	-0.136843000	-0.000558000
6	1.846208000	-0.278144000	0.000027000	6	2.241320000	-0.292033000	0.000563000
1	1.707212000	0.807262000	0.000026000	1	2.086150000	0.791219000	0.001024000
1	5.759735000	-1.569731000	0.000042000	1	6.172453000	-1.527179000	0.000298000
6	3.199068000	-0.756705000	0.000034000	6	3.600778000	-0.750648000	0.000607000
6	4.304796000	0.046504000	0.000039000	6	4.695225000	0.068326000	0.000595000
1	3.343169000	-1.843955000	0.000034000	1	3.760674000	-1.835744000	0.000581000
1	4.182140000	1.134273000	0.000039000	1	4.557084000	1.154265000	0.000740000
6	0.769783000	-1.109983000	0.000022000	6	1.177123000	-1.139972000	-0.000128000
1	0.967885000	-2.188064000	0.000021000	1	1.391716000	-2.214976000	-0.000500000
6	-2.922325000	2.275872000	0.000047000	6	-3.543471000	-2.646471000	-0.000101000
6	-2.451847000	0.912872000	0.000027000	6	-2.565824000	-1.589029000	-0.000116000
6	-4.254262000	2.564971000	0.000038000	6	-4.880664000	-2.374341000	-0.000203000
6	-3.419803000	-0.142496000	-0.000002000	6	-3.024977000	-0.235576000	-0.000274000
6	-5.249521000	1.523235000	0.000009000	6	-5.370337000	-1.020705000	-0.000156000
6	-4.813329000	0.160848000	-0.000011000	6	-4.421658000	0.046591000	-0.000227000
1	-2.182371000	3.079899000	0.000069000	1	-3.190484000	-3.680678000	-0.000045000
6	-1.088668000	0.595172000	0.000035000	6	-1.185719000	-1.838530000	-0.000094000
6	-2.979875000	-1.502426000	-0.000021000	6	-2.073520000	0.834683000	-0.000493000
6	-5.775770000	-0.897442000	-0.000039000	6	-4.883047000	1.400119000	-0.000361000
6	-1.603917000	-1.772518000	-0.000011000	6	-0.706302000	0.537545000	-0.000671000
6	-0.642877000	-0.742768000	0.000016000	6	-0.240506000	-0.794393000	-0.000310000
1	-0.365969000	1.413183000	0.000059000	1	-0.835504000	-2.874327000	0.000068000
6	-3.971107000	-2.547360000	-0.000049000	6	-2.567339000	2.190229000	-0.000647000
1	-1.269659000	-2.813474000	-0.000025000	1	0.004619000	1.365941000	-0.000767000
6	-6.627889000	1.796990000	-0.000001000	6	-6.743490000	-0.714369000	-0.000168000
6	-7.144523000	-0.573580000	-0.000048000	6	-6.263107000	1.649780000	-0.000335000
6	-7.561917000	0.758235000	-0.000029000	6	-7.203601000	0.607136000	-0.000111000
1	-4.592404000	3.604141000	0.000053000	1	-5.608437000	-3.189646000	-0.000273000
6	-5.303864000	-2.257474000	-0.000058000	6	-3.903624000	2.458262000	-0.000655000
1	-3.631385000	-3.585930000	-0.000064000	1	-1.840657000	3.006380000	-0.000800000
1	-7.882280000	-1.379564000	-0.000070000	1	-6.610455000	2.687096000	-0.000616000
1	-8.629054000	0.990739000	-0.000036000	1	-4.257673000	3.492194000	-0.000828000
1	-6.042950000	-3.062449000	-0.000080000	1	-7.465589000	-1.535547000	-0.000326000
1	-6.964432000	2.836519000	0.000014000	6	-8.681279000	0.918736000	0.001740000
				1	-8.964935000	1.497236000	0.896956000
				1	-8.961664000	1.525473000	-0.875419000
				1	-9.288742000	0.002245000	-0.013562000

D2-C <sub>5</sub> H <sub>11</sub> E(RB3LYP) = -1325.45460791 a. u.				D2-isopropyl E(RB3LYP) = -1246.82605409 a. u.			
6	7.725450000	-0.485844000	-0.000177000	6	-6.760441000	0.341859000	-0.000072000
6	8.888181000	0.239443000	-0.000077000	6	-7.887607000	-0.437430000	0.000198000
6	8.885324000	1.669247000	0.000130000	6	-7.817260000	-1.865522000	0.000638000
7	8.844256000	2.834094000	0.000295000	7	-7.721168000	-3.027117000	0.000999000
6	10.180060000	-0.496581000	-0.000189000	6	-9.212862000	0.236849000	0.000021000
8	10.283934000	-1.706248000	-0.000355000	8	-9.373577000	1.440250000	-0.000352000
8	11.243739000	0.335882000	-0.000063000	8	-10.235976000	-0.644912000	0.000317000
1	12.032434000	-0.236234000	-0.000141000	1	-11.050898000	-0.110801000	0.000169000
6	3.939976000	-0.289062000	-0.000148000	6	-2.969842000	0.322267000	-0.000160000
1	3.797642000	0.795933000	0.000034000	1	-2.777305000	-0.754957000	0.000194000
1	7.855061000	-1.572658000	-0.000336000	1	-6.941046000	1.421366000	-0.000404000
6	5.293754000	-0.763963000	-0.000218000	6	-4.344348000	0.733654000	-0.000254000
6	6.398339000	0.041389000	-0.000096000	6	-5.409948000	-0.122496000	0.000041000
1	5.440388000	-1.850947000	-0.000383000	1	-4.541536000	1.812601000	-0.000590000
1	6.273787000	1.128972000	0.000068000	1	-5.234575000	-1.203049000	0.000373000
6	2.865821000	-1.124460000	-0.000281000	6	-1.935665000	1.206547000	-0.000449000
1	3.067867000	-2.201888000	-0.000422000	1	-2.187347000	2.273463000	-0.000718000
6	-1.872047000	-2.576591000	0.000173000	6	2.729572000	2.877363000	0.000349000
6	-0.881923000	-1.531109000	0.000002000	6	1.789298000	1.786329000	0.000017000
6	-3.206078000	-2.288125000	0.000247000	6	4.075408000	2.652166000	0.000462000
6	-1.325297000	-0.172552000	-0.000089000	6	2.295289000	0.449741000	-0.000184000
6	-3.679963000	-0.928984000	0.000155000	6	4.611946000	1.316267000	0.000241000
6	-2.718538000	0.125292000	-0.000015000	6	3.700987000	0.216663000	-0.000067000
1	-1.531685000	-3.615022000	0.000243000	1	2.340574000	3.898581000	0.000505000
6	0.495532000	-1.796261000	-0.000080000	6	0.401340000	1.987344000	-0.000107000
6	-0.362021000	0.887150000	-0.000265000	6	1.382158000	-0.653329000	-0.000524000
6	-3.165366000	1.483614000	-0.000115000	6	4.210221000	-1.119005000	-0.000293000
6	1.001564000	0.574653000	-0.000334000	6	0.005231000	-0.404245000	-0.000624000
6	1.452265000	-0.762809000	-0.000232000	6	-0.506764000	0.910555000	-0.000393000
1	0.833995000	-2.835939000	-0.000012000	1	0.015118000	3.010229000	0.000049000
6	-0.841146000	2.248343000	-0.000369000	6	1.923610000	-1.990497000	-0.000762000
1	1.721914000	1.394833000	-0.000495000	1	-0.676290000	-1.256951000	-0.000935000
6	-5.051638000	-0.609875000	0.000226000	6	5.994324000	1.056540000	0.000347000
6	-4.541865000	1.746009000	-0.000038000	6	5.598775000	-1.321360000	-0.000184000
6	-5.498754000	0.716032000	0.000134000	6	6.503984000	-0.247553000	0.000145000
1	-3.943398000	-3.094884000	0.000377000	1	4.774262000	3.492405000	0.000722000
6	-2.174248000	2.531267000	-0.000295000	6	3.268678000	-2.210923000	-0.000651000
1	-0.105396000	3.056349000	-0.000506000	1	1.226355000	-2.831921000	-0.001038000

1	-4.878029000	2.787292000	-0.000115000	1	5.972204000	-2.348561000	-0.000330000
1	-2.516815000	3.569081000	-0.000373000	1	3.658935000	-3.231781000	-0.000842000
1	-5.769975000	-1.431220000	0.000356000	1	6.687225000	1.902858000	0.000580000
6	-6.971844000	1.090541000	0.000215000	6	8.009280000	-0.486958000	0.000288000
1	-7.161579000	1.736083000	-0.877315000	1	8.489117000	0.507136000	0.000330000
1	-7.161475000	1.736116000	0.877745000	6	8.472543000	-1.222998000	-1.269558000
6	-7.983580000	-0.057892000	0.000298000	6	8.472235000	-1.222897000	1.270341000
1	-7.817893000	-0.700510000	-0.883456000	1	8.171638000	-0.679834000	2.180222000
1	-7.817820000	-0.700451000	0.884082000	1	8.042479000	-2.236976000	1.327436000
6	-9.436035000	0.431333000	0.000345000	1	9.569766000	-1.326505000	1.279746000
1	-9.604821000	1.076967000	-0.882252000	1	8.042854000	-2.237107000	-1.326673000
1	-9.604742000	1.077030000	0.882911000	1	9.570077000	-1.326592000	-1.278765000
6	-10.465189000	-0.703873000	0.000431000	1	8.172136000	-0.680074000	-2.179592000
1	-10.295263000	-1.348332000	-0.881856000				
1	-10.295186000	-1.348268000	0.882751000				
6	-11.913006000	-0.208185000	0.000477000				
1	-12.124616000	0.410021000	-0.888656000				
1	-12.124538000	0.410086000	0.889582000				
1	-12.627406000	-1.047019000	0.000539000				
D2-t-but E(RB3LYP) = -1286.13661914 a. u.				D2-OH E(RB3LYP) = -1204.10771937 a. u.			
6	7.088336000	-0.360998000	-0.000016000	6	-6.016413000	-0.445604000	0.000043000
6	8.219790000	0.412094000	0.000154000	6	-7.170803000	0.293087000	-0.000059000
6	8.157313000	1.840548000	0.000374000	6	-7.151227000	1.722740000	-0.000242000
7	8.067694000	3.002664000	0.000550000	7	-7.096240000	2.887029000	-0.000393000
6	9.541298000	-0.269439000	0.000107000	6	-8.471055000	-0.427847000	0.000028000
8	9.695450000	-1.473709000	-0.000075000	8	-8.589021000	-1.636241000	0.000167000
8	10.569266000	0.606684000	0.000295000	8	-9.525063000	0.416896000	-0.000107000
1	11.381210000	0.068062000	0.000249000	1	-10.320291000	-0.146100000	-0.000052000
6	3.297927000	-0.320603000	-0.000148000	6	-2.229158000	-0.290962000	0.000054000
1	3.111361000	0.757665000	0.000016000	1	-2.075493000	0.792524000	-0.000098000
1	7.263025000	-1.441478000	-0.000177000	1	-6.158539000	-1.530853000	0.000183000
6	4.670118000	-0.739559000	-0.000168000	6	-3.587773000	-0.751140000	0.000103000
6	5.740432000	0.110729000	0.000002000	6	-4.683519000	0.066418000	-0.000014000
1	4.861375000	-1.819576000	-0.000326000	1	-3.746331000	-1.836451000	0.000245000
1	5.570975000	1.192227000	0.000161000	1	-4.546753000	1.152540000	-0.000156000
6	2.258822000	-1.199127000	-0.000297000	6	-1.163510000	-1.137485000	0.000172000
1	2.504550000	-2.267431000	-0.000414000	1	-1.376824000	-2.212751000	0.000291000
6	-2.417290000	-2.842143000	0.000133000	6	3.558813000	-2.640515000	-0.000136000

6	-1.469256000	-1.757924000	-0.000069000	6	2.580046000	-1.583233000	-0.000018000
6	-3.761802000	-2.607227000	0.000223000	6	4.895399000	-2.370375000	-0.000186000
6	-1.966544000	-0.418393000	-0.000203000	6	3.039982000	-0.229701000	0.000046000
6	-4.289311000	-1.267679000	0.000083000	6	5.387456000	-1.015680000	-0.000121000
6	-3.370483000	-0.177400000	-0.000139000	6	4.435377000	0.053300000	-0.000002000
1	-2.035805000	-3.866184000	0.000203000	1	3.205931000	-3.674809000	-0.000186000
6	-0.082233000	-1.966935000	-0.000121000	6	1.201368000	-1.833731000	0.000038000
6	-1.047908000	0.679890000	-0.000395000	6	2.086370000	0.838682000	0.000168000
6	-3.873986000	1.159291000	-0.000278000	6	4.894566000	1.407000000	0.000069000
6	0.327356000	0.423008000	-0.000433000	6	0.718897000	0.540626000	0.000214000
6	0.831612000	-0.895148000	-0.000287000	6	0.253319000	-0.790680000	0.000142000
1	0.298374000	-2.991923000	-0.000020000	1	0.852607000	-2.870051000	-0.000009000
6	-1.583302000	2.020017000	-0.000547000	6	2.578447000	2.193489000	0.000243000
1	1.014006000	1.271583000	-0.000598000	1	0.007914000	1.369008000	0.000328000
6	-5.672322000	-1.003307000	0.000157000	6	6.757508000	-0.719507000	-0.000168000
6	-5.260562000	1.366429000	-0.000196000	6	6.274555000	1.663508000	0.000018000
6	-6.181468000	0.302106000	0.000022000	6	7.196891000	0.609683000	-0.000100000
1	-4.466157000	-3.442951000	0.000370000	1	5.622679000	-3.185773000	-0.000277000
6	-2.927185000	2.247240000	-0.000506000	6	3.914773000	2.463726000	0.000194000
1	-0.881917000	2.858010000	-0.000680000	1	1.851659000	3.009566000	0.000339000
1	-5.620861000	2.397499000	-0.000252000	1	6.628858000	2.699059000	0.000071000
1	-3.312211000	3.270119000	-0.000634000	1	4.266323000	3.498486000	0.000250000
1	-6.348673000	-1.858132000	0.000313000	1	7.501456000	-1.518206000	-0.000257000
6	-7.693391000	0.603552000	0.000249000	8	8.544356000	0.816825000	-0.000153000
6	-8.053038000	1.421577000	-1.261919000	1	8.716453000	1.769972000	-0.000089000
1	-7.510186000	2.378484000	-1.301386000				
1	-7.811181000	0.860193000	-2.178699000				
1	-9.131790000	1.649459000	-1.275349000				
6	-8.545784000	-0.678397000	0.000213000				
1	-8.359628000	-1.296810000	-0.892035000				
1	-8.359821000	-1.296771000	0.892522000				
1	-9.614427000	-0.412181000	0.000109000				
6	-8.052561000	1.421258000	1.262793000				
1	-9.131274000	1.649316000	1.276629000				
1	-7.810499000	0.859556000	2.179319000				
1	-7.509496000	2.378042000	1.302334000				
D2-OCH <sub>3</sub> E(RB3LYP) = -1243.40889665 a. u.				D2-OC <sub>2</sub> H <sub>5</sub> E(RB3LYP) = -1282.72902623 a. u.			
6	6.399672000	-0.371656000	0.000069000	6	6.813958000	-0.307504000	0.000008000



6	7.535746000	0.395084000	-0.000067000	6	7.936277000	0.479325000	-0.000090000
6	7.481230000	1.823814000	-0.000200000	6	7.856361000	1.906851000	-0.000236000
7	7.397908000	2.986429000	-0.000305000	7	7.752407000	3.067809000	-0.000357000
6	8.853120000	-0.293782000	-0.000077000	6	9.265622000	-0.185982000	-0.000041000
8	9.000803000	-1.498950000	0.000038000	8	9.434819000	-1.388342000	0.000072000
8	9.886293000	0.576447000	-0.000211000	8	10.283235000	0.702462000	-0.000158000
1	10.694896000	0.032851000	-0.000199000	1	11.101295000	0.173214000	-0.000123000
6	2.609833000	-0.311384000	0.000178000	6	3.023689000	-0.315715000	0.000061000
1	2.428732000	0.767850000	0.000129000	1	2.822785000	0.760009000	-0.000054000
1	6.568414000	-1.453092000	0.000162000	1	7.001953000	-1.385763000	0.000118000
6	3.979456000	-0.737247000	0.000201000	6	4.400785000	-0.716515000	0.000085000
6	5.054673000	0.107295000	0.000082000	6	5.460662000	0.147280000	-0.000020000
1	4.165111000	-1.818265000	0.000318000	1	4.606004000	-1.794000000	0.000195000
1	4.891028000	1.189690000	-0.000009000	1	5.277598000	1.226557000	-0.000128000
6	1.565914000	-1.184709000	0.000176000	6	1.995979000	-1.208145000	0.000160000
1	1.806723000	-2.254173000	0.000178000	1	2.256611000	-2.272966000	0.000245000
6	-3.115866000	-2.810960000	-0.000108000	6	-2.654502000	-2.921651000	-0.000107000
6	-2.164250000	-1.727969000	0.000016000	6	-1.723251000	-1.821090000	0.000002000
6	-4.458570000	-2.576056000	-0.000179000	6	-4.001371000	-2.711794000	-0.000141000
6	-2.659058000	-0.386625000	0.000066000	6	-2.243081000	-0.489208000	0.000084000
6	-4.985653000	-1.233703000	-0.000121000	6	-4.553435000	-1.379510000	-0.000089000
6	-4.061293000	-0.139836000	0.000005000	6	-3.649622000	-0.268752000	0.000044000
1	-2.735707000	-3.835564000	-0.000138000	1	-2.255278000	-3.938986000	-0.000163000
6	-0.780159000	-1.942427000	0.000062000	6	-0.335403000	-2.009582000	0.000043000
6	-1.734128000	0.706446000	0.000179000	6	-1.338783000	0.621046000	0.000222000
6	-4.557369000	1.198516000	0.000062000	6	-4.170997000	1.059938000	0.000198000
6	-0.358750000	0.443948000	0.000206000	6	0.041245000	0.384350000	0.000244000
6	0.140738000	-0.874387000	0.000158000	6	0.565335000	-0.924453000	0.000147000
1	-0.404166000	-2.969183000	0.000003000	1	0.059762000	-3.029117000	-0.000015000
6	-2.262232000	2.047032000	0.000236000	6	-1.892060000	1.951483000	0.000330000
1	0.330472000	1.290536000	0.000320000	1	0.714518000	1.243687000	0.000364000
6	-6.359303000	-0.969891000	-0.000181000	6	-5.931686000	-1.141035000	-0.000121000
6	-5.945627000	1.427404000	-0.000003000	6	-5.563172000	1.263105000	0.000156000
6	-6.840295000	0.349108000	-0.000123000	6	-6.438756000	0.168514000	-0.000106000
1	-5.164690000	-3.409881000	-0.000286000	1	-4.691812000	-3.558671000	-0.000217000
6	-3.605998000	2.280505000	0.000182000	6	-3.239983000	2.159599000	0.000319000
1	-1.557985000	2.882640000	0.000345000	1	-1.203653000	2.800194000	0.000438000
1	-6.305039000	2.456139000	0.000039000	1	-5.940933000	2.285136000	0.000387000
1	-3.985281000	3.305483000	0.000233000	1	-3.638481000	3.177271000	0.000393000
1	-7.085305000	-1.785053000	-0.000277000	1	-6.641993000	-1.969920000	-0.000222000
8	-8.196932000	0.472595000	-0.000193000	8	-7.796179000	0.266744000	-0.000048000

6	-8.759896000	1.776068000	-0.000083000	6	-8.401468000	1.561939000	-0.000017000
1	-8.468640000	2.346477000	0.899782000	1	-8.077351000	2.126391000	0.894019000
1	-8.468615000	2.346642000	-0.899836000	1	-8.076789000	2.126734000	-0.893613000
1	-9.848239000	1.633618000	-0.000112000	6	-9.904857000	1.360262000	-0.000505000
				1	-10.221855000	0.798627000	0.891665000
				1	-10.221339000	0.798834000	-0.892981000
				1	-10.417785000	2.334672000	-0.000516000
D2-NH <sub>2</sub> E(RB3LYP) = -1184.24159401 a. u.				D2-N(CH <sub>3</sub> ) <sub>2</sub> E(RB3LYP) = -1262.85188298 a. u.			
6	6.021580000	-0.442570000	0.000364000	6	-6.762189000	-0.383642000	0.006482000
6	7.178643000	0.292961000	0.001804000	6	-7.905268000	0.374028000	0.006218000
6	7.163195000	1.722562000	0.002954000	6	-7.862434000	1.803000000	0.001159000
7	7.111774000	2.887073000	0.003969000	7	-7.788867000	2.966352000	-0.003119000
6	8.476174000	-0.431428000	0.002282000	6	-9.216092000	-0.325192000	0.011387000
8	8.591585000	-1.640303000	0.001568000	8	-9.355166000	-1.531692000	0.015919000
8	9.533311000	0.410053000	0.003578000	8	-10.257291000	0.536284000	0.010520000
1	10.326129000	-0.156255000	0.003708000	1	-11.060393000	-0.015285000	0.014116000
6	2.235065000	-0.284305000	-0.001818000	6	-2.973608000	-0.301479000	-0.001536000
1	2.080767000	0.799070000	-0.001723000	1	-2.796856000	0.778444000	-0.005701000
1	6.161173000	-1.528176000	-0.000289000	1	-6.922837000	-1.466340000	0.010597000
6	3.592862000	-0.744433000	-0.001320000	6	-4.340083000	-0.733616000	0.002723000
6	4.690342000	0.071794000	-0.000297000	6	-5.421498000	0.104351000	0.002009000
1	3.750847000	-1.829900000	-0.001682000	1	-4.520012000	-1.815691000	0.006862000
1	4.555143000	1.158105000	0.000116000	1	-5.264780000	1.187756000	-0.002093000
6	1.169211000	-1.131687000	-0.002197000	6	-1.925177000	-1.170957000	-0.000601000
1	1.384075000	-2.206736000	-0.002116000	1	-2.162778000	-2.241249000	0.003469000
6	-3.551345000	-2.639730000	0.000786000	6	2.763542000	-2.778194000	-0.004272000
6	-2.572719000	-1.582731000	-0.001017000	6	1.805555000	-1.701921000	-0.006948000
6	-4.888304000	-2.369450000	0.001103000	6	4.105544000	-2.534432000	-0.007215000
6	-3.034714000	-0.229445000	-0.002788000	6	2.295583000	-0.358609000	-0.012555000
6	-5.381678000	-1.015137000	-0.001054000	6	4.626893000	-1.189758000	-0.014949000
6	-4.428968000	0.051803000	-0.003204000	6	3.694713000	-0.107240000	-0.017060000
1	-3.198602000	-3.674164000	0.001676000	1	2.390481000	-3.805507000	0.000533000
6	-1.193787000	-1.831593000	-0.001089000	6	0.421911000	-1.921464000	-0.003305000
6	-2.081922000	0.840509000	-0.004032000	6	1.366290000	0.731759000	-0.012461000
6	-4.894049000	1.404463000	-0.004256000	6	4.192215000	1.231877000	-0.020240000
6	-0.714926000	0.544204000	-0.003899000	6	-0.006479000	0.464797000	-0.008735000
6	-0.247053000	-0.787284000	-0.002478000	6	-0.502512000	-0.856864000	-0.004442000
1	-0.843460000	-2.867473000	0.000045000	1	0.049358000	-2.949589000	0.000814000

6	-2.577356000	2.194864000	-0.005395000	6	1.892827000	2.074776000	-0.015182000
1	-0.004670000	1.373296000	-0.005064000	1	-0.699211000	1.308621000	-0.008759000
6	-6.751107000	-0.717403000	0.000910000	6	6.002756000	-0.925906000	-0.017576000
6	-6.270642000	1.660436000	-0.002507000	6	5.572681000	1.463069000	-0.022757000
6	-7.210753000	0.612200000	-0.000174000	6	6.506073000	0.397172000	-0.030927000
1	-5.614295000	-3.186393000	0.002169000	1	4.814735000	-3.366162000	-0.004787000
6	-3.913789000	2.462738000	-0.005210000	6	3.234966000	2.312124000	-0.017958000
1	-1.851840000	3.012192000	-0.006854000	1	1.186150000	2.908494000	-0.014619000
1	-6.620930000	2.696488000	-0.007084000	1	5.916387000	2.496489000	-0.020323000
1	-4.266978000	3.496995000	-0.006602000	1	3.610980000	3.338441000	-0.019648000
1	-7.475388000	-1.536876000	-0.000762000	1	6.684405000	-1.775265000	-0.010924000
7	-8.573911000	0.888397000	-0.060922000	7	7.868009000	0.642801000	-0.053674000
1	-8.848159000	1.801033000	0.288606000	6	8.804523000	-0.459315000	0.067798000
1	-9.181775000	0.154468000	0.288539000	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
D2-PhCH <sub>3</sub> E(RB3LYP) = -1399.26883364 a. u.				D2-PhNH <sub>2</sub> E(RB3LYP) = -1415.31174049 a. u.			
6	7.970684000	0.256951000	-0.011199000	6	7.965555000	0.258597000	-0.009841000
6	9.083072000	-0.541902000	0.034482000	6	9.080090000	-0.537839000	0.035485000
6	8.986124000	-1.966281000	0.112892000	6	8.986431000	-1.962431000	0.112975000
7	8.868416000	-3.124131000	0.176546000	7	8.871553000	-3.120642000	0.175912000
6	10.420749000	0.106699000	0.000740000	6	10.415897000	0.113689000	0.002351000
8	10.603771000	1.305078000	-0.065090000	8	10.596765000	1.312577000	-0.062601000
8	11.427153000	-0.792555000	0.051900000	8	11.424780000	-0.783195000	0.052973000
1	12.251979000	-0.274581000	0.024607000	1	12.247971000	-0.262658000	0.026064000
6	4.180356000	0.307124000	-0.018307000	6	4.175503000	0.304064000	-0.017693000
1	3.968014000	-0.764773000	0.040414000	1	3.963602000	-0.767952000	0.040247000
1	8.171310000	1.331295000	-0.070181000	1	8.164044000	1.333395000	-0.068095000
6	5.562233000	0.692602000	-0.038199000	6	5.556652000	0.690564000	-0.036998000
6	6.611757000	-0.181739000	0.011165000	6	6.607791000	-0.182381000	0.011991000
1	5.779293000	1.766105000	-0.097054000	1	5.772624000	1.764369000	-0.095099000
1	6.416418000	-1.257246000	0.070206000	1	6.414052000	-1.258214000	0.070260000
6	3.162680000	1.208967000	-0.068359000	6	3.157087000	1.205628000	-0.067421000
1	3.433994000	2.269476000	-0.126055000	1	3.428427000	2.266226000	-0.124316000
6	-1.470537000	2.964497000	-0.161448000	6	-1.475992000	2.961372000	-0.160546000

6	-0.550565000	1.857272000	-0.102224000	6	-0.555625000	1.854385000	-0.101837000
6	-2.819922000	2.765566000	-0.148339000	6	-2.825360000	2.762029000	-0.147996000
6	-1.081652000	0.532185000	-0.031266000	6	-1.086984000	0.529073000	-0.032199000
6	-3.382265000	1.441426000	-0.073643000	6	-3.388045000	1.437782000	-0.074401000
6	-2.490964000	0.325768000	-0.019346000	6	-2.495866000	0.322748000	-0.020984000
1	-1.062275000	3.976611000	-0.217166000	1	-1.067964000	3.973669000	-0.215491000
6	0.840391000	2.031992000	-0.112301000	6	0.835197000	2.029014000	-0.111277000
6	-0.189257000	-0.586256000	0.027806000	6	-0.194368000	-0.589558000	0.026157000
6	-3.024547000	-0.998256000	0.046889000	6	-3.030560000	-1.000941000	0.043698000
6	1.192242000	-0.363168000	0.015409000	6	1.186989000	-0.366547000	0.014337000
6	1.728616000	0.939760000	-0.054190000	6	1.723531000	0.936591000	-0.053894000
1	1.245695000	3.046001000	-0.166476000	1	1.240652000	3.043064000	-0.164413000
6	-0.755278000	-1.911047000	0.099406000	6	-0.760944000	-1.914254000	0.096423000
1	1.857624000	-1.227309000	0.061089000	1	1.852423000	-1.230730000	0.059291000
6	-4.767435000	1.212587000	-0.060298000	6	-4.772853000	1.208800000	-0.063926000
6	-4.416003000	-1.175789000	0.056643000	6	-4.421641000	-1.178131000	0.055116000
6	-5.302663000	-0.085142000	0.004237000	6	-5.311559000	-0.088713000	0.001234000
1	-3.502942000	3.617413000	-0.193898000	1	-3.508418000	3.613929000	-0.193338000
6	-2.104260000	-2.106282000	0.109046000	6	-2.110021000	-2.109019000	0.105343000
1	-0.073849000	-2.764037000	0.145982000	1	-0.079740000	-2.767507000	0.142480000
1	-4.814627000	-2.189783000	0.133652000	1	-4.818400000	-2.192631000	0.135222000
1	-2.513982000	-3.117897000	0.163716000	1	-2.519841000	-3.120724000	0.158953000
1	-5.441030000	2.069668000	-0.128782000	1	-5.444744000	2.066913000	-0.136264000
6	-8.737505000	-1.576042000	-0.667954000	6	-8.743616000	-1.609181000	-0.635237000
6	-9.593878000	-0.715976000	0.039262000	6	-9.602787000	-0.718266000	0.037108000
6	-9.011902000	0.353726000	0.733158000	6	-9.024725000	0.383197000	0.697613000
6	-7.358456000	-1.376132000	-0.679361000	6	-7.367178000	-1.403296000	-0.641815000
6	-7.630721000	0.559916000	0.723114000	6	-7.647228000	0.581662000	0.680383000
6	-6.773678000	-0.301030000	0.016839000	6	-6.779945000	-0.303934000	0.012920000
1	-9.160426000	-2.414772000	-1.228154000	1	-9.166341000	-2.464820000	-1.168920000
1	-7.210412000	1.389192000	1.296320000	1	-7.232699000	1.431883000	1.226499000
1	-9.650029000	1.036351000	1.300727000	1	-9.666795000	1.085787000	1.235995000
1	-6.725092000	-2.049855000	-1.260684000	1	-6.734763000	-2.102574000	-1.193176000
6	-11.085744000	-0.945198000	0.046414000	7	-10.985212000	-0.886246000	-0.004247000
1	-11.497404000	-0.934153000	-0.976867000	1	-11.494815000	-0.446917000	0.756208000
1	-11.338035000	-1.926299000	0.483293000	1	-11.298586000	-1.839570000	-0.159155000
1	-11.610552000	-0.173482000	0.628599000				

**Table S11.** Cartesian coordinates (in Angstrom unit) of B3LYP/cc-pVDZ optimized geometries of TPA based D- $\pi$ -A systems.

D3 E(RB3LYP) = -1262.81666934 a. u.				D3-CH <sub>3</sub> E(RB3LYP) = -1302.13432812 a. u.			
6	6.566075000	-0.477895000	-0.168300000	6	6.841975000	-0.607304000	-0.163439000
6	7.729039000	0.177953000	0.148553000	6	8.032006000	-0.008807000	0.167520000
6	7.722488000	1.471860000	0.755940000	6	8.080515000	1.275840000	0.792319000
7	7.677758000	2.526518000	1.250651000	7	8.080533000	2.324786000	1.301079000
6	9.020757000	-0.488692000	-0.154579000	6	9.293518000	-0.728802000	-0.138750000
8	9.129674000	-1.584287000	-0.667821000	8	9.355967000	-1.821344000	-0.666427000
8	10.084376000	0.263335000	0.206745000	8	10.388487000	-0.030518000	0.237164000
1	10.872355000	-0.257650000	-0.031640000	1	11.152931000	-0.583727000	-0.005073000
6	2.782018000	-0.310637000	-0.119437000	6	3.069152000	-0.272344000	-0.130212000
1	2.629733000	0.671546000	0.338759000	1	2.957672000	0.709380000	0.340638000
1	6.699732000	-1.461653000	-0.629186000	1	6.933603000	-1.589906000	-0.637011000
6	4.136184000	-0.733810000	-0.307473000	6	4.403960000	-0.752433000	-0.317434000
6	5.239112000	-0.002719000	0.044590000	6	5.536831000	-0.076001000	0.049753000
1	4.290789000	-1.717272000	-0.768252000	1	4.517295000	-1.735618000	-0.790824000
1	5.109025000	0.981395000	0.505978000	1	5.448344000	0.906748000	0.523852000
6	1.711573000	-1.073124000	-0.485363000	6	1.967885000	-0.982097000	-0.511838000
1	1.925572000	-2.046446000	-0.942992000	1	2.141738000	-1.957710000	-0.981644000
7	-3.871877000	0.027046000	-0.015130000	7	-3.564275000	0.353277000	-0.053746000
6	-5.966600000	-1.092449000	-0.636807000	6	-5.681766000	-0.685540000	-0.747296000
6	-4.806017000	-1.039988000	0.152284000	6	-4.544174000	-0.679316000	0.076260000
6	-6.889921000	-2.124458000	-0.458827000	6	-6.646234000	-1.681722000	-0.606402000
1	-7.788542000	-2.153050000	-1.079162000	1	-7.524268000	-1.666512000	-1.258079000
6	-4.585157000	-2.037186000	1.117252000	6	-4.397912000	-1.691887000	1.035174000
6	-6.663424000	-3.122524000	0.493974000	6	-6.507046000	-2.708835000	0.342245000
1	-3.689969000	-1.993467000	1.739835000	1	-3.523345000	-1.693614000	1.688241000
1	-7.384838000	-3.931202000	0.626840000	6	-5.363904000	-2.693481000	1.154216000
6	-5.505647000	-3.074278000	1.277322000	1	-5.229623000	-3.473616000	1.908140000
1	-5.321990000	-3.842701000	2.031645000	1	-5.806311000	0.097932000	-1.496881000
1	-6.140658000	-0.319312000	-1.386881000	6	0.573261000	-0.607111000	-0.375677000
6	0.302071000	-0.757505000	-0.346416000	6	-0.429215000	-1.479489000	-0.854842000
6	-0.663060000	-1.679284000	-0.808959000	6	0.138704000	0.600542000	0.219726000
6	-0.181662000	0.437891000	0.235192000	1	-0.132258000	-2.418771000	-1.328995000
1	-0.327465000	-2.610552000	-1.272817000	1	0.870111000	1.303387000	0.622827000
1	0.520176000	1.177590000	0.624455000	6	-1.780053000	-1.173398000	-0.758958000
6	-2.025701000	-1.430994000	-0.710066000	6	-1.206587000	0.914692000	0.327723000
6	-1.539129000	0.693937000	0.346645000	1	-2.522956000	-1.867615000	-1.152160000

1	-2.739322000	-2.161601000	-1.091436000	1	-1.505490000	1.847508000	0.806396000
1	-1.876950000	1.619294000	0.813781000	6	-2.200483000	0.035056000	-0.163422000
6	-2.495022000	-0.235071000	-0.127074000	6	-4.006050000	1.710378000	-0.075994000
6	-4.366966000	1.365014000	-0.077112000	6	-4.941512000	2.162746000	0.869218000
6	-5.300125000	1.816170000	0.870679000	6	-3.529422000	2.602504000	-1.051763000
6	-3.941268000	2.238108000	-1.092386000	1	-5.314259000	1.472317000	1.627539000
1	-5.632255000	1.140294000	1.660330000	1	-2.812253000	2.252274000	-1.796059000
1	-3.224925000	1.887632000	-1.837312000	6	-5.390755000	3.484096000	0.835256000
6	-5.798768000	3.118157000	0.799385000	6	-3.972016000	3.926306000	-1.068105000
6	-4.432757000	3.543606000	-1.146293000	1	-6.118025000	3.822380000	1.576860000
1	-6.523889000	3.456248000	1.543041000	1	-3.592923000	4.608890000	-1.832124000
1	-4.093261000	4.212077000	-1.940681000	6	-4.906200000	4.374061000	-0.128400000
6	-5.365427000	3.989922000	-0.204497000	6	-7.557042000	-3.785156000	0.475636000
1	-5.752882000	5.009468000	-0.253704000	1	-7.677290000	-4.346939000	-0.466144000
				1	-7.298465000	-4.505886000	1.265272000
				1	-8.542950000	-3.355835000	0.721385000
				1	-5.255324000	5.408407000	-0.148478000
D3-C <sub>5</sub> H <sub>11</sub> E(RB3LYP) = -1459.39052995 a. u.				D3-isopropyl E(RB3LYP) = -1380.76204245 a. u.			
6	8.094959000	-1.340020000	-0.180188000	6	7.308276000	-0.147511000	-0.169989000
6	9.374809000	-0.936262000	0.108029000	6	8.376203000	0.660596000	0.130660000
6	9.650224000	0.348557000	0.670517000	6	8.200684000	1.956321000	0.708033000
7	9.836082000	1.404262000	1.128871000	7	8.018292000	3.007377000	1.178290000
6	10.491470000	-1.871323000	-0.178440000	6	9.743642000	0.160170000	-0.157986000
8	10.359712000	-2.981294000	-0.654534000	8	9.995038000	-0.923485000	-0.646290000
8	11.695197000	-1.351296000	0.151142000	8	10.700516000	1.051589000	0.184995000
1	12.351099000	-2.035657000	-0.073632000	1	11.549486000	0.631236000	-0.042272000
6	4.433047000	-0.373742000	-0.118771000	6	3.534654000	-0.471417000	-0.120730000
1	4.496746000	0.633004000	0.305872000	1	3.255260000	0.493015000	0.314851000
1	8.011294000	-2.344252000	-0.607627000	1	7.569085000	-1.116047000	-0.608269000
6	5.664558000	-1.079486000	-0.298398000	6	4.932296000	-0.719461000	-0.300638000
6	6.901843000	-0.587578000	0.022738000	6	5.930793000	0.156501000	0.033173000
1	5.602260000	-2.088068000	-0.725590000	1	5.214051000	-1.684992000	-0.738751000
1	6.988608000	0.416378000	0.450448000	1	5.673296000	1.125846000	0.471880000
6	3.221158000	-0.904605000	-0.453307000	6	2.572572000	-1.374989000	-0.467230000
1	3.220076000	-1.915699000	-0.878125000	1	2.912096000	-2.322725000	-0.902276000
7	-1.999086000	1.360979000	0.004454000	7	-3.106139000	-0.997852000	-0.010684000
6	-4.268322000	0.658449000	-0.626265000	6	-5.053634000	-2.367418000	-0.608525000
6	-3.135691000	0.512428000	0.183914000	6	-3.900706000	-2.169979000	0.169065000

6	-5.388080000	-0.156643000	-0.434231000	6	-5.843524000	-3.502618000	-0.417005000
1	-6.252586000	-0.012411000	-1.083590000	1	-6.737496000	-3.643224000	-1.028882000
6	-3.146252000	-0.469891000	1.189089000	6	-3.553203000	-3.127482000	1.137365000
6	-5.408859000	-1.148559000	0.556130000	6	-5.489977000	-4.460427000	0.538417000
1	-2.274818000	-0.588484000	1.835661000	1	-2.665215000	-2.971965000	1.752388000
6	-4.261651000	-1.285678000	1.359118000	6	-4.340011000	-4.267279000	1.310968000
1	-4.248973000	-2.043036000	2.148252000	1	-4.058357000	-5.002960000	2.067829000
1	-4.274538000	1.418485000	-1.409590000	1	-5.326896000	-1.625270000	-1.360328000
6	1.912036000	-0.294757000	-0.319180000	6	1.134272000	-1.242199000	-0.333252000
6	0.768661000	-1.006170000	-0.745899000	6	0.297251000	-2.292719000	-0.770786000
6	1.697258000	0.993995000	0.224089000	6	0.498255000	-0.105729000	0.219628000
1	0.894997000	-2.002014000	-1.179037000	1	0.751470000	-3.183437000	-1.212994000
1	2.543593000	1.580724000	0.585911000	1	1.097608000	0.728760000	0.588185000
6	-0.509730000	-0.473123000	-0.649530000	6	-1.086009000	-2.221860000	-0.674186000
6	0.426093000	1.534582000	0.332210000	6	-0.880879000	-0.025622000	0.327969000
1	-1.365722000	-1.048788000	-1.002108000	1	-1.697892000	-3.048274000	-1.036356000
1	0.296898000	2.524534000	0.770282000	1	-1.336840000	0.859704000	0.771730000
6	-0.710494000	0.814047000	-0.106436000	6	-1.708030000	-1.083176000	-0.118990000
6	-2.208547000	2.770698000	-0.075030000	6	-3.766402000	0.266992000	-0.092647000
6	-3.037938000	3.413624000	0.858739000	6	-4.728745000	0.628195000	0.863832000
6	-1.607476000	3.527622000	-1.095180000	6	-3.479728000	1.162137000	-1.133554000
1	-3.507258000	2.828419000	1.651175000	1	-4.960404000	-0.060150000	1.678578000
1	-0.972730000	3.030498000	-1.830658000	1	-2.741392000	0.891139000	-1.890426000
6	-3.260539000	4.788861000	0.769974000	6	-5.386278000	1.854328000	0.773905000
6	-1.822832000	4.905073000	-1.166650000	6	-4.134071000	2.393778000	-1.201084000
1	-3.907427000	5.275770000	1.503323000	1	-6.129907000	2.105449000	1.534076000
1	-1.349036000	5.481021000	-1.964877000	1	-3.894082000	3.076889000	-2.020481000
6	-2.651667000	5.542972000	-0.238135000	6	-5.101444000	2.767127000	-0.256307000
1	-2.823315000	6.619415000	-0.301139000	1	-6.107098000	-5.349661000	0.681952000
6	-6.596032000	-2.065165000	0.796361000	6	-5.810681000	4.111549000	-0.352389000
1	-6.891724000	-1.976903000	1.858421000	1	-5.406574000	4.621032000	-1.244732000
1	-6.255521000	-3.111052000	0.679654000	6	-5.511940000	5.005709000	0.864419000
6	-7.830440000	-1.845979000	-0.081885000	6	-7.326780000	3.947542000	-0.561224000
1	-8.190104000	-0.807305000	0.034216000	1	-7.544846000	3.338323000	-1.452642000
1	-7.555411000	-1.959116000	-1.146372000	1	-7.801034000	3.456311000	0.305020000
6	-8.972360000	-2.813842000	0.246751000	1	-7.809835000	4.930044000	-0.691193000
1	-9.249994000	-2.704132000	1.312244000	1	-5.902893000	4.561480000	1.795239000
1	-8.613850000	-3.854643000	0.134413000	1	-5.983603000	5.995051000	0.745080000
6	-10.217407000	-2.611579000	-0.623286000	1	-4.428629000	5.156559000	0.994438000
1	-10.574479000	-1.571206000	-0.510204000				
1	-9.938553000	-2.721327000	-1.687649000				

6	-11.353194000	-3.581346000	-0.289504000				
1	-11.678966000	-3.470788000	0.758933000				
1	-11.038068000	-4.629776000	-0.427561000				
1	-12.232363000	-3.410510000	-0.931269000				
D3-t-but E(RB3LYP) = -1420.07278757 a. u.				D3-OH E(RB3LYP) = -1338.04286702 a. u.			
6	-7.487911000	-0.060727000	0.184688000	6	6.807551000	-0.406214000	-0.163510000
6	-8.530918000	0.769802000	-0.141359000	6	7.943748000	0.303515000	0.136154000
6	-8.317614000	2.032387000	-0.776529000	6	7.885056000	1.608405000	0.716460000
7	-8.104609000	3.055110000	-1.294021000	7	7.797604000	2.670402000	1.189427000
6	-9.911411000	0.329801000	0.181445000	6	9.260548000	-0.315530000	-0.156661000
8	-10.194328000	-0.722298000	0.719042000	8	9.414048000	-1.416347000	-0.647375000
8	-10.841029000	1.237896000	-0.191490000	8	10.293725000	0.486880000	0.185286000
1	-11.701320000	0.857300000	0.061768000	1	11.101287000	-0.006925000	-0.045075000
6	-3.728123000	-0.515404000	0.116397000	6	3.020352000	-0.397077000	-0.108148000
1	-3.420859000	0.419048000	-0.363513000	1	2.826810000	0.587618000	0.328730000
1	-7.776813000	-0.999749000	0.667335000	1	6.980828000	-1.393199000	-0.603997000
6	-5.131407000	-0.707596000	0.319065000	6	4.390353000	-0.766318000	-0.290347000
6	-6.103140000	0.186672000	-0.043996000	6	5.462929000	0.017835000	0.042869000
1	-5.441099000	-1.642940000	0.801563000	1	4.585593000	-1.752245000	-0.730195000
1	-5.817538000	1.126615000	-0.527046000	1	5.292657000	1.005443000	0.483362000
6	-2.793427000	-1.434961000	0.494450000	6	1.982398000	-1.212896000	-0.454452000
1	-3.160153000	-2.350590000	0.973914000	1	2.237810000	-2.186204000	-0.890639000
7	2.890352000	-1.266994000	-0.018584000	7	-3.640816000	-0.338269000	-0.000017000
6	4.791706000	-2.675375000	0.635302000	6	-5.730513000	-1.462243000	-0.626066000
6	3.644320000	-2.472292000	-0.148908000	6	-4.552906000	-1.426148000	0.139416000
6	5.541255000	-3.844545000	0.492724000	6	-6.637532000	-2.512098000	-0.471058000
1	6.431420000	-3.989440000	1.109135000	1	-7.548376000	-2.526660000	-1.074028000
6	3.261049000	-3.458322000	-1.073859000	6	-4.302958000	-2.458142000	1.060799000
6	5.152061000	-4.830275000	-0.419607000	6	-6.380953000	-3.544613000	0.436358000
1	2.377054000	-3.298998000	-1.693656000	1	-3.397306000	-2.428463000	1.668901000
6	4.007429000	-4.631352000	-1.198457000	6	-5.208248000	-3.511673000	1.197985000
1	3.698380000	-5.389240000	-1.921978000	1	-5.000460000	-4.305980000	1.918663000
1	5.092355000	-1.910831000	1.353476000	1	-5.930599000	-0.661847000	-1.340119000
6	-1.352875000	-1.356653000	0.343210000	6	0.561638000	-0.955739000	-0.319370000
6	-0.546890000	-2.413386000	0.822296000	6	-0.364382000	-1.928966000	-0.757227000
6	-0.684859000	-0.268517000	-0.266194000	6	0.026492000	0.231452000	0.233475000
1	-1.026205000	-3.267507000	1.308074000	1	0.010345000	-2.855272000	-1.200910000
1	-1.259759000	0.567419000	-0.668860000	1	0.695978000	1.011618000	0.600365000



6	0.837008000	-2.392797000	0.712844000	6	-1.735913000	-1.738978000	-0.659794000
6	0.695194000	-0.239141000	-0.387964000	6	-1.340370000	0.431324000	0.342167000
1	1.424628000	-3.221604000	1.108207000	1	-2.416247000	-2.508853000	-1.024135000
1	1.175953000	0.609050000	-0.875886000	1	-1.716857000	1.354067000	0.784071000
6	1.491232000	-1.301576000	0.101928000	6	-2.257555000	-0.550763000	-0.102853000
6	3.591382000	-0.022161000	-0.003660000	6	-4.171678000	0.990638000	-0.044647000
6	4.563707000	0.260775000	-0.970556000	6	-5.016121000	1.451954000	0.974082000
6	3.335776000	0.937226000	0.989729000	6	-3.870451000	1.848444000	-1.116030000
1	4.777320000	-0.472670000	-1.750113000	1	-5.258451000	0.794697000	1.810907000
1	2.589418000	0.731504000	1.759217000	1	-3.219363000	1.496313000	-1.918244000
6	5.262767000	1.470781000	-0.942085000	6	-5.553642000	2.738874000	0.922776000
6	4.028963000	2.145421000	0.996090000	6	-4.388412000	3.139923000	-1.161991000
1	6.010409000	1.645498000	-1.715399000	1	-6.214140000	3.083933000	1.723939000
1	3.800629000	2.864596000	1.785415000	1	-4.156360000	3.811187000	-1.990383000
6	5.013134000	2.447289000	0.034887000	6	-5.238742000	3.593079000	-0.142702000
1	5.737608000	-5.745844000	-0.524787000	8	-5.724463000	4.863015000	-0.245764000
6	5.758871000	3.793557000	0.088430000	1	-6.291066000	5.045891000	0.518236000
6	4.740411000	4.950474000	-0.038091000	1	-7.090205000	-4.366706000	0.551391000
1	4.195783000	4.894405000	-0.994378000				
1	3.996433000	4.933679000	0.773294000				
1	5.257622000	5.923470000	0.003769000				
6	6.505795000	3.913772000	1.437372000				
1	5.816817000	3.864098000	2.294717000				
1	7.244904000	3.104658000	1.552905000				
1	7.041045000	4.876153000	1.495184000				
6	6.789755000	3.934075000	-1.046188000				
1	7.296429000	4.908978000	-0.968508000				
1	7.565668000	3.153767000	-0.996472000				
1	6.317082000	3.885866000	-2.039982000				
D3-OCH <sub>3</sub> E(RB3LYP) = -1377.34438563 a. u.				D3-OC <sub>2</sub> H <sub>5</sub> E(RB3LYP) = -1416.66453642 a. u.			
6	7.069299000	-0.275280000	-0.140362000	6	7.330900000	-0.074721000	-0.141137000
6	8.168899000	0.496684000	0.141904000	6	8.383665000	0.759382000	0.143180000
6	8.044961000	1.815402000	0.679043000	6	8.182871000	2.068327000	0.680975000
7	7.904434000	2.886833000	1.116646000	7	7.980009000	3.129546000	1.119025000
6	9.515215000	-0.068522000	-0.123725000	6	9.760758000	0.273244000	-0.120766000
8	9.723818000	-1.176106000	-0.577582000	8	10.033879000	-0.820077000	-0.575013000
8	10.507266000	0.792419000	0.197291000	8	10.700913000	1.189862000	0.202453000
1	11.338592000	0.329985000	-0.012718000	1	11.557870000	0.776349000	-0.006538000

6	3.285715000	-0.443794000	-0.104739000	6	3.563486000	-0.462359000	-0.109506000
1	3.043027000	0.544088000	0.299138000	1	3.263591000	0.509615000	0.294532000
1	7.291828000	-1.266658000	-0.547607000	1	7.610952000	-1.051284000	-0.548692000
6	4.672661000	-0.753342000	-0.267925000	6	4.966108000	-0.690808000	-0.271728000
6	5.704943000	0.091040000	0.045185000	6	5.947453000	0.211854000	0.042834000
1	4.917137000	-1.742533000	-0.674606000	1	5.267930000	-1.663978000	-0.678554000
1	5.485326000	1.083129000	0.452522000	1	5.670247000	1.189316000	0.450411000
6	2.289591000	-1.318578000	-0.429727000	6	2.619946000	-1.393563000	-0.434924000
1	2.593572000	-2.292154000	-0.832952000	1	2.980156000	-2.347868000	-0.837923000
7	-3.371013000	-0.697628000	-0.030607000	7	-3.066825000	-1.104499000	-0.031367000
6	-5.399533000	-1.940442000	-0.632531000	6	-5.022355000	-2.462120000	-0.626494000
6	-4.231262000	-1.822841000	0.139074000	6	-3.859844000	-2.277605000	0.140593000
6	-6.256336000	-3.027165000	-0.449251000	6	-5.814343000	-3.596606000	-0.440470000
1	-7.160508000	-3.105157000	-1.057368000	1	-6.714880000	-3.726262000	-1.045177000
6	-3.939618000	-2.811101000	1.095341000	6	-3.508118000	-3.247801000	1.095361000
6	-5.957868000	-4.016234000	0.493240000	6	-5.455810000	-4.567075000	0.500224000
1	-3.041458000	-2.718082000	1.708157000	1	-2.614589000	-3.103082000	1.704889000
6	-4.794434000	-3.902102000	1.261090000	6	-4.297934000	-4.386262000	1.263778000
1	-4.554759000	-4.661692000	2.008800000	1	-4.011974000	-5.130876000	2.010287000
1	-5.631899000	-1.173888000	-1.373434000	1	-5.301585000	-1.709965000	-1.365937000
6	0.857578000	-1.124941000	-0.310041000	6	1.179179000	-1.283640000	-0.315221000
6	-0.018708000	-2.154683000	-0.720440000	6	0.364310000	-2.363513000	-0.723440000
6	0.263400000	0.052714000	0.201435000	6	0.517389000	-0.141867000	0.194680000
1	0.402215000	-3.075981000	-1.131989000	1	0.838137000	-3.259205000	-1.134024000
1	0.892978000	0.875136000	0.546029000	1	1.097982000	0.716685000	0.537172000
6	-1.398171000	-2.027027000	-0.635576000	6	-1.020145000	-2.316851000	-0.637241000
6	-1.111988000	0.190935000	0.297191000	6	-0.863612000	-0.084251000	0.291461000
1	-2.039110000	-2.839637000	-0.977858000	1	-1.612660000	-3.166191000	-0.977590000
1	-1.534567000	1.108305000	0.707438000	1	-1.338898000	0.807540000	0.700369000
6	-1.979015000	-0.847489000	-0.119941000	6	-1.668734000	-1.172624000	-0.122589000
6	-3.963418000	0.603107000	-0.116141000	6	-3.734259000	0.159700000	-0.116646000
6	-4.835546000	1.053941000	0.880223000	6	-4.624812000	0.562435000	0.883989000
6	-3.694389000	1.443764000	-1.211556000	6	-3.521115000	1.011351000	-1.215633000
1	-5.053133000	0.409870000	1.734123000	1	-4.799442000	-0.090671000	1.740928000
1	-3.021377000	1.101373000	-1.999785000	1	-2.834240000	0.706480000	-2.007341000
6	-5.438424000	2.313164000	0.794835000	6	-5.300039000	1.784370000	0.799586000
6	-4.274396000	2.703570000	-1.294737000	6	-4.173809000	2.235166000	-1.297950000
1	-6.115341000	2.629983000	1.587518000	1	-5.989012000	2.063068000	1.596014000
1	-4.071239000	3.363710000	-2.139620000	1	-4.014196000	2.903351000	-2.145866000
6	-5.155606000	3.150470000	-0.294103000	6	-5.073595000	2.634488000	-0.293331000
8	-5.676088000	4.395994000	-0.477060000	8	-5.665981000	3.846225000	-0.476018000

6	-6.568776000	4.903415000	0.502953000	6	-6.588961000	4.319949000	0.507014000
1	-7.472992000	4.275501000	0.595839000	1	-6.085328000	4.392383000	1.489068000
1	-6.084333000	4.986826000	1.492253000	1	-7.427165000	3.605404000	0.608663000
1	-6.858676000	5.904350000	0.157984000	6	-7.084628000	5.678243000	0.048520000
1	-6.627843000	-4.867367000	0.630367000	1	-7.585559000	5.599472000	-0.928629000
				1	-6.246378000	6.385172000	-0.048829000
				1	-7.802468000	6.085636000	0.777442000
				1	-6.074979000	-5.455530000	0.639621000
D3-NH <sub>2</sub> E(RB3LYP) = -1318.17672570 a. u.				D3-N(CH <sub>3</sub> ) <sub>2</sub> E(RB3LYP) = -1396.78728931 a. u.			
6	6.840172000	-0.601923000	-0.151992000	6	7.348366000	-0.849979000	-0.169609000
6	8.033511000	0.003770000	0.155909000	6	8.584227000	-0.347295000	0.156355000
6	8.087403000	1.308382000	0.737092000	6	8.737074000	0.932509000	0.773860000
7	8.091846000	2.373824000	1.210499000	7	8.822481000	1.980840000	1.276908000
6	9.291386000	-0.729716000	-0.128794000	6	9.782273000	-1.167636000	-0.147513000
8	9.350205000	-1.839800000	-0.619574000	8	9.756867000	-2.264935000	-0.669169000
8	10.390151000	-0.022820000	0.220668000	8	10.931547000	-0.558064000	0.222667000
1	11.151405000	-0.587185000	-0.005129000	1	11.647275000	-1.173414000	-0.018262000
6	3.068586000	-0.260473000	-0.122863000	6	3.614293000	-0.220295000	-0.136006000
1	2.958163000	0.736990000	0.313933000	1	3.578769000	0.770053000	0.328615000
1	6.928191000	-1.600195000	-0.592383000	1	7.360462000	-1.839407000	-0.637736000
6	4.401795000	-0.747516000	-0.295902000	6	4.906602000	-0.803053000	-0.320583000
6	5.537442000	-0.060981000	0.045726000	6	6.090827000	-0.215910000	0.041668000
1	4.513125000	-1.746483000	-0.735697000	1	4.942453000	-1.794973000	-0.788148000
1	5.451762000	0.937482000	0.486324000	1	6.080850000	0.773508000	0.510009000
6	1.965585000	-0.982973000	-0.477595000	6	2.460407000	-0.845998000	-0.513193000
1	2.139137000	-1.974331000	-0.913527000	1	2.559760000	-1.834996000	-0.976925000
7	-3.566027000	0.356936000	-0.050798000	7	-2.954327000	0.899845000	-0.063259000
6	-5.596971000	-0.789592000	-0.843753000	6	-5.058614000	-0.069138000	-0.904066000
6	-4.536976000	-0.690558000	0.069070000	6	-4.003857000	-0.073153000	0.018236000
6	-6.554123000	-1.793650000	-0.718927000	6	-6.091479000	-0.999091000	-0.821936000
1	-7.372121000	-1.852648000	-1.441857000	1	-6.886477000	-0.955584000	-1.564540000
6	-4.458024000	-1.627644000	1.110306000	6	-4.009195000	-1.047272000	1.026018000
6	-6.472737000	-2.745615000	0.316525000	6	-6.110317000	-1.987708000	0.193622000
1	-3.643425000	-1.558224000	1.833891000	1	-3.195940000	-1.070434000	1.754318000
6	-5.402783000	-2.644018000	1.227968000	6	-5.027187000	-1.993497000	1.108197000
1	-5.319329000	-3.367032000	2.043812000	1	-4.980794000	-2.734681000	1.904369000

1	-5.674141000	-0.064778000	-1.656417000	1	-5.071289000	0.677729000	-1.700387000
6	0.572244000	-0.604606000	-0.352272000	6	1.099842000	-0.366291000	-0.380153000
6	-0.431705000	-1.493561000	-0.797434000	6	0.032819000	-1.162310000	-0.854087000
6	0.137206000	0.622968000	0.201913000	6	0.756806000	0.874136000	0.209282000
1	-0.135577000	-2.449677000	-1.237402000	1	0.257378000	-2.124984000	-1.321369000
1	0.868955000	1.339308000	0.580061000	1	1.539209000	1.520679000	0.611103000
6	-1.782219000	-1.185898000	-0.708606000	6	-1.290476000	-0.755086000	-0.759799000
6	-1.207225000	0.940998000	0.300660000	6	-0.559669000	1.291244000	0.313375000
1	-2.525761000	-1.895462000	-1.071634000	1	-2.084562000	-1.394624000	-1.145108000
1	-1.503953000	1.889150000	0.749309000	1	-0.785216000	2.245590000	0.789425000
6	-2.203745000	0.044715000	-0.158277000	6	-1.620001000	0.488093000	-0.175136000
6	-4.028062000	1.705594000	-0.066500000	6	-3.312595000	2.279481000	-0.035602000
6	-5.010580000	2.124599000	0.846601000	6	-4.271071000	2.740097000	0.883027000
6	-3.535309000	2.624322000	-1.010200000	6	-2.742086000	3.190040000	-0.942777000
1	-5.400125000	1.414134000	1.577259000	1	-4.721566000	2.036344000	1.584500000
1	-2.784861000	2.301886000	-1.733845000	1	-2.010596000	2.836660000	-1.671358000
6	-5.485169000	3.436991000	0.816036000	6	-4.645057000	4.084862000	0.894221000
6	-4.005239000	3.938577000	-1.023475000	6	-3.111665000	4.535697000	-0.914257000
1	-6.247975000	3.747522000	1.533833000	1	-5.390456000	4.427332000	1.615779000
1	-3.612377000	4.640078000	-1.763109000	1	-2.659287000	5.230259000	-1.625945000
6	-4.983290000	4.353043000	-0.113659000	6	-4.065521000	4.991714000	0.001343000
7	-7.386912000	-3.794611000	0.399210000	7	-7.145698000	-2.904149000	0.292671000
1	-8.290720000	-3.611126000	-0.025689000	6	-8.135498000	-2.984491000	-0.765824000
1	-7.489349000	-4.203060000	1.323273000	1	-7.698069000	-3.258884000	-1.746658000
1	-5.353254000	5.380159000	-0.131476000	1	-8.883848000	-3.742653000	-0.501521000
				1	-8.666286000	-2.025616000	-0.892060000
				6	-7.038238000	-4.008432000	1.228403000
				1	-7.953947000	-4.611526000	1.179565000
				1	-6.176340000	-4.672196000	1.015805000
				1	-6.935046000	-3.647197000	2.265705000
				1	-4.357017000	6.043829000	0.016200000
D3-PhCH <sub>3</sub> E(RB3LYP) = -1533.20535533 a. u.				D3-PhNH <sub>2</sub> E(RB3LYP) = -1549.24808161 a. u.			
6	8.177233000	-1.408663000	-0.177636000	6	8.173025000	-1.403549000	-0.176926000
6	9.450725000	-1.094811000	0.226183000	6	9.449587000	-1.085777000	0.215170000
6	9.733193000	0.091053000	0.972574000	6	9.737835000	0.109907000	0.943334000
7	9.925100000	1.067394000	1.580029000	7	9.934555000	1.094316000	1.536129000
6	10.553395000	-2.022921000	-0.130265000	6	10.548707000	-2.019942000	-0.134616000
8	10.414407000	-3.052482000	-0.759922000	8	10.405324000	-3.058256000	-0.749001000

8	11.752110000	-1.596536000	0.326652000	8	11.750984000	-1.588920000	0.309149000
1	12.399142000	-2.267449000	0.043202000	1	12.394956000	-2.264912000	0.030940000
6	4.548025000	-0.323445000	-0.163568000	6	4.544696000	-0.316733000	-0.158931000
1	4.620218000	0.613392000	0.397720000	1	4.619460000	0.628120000	0.388405000
1	8.086882000	-2.341929000	-0.742437000	1	8.078558000	-2.344533000	-0.728113000
6	5.765485000	-1.044415000	-0.378232000	6	5.760594000	-1.040581000	-0.369476000
6	6.997673000	-0.646884000	0.067711000	6	6.995818000	-0.637593000	0.064158000
1	5.695440000	-1.982682000	-0.942396000	1	5.687397000	-1.986779000	-0.919901000
1	7.091509000	0.285894000	0.632973000	1	7.093285000	0.303013000	0.615665000
6	3.340076000	-0.758034000	-0.625589000	6	3.334107000	-0.758179000	-0.608646000
1	3.329699000	-1.701963000	-1.183775000	1	3.321617000	-1.710107000	-1.153125000
7	-1.823551000	1.624826000	-0.111950000	7	-1.828271000	1.626817000	-0.105199000
6	-4.116958000	1.128246000	-0.840435000	6	-4.103674000	1.097223000	-0.870788000
6	-2.993112000	0.810432000	-0.060979000	6	-2.997093000	0.807583000	-0.057448000
6	-5.266621000	0.343617000	-0.775232000	6	-5.250398000	0.307787000	-0.810925000
1	-6.115741000	0.598300000	-1.412666000	1	-6.084045000	0.538540000	-1.477237000
6	-3.053036000	-0.312551000	0.781036000	6	-3.071072000	-0.290800000	0.814396000
6	-5.338168000	-0.790925000	0.055364000	6	-5.338704000	-0.802722000	0.051574000
1	-2.195961000	-0.560869000	1.409355000	1	-2.226634000	-0.516783000	1.468049000
6	-4.202009000	-1.098874000	0.828547000	6	-4.218093000	-1.080281000	0.859846000
1	-4.231348000	-1.949321000	1.512733000	1	-4.258961000	-1.909273000	1.569340000
1	-4.082540000	1.992022000	-1.506392000	1	-4.057331000	1.941985000	-1.560272000
6	2.044963000	-0.121938000	-0.472247000	6	2.039922000	-0.120986000	-0.458435000
6	0.903533000	-0.728152000	-1.042460000	6	0.895772000	-0.735666000	-1.014404000
6	1.843772000	1.091661000	0.226442000	6	1.840857000	1.102385000	0.224092000
1	1.021008000	-1.662006000	-1.598600000	1	1.011027000	-1.677567000	-1.557355000
1	2.688815000	1.594442000	0.700230000	1	2.687667000	1.611920000	0.687478000
6	-0.361055000	-0.164791000	-0.934700000	6	-0.368489000	-0.171835000	-0.908772000
6	0.585629000	1.660168000	0.347158000	6	0.583388000	1.672254000	0.342069000
1	-1.215747000	-0.655863000	-1.400535000	1	-1.225215000	-0.670523000	-1.362462000
1	0.464465000	2.589213000	0.904832000	1	0.464739000	2.608641000	0.887771000
6	-0.548097000	1.045317000	-0.233973000	6	-0.553494000	1.049139000	-0.225498000
6	-1.974039000	3.043546000	-0.046034000	6	-1.986198000	3.043974000	-0.037035000
6	-2.796119000	3.620883000	0.935534000	6	-2.827275000	3.613768000	0.933013000
6	-1.316668000	3.874618000	-0.968679000	6	-1.320858000	3.882447000	-0.947615000
1	-3.307237000	2.977344000	1.653461000	1	-3.346005000	2.964899000	1.640523000
1	-0.686088000	3.428543000	-1.739667000	1	-0.676514000	3.443019000	-1.710963000
6	-2.957584000	5.006543000	0.988470000	6	-2.998139000	4.998159000	0.987428000
6	-1.471068000	5.260290000	-0.898188000	6	-1.485289000	5.266784000	-0.875578000
1	-3.599411000	5.442814000	1.757237000	1	-3.654705000	5.427959000	1.747414000
1	-0.954169000	5.895091000	-1.621473000	1	-0.962025000	5.906798000	-1.589709000

6	-2.293636000	5.833610000	0.076904000	6	-2.325831000	5.832425000	0.088650000
6	-6.562665000	-1.628088000	0.115807000	6	-6.559299000	-1.642251000	0.108019000
6	-7.845717000	-1.053036000	0.031163000	6	-7.843063000	-1.086283000	-0.052197000
6	-6.486462000	-3.024353000	0.260005000	6	-6.487901000	-3.031606000	0.325845000
1	-7.945746000	0.031291000	-0.053758000	1	-7.949291000	-0.008443000	-0.193519000
1	-5.509243000	-3.510396000	0.301781000	1	-5.512083000	-3.510941000	0.430889000
6	-8.993974000	-1.840374000	0.088392000	6	-8.992699000	-1.869198000	0.002000000
6	-7.640337000	-3.808833000	0.317206000	6	-7.630575000	-3.824608000	0.379829000
1	-9.974637000	-1.359666000	0.029091000	1	-9.973498000	-1.400481000	-0.117116000
1	-7.544617000	-4.893027000	0.421130000	1	-7.535184000	-4.902794000	0.535293000
6	-8.916457000	-3.235503000	0.232618000	6	-8.909869000	-3.258229000	0.218632000
6	-10.167801000	-4.077406000	0.293172000	7	-10.052554000	-4.056553000	0.209369000
1	-10.769055000	-3.968669000	-0.625368000	1	-10.914783000	-3.573328000	0.442325000
1	-9.931287000	-5.144688000	0.415407000	1	-9.969406000	-4.930371000	0.720059000
1	-10.812557000	-3.776489000	1.136165000	1	-2.457388000	6.915193000	0.137759000
1	-2.417474000	6.917360000	0.124954000				

**Table S12.** Cartesian coordinates (in Angstrom unit) of B3LYP/cc-pVDZ optimized geometries of carbazol based D- $\pi$ -A systems.

D4 E(RB3LYP) = -1030.57760506 a. u.	D4-CH <sub>3</sub> E(RB3LYP) = -1069.89531958 a. u.						
6	-5.150890000	-0.476250000	0.000073000	6	-5.601120000	-0.487101000	0.000050000
6	-6.364139000	0.162248000	0.000082000	6	-6.819223000	0.142827000	0.000093000
6	-6.465597000	1.588293000	0.000079000	6	-6.930963000	1.568046000	0.000094000
7	-6.510395000	2.753065000	0.000064000	7	-6.983431000	2.732532000	0.000098000
6	-7.598148000	-0.665882000	0.000100000	6	-8.046951000	-0.693958000	0.000145000
8	-7.614119000	-1.880162000	-0.000040000	8	-8.054659000	-1.908441000	0.000159000
8	-8.720420000	0.086325000	-0.000064000	8	-9.174945000	0.050001000	0.000195000
1	-9.464481000	-0.542732000	-0.000170000	1	-9.914021000	-0.584820000	0.000234000
6	-1.389875000	-0.012716000	0.000050000	6	-1.843341000	0.000262000	-0.000099000
1	-1.322073000	1.079252000	0.000042000	1	-1.781801000	1.092633000	-0.000097000
1	-5.201575000	-1.569604000	0.000078000	1	-5.644198000	-1.580820000	0.000057000
6	-2.706010000	-0.580125000	0.000061000	6	-3.155668000	-0.574910000	-0.000046000
6	-3.866016000	0.144728000	0.000065000	6	-4.320776000	0.142399000	-0.000001000
1	-2.776500000	-1.674789000	0.000066000	1	-3.219374000	-1.670052000	-0.000040000
1	-3.819306000	1.238379000	0.000060000	1	-4.281265000	1.236361000	-0.000002000
6	2.141065000	-1.296694000	-0.000029000	6	1.695184000	-1.265023000	-0.000249000
6	3.471949000	-0.882467000	-0.000046000	6	3.023348000	-0.843932000	-0.000261000
6	3.830269000	0.495580000	0.000004000	6	3.375218000	0.536488000	-0.000239000

6	2.809130000	1.461474000	0.000073000	6	2.348537000	1.496843000	-0.000291000
6	1.482493000	1.056426000	0.000088000	6	1.024019000	1.084611000	-0.000257000
6	1.123915000	-0.321011000	0.000036000	6	0.672273000	-0.294605000	-0.000207000
7	4.633398000	-1.637992000	-0.000106000	7	4.189618000	-1.592986000	-0.000563000
6	5.276441000	0.551186000	-0.000029000	6	4.820139000	0.597646000	-0.000128000
1	1.880932000	-2.358040000	-0.000067000	1	1.440601000	-2.327789000	-0.000269000
1	3.055605000	2.525319000	0.000117000	1	2.589232000	2.562060000	-0.000319000
1	0.698833000	1.814528000	0.000148000	1	0.236324000	1.838627000	-0.000267000
6	-0.259826000	-0.773559000	0.000046000	6	-0.708521000	-0.754204000	-0.000148000
1	-0.391869000	-1.862077000	0.000047000	1	-0.834767000	-1.843482000	-0.000138000
6	7.098987000	-1.112258000	-0.000146000	6	6.651374000	-1.057304000	0.000115000
6	8.006610000	-0.053540000	-0.000124000	6	7.577317000	-0.010549000	0.000296000
6	5.735427000	-0.797089000	-0.000098000	6	5.286412000	-0.745550000	-0.000090000
1	9.077112000	-0.269904000	-0.000160000	6	7.116901000	1.329993000	0.000186000
6	7.572001000	1.287401000	-0.000056000	1	7.852353000	2.138292000	0.000285000
1	8.311340000	2.090556000	-0.000040000	6	5.762060000	1.640092000	-0.000024000
6	6.213990000	1.596523000	-0.000008000	1	5.435473000	2.682460000	-0.000094000
1	5.882461000	2.637194000	0.000045000	1	6.989751000	-2.096517000	0.000144000
1	7.442272000	-2.149058000	-0.000199000	1	4.233823000	-2.602211000	0.001291000
1	4.671876000	-2.647449000	-0.000154000	6	9.060746000	-0.291710000	0.000637000
				1	9.549290000	0.147251000	0.886962000
				1	9.270480000	-1.371446000	0.000238000
				1	9.549832000	0.147987000	-0.885020000
D4-C <sub>5</sub> H <sub>11</sub> E(RB3LYP) = -1227.15157794 a. u.				D4-isopropyl E(RB3LYP) = -1148.52265162 a. u.			
6	7.359206000	-0.769040000	-0.000026000	6	-6.406066000	-0.541602000	0.000006000
6	8.631642000	-0.257419000	0.000088000	6	-7.638718000	0.059220000	0.000034000
6	8.877976000	1.150776000	0.000259000	6	-7.784286000	1.481392000	0.000061000
7	9.040661000	2.305047000	0.000398000	7	-7.864433000	2.644295000	0.000083000
6	9.774416000	-1.206750000	0.000030000	6	-8.846299000	-0.806513000	0.000037000
8	9.667121000	-2.416550000	-0.000114000	8	-8.825095000	-2.020811000	0.000016000
8	10.967967000	-0.573130000	0.000156000	8	-9.991568000	-0.089511000	0.000066000
1	11.643374000	-1.275301000	0.000105000	1	-10.715453000	-0.741608000	0.000065000
6	3.664482000	0.071576000	-0.000079000	6	-2.660911000	0.035241000	-0.000034000
1	3.706439000	1.164871000	0.000047000	1	-2.625469000	1.128770000	-0.000019000
1	7.298497000	-1.861924000	-0.000154000	1	-6.423111000	-1.636033000	-0.000012000
6	4.916443000	-0.625019000	-0.000110000	6	-3.959216000	-0.571129000	-0.000027000
6	6.144326000	-0.021203000	0.000007000	6	-5.141001000	0.118233000	0.000000000
1	4.876318000	-1.721290000	-0.000235000	1	-3.996771000	-1.667472000	-0.000044000

1	6.208524000	1.071589000	0.000132000	1	-5.127562000	1.212827000	0.000017000
6	0.022182000	-0.853912000	-0.000136000	6	0.906711000	-1.145415000	-0.000103000
6	-1.260319000	-0.309405000	-0.000102000	6	2.224626000	-0.693159000	-0.000104000
6	-1.480299000	1.098362000	-0.000111000	6	2.543063000	0.695146000	-0.000076000
6	-0.367348000	1.957422000	-0.000155000	6	1.494347000	1.630893000	-0.000060000
6	0.912249000	1.421928000	-0.000182000	6	0.179678000	1.187601000	-0.000053000
6	1.132226000	0.015576000	-0.000167000	6	-0.138943000	-0.199407000	-0.000068000
7	-2.492087000	-0.944481000	-0.000054000	7	3.407967000	-1.414817000	-0.000192000
6	-2.912672000	1.295071000	-0.000090000	6	3.986693000	0.791064000	-0.000054000
1	0.175366000	-1.935976000	-0.000131000	1	0.677259000	-2.213878000	-0.000125000
1	-0.506353000	3.040617000	-0.000179000	1	1.710016000	2.701456000	-0.000047000
1	1.767656000	2.098170000	-0.000235000	1	-0.625609000	1.922778000	-0.000033000
6	2.463312000	-0.572267000	-0.000188000	6	-1.508500000	-0.691925000	-0.000058000
1	2.486140000	-1.668614000	-0.000291000	1	-1.608658000	-1.783899000	-0.000073000
6	-4.892462000	-0.183975000	0.000028000	6	5.854825000	-0.822780000	0.000000000
6	-5.718945000	0.942888000	0.000028000	6	6.760676000	0.246122000	0.000064000
6	-3.503959000	0.003336000	-0.000026000	6	4.485867000	-0.542134000	-0.000061000
6	-5.131133000	2.234702000	-0.000056000	6	6.266681000	1.571906000	0.000053000
1	-5.788985000	3.107618000	-0.000074000	1	6.982549000	2.397357000	0.000094000
6	-3.754940000	2.420286000	-0.000112000	6	4.902771000	1.853052000	-0.000011000
1	-3.334735000	3.428563000	-0.000165000	1	4.553995000	2.888185000	-0.000016000
1	-5.310855000	-1.191313000	0.000047000	1	6.206967000	-1.857006000	-0.000019000
1	-2.631711000	-1.944975000	-0.000081000	1	3.475264000	-2.422735000	0.000276000
6	-7.234784000	0.843778000	0.000098000	6	8.264429000	-0.005221000	0.000136000
1	-7.615238000	1.399534000	-0.877162000	1	8.750926000	0.985418000	0.000247000
1	-7.615170000	1.399582000	0.877363000	6	8.724950000	-0.743612000	-1.269452000
6	-7.843884000	-0.560172000	0.000162000	6	8.724800000	-0.743830000	1.269646000
1	-7.488335000	-1.120419000	-0.883872000	1	8.425635000	-0.200245000	2.179662000
1	-7.488418000	-1.120319000	0.884289000	1	8.290688000	-1.756305000	1.325944000
6	-9.376431000	-0.542762000	0.000116000	1	9.821987000	-0.852261000	1.279966000
1	-9.735893000	0.019477000	-0.882432000	1	8.290836000	-1.756073000	-1.325975000
1	-9.735927000	0.019483000	0.882647000	1	9.822138000	-0.852044000	-1.279656000
6	-10.006121000	-1.939763000	0.000102000	1	8.425893000	-0.199861000	-2.179404000
1	-9.645967000	-2.500556000	-0.882292000				
1	-9.645934000	-2.500591000	0.882461000				
6	-11.536200000	-1.914150000	0.000131000				
1	-11.927784000	-1.390856000	-				
	0.888874000						
1	-11.927752000	-1.390916000	0.889185000				
1	-11.957748000	-2.932143000	0.000103000				



D4-t-but E(RB3LYP) = -1187.83287967 a. u.				D4-OH E(RB3LYP) = -1105.80408310 a. u.			
6	6.782666000	-0.515359000	0.000035000	6	5.586918000	-0.485158000	-0.000019000
6	8.009573000	0.097125000	0.000304000	6	6.805999000	0.143484000	-0.000005000
6	8.141648000	1.520614000	0.000566000	6	6.919266000	1.568518000	0.000018000
7	8.210780000	2.684224000	0.000776000	7	6.973080000	2.732975000	0.000039000
6	9.225297000	-0.757116000	0.000317000	6	8.032530000	-0.694517000	-0.000016000
8	9.215618000	-1.971564000	0.000068000	8	8.039242000	-1.909121000	0.000005000
8	10.363729000	-0.029292000	0.000567000	8	9.161626000	0.048043000	0.000046000
1	11.093748000	-0.674514000	0.000530000	1	9.899657000	-0.587962000	0.000070000
6	3.032195000	0.025805000	-0.000313000	6	1.829624000	0.003439000	-0.000022000
1	2.986288000	1.118943000	-0.000172000	1	1.767939000	1.095822000	-0.000005000
1	6.810097000	-1.609580000	-0.000152000	1	5.629049000	-1.578925000	-0.000037000
6	4.336219000	-0.568153000	-0.000265000	6	3.141497000	-0.571589000	-0.000029000
6	5.511396000	0.132427000	-0.000014000	6	4.307363000	0.145119000	-0.000014000
1	4.384218000	-1.664089000	-0.000444000	1	3.204991000	-1.666780000	-0.000046000
1	5.487544000	1.226842000	0.000155000	1	4.268495000	1.239104000	0.000003000
6	-0.523933000	-1.189042000	-0.000419000	6	-1.709626000	-1.264502000	0.000001000
6	-1.846237000	-0.749675000	-0.000451000	6	-3.036218000	-0.843884000	0.000010000
6	-2.177642000	0.635718000	-0.000542000	6	-3.391289000	0.535392000	-0.000009000
6	-1.138165000	1.581512000	-0.000760000	6	-2.365227000	1.496384000	-0.000037000
6	0.180816000	1.150934000	-0.000760000	6	-1.040052000	1.084835000	-0.000047000
6	0.512562000	-0.232920000	-0.000559000	6	-0.685954000	-0.293133000	-0.000028000
7	-3.022429000	-1.482815000	-0.000481000	7	-4.204257000	-1.595469000	0.000055000
6	-3.622237000	0.717151000	-0.000486000	6	-4.835645000	0.594287000	0.000011000
1	-0.284057000	-2.255212000	-0.000331000	1	-1.454585000	-2.327195000	0.000017000
1	-1.364333000	2.649902000	-0.000937000	1	-2.606181000	2.561521000	-0.000052000
1	0.979013000	1.893795000	-0.000971000	1	-0.253430000	1.840050000	-0.000072000
6	1.886785000	-0.712341000	-0.000504000	6	0.694478000	-0.751314000	-0.000033000
1	1.997383000	-1.803306000	-0.000613000	1	0.821537000	-1.840552000	-0.000045000
6	-5.473543000	-0.913146000	-0.000076000	6	-6.663132000	-1.068601000	-0.000008000
6	-6.401846000	0.140106000	-0.000067000	6	-7.573586000	-0.007078000	-0.000008000
6	-4.108761000	-0.619693000	-0.000289000	6	-5.300330000	-0.750970000	0.000022000
6	-5.915708000	1.470052000	-0.000362000	6	-7.134388000	1.336994000	0.000029000
1	-6.619233000	2.300855000	-0.000645000	1	-7.890407000	2.122953000	0.000093000
6	-4.553094000	1.763932000	-0.000597000	6	-5.778858000	1.636102000	0.000011000
1	-4.219885000	2.804216000	-0.000895000	1	-5.452675000	2.678323000	0.000017000
1	-5.805303000	-1.953326000	-0.000082000	1	-7.008584000	-2.106177000	-0.000128000
1	-3.079813000	-2.491327000	0.000196000	1	-4.245893000	-2.604730000	0.000033000

6	-7.909861000	-0.184990000	0.000516000	8	-8.923060000	-0.203432000	-0.000050000
6	-8.784402000	1.082291000	0.000612000	1	-9.104362000	-1.154779000	0.000528000
1	-8.608572000	1.704194000	0.892373000				
1	-8.609632000	1.703850000	-0.891603000				
1	-9.848323000	0.797034000	0.001168000				
6	-8.259624000	-1.008742000	-1.260859000				
1	-8.023696000	-0.445423000	-2.178024000				
1	-7.704571000	-1.958845000	-1.299223000				
1	-9.335542000	-1.250222000	-1.275564000				
6	-8.258758000	-1.007674000	1.263166000				
1	-9.334718000	-1.248584000	1.278047000				
1	-7.703957000	-1.957884000	1.301571000				
1	-8.021960000	-0.443235000	2.179308000				
D4-OCH <sub>3</sub> E(RB3LYP) = -1145.10585530 a. u.				D4-OC <sub>2</sub> H <sub>5</sub> E(RB3LYP) = -1184.42598167 a. u.			
6	6.002656000	-0.529413000	-0.000039000	6	6.455166000	-0.565540000	-0.000055000
6	7.234445000	0.074263000	-0.000061000	6	7.694821000	0.021964000	-0.000079000
6	7.376743000	1.496668000	-0.000097000	6	7.855736000	1.442373000	-0.000118000
7	7.454170000	2.659809000	-0.000127000	7	7.948409000	2.604405000	-0.000149000
6	8.443489000	-0.788474000	-0.000045000	6	8.892396000	-0.856489000	-0.000064000
8	8.425671000	-2.003022000	-0.000036000	8	8.858782000	-2.070728000	-0.000050000
8	9.587660000	-0.069154000	-0.000094000	8	10.045966000	-0.152248000	-0.000110000
1	10.312339000	-0.720316000	-0.000098000	1	10.761948000	-0.812954000	-0.000112000
6	2.255988000	0.033994000	-0.000028000	6	2.716121000	0.046028000	-0.000040000
1	2.215674000	1.127369000	-0.000054000	1	2.689679000	1.139826000	-0.000067000
1	6.022604000	-1.623817000	-0.000011000	1	6.460846000	-1.660114000	-0.000026000
6	3.556085000	-0.566747000	-0.000022000	6	4.008362000	-0.571228000	-0.000035000
6	4.736231000	0.126477000	-0.000047000	6	5.197437000	0.106704000	-0.000062000
1	3.597839000	-1.663000000	0.000005000	1	4.036055000	-1.667934000	-0.000006000
1	4.719308000	1.221021000	-0.000074000	1	5.194670000	1.201375000	-0.000091000
6	-1.307099000	-1.165105000	0.000044000	6	-0.861819000	-1.108310000	0.000039000
6	-2.625535000	-0.719075000	0.000044000	6	-2.174557000	-0.645946000	0.000041000
6	-2.953862000	0.667315000	-0.000002000	6	-2.485596000	0.744541000	-0.000006000
6	-1.909028000	1.608316000	-0.000050000	6	-1.429045000	1.672392000	-0.000057000
6	-0.592321000	1.171151000	-0.000050000	6	-0.117873000	1.218864000	-0.000059000
6	-0.264956000	-0.213744000	-0.000003000	6	0.192198000	-0.170007000	-0.000011000
7	-3.807641000	-1.446738000	0.000085000	7	-3.365635000	-1.358697000	0.000085000
6	-4.396065000	0.753335000	0.000013000	6	-3.926533000	0.848502000	0.000011000
1	-1.072536000	-2.232530000	0.000079000	1	-0.640556000	-2.178580000	0.000076000

1	-2.129281000	2.677941000	-0.000087000	1	-1.635948000	2.744686000	-0.000095000
1	0.208954000	1.910821000	-0.000089000	1	0.692577000	1.948480000	-0.000100000
6	1.106137000	-0.698458000	-0.000001000	6	1.557006000	-0.671817000	-0.000010000
1	1.212061000	-1.789972000	0.000027000	1	1.649206000	-1.764585000	0.000019000
6	-6.256005000	-0.882536000	0.000097000	6	-5.806712000	-0.764523000	0.000100000
6	-7.147968000	0.195600000	0.000069000	6	-6.686570000	0.324122000	0.000072000
6	-4.887261000	-0.580136000	0.000068000	6	-4.434492000	-0.478645000	0.000068000
6	-6.679079000	1.533908000	0.000015000	6	-6.199794000	1.656467000	0.000015000
1	-7.424285000	2.330209000	-0.000004000	1	-6.934954000	2.462077000	-0.000004000
6	-5.322046000	1.812843000	-0.000013000	6	-4.839600000	1.919161000	-0.000016000
1	-4.979149000	2.849684000	-0.000055000	1	-4.484287000	2.951830000	-0.000060000
1	-6.598201000	-1.916597000	0.000139000	1	-6.160701000	-1.794505000	0.000144000
1	-3.869859000	-2.454960000	0.000125000	1	-3.440527000	-2.366049000	0.000126000
8	-8.504083000	0.066762000	0.000092000	8	-8.043058000	0.212113000	0.000097000
6	-9.059994000	-1.237952000	0.000145000	6	-8.633034000	-1.088140000	0.000152000
1	-8.764584000	-1.807081000	-0.899625000	1	-8.301285000	-1.649193000	0.893993000
1	-8.764564000	-1.807017000	0.899949000	1	-8.301308000	-1.649258000	-0.893656000
1	-10.149351000	-1.103319000	0.000152000	6	-10.139100000	-0.906146000	0.000165000
				1	-10.462884000	-0.348618000	-0.892081000
				1	-10.462861000	-0.348552000	0.892379000
				1	-10.639737000	-1.886945000	0.000208000
D4-NH <sub>2</sub> E(RB3LYP) = -1085.93813684 a. u.				D4-N(CH <sub>3</sub> ) <sub>2</sub> E(RB3LYP) = -1164.54853724 a. u.			
6	5.592445000	-0.483041000	-0.000126000	6	6.420738000	-0.500569000	0.003811000
6	6.814115000	0.142131000	0.001893000	6	7.649726000	0.110956000	0.006941000
6	6.931421000	1.566708000	0.004135000	6	7.782973000	1.534054000	0.008375000
7	6.988325000	2.731096000	0.006042000	7	7.852983000	2.697774000	0.009487000
6	8.037458000	-0.699013000	0.001829000	6	8.863207000	-0.743606000	0.008889000
8	8.041676000	-1.913893000	0.000324000	8	8.854378000	-1.958607000	0.007954000
8	9.169531000	0.039932000	0.003900000	8	10.003890000	-0.017560000	0.011967000
1	9.904657000	-0.599354000	0.003694000	1	10.731275000	-0.665598000	0.013047000
6	1.836555000	0.010186000	-0.002270000	6	2.670502000	0.031053000	-0.003730000
1	1.774927000	1.102575000	-0.001275000	1	2.619384000	1.123985000	-0.003253000
1	5.631941000	-1.576938000	-0.001614000	1	6.448284000	-1.594847000	0.003040000
6	3.147097000	-0.565316000	-0.002102000	6	3.974779000	-0.557187000	-0.001384000
6	4.315015000	0.149526000	-0.000403000	6	5.150577000	0.145434000	0.001552000
1	3.209569000	-1.660638000	-0.003331000	1	4.026191000	-1.653122000	-0.001976000
1	4.277953000	1.243573000	0.000872000	1	5.125002000	1.239811000	0.002240000
6	-1.703271000	-1.260346000	-0.002678000	6	-0.881475000	-1.207255000	-0.011019000

6	-3.029590000	-0.841633000	-0.002395000	6	-2.203691000	-0.776965000	-0.013262000
6	-3.386404000	0.538435000	-0.003233000	6	-2.548034000	0.606977000	-0.013738000
6	-2.360380000	1.499893000	-0.004021000	6	-1.513088000	1.559066000	-0.011509000
6	-1.034725000	1.089623000	-0.004008000	6	-0.191193000	1.136824000	-0.009092000
6	-0.679132000	-0.287902000	-0.003392000	6	0.151988000	-0.243915000	-0.008844000
7	-4.197220000	-1.593528000	-0.001277000	7	-3.378134000	-1.517665000	-0.015329000
6	-4.829280000	0.595093000	-0.003565000	6	-3.989450000	0.675411000	-0.016593000
1	-1.447094000	-2.322842000	-0.002345000	1	-0.634690000	-2.272014000	-0.010749000
1	-2.602032000	2.564944000	-0.005017000	1	-1.745237000	2.626247000	-0.011797000
1	-0.248743000	1.845603000	-0.004831000	1	0.601712000	1.885580000	-0.007413000
6	0.700363000	-0.744605000	-0.003374000	6	1.526604000	-0.712895000	-0.006386000
1	0.828240000	-1.833835000	-0.004134000	1	1.644489000	-1.803296000	-0.006661000
6	-6.654414000	-1.073580000	0.001256000	6	-5.827891000	-0.982849000	-0.017464000
6	-7.585269000	-0.021780000	-0.000030000	6	-6.768476000	0.073193000	-0.023892000
6	-5.295802000	-0.750597000	-0.002650000	6	-4.469748000	-0.663833000	-0.017974000
6	-7.131024000	1.325674000	-0.002059000	6	-6.290176000	1.421363000	-0.015349000
1	-7.871072000	2.129621000	-0.007703000	1	-6.999763000	2.246067000	-0.010594000
6	-5.777708000	1.631497000	-0.002990000	6	-4.934332000	1.713665000	-0.013925000
1	-5.457487000	2.675775000	-0.001781000	1	-4.610892000	2.757066000	-0.008202000
1	-6.991157000	-2.113268000	0.000036000	1	-6.141999000	-2.025049000	-0.013531000
1	-4.238361000	-2.602766000	-0.005409000	1	-3.428531000	-2.526446000	-0.017322000
7	-8.951485000	-0.286146000	-0.062230000	7	-8.127443000	-0.188245000	-0.040425000
1	-9.549093000	0.451159000	0.298067000	6	-9.085429000	0.897229000	0.069146000
1	-9.234067000	-1.197582000	0.284317000	1	-8.983651000	1.616900000	-0.761806000
				1	-10.101169000	0.484187000	0.027078000
				1	-8.984217000	1.460280000	1.016755000
				6	-8.597968000	-1.556831000	0.045833000
				1	-9.694249000	-1.567080000	0.003220000
				1	-8.224349000	-2.168048000	-0.795099000
				1	-8.286441000	-2.054260000	0.985208000
D4-PhCH <sub>3</sub> E(RB3LYP) = -1300.96594988 a. u.				D4-PhNH <sub>2</sub> E(RB3LYP) = -1317.00868434 a. u.			
6	7.736937000	-0.574422000	0.058760000	6	7.731377000	-0.571620000	0.058138000
6	8.973052000	0.016808000	0.006671000	6	8.969103000	0.017332000	0.008097000
6	9.127051000	1.432188000	-0.122822000	6	9.125994000	1.432624000	-0.118033000
7	9.214076000	2.589747000	-0.228805000	7	9.215513000	2.590288000	-0.221237000
6	10.175545000	-0.852314000	0.088404000	6	10.169408000	-0.854113000	0.088514000
8	10.146948000	-2.061373000	0.199095000	8	10.138979000	-2.063537000	0.196460000

8	11.324964000	-0.144880000	0.025658000	8	11.320734000	-0.149051000	0.027927000
1	12.045079000	-0.798293000	0.086793000	1	12.038887000	-0.804674000	0.087967000
6	3.995489000	0.022871000	-0.002224000	6	3.990796000	0.028501000	-0.003113000
1	3.967391000	1.112051000	-0.101995000	1	3.962474000	1.117864000	-0.100764000
1	7.747444000	-1.664359000	0.158666000	1	7.740041000	-1.661813000	0.155607000
6	5.289852000	-0.589205000	0.055998000	6	5.284511000	-0.583743000	0.054271000
6	6.475840000	0.090140000	-0.004257000	6	6.471662000	0.094584000	-0.004045000
1	5.320421000	-1.681174000	0.156070000	1	5.314507000	-1.675981000	0.152084000
1	6.469147000	1.180234000	-0.104134000	1	6.466178000	1.184889000	-0.101619000
6	0.419861000	-1.128666000	0.096182000	6	0.415394000	-1.126180000	0.093594000
6	-0.894729000	-0.668860000	0.051951000	6	-0.899321000	-0.667961000	0.050060000
6	-1.203218000	0.716226000	-0.074370000	6	-1.209667000	0.717375000	-0.074799000
6	-0.147393000	1.640995000	-0.156175000	6	-0.154415000	1.643062000	-0.155707000
6	1.163550000	1.189930000	-0.112819000	6	1.157100000	1.193384000	-0.112994000
6	1.472191000	-0.193921000	0.013326000	6	1.467379000	-0.190208000	0.011590000
7	-2.083206000	-1.378986000	0.113984000	7	-2.087287000	-1.379011000	0.111491000
6	-2.644904000	0.821931000	-0.086082000	6	-2.650959000	0.821372000	-0.086334000
1	0.641447000	-2.194332000	0.193372000	1	0.638202000	-2.191757000	0.189554000
1	-0.355149000	2.708679000	-0.253328000	1	-0.363272000	2.710654000	-0.251746000
1	1.974267000	1.916252000	-0.177064000	1	1.967074000	1.920648000	-0.176650000
6	2.838227000	-0.693721000	0.061366000	6	2.833210000	-0.688590000	0.058867000
1	2.930829000	-1.781787000	0.160981000	1	2.926686000	-1.776818000	0.156518000
6	-4.524199000	-0.771848000	0.058153000	6	-4.528859000	-0.774706000	0.058895000
6	-5.423988000	0.301764000	-0.032932000	6	-5.433138000	0.296221000	-0.033604000
6	-3.153982000	-0.502108000	0.030267000	6	-3.159310000	-0.502938000	0.028613000
6	-4.918477000	1.623581000	-0.150265000	6	-4.926262000	1.618929000	-0.151509000
1	-5.624046000	2.449748000	-0.249991000	1	-5.631644000	2.444829000	-0.254704000
6	-3.554073000	1.887834000	-0.177746000	6	-3.562802000	1.885581000	-0.176869000
1	-3.196616000	2.914962000	-0.278526000	1	-3.207405000	2.913550000	-0.277305000
1	-4.890517000	-1.793200000	0.178467000	1	-4.891470000	-1.796965000	0.182805000
1	-2.158548000	-2.382070000	0.207060000	1	-2.161700000	-2.382292000	0.202535000
6	-9.139615000	0.698380000	0.687941000	6	-9.154181000	0.719242000	0.653162000
6	-9.702262000	-0.414648000	0.048385000	6	-9.710899000	-0.422295000	0.044608000
6	-8.830551000	-1.288798000	-0.621794000	6	-8.835050000	-1.322424000	-0.592406000
6	-7.763235000	0.932864000	0.661401000	6	-7.781438000	0.946692000	0.621262000
6	-7.456267000	-1.060056000	-0.650167000	6	-7.463391000	-1.086440000	-0.615105000
6	-6.889661000	0.057790000	-0.007326000	6	-6.896227000	0.051770000	-0.010401000
1	-9.789568000	1.393926000	1.225728000	1	-9.809516000	1.431548000	1.162075000
1	-6.811725000	-1.745496000	-1.205026000	1	-6.818388000	-1.793466000	-1.141569000
1	-9.237920000	-2.161274000	-1.140637000	1	-9.240950000	-2.208752000	-1.087866000
1	-7.358682000	1.796949000	1.192671000	1	-7.383956000	1.828997000	1.127339000

6	-11.189476000	-0.671706000	0.070151000	7	-11.090479000	-0.620658000	0.015938000
1	-11.609471000	-0.678605000	-	1	-11.605056000	-0.159518000	0.760128000
	0.949993000			1	-11.382735000	-1.587284000	-0.091357000
1	-11.420608000	-1.652522000	0.518958000				
1	-11.723952000	0.096813000	0.647783000				

**Table S13.** Cartesian coordinates (in Angstrom unit) of B3LYP/cc-pVDZ optimized geometries of phenothiazine based D- $\pi$ -A systems.

D5 E(RB3LYP) = -1507.38398515 a. u.				D5-CH <sub>3</sub> E(RB3LYP) = -1546.70173579 a. u.			
6	6.141109000	-0.541743000	0.085383000	6	6.466391000	-0.625560000	0.090000000
6	7.364454000	0.075858000	0.148669000	6	7.706668000	-0.049751000	0.202995000
6	7.489787000	1.499859000	0.150699000	6	7.874022000	1.367470000	0.285500000
7	7.551831000	2.663950000	0.150188000	7	7.970777000	2.527408000	0.350327000
6	8.581652000	-0.772685000	0.216346000	6	8.896818000	-0.937203000	0.239092000
8	8.577629000	-1.987236000	0.219827000	8	8.857026000	-2.149554000	0.175544000
8	9.715795000	-0.039868000	0.274087000	8	10.051497000	-0.243671000	0.352131000
1	10.447033000	-0.682374000	0.314937000	1	10.762307000	-0.909782000	0.366810000
6	2.395601000	-0.009259000	-0.116688000	6	2.741250000	0.027081000	-0.130394000
1	2.350179000	1.084335000	-0.122523000	1	2.726471000	1.120241000	-0.077341000
1	6.172564000	-1.635852000	0.090577000	1	6.465656000	-1.718758000	0.035100000
6	3.697294000	-0.601607000	-0.044972000	6	4.024224000	-0.605622000	-0.074495000
6	4.870186000	0.101389000	0.015519000	6	5.216177000	0.058047000	0.039461000
1	3.746413000	-1.697440000	-0.038935000	1	4.042035000	-1.701150000	-0.127911000
1	4.843659000	1.195785000	0.010694000	1	5.221416000	1.151374000	0.094441000
6	1.249667000	-0.745504000	-0.175721000	6	1.575950000	-0.671939000	-0.244184000
1	1.354397000	-1.836881000	-0.165966000	1	1.650623000	-1.764791000	-0.292461000
6	-1.793876000	1.512487000	-0.324659000	6	-1.402144000	1.674790000	-0.310044000
6	-2.860144000	0.584300000	-0.371616000	6	-2.493044000	0.780653000	-0.422204000
7	-4.199389000	1.001641000	-0.418955000	7	-3.817945000	1.236743000	-0.464759000
6	-2.507729000	-0.787598000	-0.388602000	6	-2.177422000	-0.598155000	-0.509573000
16	-3.743149000	-2.035230000	-0.693284000	16	-3.438968000	-1.794849000	-0.900268000
6	-5.151861000	-1.229450000	0.043896000	6	-4.842259000	-0.991553000	-0.149649000
6	-5.261146000	0.178944000	0.039409000	6	-4.910595000	0.417298000	-0.074944000
6	-0.466480000	1.105337000	-0.278300000	6	-0.087379000	1.228965000	-0.267959000
6	-1.178786000	-1.187320000	-0.298201000	6	-0.861237000	-1.038492000	-0.423412000
6	-6.190260000	-2.030420000	0.525708000	6	-5.910346000	-1.788399000	0.262492000
6	-6.471336000	0.733200000	0.498883000	6	-6.115155000	0.968831000	0.393893000

6	-7.522201000	-0.075226000	0.942013000	6	-7.194234000	0.160828000	0.767123000
6	-7.386902000	-1.461555000	0.968030000	6	-7.115270000	-1.232456000	0.719420000
1	-6.059102000	-3.114585000	0.528248000	1	-5.802027000	-2.874502000	0.201103000
1	-6.609308000	1.811584000	0.518920000	1	-6.232028000	2.046745000	0.478742000
1	-8.446525000	0.397203000	1.280463000	1	-8.111650000	0.640966000	1.115983000
1	-8.198145000	-2.098115000	1.325267000	6	0.224914000	-0.144117000	-0.308747000
6	-0.116809000	-0.258792000	-0.248852000	1	-1.578215000	2.745840000	-0.248131000
1	-1.998659000	2.580151000	-0.319102000	1	0.707291000	1.971821000	-0.185473000
1	0.308165000	1.872907000	-0.248890000	1	-0.666522000	-2.112526000	-0.476666000
1	-0.955244000	-2.257013000	-0.295561000	6	-4.066326000	2.666843000	-0.693083000
6	-4.489102000	2.408712000	-0.729873000	1	-3.333346000	3.009025000	-1.438653000
1	-3.776303000	2.721854000	-1.507079000	1	-5.049980000	2.747801000	-1.178264000
1	-5.481404000	2.434715000	-1.203351000	6	-4.017033000	3.576614000	0.543285000
6	-4.445291000	3.395391000	0.446318000	1	-3.033283000	3.557135000	1.034339000
1	-3.455020000	3.430405000	0.923035000	1	-4.761939000	3.290040000	1.299480000
1	-5.172577000	3.140418000	1.230426000	1	-4.223569000	4.616116000	0.240020000
1	-4.681207000	4.408372000	0.081120000	6	-8.265508000	-2.116593000	1.134197000
				1	-8.615201000	-2.741991000	0.295331000
				1	-7.972580000	-2.802460000	1.946792000
				1	-9.120760000	-1.522299000	1.488059000
D5-C <sub>5</sub> H <sub>11</sub> E(RB3LYP) = -1703.95800820 a. u.				D5-isopropyl E(RB3LYP) = -1625.32940691 a. u.			
6	-7.961865000	-0.975005000	-0.185561000	6	7.109217000	-0.751578000	0.099269000
6	-9.230072000	-0.541907000	-0.480350000	6	8.365768000	-0.233209000	0.286393000
6	-9.496613000	0.814233000	-0.845238000	6	8.581010000	1.165871000	0.485340000
7	-9.674962000	1.928235000	-1.138887000	7	8.717089000	2.312674000	0.644558000
6	-10.344269000	-1.521288000	-0.413731000	6	9.522381000	-1.164605000	0.279306000
8	-10.218636000	-2.691847000	-0.114567000	8	9.441331000	-2.365865000	0.118593000
8	-11.536179000	-0.965562000	-0.726325000	8	10.697571000	-0.525771000	0.473923000
1	-12.191851000	-1.682455000	-0.653419000	1	11.383704000	-1.217083000	0.452046000
6	-4.322750000	0.031465000	0.121791000	6	3.416591000	0.055759000	-0.153122000
1	-4.385842000	1.092022000	-0.141395000	1	3.439694000	1.141061000	-0.013041000
1	-7.883293000	-2.034017000	0.079816000	1	7.071174000	-1.836268000	-0.042493000
6	-5.547034000	-0.710320000	0.114809000	6	4.674280000	-0.627239000	-0.119090000
6	-6.773662000	-0.187150000	-0.195185000	6	5.885784000	-0.019821000	0.074621000
1	-5.486732000	-1.773451000	0.378412000	1	4.654365000	-1.715021000	-0.259389000
1	-6.856640000	0.871529000	-0.461137000	1	5.928442000	1.064799000	0.216759000
6	-3.119964000	-0.528752000	0.436774000	6	2.230172000	-0.587484000	-0.348481000
1	-3.116148000	-1.595108000	0.691981000	1	2.266696000	-1.675077000	-0.482813000

6	-0.338508000	2.039085000	0.215951000	6	-0.658863000	1.868066000	-0.288200000
6	0.805183000	1.281317000	0.562741000	6	-1.778057000	1.027859000	-0.496108000
7	2.085349000	1.851231000	0.590753000	7	-3.084487000	1.535589000	-0.528392000
6	0.587746000	-0.078194000	0.899492000	6	-1.510428000	-0.350345000	-0.689474000
16	1.902486000	-1.064564000	1.588358000	16	-2.804709000	-1.462527000	-1.204560000
6	3.293822000	-0.298432000	0.778603000	6	-4.194897000	-0.669082000	-0.419505000
6	3.262063000	1.071232000	0.433870000	6	-4.213577000	0.727537000	-0.229554000
6	-1.609637000	1.480259000	0.186008000	6	0.637608000	1.370763000	-0.254338000
6	-0.682118000	-0.639984000	0.825245000	6	-0.213552000	-0.845814000	-0.610668000
6	4.446135000	-1.060057000	0.593216000	6	-5.303049000	-1.456280000	-0.094887000
6	4.453935000	1.624304000	-0.061290000	6	-5.409357000	1.284102000	0.262200000
6	5.617456000	0.859103000	-0.206354000	6	-6.523644000	0.491954000	0.545816000
6	5.640252000	-0.501386000	0.107552000	6	-6.495669000	-0.898379000	0.383332000
1	4.415592000	-2.120127000	0.859729000	1	-5.232987000	-2.536953000	-0.243855000
1	4.497260000	2.672481000	-0.348176000	1	-5.487696000	2.355297000	0.433597000
1	6.511288000	1.353936000	-0.587332000	1	-7.425683000	0.984410000	0.915454000
6	-1.820700000	0.117844000	0.475727000	6	0.901025000	-0.005395000	-0.399828000
1	-0.238859000	3.090127000	-0.043550000	1	-0.797745000	2.936560000	-0.143173000
1	-2.449292000	2.121619000	-0.085645000	1	1.456257000	2.073905000	-0.094526000
1	-0.799509000	-1.697247000	1.075716000	1	-0.056413000	-1.918643000	-0.747191000
6	2.209044000	3.314590000	0.545567000	6	-3.276631000	2.987583000	-0.645966000
1	1.399980000	3.728748000	1.165292000	1	-2.515375000	3.360285000	-1.347313000
1	3.145744000	3.573088000	1.060579000	1	-4.245578000	3.143647000	-1.142271000
6	2.183114000	3.960706000	-0.847457000	6	-3.222702000	3.794330000	0.659793000
1	1.242473000	3.760143000	-1.380627000	1	-2.251830000	3.699081000	1.167314000
1	3.001290000	3.599903000	-1.487175000	1	-3.994600000	3.477388000	1.375739000
1	2.288244000	5.053283000	-0.745320000	1	-3.384627000	4.861587000	0.436287000
6	6.864970000	-1.385459000	-0.046411000	6	-7.696015000	-1.778007000	0.706086000
1	6.602004000	-2.230919000	-0.709101000	1	-7.396721000	-2.818123000	0.487839000
1	7.087115000	-1.846500000	0.934030000	6	-8.904911000	-1.447922000	-0.187465000
6	8.134544000	-0.715438000	-0.577775000	6	-8.072330000	-1.709062000	2.196904000
1	7.932201000	-0.267143000	-1.567588000	1	-7.219114000	-1.980737000	2.838246000
1	8.419836000	0.120625000	0.086517000	1	-8.396892000	-0.694247000	2.482402000
6	9.313445000	-1.687292000	-0.697667000	1	-8.903000000	-2.398584000	2.420842000
1	9.029858000	-2.526503000	-1.360699000	1	-9.267025000	-0.421303000	-0.009560000
1	9.516693000	-2.139940000	0.291342000	1	-9.741441000	-2.135577000	0.019854000
6	10.594679000	-1.035073000	-1.227829000	1	-8.648627000	-1.532317000	-1.255349000
1	10.390075000	-0.582803000	-2.215908000				
1	10.876962000	-0.196756000	-0.564308000				
6	11.767103000	-2.011546000	-1.345227000				
1	11.528658000	-2.842844000	-2.030520000				



1	12.019323000	-2.453846000	-0.366295000			
1	12.671821000	-1.512937000	-1.728512000			
D5-t-but E(RB3LYP) = -1664.64042510 a. u.				D5-OH E(RB3LYP) = -1582.60895224 a. u.		
6	7.349013000	-0.820006000	0.091177000	6	6.459515000	-0.615463000 0.091964000
6	8.617913000	-0.336622000	0.288409000	6	7.698960000	-0.036147000 0.198483000
6	8.867986000	1.053164000	0.510451000	6	7.863467000	1.382072000 0.267865000
7	9.032641000	2.193425000	0.688550000	7	7.957810000	2.542782000 0.321989000
6	9.750723000	-1.296611000	0.267609000	6	8.890758000	-0.920694000 0.241512000
8	9.639769000	-2.492674000	0.087191000	8	8.853643000	-2.133727000 0.189097000
8	10.941294000	-0.690821000	0.474087000	8	10.044340000	-0.223904000 0.347110000
1	11.609849000	-1.398746000	0.441774000	1	10.756235000	-0.888696000 0.367153000
6	3.678564000	0.084916000	-0.153379000	6	2.732967000	0.026904000 -0.130685000
1	3.729138000	1.166825000	0.004561000	1	2.715823000	1.120471000 -0.087544000
1	7.283854000	-1.900936000	-0.068322000	1	6.461020000	-1.709124000 0.047069000
6	4.918347000	-0.630432000	-0.128609000	6	4.017112000	-0.602313000 -0.070321000
6	6.144518000	-0.057234000	0.076797000	6	5.208024000	0.064881000 0.036413000
1	4.871040000	-1.714917000	-0.286735000	1	4.037301000	-1.698256000 -0.113740000
1	6.214364000	1.023495000	0.236706000	1	5.210945000	1.158677000 0.081391000
6	2.476433000	-0.524339000	-0.361255000	6	1.568770000	-0.675695000 -0.236859000
1	2.485225000	-1.610163000	-0.513410000	1	1.645940000	-1.768788000 -0.275038000
6	-0.348080000	2.003913000	-0.266157000	6	-1.413916000	1.664318000 -0.320745000
6	-1.488291000	1.196676000	-0.490444000	6	-2.503981000	0.766688000 -0.419639000
7	-2.780604000	1.739442000	-0.518359000	7	-3.828368000	1.216423000 -0.462066000
6	-1.256233000	-0.184955000	-0.704691000	6	-2.184705000	-0.612349000 -0.496793000
16	-2.577249000	-1.255649000	-1.238187000	16	-3.441563000	-1.817148000 -0.881432000
6	-3.950320000	-0.437958000	-0.446694000	6	-4.849052000	-1.016401000 -0.139842000
6	-3.932186000	0.958103000	-0.238343000	6	-4.918951000	0.392517000 -0.063010000
6	0.934899000	1.472689000	-0.237585000	6	-0.098547000	1.221265000 -0.277773000
6	0.027423000	-0.714872000	-0.631874000	6	-0.867837000	-1.049430000 -0.409444000
6	-5.077283000	-1.199289000	-0.140528000	6	-5.910250000	-1.822373000 0.269810000
6	-5.116060000	1.533024000	0.250171000	6	-6.120554000	0.941813000 0.413528000
6	-6.254715000	0.763701000	0.516312000	6	-7.203315000	0.140097000 0.788987000
6	-6.267442000	-0.623094000	0.338968000	6	-7.103563000	-1.250323000 0.726816000
1	-5.018082000	-2.276410000	-0.308689000	1	-5.829508000	-2.909056000 0.216073000
1	-5.173540000	2.603009000	0.436770000	1	-6.237617000	2.019273000 0.502170000
1	-7.138349000	1.284184000	0.883715000	1	-8.122397000	0.614351000 1.143927000
6	1.162892000	0.092708000	-0.405413000	6	0.216903000	-0.151736000 -0.304815000
1	-0.459484000	3.073111000	-0.103675000	1	-1.592231000	2.735628000 -0.269286000

1	1.771046000	2.151621000	-0.064260000	1	0.694989000	1.966384000	-0.204959000
1	0.157021000	-1.789128000	-0.785118000	1	-0.670746000	-2.123440000	-0.454345000
6	-2.933586000	3.198196000	-0.605855000	6	-4.085766000	2.641604000	-0.704754000
1	-2.159152000	3.565697000	-1.295293000	1	-3.357710000	2.981011000	-1.456604000
1	-3.895516000	3.390304000	-1.103061000	1	-5.071973000	2.711742000	-1.186995000
6	-2.865509000	3.973500000	0.718024000	6	-4.036494000	3.566025000	0.521089000
1	-1.900176000	3.840665000	1.227714000	1	-3.050513000	3.556989000	1.007945000
1	-3.649594000	3.660542000	1.422360000	1	-4.776158000	3.284799000	1.284556000
1	-2.997926000	5.049520000	0.518424000	1	-4.249576000	4.601016000	0.207047000
6	-7.490279000	-1.508611000	0.637405000	8	-8.109730000	-2.098600000	1.088600000
6	-7.118593000	-2.552656000	1.715822000	1	-8.868209000	-1.574771000	1.385453000
1	-6.291727000	-3.202744000	1.390360000				
1	-6.809874000	-2.060553000	2.652101000				
1	-7.983516000	-3.199556000	1.938201000				
6	-8.685465000	-0.686776000	1.152941000				
1	-8.448604000	-0.161275000	2.091629000				
1	-9.019375000	0.060235000	0.415453000				
1	-9.536889000	-1.355800000	1.354447000				
6	-7.926037000	-2.238816000	-0.654229000				
1	-8.800313000	-2.880956000	-0.455965000				
1	-8.202411000	-1.518688000	-1.441136000				
1	-7.125585000	-2.880962000	-1.053294000				
D5-OCH <sub>3</sub> E(RB3LYP) = -1621.91065765 a. u.				D5-OC <sub>2</sub> H <sub>5</sub> E(RB3LYP) = -1661.23080517 a. u.			
6	6.806039000	-0.676901000	0.115016000	6	-7.150429000	-0.791264000	-0.120031000
6	8.053841000	-0.124925000	0.262343000	6	-8.411032000	-0.286293000	-0.318634000
6	8.242482000	1.286362000	0.388314000	6	-8.637977000	1.108741000	-0.532029000
7	8.356676000	2.442254000	0.488175000	7	-8.783705000	2.252716000	-0.702910000
6	9.228747000	-1.032241000	0.289659000	6	-9.558775000	-1.227967000	-0.308676000
8	9.170927000	-2.241571000	0.190459000	8	-9.468043000	-2.427018000	-0.136167000
8	10.392857000	-0.361411000	0.439331000	8	-10.739070000	-0.602028000	-0.515507000
1	11.092222000	-1.039645000	0.444791000	1	-11.418442000	-1.299853000	-0.490509000
6	3.095293000	0.040484000	-0.139102000	6	-3.466561000	0.049992000	0.143840000
1	3.096245000	1.131804000	-0.054954000	1	-3.497787000	1.133714000	-0.006552000
1	6.788892000	-1.767936000	0.028484000	1	-7.103406000	-1.874195000	0.032220000
6	4.367186000	-0.613349000	-0.083411000	6	-4.717901000	-0.643586000	0.109810000
6	5.567857000	0.027710000	0.066487000	6	-5.934016000	-0.048663000	-0.095956000
1	4.369016000	-1.707083000	-0.168086000	1	-4.689556000	-1.729827000	0.260482000
1	5.589260000	1.118805000	0.153052000	1	-5.985347000	1.034159000	-0.248578000

6	1.920949000	-0.636956000	-0.289139000	6	-2.275475000	-0.581670000	0.351236000
1	1.980151000	-1.729037000	-0.367646000	1	-2.304141000	-1.668263000	0.495506000
6	-1.020068000	1.756065000	-0.327789000	6	0.593440000	1.896349000	0.280835000
6	-2.123572000	0.882169000	-0.478574000	6	1.719744000	1.066944000	0.499636000
7	-3.438857000	1.357276000	-0.524309000	7	3.019660000	1.583051000	0.531887000
6	-1.826404000	-0.498484000	-0.603679000	6	1.461092000	-0.311680000	0.706959000
16	-3.096351000	-1.666256000	-1.052613000	16	2.757699000	-1.410516000	1.244916000
6	-4.502938000	-0.868410000	-0.305550000	6	4.151368000	-0.619077000	0.467138000
6	-4.550972000	0.539217000	-0.177565000	6	4.160082000	0.778318000	0.251330000
6	0.286759000	1.288992000	-0.281578000	6	-0.698322000	1.388283000	0.246705000
6	-0.518433000	-0.961127000	-0.513314000	6	0.168654000	-0.818027000	0.628428000
6	-5.584958000	-1.665344000	0.054294000	6	5.261324000	-1.404022000	0.171745000
6	-5.751423000	1.088517000	0.295511000	6	5.350772000	1.332237000	-0.240659000
6	-6.860631000	0.297012000	0.623454000	6	6.487070000	0.555498000	-0.504331000
6	-6.781972000	-1.092660000	0.511823000	6	6.448398000	-0.826795000	-0.306307000
1	-5.525712000	-2.750916000	-0.037760000	1	5.231917000	-2.482946000	0.331495000
1	-5.851731000	2.164007000	0.422086000	1	5.421681000	2.400208000	-0.433628000
1	-7.766326000	0.789101000	0.974834000	1	7.382491000	1.052103000	-0.874824000
6	0.579491000	-0.087275000	-0.357383000	6	-0.951884000	0.011103000	0.403848000
1	-1.181121000	2.827516000	-0.237133000	1	0.724458000	2.964509000	0.125924000
1	1.091363000	2.016816000	-0.167096000	1	-1.521982000	2.083173000	0.076603000
1	-0.338725000	-2.035919000	-0.596561000	1	0.019145000	-1.890519000	0.776100000
6	-3.666601000	2.795552000	-0.714278000	6	3.202882000	3.036573000	0.632995000
1	-2.919481000	3.151140000	-1.439424000	1	2.435850000	3.414835000	1.325139000
1	-4.642780000	2.902687000	-1.209785000	1	4.168620000	3.203808000	1.132269000
6	-3.623039000	3.668853000	0.548575000	6	3.151461000	3.826666000	-0.683224000
1	-2.645900000	3.623100000	1.051034000	1	2.183134000	3.719953000	-1.193415000
1	-4.380663000	3.369730000	1.287196000	1	3.927694000	3.504216000	-1.392079000
1	-3.813332000	4.719209000	0.273230000	1	3.307234000	4.897555000	-0.472967000
8	-7.781902000	-1.969675000	0.811581000	8	7.476773000	-1.689821000	-0.537533000
6	-9.012263000	-1.441575000	1.280845000	6	8.711631000	-1.165905000	-1.028246000
1	-8.883152000	-0.883967000	2.225957000	1	9.113402000	-0.422825000	-0.313916000
1	-9.483833000	-0.778693000	0.533095000	1	8.542926000	-0.650565000	-1.992493000
1	-9.664783000	-2.306214000	1.458708000	6	9.667264000	-2.332080000	-1.194946000
				1	9.262287000	-3.067056000	-1.907513000
				1	9.832829000	-2.839399000	-0.232042000
				1	10.637980000	-1.976007000	-1.573860000

D5-NH <sub>2</sub> E(RB3LYP) = -1562.74278223 a. u.				D5-N(CH <sub>3</sub> ) <sub>2</sub> E(RB3LYP) = -1641.35353649 a. u.			
6	6.459886000	-0.618717000	0.091685000	6	-7.079002000	-0.760229000	-0.107987000
6	7.702068000	-0.044935000	0.202345000	6	-8.344301000	-0.252474000	-0.270550000
6	7.872416000	1.372200000	0.277450000	6	-8.578473000	1.148932000	-0.425556000
7	7.971712000	2.532317000	0.336327000	7	-8.730100000	2.298287000	-0.549092000
6	8.889576000	-0.934388000	0.243853000	6	-9.488160000	-1.197747000	-0.283399000
8	8.848066000	-2.147281000	0.187103000	8	-9.392114000	-2.402647000	-0.159713000
8	10.046442000	-0.243140000	0.353707000	8	-10.673686000	-0.568936000	-0.450272000
1	10.754819000	-0.911662000	0.372235000	1	-11.349493000	-1.270568000	-0.444140000
6	2.735906000	0.034498000	-0.133775000	6	-3.394109000	0.077429000	0.143712000
1	2.720498000	1.127950000	-0.087303000	1	-3.427640000	1.166304000	0.037563000
1	6.457347000	-1.712220000	0.042706000	1	-7.027045000	-1.848207000	0.000577000
6	4.018005000	-0.597331000	-0.073924000	6	-4.644338000	-0.615636000	0.097132000
6	5.211381000	0.065898000	0.036752000	6	-5.864839000	-0.015974000	-0.069631000
1	4.035609000	-1.693224000	-0.121053000	1	-4.612744000	-1.707050000	0.203824000
1	5.217663000	1.159515000	0.085524000	1	-5.920298000	1.071937000	-0.178253000
6	1.570014000	-0.666029000	-0.243219000	6	-2.199504000	-0.561119000	0.311109000
1	1.646225000	-1.759159000	-0.284258000	1	-2.226815000	-1.652772000	0.411273000
6	-1.409409000	1.676882000	-0.325092000	6	0.667808000	1.918291000	0.310201000
6	-2.501493000	0.780243000	-0.422398000	6	1.797623000	1.080313000	0.478080000
7	-3.823311000	1.229906000	-0.459759000	7	3.096090000	1.592044000	0.512022000
6	-2.182952000	-0.599938000	-0.502941000	6	1.540670000	-0.306915000	0.631822000
16	-3.440513000	-1.801217000	-0.897809000	16	2.843105000	-1.424539000	1.115693000
6	-4.849490000	-1.003530000	-0.153522000	6	4.229774000	-0.605206000	0.349988000
6	-4.915587000	0.401945000	-0.067215000	6	4.232664000	0.793961000	0.190694000
6	-0.094893000	1.232461000	-0.283288000	6	-0.623895000	1.411703000	0.271024000
6	-0.866659000	-1.037710000	-0.416728000	6	0.247497000	-0.809083000	0.547890000
6	-5.911214000	-1.811580000	0.253608000	6	5.332951000	-1.389167000	0.014619000
6	-6.117039000	0.945024000	0.420432000	6	5.425433000	1.358749000	-0.289998000
6	-7.196210000	0.142585000	0.793190000	6	6.548899000	0.589703000	-0.594185000
6	-7.114039000	-1.255930000	0.723686000	6	6.530172000	-0.815693000	-0.472168000
1	-5.805976000	-2.896767000	0.178449000	1	5.248887000	-2.465262000	0.156119000
1	-6.232815000	2.021954000	0.521007000	1	5.505513000	2.434090000	-0.434755000
1	-8.112053000	0.617473000	1.153256000	1	7.439513000	1.106925000	-0.945887000
6	0.219544000	-0.141178000	-0.310900000	6	-0.876202000	0.028556000	0.372209000
1	-1.586925000	2.748368000	-0.273021000	1	0.797358000	2.992153000	0.198834000
1	0.699610000	1.976656000	-0.210887000	1	-1.449714000	2.112795000	0.141343000
1	-0.670171000	-2.111754000	-0.464640000	1	0.099055000	-1.886745000	0.653301000
				6	3.285625000	3.039944000	0.662426000

6	-4.082267000	2.655885000	-0.693975000	1	2.528114000	3.397442000	1.375807000
1	-3.357286000	3.000922000	-1.446382000	1	4.257557000	3.186909000	1.155884000
1	-5.070492000	2.727966000	-1.171512000	6	3.222410000	3.873252000	-0.626180000
6	-4.029063000	3.571959000	0.537869000	1	2.247566000	3.786411000	-1.127844000
1	-3.041057000	3.560173000	1.020753000	1	3.989346000	3.570020000	-1.353449000
1	-4.765935000	3.284009000	1.301563000	1	3.385143000	4.936274000	-0.383530000
1	-4.244273000	4.609047000	0.232176000	7	7.623147000	-1.600745000	-0.818771000
7	-8.203922000	-2.069627000	1.042754000	6	7.630195000	-3.006905000	-0.458933000
1	-8.859464000	-1.653460000	1.697993000	1	7.580995000	-3.176964000	0.635973000
1	-7.955428000	-3.011004000	1.333252000	1	6.782423000	-3.540049000	-0.920215000
				1	8.551667000	-3.469179000	-0.836268000
				6	8.896339000	-0.957295000	-1.085339000
				1	9.292044000	-0.397081000	-0.213658000
				1	9.633238000	-1.721374000	-1.365278000
				1	8.816659000	-0.252161000	-1.929424000
D5-PhCH <sub>3</sub> E(RB3LYP) = -1777.77268048 a. u.				D5-PhNH <sub>2</sub> E(RB3LYP) = -1793.81532069 a. u.			
6	-8.044786000	-1.131819000	-0.057993000	6	-8.042173000	-1.124496000	-0.060535000
6	-9.338162000	-0.769857000	-0.337955000	6	-9.336468000	-0.762283000	-0.337581000
6	-9.677961000	0.559490000	-0.738932000	6	-9.677609000	0.568372000	-0.732816000
7	-9.916443000	1.653582000	-1.063081000	7	-9.917286000	1.663594000	-1.052371000
6	-10.401906000	-1.799167000	-0.216170000	6	-10.399075000	-1.792519000	-0.218730000
8	-10.212909000	-2.951936000	0.116511000	8	-10.209429000	-2.946728000	0.109047000
8	-11.625434000	-1.311564000	-0.519479000	8	-11.623677000	-1.304684000	-0.518403000
1	-12.244128000	-2.056147000	-0.409905000	1	-12.241168000	-2.050516000	-0.410798000
6	-4.453994000	0.060023000	0.136834000	6	-4.451237000	0.065512000	0.135966000
1	-4.575308000	1.107116000	-0.157987000	1	-4.571849000	1.114040000	-0.153988000
1	-7.909082000	-2.176677000	0.238545000	1	-7.905717000	-2.170518000	0.231575000
6	-5.640104000	-0.740790000	0.180235000	6	-5.637401000	-0.734524000	0.176858000
6	-6.896858000	-0.288016000	-0.118667000	6	-6.894826000	-0.280445000	-0.118876000
1	-5.521867000	-1.790590000	0.475615000	1	-5.519327000	-1.785680000	0.467576000
1	-7.037270000	0.756235000	-0.415734000	1	-7.035522000	0.765064000	-0.411339000
6	-3.218861000	-0.429823000	0.442634000	6	-3.215874000	-0.426864000	0.438555000
1	-3.156297000	-1.485788000	0.731082000	1	-3.154465000	-1.484287000	0.722019000
6	-0.574708000	2.264546000	0.081479000	6	-0.569043000	2.265467000	0.088251000
6	0.611337000	1.576060000	0.428129000	6	0.617145000	1.573497000	0.429398000
7	1.862699000	2.210482000	0.411359000	7	1.868328000	2.205109000	0.413401000
6	0.470153000	0.219162000	0.810553000	6	0.474215000	0.214625000	0.806433000
16	1.847836000	-0.677963000	1.498613000	16	1.849946000	-0.686698000	1.492660000

6	3.178499000	0.130247000	0.628871000	6	3.183539000	0.122577000	0.627613000
6	3.071700000	1.487211000	0.253390000	6	3.077735000	1.479636000	0.254372000
6	-1.816616000	1.642476000	0.095807000	6	-1.811610000	1.645167000	0.101044000
6	-0.771037000	-0.407393000	0.780927000	6	-0.767886000	-0.409630000	0.774868000
6	4.362556000	-0.581608000	0.440483000	6	4.367524000	-0.590000000	0.441475000
6	4.227958000	2.089426000	-0.276841000	6	4.234555000	2.080148000	-0.275708000
6	5.421044000	1.381202000	-0.425983000	6	5.426287000	1.370115000	-0.427473000
6	5.518848000	0.025343000	-0.081726000	6	5.525710000	0.013672000	-0.082476000
1	4.393451000	-1.626178000	0.756259000	1	4.396995000	-1.633753000	0.760089000
1	4.210161000	3.128451000	-0.597296000	1	4.218237000	3.119452000	-0.595764000
1	6.280557000	1.894839000	-0.860092000	1	6.284535000	1.883630000	-0.864322000
6	-1.952857000	0.281554000	0.432755000	6	-1.949425000	0.282519000	0.431110000
1	-0.533099000	3.310272000	-0.212965000	1	-0.526317000	3.312631000	-0.200944000
1	-2.692608000	2.232154000	-0.178063000	1	-2.687202000	2.237398000	-0.168685000
1	-0.829945000	-1.460706000	1.066073000	1	-0.828153000	-1.464089000	1.055573000
6	1.910303000	3.677125000	0.327084000	6	1.919218000	3.671482000	0.332648000
1	1.092173000	4.064892000	0.951825000	1	1.102982000	4.060398000	0.959259000
1	2.841242000	3.996548000	0.817736000	1	2.851827000	3.987438000	0.822337000
6	1.826070000	4.284356000	-1.080851000	6	1.834547000	4.281827000	-1.073970000
1	0.887366000	4.023033000	-1.590573000	1	0.894251000	4.024038000	-1.582629000
1	2.649686000	3.948976000	-1.727421000	1	2.656269000	3.944990000	-1.722186000
1	1.877377000	5.383080000	-1.008026000	1	1.889115000	5.380313000	-0.999303000
6	7.949387000	-2.806677000	-0.813405000	6	7.951347000	-2.832988000	-0.790302000
6	9.200861000	-2.206383000	-0.597661000	6	9.205366000	-2.221380000	-0.599780000
6	9.215891000	-0.859922000	-0.208741000	6	9.226393000	-0.861306000	-0.235352000
6	6.764723000	-2.091786000	-0.648313000	6	6.773032000	-2.111342000	-0.621470000
6	8.031667000	-0.139268000	-0.040371000	6	8.041823000	-0.149155000	-0.069762000
6	6.778980000	-0.738848000	-0.257193000	6	6.783117000	-0.751283000	-0.257503000
1	7.901944000	-3.853637000	-1.126247000	1	7.904494000	-3.885840000	-1.082049000
1	8.082652000	0.900064000	0.291476000	1	8.097739000	0.897295000	0.238230000
1	10.173193000	-0.365278000	-0.023330000	1	10.185634000	-0.364211000	-0.066381000
1	5.811334000	-2.584413000	-0.851829000	1	5.820437000	-2.612766000	-0.806448000
6	10.477047000	-2.991083000	-0.782010000	7	10.386221000	-2.955375000	-0.704201000
1	10.501657000	-3.877041000	-0.125330000	1	11.212877000	-2.407311000	-0.922413000
1	10.575993000	-3.356842000	-1.818166000	1	10.325662000	-3.780964000	-1.292463000
1	11.363359000	-2.380075000	-0.555874000				

**Table S14.** Cartesian coordinates (in Angstrom unit) of B3LYP/cc-pVDZ optimized geometries of coumarin based D- $\pi$ -A systems.

D6 E(RB3LYP) = -1010.12941408 a. u.				D6-CH <sub>3</sub> E(RB3LYP) = -1049.44836104 a. u.			
6	3.036412000	-1.857466000	0.000004000	6	2.560347000	1.992917000	0.000032000
6	2.085262000	-0.721198000	0.000011000	6	1.639009000	0.833865000	0.000150000
6	2.573182000	0.559450000	0.000022000	6	2.160379000	-0.434990000	0.000289000
6	3.979431000	0.832390000	0.000015000	6	3.570853000	-0.670491000	0.000199000
6	4.861847000	-0.268623000	0.000008000	6	4.425923000	0.450059000	-0.000033000
6	6.247219000	-0.089700000	-0.000008000	6	5.815590000	0.307995000	-0.000158000
6	6.761830000	1.205162000	-0.000016000	6	6.390228000	-0.965452000	-0.000053000
6	5.904393000	2.320063000	-0.000007000	6	5.541120000	-2.097125000	0.000193000
6	4.528751000	2.134328000	0.000007000	6	4.163807000	-1.954189000	0.000311000
1	1.886365000	1.409792000	0.000031000	1	1.494909000	-1.302201000	0.000460000
1	3.851645000	2.991726000	0.000013000	1	3.516225000	-2.834219000	0.000498000
1	6.320881000	3.328700000	-0.000013000	1	5.982022000	-3.096582000	0.000290000
1	6.893036000	-0.968457000	-0.000014000	1	6.430573000	1.209401000	-0.000325000
8	4.391400000	-1.548787000	0.000021000	8	3.924643000	1.717695000	-0.000121000
8	2.731997000	-3.024822000	-0.000034000	8	2.229144000	3.153066000	-0.000275000
6	-4.176767000	-0.416117000	-0.000005000	6	-4.612834000	0.370127000	0.000044000
6	-5.325903000	0.328841000	-0.000006000	6	-5.744563000	-0.401771000	-0.000048000
6	-5.297558000	1.758515000	-0.000008000	6	-5.682343000	-1.830306000	-0.000211000
7	-5.234193000	2.922273000	-0.000013000	7	-5.592422000	-2.992365000	-0.000344000
6	-6.632263000	-0.384743000	-0.000006000	6	-7.066841000	0.280557000	0.000025000
8	-6.755212000	-1.591877000	0.000010000	8	-7.219081000	1.484534000	0.000169000
8	-7.679177000	0.467357000	0.000009000	8	-8.093907000	-0.595896000	-0.000072000
1	-8.479846000	-0.088099000	0.000022000	1	-8.906872000	-0.058665000	-0.000008000
6	-0.390367000	-0.252043000	-0.000001000	6	-0.823870000	0.300059000	0.000051000
1	-0.247767000	0.834014000	-0.000004000	1	-0.653448000	-0.781939000	-0.000091000
1	-4.322366000	-1.500783000	-0.000004000	1	-4.784355000	1.451018000	0.000167000
6	-1.745978000	-0.721911000	-0.000003000	6	-2.190489000	0.735210000	0.000097000
6	-2.841906000	0.094364000	-0.000005000	6	-3.266532000	-0.107737000	-0.000007000
1	-1.896950000	-1.807757000	-0.000003000	1	-2.368715000	1.816996000	0.000225000
1	-2.705673000	1.180653000	-0.000007000	1	-3.103774000	-1.190369000	-0.000134000
6	0.679387000	-1.093063000	0.000006000	6	0.224435000	1.168347000	0.000163000
1	0.502281000	-2.171772000	0.000010000	1	0.018949000	2.242074000	0.000255000
1	7.843848000	1.351610000	-0.000030000	6	7.887307000	-1.141848000	-0.000280000
				1	8.217285000	-1.710573000	0.885196000
				1	8.217151000	-1.709136000	-0.886740000

				1	8.411446000	-0.175791000	0.000436000
D6-C <sub>5</sub> H <sub>11</sub> E(RB3LYP) = -1206.70441262 a. u.				D6-isopropyl E(RB3LYP) = -1128.07595004 a. u.			
6	0.447249000	2.620052000	0.000096000	6	-1.749673000	2.057336000	-0.000075000
6	-0.302076000	1.342102000	-0.000084000	6	-0.842431000	0.886316000	-0.000257000
6	0.392500000	0.159464000	-0.000222000	6	-1.379433000	-0.375592000	-0.000442000
6	1.822283000	0.125514000	-0.000150000	6	-2.793226000	-0.593196000	-0.000329000
6	2.512598000	1.357219000	0.000056000	6	-3.635673000	0.538969000	-0.000014000
6	3.903829000	1.409936000	0.000145000	6	-5.024181000	0.416357000	0.000154000
6	4.659502000	0.228920000	0.000029000	6	-5.619506000	-0.851453000	0.000001000
6	3.978295000	-1.007252000	-0.000182000	6	-4.784071000	-1.989898000	-0.000319000
6	2.590340000	-1.057296000	-0.000271000	6	-3.402073000	-1.866643000	-0.000480000
1	-0.143650000	-0.793156000	-0.000406000	1	-0.725440000	-1.251478000	-0.000674000
1	2.075242000	-2.020918000	-0.000433000	1	-2.767554000	-2.756145000	-0.000718000
1	4.541710000	-1.939891000	-0.000277000	1	-5.237596000	-2.983517000	-0.000438000
1	4.386413000	2.389378000	0.000305000	1	-5.618688000	1.331011000	0.000397000
8	1.835346000	2.542212000	0.000168000	8	-3.116187000	1.800988000	0.000123000
8	-0.046683000	3.721037000	0.000168000	8	-1.401746000	3.212728000	0.000310000
6	-6.426427000	0.003694000	-0.000067000	6	5.403135000	0.345001000	-0.000175000
6	-7.438615000	-0.919528000	0.000023000	6	6.525159000	-0.440913000	-0.000087000
6	-7.176348000	-2.325149000	0.000215000	6	6.445216000	-1.868568000	0.000109000
7	-6.924147000	-3.463077000	0.000371000	7	6.340901000	-3.029420000	0.000254000
6	-8.843538000	-0.429817000	-0.000087000	6	7.855833000	0.224927000	-0.000215000
8	-9.163671000	0.740796000	-0.000211000	8	8.023034000	1.426914000	0.000148000
8	-9.737356000	-1.441913000	0.000068000	8	8.871911000	-0.664235000	0.000516000
1	-10.617649000	-1.024068000	0.000019000	1	9.691500000	-0.137164000	0.000852000
6	-2.665314000	0.467038000	-0.000016000	6	1.613611000	0.322124000	-0.000156000
1	-2.344218000	-0.580175000	0.000155000	1	1.429592000	-0.757630000	0.000014000
1	-6.748085000	1.049784000	-0.000215000	1	5.588091000	1.423675000	-0.000324000
6	-4.079461000	0.705607000	-0.000091000	6	2.985539000	0.740243000	-0.000222000
6	-5.026435000	-0.280229000	0.000014000	6	4.050967000	-0.116065000	-0.000108000
1	-4.408047000	1.751593000	-0.000243000	1	3.177230000	1.819719000	-0.000372000
1	-4.713106000	-1.329233000	0.000164000	1	3.874724000	-1.196582000	0.000040000
6	-1.749565000	1.474237000	-0.000128000	6	0.576220000	1.203378000	-0.000279000
1	-2.104010000	2.508392000	-0.000236000	1	0.794793000	2.274517000	-0.000384000
6	6.173697000	0.335271000	0.000138000	6	-7.133924000	-1.004942000	0.000181000
1	6.472385000	0.938647000	0.877275000	1	-7.343077000	-2.088492000	-0.000004000
1	6.472491000	0.938941000	-0.876761000	6	-7.767453000	-0.409206000	-1.270198000
6	6.966226000	-0.974222000	-0.000033000	6	-7.767093000	-0.409709000	1.270976000
1	6.690532000	-1.577423000	0.883914000	1	-7.337642000	-0.856759000	2.181293000



1	6.690625000	-1.577135000	-0.884205000	1	-7.611445000	0.680534000	1.325374000
6	8.481828000	-0.746048000	0.000086000	1	-8.854047000	-0.591687000	1.280056000
1	8.760481000	-0.139988000	0.882801000	1	-7.611825000	0.681059000	-1.324208000
1	8.760576000	-0.139700000	-0.882401000	1	-8.854409000	-0.591184000	-1.279042000
6	9.296222000	-2.044051000	-0.000082000	1	-7.338259000	-0.855893000	-2.180814000
1	9.016026000	-2.648781000	0.882166000				
1	9.016122000	-2.648493000	-0.882557000				
6	10.808260000	-1.808722000	0.000039000				
1	11.124508000	-1.237214000	0.889291000				
1	11.124605000	-1.236925000	-0.888992000				
1	11.364687000	-2.759580000	-0.000085000				
D6-t-but E(RB3LYP) = -1167.38696880 a. u.				D6-OH E(RB3LYP) = -1085.35885521 a. u.			
6	-1.352931000	2.213410000	-0.000209000	6	2.576676000	1.984281000	0.000204000
6	-0.481001000	1.016251000	-0.000090000	6	1.655919000	0.828833000	-0.000151000
6	-1.055412000	-0.229502000	0.000117000	6	2.177803000	-0.442099000	-0.000435000
6	-2.474643000	-0.403216000	0.000088000	6	3.584027000	-0.681682000	-0.000294000
6	-3.281614000	0.750092000	-0.000046000	6	4.443203000	0.439364000	0.000148000
6	-4.676784000	0.672668000	-0.000065000	6	5.830414000	0.299531000	0.000318000
6	-5.319302000	-0.569600000	0.000054000	6	6.382708000	-0.985500000	0.000041000
6	-4.510510000	-1.734495000	0.000178000	6	5.548722000	-2.125683000	-0.000411000
6	-3.128453000	-1.656144000	0.000201000	6	4.175615000	-1.967694000	-0.000577000
1	-0.427729000	-1.124442000	0.000274000	1	1.510155000	-1.307625000	-0.000811000
1	-2.525021000	-2.567061000	0.000305000	1	3.526095000	-2.845910000	-0.000924000
1	-4.979630000	-2.719108000	0.000258000	1	6.012915000	-3.112201000	-0.000620000
1	-5.227733000	1.611241000	-0.000176000	1	6.453358000	1.196421000	0.000658000
8	-2.726911000	1.996540000	-0.000159000	8	3.945533000	1.705093000	0.000413000
8	-0.971872000	3.358411000	-0.000075000	8	2.255137000	3.146724000	0.000370000
6	5.745732000	0.290238000	0.000034000	6	-4.596050000	0.374119000	-0.000126000
6	6.844281000	-0.528282000	-0.000037000	6	-5.731169000	-0.393557000	0.000071000
6	6.722422000	-1.952963000	-0.000203000	6	-5.674355000	-1.822233000	0.000492000
7	6.584116000	-3.110266000	-0.000339000	7	-5.587551000	-2.984578000	0.000836000
6	8.193862000	0.098126000	0.000065000	6	-7.050309000	0.293630000	-0.000169000
8	8.396457000	1.294683000	0.000278000	8	-7.198571000	1.498294000	-0.000543000
8	9.183449000	-0.820509000	0.000061000	8	-8.081295000	-0.578656000	0.000049000
1	10.018093000	-0.317630000	0.000193000	1	-8.891618000	-0.037512000	-0.000142000
6	1.957205000	0.379196000	-0.000044000	6	-0.807626000	0.295066000	-0.000006000
1	1.741318000	-0.694649000	-0.000192000	1	-0.638729000	-0.787212000	0.000363000

1	5.962291000	1.363017000	0.000164000	1	-4.763870000	1.455622000	-0.000452000
6	3.340855000	0.756500000	0.000032000	6	-2.172899000	0.732284000	-0.000174000
6	4.380665000	-0.130829000	-0.000049000	6	-3.251797000	-0.107767000	0.000056000
1	3.564338000	1.829860000	0.000165000	1	-2.348907000	1.814485000	-0.000513000
1	4.172672000	-1.205687000	-0.000180000	1	-3.092148000	-1.190853000	0.000388000
6	0.946345000	1.290876000	0.000043000	6	0.242264000	1.162301000	-0.000246000
1	1.196767000	2.355027000	0.000131000	1	0.036228000	2.236026000	-0.000483000
6	-6.851971000	-0.702614000	0.000005000	8	7.719643000	-1.205481000	0.000179000
6	-7.556758000	0.665611000	-0.000316000	1	8.186921000	-0.356149000	0.000505000
1	-7.303379000	1.259649000	0.891744000				
1	-7.303364000	1.259241000	-0.892643000				
1	-8.648039000	0.519115000	-0.000295000				
6	-7.294800000	-1.478475000	-1.263046000				
1	-6.993781000	-0.946873000	-2.179912000				
1	-6.860124000	-2.489074000	-1.301041000				
1	-8.391737000	-1.586588000	-1.275835000				
6	-7.294945000	-1.477950000	1.263329000				
1	-8.391888000	-1.586009000	1.276062000				
1	-6.860322000	-2.488554000	1.301771000				
1	-6.993986000	-0.945992000	2.180008000				
D6-OCH <sub>3</sub> E(RB3LYP) = -1124.65952465 a. u.				D6-OC <sub>2</sub> H <sub>5</sub> E(RB3LYP) = -1163.97984340 a. u.			
6	2.091174000	2.184269000	-0.000162000	6	-1.595204000	2.290727000	0.000148000
6	1.213618000	0.993348000	0.000103000	6	-0.745217000	1.080114000	-0.000115000
6	1.782930000	-0.256272000	0.000309000	6	-1.343265000	-0.156241000	-0.000363000
6	3.197944000	-0.439974000	0.000203000	6	-2.761728000	-0.307599000	-0.000309000
6	4.016984000	0.715025000	-0.000121000	6	-3.554348000	0.865676000	-0.000006000
6	5.402463000	0.627412000	-0.000242000	6	-4.941376000	0.809026000	0.000085000
6	6.011202000	-0.636875000	-0.000040000	6	-5.580352000	-0.440696000	-0.000139000
6	5.220092000	-1.808107000	0.000290000	6	-4.814609000	-1.629665000	-0.000453000
6	3.836852000	-1.697228000	0.000410000	6	-3.429496000	-1.549965000	-0.000534000
1	1.149609000	-1.147281000	0.000586000	1	-0.730309000	-1.061387000	-0.000629000
1	3.222383000	-2.600434000	0.000664000	1	-2.835605000	-2.466879000	-0.000778000
1	5.680488000	-2.794490000	0.000451000	1	-5.296595000	-2.605526000	-0.000644000
1	6.013706000	1.529333000	-0.000490000	1	-5.531638000	1.724834000	0.000325000
8	3.466681000	1.961744000	-0.000317000	8	-2.975921000	2.099508000	0.000205000
8	1.719284000	3.331932000	-0.000247000	8	-1.197573000	3.429692000	0.000304000
6	-5.016118000	0.299434000	0.000104000	6	5.466623000	0.241703000	0.000026000
6	-6.120902000	-0.511590000	-0.000040000	6	6.552549000	-0.594563000	0.000151000

6	-6.008712000	-1.936969000	-0.000353000	6	6.407455000	-2.016954000	0.000361000
7	-5.876748000	-3.095082000	-0.000609000	7	6.250132000	-3.171907000	0.000536000
6	-7.465499000	0.123844000	0.000143000	6	7.911291000	0.009648000	0.000068000
8	-7.660670000	1.321843000	0.000391000	8	8.134303000	1.202824000	-0.000364000
8	-8.462094000	-0.787764000	-0.000054000	8	8.886697000	-0.924730000	-0.000088000
1	-9.292571000	-0.278110000	0.000065000	1	9.728598000	-0.434195000	-0.000361000
6	-1.227649000	0.366272000	0.000006000	6	1.680853000	0.396708000	0.000016000
1	-1.017471000	-0.708764000	-0.000267000	1	1.445564000	-0.673060000	0.000206000
1	-5.225600000	1.373649000	0.000348000	1	5.700907000	1.310786000	-0.000135000
6	-2.608458000	0.750842000	0.000135000	6	3.070169000	0.748897000	-0.000041000
6	-3.654455000	-0.130095000	-0.000033000	6	4.095493000	-0.156127000	0.000095000
1	-2.825831000	1.825503000	0.000386000	1	3.312654000	1.818207000	-0.000207000
1	-3.453130000	-1.206217000	-0.000280000	1	3.869204000	-1.227283000	0.000259000
6	-0.211416000	1.272955000	0.000180000	6	0.685876000	1.326782000	-0.000129000
1	-0.457805000	2.338151000	0.000356000	1	0.956846000	2.385984000	-0.000232000
8	7.364550000	-0.628465000	-0.000181000	8	-6.931670000	-0.401705000	-0.000059000
6	8.061951000	-1.869818000	0.000024000	6	-7.675725000	-1.628628000	0.000076000
1	7.830728000	-2.463577000	0.901069000	1	-7.411336000	-2.220915000	0.894638000
1	7.830558000	-2.463969000	-0.900720000	1	-7.411853000	-2.220801000	-0.894716000
1	9.128181000	-1.611377000	-0.000133000	6	-9.147278000	-1.263742000	0.000513000
				1	-9.401732000	-0.671961000	-0.891975000
				1	-9.401252000	-0.672137000	0.893253000
				1	-9.761326000	-2.177646000	0.000585000
D6-NH <sub>2</sub> E(RB3LYP) = -1065.49481684 a. u.				D6-N(CH <sub>3</sub> ) <sub>2</sub> E(RB3LYP) = -1144.10660149 a. u.			
6	-2.567033000	1.987873000	0.000252000	6	1.715480000	2.148615000	0.000044000
6	-1.648635000	0.832351000	-0.001747000	6	0.833657000	0.965080000	0.000030000
6	-2.174755000	-0.439612000	-0.003076000	6	1.400361000	-0.290614000	0.000023000
6	-3.577139000	-0.675716000	-0.003545000	6	2.808019000	-0.480419000	0.000038000
6	-4.439581000	0.446636000	-0.003231000	6	3.636139000	0.666493000	0.000077000
6	-5.822727000	0.312429000	-0.001232000	6	5.021707000	0.582675000	0.000063000
6	-6.397902000	-0.971867000	-0.001176000	6	5.656259000	-0.683252000	0.000028000
6	-5.547272000	-2.111320000	-0.001446000	6	4.829110000	-1.849859000	-0.000027000
6	-4.175392000	-1.958669000	-0.002441000	6	3.453666000	-1.739359000	-0.000017000
1	-1.507914000	-1.305963000	-0.003875000	1	0.761412000	-1.177774000	-0.000002000
1	-3.529895000	-2.840101000	-0.000893000	1	2.840876000	-2.644010000	-0.000063000
1	-5.990049000	-3.109773000	-0.004329000	1	5.278059000	-2.840812000	-0.000097000
1	-6.439807000	1.212348000	-0.002174000	1	5.581847000	1.514573000	0.000096000
8	-3.936566000	1.711586000	-0.001076000	8	3.092391000	1.916340000	0.000138000

8	-2.244482000	3.150774000	0.003166000	8	1.355920000	3.301121000	0.000009000
6	4.600972000	0.367664000	-0.000008000	6	-5.397493000	0.306177000	-0.000033000
6	5.738998000	-0.397658000	0.000691000	6	-6.513200000	-0.492243000	-0.000010000
6	5.685211000	-1.826263000	0.000586000	6	-6.417616000	-1.918563000	0.000044000
7	5.600891000	-2.988921000	0.000563000	7	-6.299306000	-3.078317000	0.000093000
6	7.055335000	0.291921000	0.001738000	6	-7.848563000	0.158288000	-0.000046000
8	7.202732000	1.497121000	0.002125000	8	-8.032003000	1.358738000	-0.000095000
8	8.089626000	-0.577709000	0.002217000	8	-8.857596000	-0.741082000	-0.000021000
1	8.897285000	-0.032749000	0.002808000	1	-9.680215000	-0.219050000	-0.000049000
6	0.813588000	0.290070000	-0.001967000	6	-1.610060000	0.344324000	0.000009000
1	0.642435000	-0.791846000	-0.003037000	1	-1.404919000	-0.731656000	0.000047000
1	4.767195000	1.449467000	0.000335000	1	-5.595685000	1.382606000	-0.000076000
6	2.178049000	0.724942000	-0.001160000	6	-2.986637000	0.736434000	-0.000024000
6	3.258473000	-0.114981000	-0.001063000	6	-4.041795000	-0.135914000	-0.000002000
1	2.355005000	1.807117000	-0.000436000	1	-3.196844000	1.812702000	-0.000073000
1	3.099162000	-1.198114000	-0.001713000	1	-3.849823000	-1.213737000	0.000041000
6	-0.235848000	1.159880000	-0.001326000	6	-0.587786000	1.246946000	0.000002000
1	-0.026096000	2.233052000	-0.000208000	1	-0.831738000	2.312931000	-0.000025000
7	-7.763935000	-1.128587000	-0.050677000	7	7.024347000	-0.787153000	0.000041000
1	-8.338890000	-0.335318000	0.207162000	6	7.665551000	-2.092913000	-0.000028000
1	-8.143668000	-2.025801000	0.226614000	1	7.396781000	-2.684386000	0.893220000
				1	7.397277000	-2.684111000	-0.893620000
				1	8.753691000	-1.957340000	0.000312000
				6	7.846220000	0.412978000	-0.000192000
				1	8.904309000	0.125306000	-0.000249000
				1	7.660853000	1.036320000	-0.892954000
				1	7.661016000	1.036544000	0.892445000
D5-PhCH <sub>3</sub> E(RB3LYP) = -1280.51898449 a. u.				D5-PhNH <sub>2</sub> E(RB3LYP) = -1296.56297716 a. u.			
6	0.361398000	2.289071000	-0.140138000	6	0.366582000	2.287305000	-0.133333000
6	-0.483619000	1.075327000	-0.061296000	6	-0.477529000	1.073955000	-0.057588000
6	0.118757000	-0.155213000	0.018884000	6	0.126426000	-0.157595000	0.019750000
6	1.540452000	-0.297918000	0.026933000	6	1.545956000	-0.299886000	0.027709000
6	2.323317000	0.873835000	-0.044756000	6	2.329968000	0.872321000	-0.039793000
6	3.715621000	0.824796000	-0.046603000	6	3.721127000	0.824281000	-0.043076000
6	4.379850000	-0.409758000	0.026672000	6	4.391023000	-0.409650000	0.027735000
6	3.600477000	-1.591917000	0.100794000	6	3.607829000	-1.592170000	0.098716000
6	2.217017000	-1.536426000	0.101016000	6	2.225418000	-1.537931000	0.097609000
1	-0.488732000	-1.062031000	0.077717000	1	-0.481283000	-1.064509000	0.076046000

1	1.629742000	-2.455181000	0.169000000	1	1.639378000	-2.457750000	0.163269000
1	4.099061000	-2.557972000	0.187499000	1	4.104074000	-2.559218000	0.186383000
1	4.264322000	1.762718000	-0.132821000	1	4.265816000	1.764312000	-0.130052000
8	1.739468000	2.104493000	-0.126491000	8	1.745019000	2.103158000	-0.118600000
8	-0.045641000	3.422618000	-0.214431000	8	-0.039770000	3.421693000	-0.205918000
6	-6.692208000	0.214132000	-0.013724000	6	-6.685276000	0.213201000	-0.014091000
6	-7.772994000	-0.626282000	0.037165000	6	-7.769177000	-0.624374000	0.034318000
6	-7.620736000	-2.045282000	0.125094000	6	-7.621107000	-2.043887000	0.119274000
7	-7.456743000	-3.197016000	0.196570000	7	-7.460696000	-3.196348000	0.188296000
6	-9.135685000	-0.030181000	-0.001169000	6	-9.129329000	-0.024518000	-0.003607000
8	-9.363841000	1.159486000	-0.075007000	8	-9.355128000	1.166009000	-0.075168000
8	-10.105405000	-0.968043000	0.055692000	8	-10.102646000	-0.959502000	0.050724000
1	-10.950594000	-0.484085000	0.024799000	1	-10.945597000	-0.471739000	0.020270000
6	-2.906730000	0.385003000	-0.020535000	6	-2.900229000	0.380426000	-0.018731000
1	-2.667362000	-0.681823000	0.045825000	1	-2.660473000	-0.686419000	0.045625000
1	-6.931739000	1.279958000	-0.080036000	1	-6.922263000	1.279758000	-0.078288000
6	-4.297952000	0.731367000	-0.043368000	6	-4.290585000	0.726851000	-0.041406000
6	-5.318512000	-0.176620000	0.011956000	6	-5.313120000	-0.180021000	0.011550000
1	-4.544618000	1.797547000	-0.109811000	1	-4.536637000	1.793380000	-0.105788000
1	-5.087364000	-1.244664000	0.078481000	1	-5.083563000	-1.248527000	0.076014000
6	-1.915929000	1.317191000	-0.077711000	6	-1.909095000	1.313412000	-0.073750000
1	-2.190150000	2.373382000	-0.144244000	1	-2.184688000	2.369476000	-0.138198000
6	8.708519000	-0.593212000	0.026573000	6	8.718676000	-0.591807000	0.027502000
6	8.025168000	0.464117000	0.650674000	6	8.037332000	0.506395000	0.591303000
6	7.940020000	-1.587584000	-0.594597000	6	7.947365000	-1.629312000	-0.534727000
1	8.594909000	1.250506000	1.153300000	1	8.609759000	1.318198000	1.047782000
1	8.441619000	-2.418878000	-1.096792000	1	8.449142000	-2.488229000	-0.988237000
6	6.633994000	0.526828000	0.650752000	6	6.648713000	0.560807000	0.586533000
6	6.545300000	-1.533350000	-0.593169000	6	6.558692000	-1.568123000	-0.526322000
1	6.137440000	1.350739000	1.167394000	1	6.158594000	1.417595000	1.053069000
1	5.982419000	-2.313225000	-1.110106000	1	5.998606000	-2.378681000	-0.996743000
6	5.861391000	-0.473384000	0.028075000	6	5.867609000	-0.472880000	0.030594000
6	10.216372000	-0.645618000	0.028870000	7	10.102713000	-0.676976000	0.079622000
1	10.614514000	-0.640136000	1.057350000	1	10.597230000	0.204280000	0.171886000
1	10.590829000	-1.549458000	-0.473485000	1	10.534377000	-1.290326000	-0.603793000
1	10.646528000	0.229766000	-0.486512000				