

Design and DFT study of nitrogen-rich donor systems for improved photovoltaic performance in dye-sensitized solar cells

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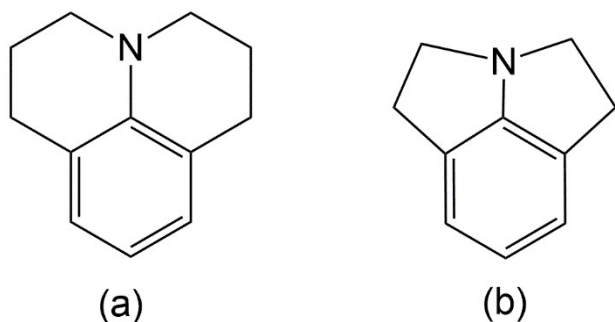


Fig. S1 ChemDraw of a) Julolidine b) 1,2,4,5-tetrahydropyrrolo[3,2,1-hi] indole

Table 1 Cartesian coordinates (in Angstrom unit) of B3LYP/cc-pVDZ geometries of D1 – D18 donor systems.

D1 E(RB3LYP) = -754.584057965 a. u.				D2 E(RB3LYP) = -770.614550367 a. u.			
6	-2.501997000	0.615533000	0.302857000	6	-2.499054000	0.659587000	0.225476000
6	-1.211325000	-0.153833000	0.069154000	6	-1.218420000	-0.145708000	0.064067000
6	-2.441235000	1.921579000	-0.494820000	6	-2.368849000	1.965985000	-0.564511000
6	0.001333000	0.585590000	-0.031049000	6	0.004575000	0.560541000	-0.001637000
6	-1.244186000	2.757753000	-0.058247000	6	-1.173021000	2.769214000	-0.066837000
7	-0.011091000	1.979202000	0.056485000	7	0.026541000	1.955528000	0.069513000
6	-1.189263000	-1.551481000	-0.052876000	6	-1.226017000	-1.551029000	-0.014151000
6	1.225308000	-0.105249000	-0.196813000	6	1.229650000	-0.153758000	-0.130510000
6	1.209709000	2.717918000	-0.230292000	6	1.273235000	2.691216000	0.092461000
6	1.221883000	-1.501852000	-0.350870000	6	1.213749000	-1.559648000	-0.154201000
6	0.026101000	-2.214841000	-0.277500000	6	-0.011818000	-2.234251000	-0.112326000
6	2.571681000	0.597977000	-0.169237000	7	2.428225000	0.589056000	-0.210968000
1	-3.361505000	2.512869000	-0.356079000	1	-3.279611000	2.579605000	-0.466829000
6	2.427794000	2.026506000	0.365949000	6	2.419575000	1.811870000	0.573371000
1	2.308513000	1.994229000	1.463295000	1	2.311476000	1.617243000	1.663032000
1	-1.464791000	3.248426000	0.911103000	1	-1.417836000	3.245764000	0.905845000
1	1.104187000	3.727100000	0.200017000	1	1.165865000	3.559375000	0.771670000
1	-2.363775000	1.681282000	-1.569622000	1	-2.244570000	1.729223000	-1.635607000
1	3.334386000	2.616024000	0.153261000	1	3.368098000	2.347183000	0.420847000
1	-1.080714000	3.571715000	-0.787843000	1	-0.961202000	3.596950000	-0.770413000
1	1.344955000	2.851046000	-1.327086000	1	1.518397000	3.094001000	-0.912536000
6	2.547470000	-2.162248000	-0.646329000	6	2.518325000	-2.329653000	-0.205842000
1	2.448830000	-3.258735000	-0.628928000	1	2.410642000	-3.274110000	0.351644000
6	3.675311000	-1.705825000	0.305494000	6	3.674020000	-1.496883000	0.353267000
1	3.646076000	-2.317927000	1.221474000	1	3.544192000	-1.350387000	1.439976000
1	4.646966000	-1.912911000	-0.172079000				
6	3.566225000	-0.210964000	0.693741000				
1	3.224952000	-0.129476000	1.739595000				
1	4.557527000	0.271527000	0.652952000				

6	-2.47053000	-2.366649000	0.010853000	1	4.638684000	-2.007869000	0.200475000
1	-2.283468000	-3.297451000	0.572062000	6	3.687857000	-0.139178000	-0.352710000
6	-3.652536000	-1.603825000	0.614323000	1	4.497378000	0.498189000	0.033344000
1	-3.515779000	-1.501332000	1.706365000	1	3.896294000	-0.302985000	-1.428589000
1	-4.585644000	-2.170886000	0.463358000	6	-2.529713000	-2.331012000	-0.020090000
6	-3.751563000	-0.213160000	-0.013884000	1	-2.407120000	-3.260563000	0.561086000
1	-3.857764000	-0.314319000	-1.110557000	6	-3.723054000	-1.525486000	0.501857000
1	-4.648250000	0.320495000	0.343929000	1	-3.646730000	-1.407103000	1.598322000
1	0.034057000	-3.302532000	-0.393571000	1	-4.661744000	-2.069304000	0.305839000
1	-2.548766000	0.889294000	1.377437000	6	-3.748895000	-0.142916000	-0.152601000
1	2.975385000	0.650718000	-1.200703000	1	-3.793698000	-0.259137000	-1.251981000
1	2.836995000	-1.896438000	-1.680743000	1	-4.650995000	0.418387000	0.144652000
1	-2.735816000	-2.684709000	-1.015761000	1	-0.012485000	-3.328216000	-0.140789000
				1	-2.595644000	0.934448000	1.296638000
				1	2.751696000	-2.613506000	-1.249749000
				1	-2.747333000	-2.652625000	-
					1.057176000		
D3 E(RB3LYP) = -786.644225965 a. u.				D4 E(RB3LYP) = -802.677715342 a. u.			
7	-2.436483000	0.593885000	0.138505000	7	-2.428649000	0.605456000	0.099802000
6	-1.232666000	-0.145090000	0.057042000	6	-1.219982000	-0.142871000	0.019367000
6	-2.335033000	1.971474000	-0.305724000	6	-2.358830000	1.906278000	-0.541361000
6	-0.001282000	0.548052000	0.121034000	6	0.009838000	0.564956000	-0.021441000
6	-1.204656000	2.651836000	0.464888000	6	-1.217770000	2.713413000	0.062900000
7	0.060131000	1.949204000	0.302072000	7	0.018572000	1.962710000	0.009738000
6	-1.239108000	-1.553535000	-0.054317000	6	-1.216078000	-1.550641000	0.017968000
6	1.225453000	-0.150925000	-0.002865000	6	1.235406000	-0.144448000	-0.064335000
6	1.117966000	2.578158000	-0.471651000	6	1.264637000	2.685901000	-0.110938000
6	1.213706000	-1.556446000	-0.138180000	6	1.223202000	-1.554663000	-0.099301000
6	-0.014545000	-2.220201000	-0.133165000	6	0.001565000	-2.231605000	-0.052989000
7	2.426406000	0.561158000	0.051782000	7	2.465670000	0.572559000	-0.071736000
1	-3.290884000	2.479294000	-0.098599000	1	-3.310675000	2.434203000	-0.372493000
6	2.459258000	2.009950000	-0.018327000	6	2.396826000	1.892870000	0.528074000
1	2.726086000	2.442242000	0.966810000	1	2.236013000	1.843455000	1.628418000
1	-1.482456000	2.677689000	1.534251000	1	-1.478267000	2.993614000	1.104326000
1	1.108151000	3.662647000	-0.287816000	1	1.167110000	3.655012000	0.406836000
1	-2.145956000	2.046017000	-1.400648000	1	-2.213242000	1.820943000	-1.641907000
1	3.243507000	2.326005000	-0.734670000	1	3.355778000	2.407249000	0.354399000
1	-1.082946000	3.691718000	0.126147000	1	-1.096308000	3.649834000	-0.509453000
1	0.991053000	2.416286000	-1.564736000	1	1.517765000	2.899332000	-1.170742000
6	2.523526000	-2.304570000	-0.255464000	7	2.429425000	-2.299286000	-0.213973000
1	2.414405000	-3.322075000	0.153784000	1	2.529839000	-2.966884000	0.547191000

6	3.640554000	-1.548359000	0.468326000	6	3.638461000	-1.520693000	-0.437753000
1	3.439957000	-1.538613000	1.553546000	1	4.513074000	-2.126376000	-0.157325000
1	4.617132000	-2.035274000	0.315444000	1	3.727470000	-1.289126000	-1.514322000
6	3.710621000	-0.111809000	-0.043266000	6	3.626064000	-0.203771000	0.337671000
1	4.444962000	0.462849000	0.548910000	1	3.619103000	-0.416654000	1.431414000
1	4.082227000	-0.106413000	-1.092697000	1	4.533085000	0.385495000	0.120550000
6	-2.546006000	-2.320810000	-0.113076000	6	-2.519322000	-2.325687000	0.062720000
1	-2.461984000	-3.251932000	0.472444000	1	-2.402690000	-3.213557000	0.706373000
6	-3.718165000	-1.477093000	0.393153000	6	-3.676503000	-1.455016000	0.555759000
1	-3.661874000	-1.364109000	1.489337000	1	-3.575596000	-1.262223000	1.637568000
1	-4.680496000	-1.958854000	0.156913000	1	-4.643352000	-1.958715000	0.396361000
6	-3.663638000	-0.091293000	-0.242428000	6	-3.660169000	-0.120994000	-0.182269000
1	-3.751399000	-0.186332000	-1.349340000	1	-3.783935000	-0.302312000	-1.275443000
1	-4.511883000	0.527528000	0.094313000	1	-4.504501000	0.513322000	0.135283000
1	-0.017305000	-3.312162000	-0.211861000	1	0.009044000	-3.324142000	-0.091704000
1	2.805352000	-2.427449000	-1.319478000	1	-2.758910000	-2.710718000	-0.946581000
1	-2.751928000	-2.634819000	-1.154443000				
D5 E(RB3LYP) = -818.710617893 a. u.				D6 E(RB3LYP) = -597.236036813 a. u.			
7	-2.449530000	0.581040000	0.118805000	6	-2.228239000	0.826588000	-0.179758000
6	-1.222565000	-0.143985000	0.024012000	6	-1.199390000	-0.068665000	-0.807557000
6	-2.401723000	1.885242000	-0.517075000	6	0.000001000	0.596246000	-0.916739000
6	-0.001440000	0.564561000	-0.034174000	6	-1.305619000	2.010046000	0.339268000
6	-1.251840000	2.695534000	0.070605000	7	0.000001000	1.899548000	-0.408554000
7	-0.008573000	1.960814000	-0.027334000	6	-1.216062000	-1.397654000	-0.381444000
6	-1.211253000	-1.553750000	0.018462000	6	1.199391000	-0.068666000	-0.807559000
6	1.230928000	-0.135857000	-0.075851000	6	1.305624000	2.010049000	0.339262000
6	1.234151000	2.698270000	-0.104344000	6	1.216061000	-1.397656000	-0.381441000
6	1.222569000	-1.542775000	-0.102180000	6	0.000000000	-2.102301000	-0.215138000
6	0.006309000	-2.236302000	-0.055876000	6	2.228241000	0.826585000	-0.179757000
7	2.458688000	0.596436000	-0.090896000	1	-1.108746000	1.902548000	1.425347000
1	-3.353330000	2.407028000	-0.326447000	1	1.108754000	1.902563000	1.425343000
6	2.364737000	1.902703000	0.536302000	1	-1.763332000	2.996339000	0.174581000
1	2.185070000	1.827215000	1.633029000	1	1.763339000	2.996339000	0.174565000
1	-1.489133000	2.957737000	1.122655000	6	2.566750000	-1.605131000	0.294502000
1	1.117485000	3.654332000	0.433938000	1	2.538438000	-2.351814000	1.103221000
1	-2.275056000	1.807147000	-1.620450000	6	2.901271000	-0.162916000	0.827120000
1	3.319764000	2.432673000	0.390284000	1	2.442743000	-0.039429000	1.823370000
1	-1.155261000	3.641347000	-0.490544000	1	3.985053000	-0.002461000	0.939727000
1	1.503287000	2.938335000	-1.153847000	6	-2.566751000	-1.605129000	0.294502000
7	2.431112000	-2.280788000	-0.218764000	1	-2.538437000	-2.351808000	1.103225000
1	2.530352000	-2.957831000	0.534008000	1	-3.335518000	-1.933006000	-0.428280000
				6	-2.901277000	-0.162913000	0.827115000
				1	-3.985060000	-0.002458000	0.939711000
				1	-2.442760000	-0.039423000	1.823369000

6	3.639074000	-1.495995000	-0.431789000	1	-0.000001000	-3.091645000	0.250203000
1	4.513257000	-2.097415000	-0.140818000	1	-2.971115000	1.229770000	-0.890253000
1	3.737989000	-1.266585000	-1.507881000	1	2.971123000	1.229762000	-0.890249000
6	3.613279000	-0.176731000	0.339930000	1	3.335518000	-1.933001000	-0.428281000
1	3.587792000	-0.388606000	1.434178000				
1	4.523984000	0.411664000	0.136314000				
7	-2.432691000	-2.260956000	0.017668000				
1	-2.340452000	-3.193709000	0.409523000				
6	-3.590182000	-1.534962000	0.514935000				
1	-3.560721000	-1.359682000	1.611141000				
1	-4.500614000	-2.111466000	0.286781000				
6	-3.644718000	-0.187854000	-0.196341000				
1	-3.752433000	-0.363415000	-1.289338000				
1	-4.525314000	0.384023000	0.140837000				
1	0.016321000	-3.327195000	-0.119406000				
D7 E(RB3LYP) = -613.258437915 a. u.				D8 E(RB3LYP) = -629.280856933 a. u.			
6	-2.176727000	0.883125000	-0.151777000	7	-2.125210000	0.784142000	-0.182671000
6	-1.193210000	-0.043093000	-0.808257000	6	-1.171674000	-0.073348000	-0.760919000
6	0.012233000	0.594622000	-0.952619000	6	0.000078000	0.594379000	-0.998038000
6	-1.194619000	2.010042000	0.388746000	6	-1.311395000	1.967045000	0.284978000
7	0.070293000	1.900512000	-0.432793000	7	0.000133000	1.902846000	-0.457871000
6	-1.255768000	-1.378748000	-0.397716000	6	-1.224723000	-1.416724000	-0.384504000
6	1.179823000	-0.099302000	-0.760884000	6	1.171683000	-0.073500000	-0.760931000
6	1.418894000	1.957366000	0.234915000	6	1.312016000	1.967278000	0.284429000
6	1.183863000	-1.434069000	-0.365990000	6	1.224532000	-1.416949000	-0.384489000
6	-0.055369000	-2.104668000	-0.217856000	6	-0.000125000	-2.106762000	-0.217307000
7	2.177726000	0.730277000	-0.211753000	7	2.125416000	0.783787000	-0.182602000
1	-0.950972000	1.831109000	1.455988000	1	-1.142191000	1.917840000	1.386858000
1	1.303710000	1.965701000	1.343558000	1	1.143176000	1.919014000	1.386356000
1	-1.624995000	3.018106000	0.300416000	1	-1.834316000	2.905269000	0.051839000
1	1.958488000	2.866563000	-0.066820000	1	1.835106000	2.905142000	0.050252000
6	2.529179000	-1.613872000	0.325643000	6	2.572375000	-1.555349000	0.312044000
1	2.507649000	-2.316351000	1.172284000	1	2.573404000	-2.270103000	1.148790000
6	2.846671000	-0.145920000	0.789382000	6	2.825677000	-0.084350000	0.805083000
1	2.413372000	0.034666000	1.794876000	1	2.379312000	0.060278000	1.810509000
1	3.928094000	0.050093000	0.841316000	1	3.897046000	0.158224000	0.866388000
6	-2.611255000	-1.544909000	0.280669000	6	-2.572424000	-1.555155000	0.312153000
1	-2.608179000	-2.302191000	1.080142000	1	-2.572905000	-2.269430000	1.149328000
1	-3.400780000	-1.830892000	-0.437694000	1	-3.374438000	-1.855156000	-0.385122000
				6	-2.826301000	-0.083931000	0.804554000
				1	-3.897791000	0.158449000	0.864569000
				1	-2.381132000	0.061354000	1.810374000

6	-2.884672000	-0.098711000	0.839411000	1	-0.000242000	-3.107561000	0.225252000
1	-3.960509000	0.104998000	0.957931000	1	3.374287000	-1.854557000	-0.385708000
1	-2.419239000	-0.011179000	1.836198000				
1	-0.080962000	-3.100413000	0.233911000				
1	-2.904630000	1.340011000	-0.845106000				
1	3.308555000	-1.956923000	-0.377192000				
D9 E(RB3LYP) = -645.303391079 a. u.				D10 E(RB3LYP) = -661.327505080 a. u.			
7	-2.118760000	0.818370000	-0.193776000	7	-2.153558000	0.789737000	-0.217856000
6	-1.173996000	-0.055687000	-0.786056000	6	-1.193245000	-0.059713000	-0.845480000
6	0.015205000	0.597404000	-0.993892000	6	-0.000024000	0.597508000	-0.988371000
6	-1.279093000	1.971104000	0.301397000	6	-1.310504000	1.895253000	0.368985000
7	0.040933000	1.889517000	-0.425689000	7	-0.000035000	1.865183000	-0.377055000
6	-1.225021000	-1.389461000	-0.388859000	6	-1.210172000	-1.363808000	-0.356374000
6	1.185184000	-0.078903000	-0.804303000	6	1.193239000	-0.059686000	-0.845525000
6	1.345485000	1.907564000	0.333914000	6	1.310178000	1.894990000	0.369423000
6	1.210805000	-1.398597000	-0.359403000	6	1.210192000	-1.363725000	-0.356269000
6	-0.007149000	-2.097182000	-0.200873000	6	0.000025000	-2.081456000	-0.179265000
7	2.158014000	0.750087000	-0.200472000	7	2.153463000	0.789912000	-0.217862000
1	-1.120241000	1.902425000	1.403594000	1	-1.140108000	1.738705000	1.462088000
1	1.166232000	1.794797000	1.430640000	1	1.139424000	1.737801000	1.462396000
1	-1.774316000	2.926592000	0.077916000	1	-1.806735000	2.865559000	0.227136000
1	1.875528000	2.853915000	0.158598000	1	1.806376000	2.865428000	0.228328000
7	2.482883000	-1.552454000	0.271364000	7	2.464622000	-1.520134000	0.287901000
1	2.474631000	-2.219008000	1.041893000	1	2.436392000	-2.157840000	1.081669000
6	2.857168000	-0.170447000	0.732178000	6	2.891777000	-0.129893000	0.682370000
1	2.531375000	0.028574000	1.781265000	1	2.652275000	0.092323000	1.748137000
1	3.949002000	-0.044830000	0.676719000	1	3.979279000	-0.028825000	0.545501000
6	-2.572332000	-1.523789000	0.306627000	7	-2.464735000	-1.520242000	0.287616000
1	-2.572755000	-2.234804000	1.146882000	1	-2.436701000	-2.158249000	1.081168000
1	-3.373316000	-1.827391000	-0.389992000	6	-2.891298000	-0.130010000	0.682845000
6	-2.823151000	-0.049414000	0.791515000	1	-3.978917000	-0.028747000	0.547118000
1	-3.894953000	0.193243000	0.847802000	1	-2.650605000	0.091877000	1.748445000
1	-2.383466000	0.095798000	1.799876000	1	0.000015000	-3.045982000	0.334774000
1	-0.017849000	-3.083497000	0.271350000				

D11				D12			
E(RB3LYP) = -1264.71957551 a. u.				E(RB3LYP) = -1261.07323143 a. u.			
6	0.603384000	-1.477763000	0.074369000	6	-1.213714000	-0.617858000	0.401960000
6	0.878644000	-0.100765000	-0.058584000	6	-1.077261000	0.789788000	0.418250000
6	-0.741872000	-1.891747000	0.044030000	6	-0.056428000	-1.389767000	0.175347000
6	-1.481541000	0.377095000	-0.312440000	6	1.279373000	0.609611000	-0.095754000
6	-1.802721000	-0.984745000	-0.145977000	6	1.206514000	-0.797034000	-0.057724000
6	-0.152381000	0.842002000	-0.249234000	6	0.149572000	1.425552000	0.145577000
1	1.913464000	0.240847000	-0.023155000	1	-1.948584000	1.396674000	0.677897000
1	-2.282179000	1.091572000	-0.515705000	1	2.222670000	1.089881000	-0.368031000
1	-0.970413000	-2.955124000	0.161435000	1	-0.113635000	-2.478067000	0.258148000
6	0.103711000	2.272467000	-0.472273000	6	0.306811000	2.881840000	0.157216000
1	-0.634342000	2.769857000	-1.103985000	1	1.272832000	3.252545000	0.506894000
6	1.126091000	3.061553000	-0.033978000	6	-0.613981000	3.855900000	-0.161184000
7	1.339641000	4.384958000	-0.472452000	7	-0.504952000	5.200231000	0.204926000
6	2.743732000	4.703187000	-0.233256000	6	-1.565560000	5.925902000	-0.337146000
6	3.008816000	3.919699000	1.044439000	6	-2.344143000	5.064546000	-1.027347000
7	2.149415000	2.743344000	0.885830000	7	-1.786667000	3.781192000	-0.923960000
1	4.064811000	3.632322000	1.169483000	1	-3.264044000	5.236311000	-1.576117000
1	3.394398000	4.348244000	-1.061951000	1	-1.682762000	6.988391000	-0.151147000
1	2.703130000	4.515064000	1.929815000	6	2.361559000	-1.659156000	-0.320229000
1	2.894664000	5.787042000	-0.114197000	1	2.146418000	-2.597807000	-0.835533000
6	-3.172024000	-1.505727000	-0.250979000	6	3.693348000	-1.427569000	-0.055995000
1	-3.239039000	-2.528145000	-0.626558000	7	4.751922000	-2.129393000	-0.639180000
6	-4.365786000	-0.902174000	0.017114000	6	5.962103000	-1.695227000	-0.098466000
7	-5.617744000	-1.464692000	-0.304369000	6	5.687351000	-0.728245000	0.803648000
6	-6.584231000	-0.373185000	-0.372002000	7	4.297924000	-0.534857000	0.838697000
6	-6.049272000	0.559566000	0.705103000	1	6.354001000	-0.135638000	1.421147000
7	-4.600687000	0.352612000	0.620907000	1	6.912583000	-2.096202000	-0.434711000
1	-6.314745000	1.615691000	0.539630000	6	-2.514678000	-1.206487000	0.727173000
1	-6.579089000	0.121253000	-1.367637000	1	-3.136416000	-0.622583000	1.409368000
1	-6.433578000	0.256062000	1.701033000	6	-3.038254000	-2.424519000	0.356147000
1	-7.605591000	-0.728647000	-0.166739000	7	-4.120324000	-3.045202000	0.987096000
6	1.648412000	-2.481646000	0.321128000	6	-4.439784000	-4.228379000	0.321428000
1	1.322529000	-3.338107000	0.913825000	6	-3.577034000	-4.370150000	-0.707369000
6	2.959285000	-2.495183000	-0.055435000	7	-2.689662000	-3.280913000	-0.699207000
7	3.897213000	-3.443516000	0.402023000	1	-5.234588000	-4.879975000	0.669535000
6	5.224629000	-2.858979000	0.240901000	1	-3.489015000	-5.161189000	-1.444629000
6	5.031123000	-2.035561000	-1.024477000	6	-2.022231000	2.749627000	-1.920143000
7	3.634285000	-1.605237000	-0.919126000	1	-2.306529000	1.792815000	-1.459528000
1	5.713379000	-1.173480000	-1.093197000	1	-2.827215000	3.088120000	-2.587245000

1	5.497362000	-2.210613000	1.101939000	1	-1.108424000	2.575581000	-2.514759000
1	5.181523000	-2.670616000	-1.922156000	6	0.527887000	5.712641000	1.067930000
1	5.995655000	-3.637533000	0.135669000	1	1.512316000	5.739129000	0.565773000
6	-3.888492000	0.696199000	1.846089000	1	0.267114000	6.734260000	1.377444000
1	-4.180745000	0.037867000	2.690298000	1	0.623909000	5.076230000	1.964642000
1	-2.804263000	0.627447000	1.702265000	6	-4.744697000	-2.543167000	2.184068000
1	-4.132010000	1.736004000	2.115818000	1	-5.336389000	-1.629714000	1.990490000
6	-5.708533000	-2.488792000	-1.324485000	1	-5.414926000	-3.312313000	2.592234000
1	-5.184703000	-3.401826000	-1.004776000	1	-3.978108000	-2.294439000	2.938197000
1	-6.767481000	-2.748370000	-1.471793000	6	-2.062141000	-2.804807000	-1.921077000
1	-5.278192000	-2.166697000	-2.295401000	1	-2.061484000	-3.624086000	-2.653658000
6	1.797860000	2.100975000	2.146586000	1	-2.619535000	-1.947054000	-2.339894000
1	1.245676000	1.170442000	1.972925000	6	4.584369000	-3.106926000	-1.683300000
1	2.725172000	1.851164000	2.685866000	1	4.130823000	-4.042082000	-1.306686000
1	1.186635000	2.766461000	2.791069000	1	3.926568000	-2.708241000	-2.474944000
6	0.769185000	4.829356000	-1.727193000	1	5.565577000	-3.345472000	-2.116696000
1	1.065121000	4.189066000	-2.584151000	6	3.618614000	-0.005379000	2.009162000
1	-0.329485000	4.838635000	-1.671722000	1	2.895759000	0.778148000	1.741289000
1	1.100245000	5.860543000	-1.921026000	1	3.063516000	-0.806715000	2.527714000
6	3.644410000	-4.176254000	1.625205000	1	4.373350000	0.410218000	2.691246000
1	2.771435000	-4.835470000	1.508691000	1	-1.029042000	-2.478557000	-1.740073000
1	4.514589000	-4.813543000	1.842344000				
1	3.459786000	-3.510713000	2.494095000				
6	3.029432000	-1.260975000	-2.200638000				
1	2.967437000	-2.139906000	-2.875267000				
1	2.023510000	-0.848916000	-2.062817000				
1	3.649302000	-0.491784000	-2.687734000				
D13 E(RB3LYP) = -920.568603608 a. u.				D14 E(RB3LYP) = -918.138306075 a. u			
6	-0.369417000	3.066286000	-0.292646000	6	0.383436000	-2.658782000	-1.399444000
6	-1.345109000	2.068883000	-0.349698000	6	1.348540000	-1.688742000	-1.110206000
6	0.987174000	2.745415000	-0.262498000	6	-0.953825000	-2.471220000	-1.059122000
6	0.408801000	0.405789000	-0.373580000	6	-0.376051000	-0.333901000	-0.094186000

6	1.408063000	1.396780000	-0.295991000	6	-1.372787000	-1.278981000	-0.417007000
6	-0.969308000	0.706802000	-0.385224000	6	0.988358000	-0.506479000	-0.421424000
1	-2.400612000	2.338515000	-0.412777000	1	2.376682000	-1.824823000	-1.452539000
1	0.713283000	-0.640265000	-0.456434000	6	1.944667000	0.552374000	-0.100509000
6	-1.930349000	-0.391218000	-0.537774000	1	1.551655000	1.571168000	-0.116313000
1	-1.536429000	-1.269429000	-1.051894000	6	3.294606000	0.447416000	0.162427000
6	-3.243714000	-0.464965000	-0.173163000	7	4.200998000	1.506582000	0.093995000
7	-4.106247000	-1.509461000	-0.557728000	6	5.467157000	1.071554000	0.484635000
6	-5.473958000	-1.008598000	-0.457477000	6	5.375855000	-0.241457000	0.789044000
6	-5.356636000	-0.068182000	0.733502000	7	4.049095000	-0.650648000	0.589360000
7	-3.988684000	0.445326000	0.607192000	1	6.137625000	-0.939863000	1.118658000
1	-6.095292000	0.748548000	0.719539000	1	6.324650000	1.736186000	0.479816000
1	-5.778556000	-0.458088000	-1.373601000	6	-2.775879000	-1.121191000	-0.040356000
1	-5.478494000	-0.631901000	1.681375000	1	-3.309201000	-2.044135000	0.196909000
1	-6.189777000	-1.827965000	-0.291179000	6	-3.504575000	0.038260000	0.120318000
6	2.843511000	1.098449000	-0.338044000	7	-4.705995000	0.130288000	0.824594000
1	3.455563000	1.886338000	-0.780092000	6	-5.211277000	1.426403000	0.730003000
6	3.523011000	-0.018549000	0.055245000	6	-4.346868000	2.153087000	-0.011536000
7	4.884653000	-0.243649000	-0.222425000	7	-3.281797000	1.321991000	-0.390174000
6	5.119862000	-1.681716000	-0.136138000	1	-4.375894000	3.198686000	-0.298944000
6	4.147337000	-2.073076000	0.967252000	1	-6.129522000	1.717740000	1.229061000
7	3.037293000	-1.136007000	0.767273000	6	3.473009000	-1.793898000	1.277433000
1	3.807576000	-3.118496000	0.899575000	1	2.981049000	-2.488736000	0.581940000
1	4.872259000	-2.197041000	-1.089230000	1	4.276017000	-2.320522000	1.811270000
1	4.614508000	-1.922371000	1.962319000	1	2.714247000	-1.457531000	2.004667000
1	6.168582000	-1.902118000	0.114920000	6	3.859844000	2.822396000	-0.384375000
6	2.231279000	-0.921195000	1.963684000	1	3.232865000	3.375511000	0.338303000
1	2.816119000	-0.435057000	2.771496000	1	4.781685000	3.395096000	-0.555924000
1	1.354000000	-0.303079000	1.742032000	1	3.298583000	2.747471000	-1.331586000
1	1.877061000	-1.897581000	2.329948000	6	-5.275708000	-0.956310000	1.581021000
6	5.530450000	0.467817000	-1.306541000	1	-5.688910000	-1.744074000	0.925420000
1	5.573420000	1.545831000	-1.091531000	1	-4.504386000	-1.418494000	2.220544000
1	6.565482000	0.106827000	-1.399037000	1	-6.085568000	-0.569774000	2.214959000
1	5.012680000	0.329999000	-2.278167000	6	-2.474354000	1.577817000	-1.570648000
6	-3.428098000	0.926131000	1.864921000	1	-1.397960000	1.553483000	-1.347338000
1	-2.450879000	1.396234000	1.707091000	1	-2.671343000	0.811704000	-2.340188000
1	-4.106842000	1.684002000	2.286846000	1	-2.741548000	2.566404000	-1.968800000
1	-3.315728000	0.106986000	2.604941000	1	-0.656359000	0.550397000	0.484625000
6	-3.785533000	-2.324647000	-1.711582000	1	-1.696682000	-3.233228000	-1.308915000
1	-3.633171000	-1.723851000	-2.631891000	1	0.681314000	-3.570243000	-1.926468000
1	-2.872277000	-2.910585000	-1.530387000				
1	-4.607513000	-3.035800000	-1.881334000				
1	1.737134000	3.539393000	-0.216392000				
1	-0.675403000	4.116260000	-0.281801000				
D15 E(RB3LYP) = -459.692079007 a. u.				D16 E(RB3LYP) = - 687.101823450 a. u.			
6	2.608953000	0.696402000	0.079050000	6	1.369371000	-0.939334000	-0.161517000

6	2.608929000	-0.696606000	0.079028000	6	0.706068000	-2.150176000	-0.084264000
6	1.402928000	-1.420077000	-0.026249000	6	-0.706070000	-2.150169000	-0.084328000
6	0.216405000	-0.706998000	-0.143116000	6	-1.369371000	-0.939331000	-0.161587000
6	0.216407000	0.706922000	-0.143097000	6	-0.699923000	0.323777000	-0.200889000
6	1.402976000	1.419938000	-0.026150000	6	0.699918000	0.323767000	-0.200911000
7	-1.108766000	-1.146371000	-0.301939000	7	-2.759492000	-0.715721000	-0.249450000
6	-1.959979000	0.000087000	0.008507000	6	-2.956711000	0.674705000	0.108757000
7	-1.108613000	1.146474000	-0.302071000	7	-1.711108000	1.318425000	-0.304356000
1	-2.878135000	0.000216000	-0.604522000	7	1.711154000	1.318392000	-0.304485000
1	-2.267447000	0.000208000	1.091501000	6	2.956685000	0.674707000	0.108884000
1	1.408088000	2.511204000	-0.008538000	7	2.759482000	-0.715721000	-0.249271000
1	3.550675000	1.241260000	0.172992000	1	-3.820368000	1.115026000	-0.419623000
1	3.550637000	-1.241495000	0.172923000	1	-3.130737000	0.795326000	1.216123000
1	1.408005000	-2.511348000	-0.008759000	1	3.130533000	0.795410000	1.216268000
6	-1.528649000	2.433656000	0.205668000	1	3.820412000	1.114983000	-0.419409000
1	-1.490111000	2.496620000	1.314955000	6	-1.590670000	2.683142000	0.156824000
1	-0.889944000	3.227023000	-0.209237000	1	-1.218149000	2.771746000	1.199705000
1	-2.561336000	2.637561000	-0.117553000	1	-0.940383000	3.272037000	-0.501895000
6	-1.528986000	-2.433530000	0.205697000	1	-2.587629000	3.147825000	0.114617000
1	-0.891244000	-3.227084000	-0.210273000	6	-3.682188000	-1.667474000	0.327733000
1	-1.489243000	-2.496921000	1.314914000	1	-3.546528000	-2.655059000	-0.137151000
1	-2.562189000	-2.636734000	-0.116365000	1	-3.561840000	-1.779117000	1.427883000
				1	-4.714833000	-1.345296000	0.121513000
				6	3.682183000	-1.667518000	0.327788000
				1	3.546463000	-2.655065000	-0.137159000
				1	4.714822000	-1.345353000	0.121525000
				1	3.561911000	-1.779257000	1.427941000
				6	1.590691000	2.683220000	0.156334000
				1	1.218538000	2.772097000	1.199320000
				1	2.587573000	3.148029000	0.113608000
				1	0.940078000	3.271781000	-0.502362000
				1	1.256083000	-3.089319000	-0.022385000
				1	-1.256100000	-3.089309000	-0.022523000
D17	E(RB3LYP) = -687.134760227 a. u.			D18	E(RB3LYP) = -765.738263527a. u.		
6	-1.188335000	-0.819800000	-0.070519000	6	-0.616158000	-2.176033000	-0.234058000
6	-0.597333000	-2.095858000	0.038999000	6	-1.395336000	-1.012275000	-0.154448000
6	-0.334298000	0.312454000	-0.069571000	6	0.769321000	-2.129507000	-0.247889000
6	0.785895000	-2.236885000	0.135673000	6	-0.731299000	0.240292000	-0.087984000
6	1.069303000	0.150059000	-0.051894000	6	1.457599000	-0.901154000	-0.176314000
6	1.641108000	-1.132917000	0.076542000	6	0.693933000	0.291385000	-0.061436000
7	-0.842247000	1.650925000	-0.157473000	7	-2.816000000	-1.127980000	-0.201390000
6	-2.193882000	1.685093000	-0.712267000	6	-3.506768000	0.134281000	-0.439883000
1	-2.142759000	1.445374000	-1.787539000	1	-4.572897000	0.009035000	-0.198192000
1	-2.596648000	2.703852000	-0.609153000	1	-3.441313000	0.390057000	-1.512947000
7	3.053335000	-1.305392000	0.165507000	7	1.345212000	1.557520000	0.069463000
1	3.397368000	-1.910406000	-0.577713000	6	2.731595000	1.542647000	-0.381656000

6	3.832860000	-0.076050000	0.270355000	1	3.204023000	2.495695000	-0.101685000
1	4.873721000	-0.289307000	-0.015430000	1	2.752255000	1.462812000	-1.481969000
1	3.839930000	0.257220000	1.323500000	7	-1.475700000	1.452999000	0.004032000
7	-2.577388000	-0.660336000	-0.223434000	6	-2.870836000	1.255385000	0.388231000
6	-3.115268000	0.673785000	-0.026859000	1	-2.917738000	0.990602000	1.459793000
1	-4.122779000	0.716827000	-0.473005000	1	-3.406895000	2.207613000	0.258558000
1	-3.226025000	0.932486000	1.050179000	7	2.863366000	-0.859956000	-0.233142000
7	1.887189000	1.290235000	-0.144276000	6	3.505616000	0.364400000	0.205277000
1	1.399688000	2.035111000	-0.642026000	1	3.545820000	0.451444000	1.314381000
6	3.254842000	1.054864000	-0.586821000	1	4.546112000	0.368727000	-0.159245000
1	3.316621000	0.765854000	-1.658214000	1	1.321477000	-3.064797000	-0.318130000
1	3.837418000	1.981038000	-0.453703000	1	-1.117259000	-3.141721000	-0.321532000
1	1.222677000	-3.231326000	0.257246000	6	-1.313605000	2.384371000	-1.116733000
1	-1.219077000	-2.988708000	0.072800000	1	-1.795144000	2.026580000	-2.050652000
6	-0.714024000	2.418919000	1.088869000	1	-1.761796000	3.354336000	-0.846058000
1	-0.976098000	3.471955000	0.893071000	1	-0.244156000	2.536513000	-1.305244000
1	-1.362290000	2.042036000	1.906451000	6	1.158960000	2.222378000	1.362062000
1	0.328375000	2.380480000	1.433365000	1	1.529630000	3.258309000	1.291888000
6	-3.456060000	-1.761194000	0.111804000	1	0.087775000	2.253529000	1.597168000
1	-4.492338000	-1.464326000	-0.106834000	1	1.692867000	1.716213000	2.193741000
1	-3.232419000	-2.648829000	-0.500727000	6	3.614339000	-2.082106000	-0.034950000
1	-3.400444000	-2.062177000	1.179599000	1	3.451878000	-2.545411000	0.961582000
				1	3.364327000	-2.833254000	-0.800729000
				1	4.685674000	-1.855447000	-0.135749000
				6	-3.424312000	-1.929333000	0.858264000
				1	-3.432935000	-1.421914000	1.848173000
				1	-4.464830000	-2.168504000	0.585010000
				1	-2.883308000	-2.876881000	0.978189000
				6	-0.702225000	-2.123871000	0.003364000
				6	-1.417911000	-0.929920000	-0.029312000
				6	0.701938000	-2.123890000	-0.003626000
				6	-0.699721000	0.306960000	-0.059068000
				6	1.417856000	-0.930072000	0.029702000
				6	0.699768000	0.306946000	0.059569000
				7	-2.824942000	-0.906513000	-0.005858000
				6	-3.451773000	0.322374000	0.225055000
				1	-4.500617000	0.280071000	0.518583000
				7	1.405593000	1.545968000	0.179750000
				6	2.787727000	1.483871000	-0.140032000
				1	3.282763000	2.437409000	-0.330508000
				7	-1.405510000	1.546033000	-0.179579000
				6	-2.787759000	1.484125000	0.139600000
				1	-3.282842000	2.437816000	0.329191000
				7	2.824864000	-0.906764000	0.006638000
				6	3.451619000	0.322014000	-0.225355000
				1	4.500306000	0.279479000	-0.519418000
				1	-1.222181000	-3.080366000	0.011344000
				1	1.221788000	-3.080446000	-0.012217000

	6	-1.109640000	2.341937000	-1.377476000
	1	-1.474719000	1.857223000	-2.305129000
	1	-1.607998000	3.319833000	-1.281315000
	1	-0.026529000	2.506021000	-1.448387000
	6	-3.562321000	-2.134800000	0.189717000
	1	-3.296186000	-2.643815000	1.137613000
	1	-4.636387000	-1.906975000	0.206256000
	1	-3.382294000	-2.844880000	-0.635524000
	6	1.110237000	2.342464000	1.377274000
	1	1.608525000	3.320306000	1.280376000
	1	0.027161000	2.506469000	1.448631000
	1	1.475690000	1.858295000	2.305124000
	6	3.562087000	-2.135005000	-0.189808000
	1	3.381462000	-2.845730000	0.634752000
	1	3.296468000	-2.643091000	-1.138326000
	1	4.636241000	-1.907494000	-0.205336000

Table 2 Cartesian coordinates (in Angstrom unit) of B3LYP/cc-pVDZ geometries of D1- π -A – D18- π -A systems.

D1- π -A E(RB3LYP) = -1267.64924217 a. u.				D2- π -A E(RB3LYP) = -1283.68206001 a. u.			
6	3.306086000	2.607548000	0.377940000	6	4.174802000	2.281580000	-0.087193000
6	2.707260000	1.219216000	0.187547000	6	3.138858000	1.169702000	0.050669000
6	4.356573000	2.836461000	-0.712666000	6	5.211363000	1.880414000	-1.139884000
6	3.622037000	0.171621000	-0.133013000	6	3.596632000	-0.166535000	-0.088081000
6	5.465849000	1.802372000	-0.597167000	6	5.893144000	0.586766000	-0.730177000
7	4.957053000	0.449823000	-0.366713000	7	4.930878000	-0.437144000	-0.343505000
6	1.341269000	0.952722000	0.326614000	6	1.781908000	1.431062000	0.282753000
6	3.148298000	-1.163159000	-0.183776000	6	2.672870000	-1.249776000	0.046777000
6	5.867486000	-0.612816000	-0.774884000	6	5.462300000	-1.787193000	-0.320265000
6	1.777122000	-1.423793000	-0.089338000	6	1.314485000	-0.992070000	0.280132000
6	0.835444000	-0.377122000	0.141851000	6	0.841548000	0.355766000	0.343927000
6	4.096660000	-2.343234000	-0.333033000	7	3.192533000	-2.556028000	-0.074597000
1	4.794832000	3.844350000	-0.631407000	1	5.971826000	2.668755000	-1.259343000
6	5.543392000	-1.918299000	-0.068946000	6	4.539150000	-2.714765000	0.448493000
1	5.691509000	-1.779168000	1.016374000	1	4.601398000	-2.495966000	1.536477000
1	6.155544000	2.074676000	0.225702000	1	6.596158000	0.773491000	0.107460000
1	6.891858000	-0.290768000	-0.527345000	1	6.459475000	-1.767689000	0.158917000
1	3.870760000	2.768601000	-1.701290000	1	4.712089000	1.753100000	-2.116013000
1	6.243896000	-2.703375000	-0.395017000	1	4.865765000	-3.752938000	0.296437000
1	6.070881000	1.794475000	-1.522005000	1	6.500763000	0.191722000	-1.564801000
1	5.832905000	-0.749182000	-1.877047000	1	5.600288000	-2.168757000	-1.351227000
6	1.397468000	-2.867869000	-0.359385000	6	0.391901000	-2.169171000	0.549922000

1	0.324669000	-3.059256000	-0.248964000	1	-0.369745000	-1.876358000	1.286845000
6	2.194944000	-3.871310000	0.498110000	6	1.153916000	-3.401523000	1.035776000
1	1.739742000	-3.935831000	1.499549000	1	1.575684000	-3.222723000	2.040168000
1	2.094433000	-4.871645000	0.047052000	1	0.475716000	-4.266288000	1.109887000
6	3.681649000	-3.475462000	0.630088000	6	2.277720000	-3.689935000	0.047824000
1	3.883412000	-3.123341000	1.655569000	1	2.863361000	-4.571431000	0.346080000
1	4.335116000	-4.348420000	0.466532000	1	1.839031000	-3.915701000	-0.943112000
6	0.402624000	2.085028000	0.716839000	6	1.297795000	2.871523000	0.414016000
1	-0.361604000	1.702721000	1.409662000	1	0.602731000	2.956841000	1.264159000
6	1.101845000	3.301737000	1.324560000	6	2.409999000	3.907540000	0.595021000
1	1.480632000	3.057080000	2.333335000	1	2.803591000	3.860687000	1.626638000
1	0.375086000	4.120395000	1.447218000	1	1.994136000	4.918952000	0.461839000
6	2.262882000	3.723496000	0.431682000	6	3.546300000	3.643275000	-0.384212000
1	1.885824000	3.931743000	-0.587092000	1	3.157599000	3.655926000	-1.419547000
1	2.735189000	4.652242000	0.792086000	1	4.318872000	4.427632000	-0.322093000
1	3.839919000	2.605701000	1.350604000	1	4.709456000	2.369292000	0.881060000
1	4.031424000	-2.731031000	-1.369520000	1	-0.160739000	-2.445532000	-0.366257000
1	1.618540000	-3.068293000	-1.424541000	1	0.703676000	3.133014000	-0.481074000
1	-0.148450000	2.421412000	-0.180576000	6	-5.442616000	0.507343000	0.121550000
6	-5.457758000	-0.538488000	0.039470000	6	-6.661630000	-0.029187000	-0.221238000
6	-6.688970000	0.031819000	-0.179537000	6	-6.767627000	-1.298096000	-0.869517000
6	-6.823066000	1.389443000	-0.604979000	7	-6.812989000	-2.337125000	-1.397014000
7	-6.891950000	2.500638000	-0.951631000	6	-7.886267000	0.740717000	0.098061000
6	-7.898779000	-0.796737000	0.036155000	8	-7.902430000	1.825563000	0.646975000
8	-7.890491000	-1.957753000	0.396523000	8	-9.014682000	0.102067000	-0.291013000
8	-9.041762000	-0.116671000	-0.213889000	1	-9.749606000	0.688508000	-0.036577000
1	-9.765518000	-0.745941000	-0.043493000	6	-1.688779000	0.011061000	0.088235000
6	-1.708982000	0.002218000	-0.005799000	1	-1.623202000	-0.949660000	-0.423509000
1	-1.664903000	1.036793000	-0.346080000	1	-5.490922000	1.483667000	0.614380000
1	-5.484625000	-1.583913000	0.363150000	6	-3.000886000	0.541381000	0.285245000
6	-3.012955000	-0.568934000	0.133354000	6	-4.164694000	-0.075802000	-0.099477000
6	-4.190246000	0.090261000	-0.111752000	1	-3.074945000	1.516934000	0.782624000
1	-3.066441000	-1.615206000	0.460511000	1	-4.118247000	-1.051529000	-0.593734000
1	-4.165096000	1.135779000	-0.435310000	6	-0.564150000	0.695449000	0.471991000
6	-0.573176000	-0.728116000	0.225635000	1	-0.768528000	1.679931000	0.900355000
1	-0.766967000	-1.770044000	0.496256000				
D3- π -A E(RB3LYP) = -1299.71050012 a. u.				D4- π -A E(RB3LYP) = -1315.75401584 a. u.			
7	3.250219000	2.550368000	0.182907000	7	4.178061000	2.155666000	0.204692000
6	2.698491000	1.245903000	0.117102000	6	3.178806000	1.155176000	0.052668000
6	4.415233000	2.753887000	-0.660620000	6	5.463792000	1.800627000	-0.370287000
6	3.604391000	0.172015000	-0.105742000	6	3.610656000	-0.209826000	0.039846000
6	5.494800000	1.758807000	-0.278119000	6	5.963804000	0.517716000	0.267921000
7	4.958484000	0.412198000	-0.272890000	7	4.954170000	-0.518520000	0.168981000
6	1.323972000	0.994215000	0.275806000	6	1.818661000	1.456005000	-0.037009000
6	3.113725000	-1.162907000	-0.146939000	6	2.665203000	-1.246560000	-0.118492000

6	5.932022000	-0.661395000	-0.369847000	6	5.420673000	-1.892051000	0.205413000
6	1.761148000	-1.431754000	0.101345000	6	1.297110000	-0.943222000	-0.259249000
6	0.837585000	-0.347625000	0.248588000	6	0.847863000	0.410446000	-0.184707000
7	4.054704000	-2.172330000	-0.444320000	7	3.130700000	-2.591441000	-0.167014000
1	4.789403000	3.776579000	-0.502286000	1	6.176921000	2.613390000	-0.164856000
6	5.358052000	-1.965282000	0.164098000	6	4.307670000	-2.825580000	0.651835000
1	5.309373000	-1.930173000	1.273716000	1	4.097960000	-2.673757000	1.733463000
1	5.912997000	2.019939000	0.714522000	1	6.235969000	0.705036000	1.325621000
1	6.829035000	-0.382792000	0.213901000	1	6.264511000	-1.962145000	0.914329000
1	4.169622000	2.651722000	-1.740427000	1	5.407704000	1.675122000	-1.474612000
1	6.025471000	-2.792462000	-0.116311000	1	4.630320000	-3.869557000	0.518277000
1	6.322341000	1.810131000	-1.008411000	1	6.874882000	0.176933000	-0.254155000
1	6.251311000	-0.798717000	-1.421490000	1	5.796109000	-2.205571000	-0.788644000
6	1.303597000	-2.881205000	0.191286000	7	0.394988000	-1.987546000	-0.488115000
1	0.592711000	-2.999116000	1.023310000	1	-0.433969000	-1.693079000	-0.996195000
6	2.463356000	-3.856257000	0.404065000	6	0.933461000	-3.264139000	-0.930830000
1	2.861238000	-3.758549000	1.429425000	1	0.146282000	-4.028436000	-0.845707000
1	2.115764000	-4.894860000	0.283840000	1	1.278145000	-3.239646000	-1.984023000
6	3.565847000	-3.537704000	-0.599764000	6	2.107201000	-3.618167000	-0.034140000
1	4.420331000	-4.222181000	-0.496785000	1	1.749932000	-3.718749000	1.013149000
1	3.169970000	-3.666567000	-1.625479000	1	2.542081000	-4.584507000	-0.336385000
6	0.402804000	2.164485000	0.575295000	6	1.360778000	2.902192000	0.084932000
1	-0.366679000	1.854594000	1.297380000	1	0.489236000	2.964658000	0.754096000
6	1.158619000	3.379140000	1.112067000	6	2.457905000	3.827362000	0.613789000
1	1.535939000	3.178550000	2.129057000	1	2.593336000	3.674383000	1.697658000
1	0.489836000	4.251600000	1.171209000	1	2.178470000	4.881202000	0.460327000
6	2.332708000	3.681556000	0.198208000	6	3.771920000	3.524114000	-0.085610000
1	1.959862000	3.916119000	-0.824493000	1	3.663351000	3.690720000	-1.181927000
1	2.894031000	4.564478000	0.546128000	1	4.572114000	4.194778000	0.266977000
1	0.750176000	-3.167234000	-0.722138000	1	1.014214000	3.270082000	-0.899443000
1	-0.140799000	2.466755000	-0.338625000	6	-5.438064000	0.559209000	-0.107437000
6	-5.451220000	-0.530469000	0.088905000	6	-6.669536000	-0.013215000	0.118190000
6	-6.683752000	0.024539000	-0.166109000	6	-6.797256000	-1.360447000	0.575783000
6	-6.819199000	1.363840000	-0.645026000	7	-6.859296000	-2.464166000	0.947560000
7	-6.889087000	2.460711000	-1.034871000	6	-7.881165000	0.800595000	-0.127251000
6	-7.891050000	-0.800795000	0.067750000	8	-7.879535000	1.952333000	-0.518434000
8	-7.882482000	-1.947323000	0.472963000	8	-9.023402000	0.120843000	0.132749000
8	-9.035309000	-0.137269000	-0.221135000	1	-9.747647000	0.743055000	-0.059503000
1	-9.756716000	-0.764436000	-0.034178000	6	-1.689160000	0.042846000	-0.034899000
6	-1.705936000	0.026055000	0.070272000	1	-1.633282000	-0.979249000	0.345946000
1	-1.663510000	1.045911000	-0.311084000	1	-5.470006000	1.595318000	-0.459560000
1	-5.477276000	-1.562663000	0.452702000	6	-2.992003000	0.602556000	-0.192453000
6	-3.007318000	-0.545812000	0.213672000	6	-4.169748000	-0.055321000	0.068349000
6	-4.185916000	0.097324000	-0.071892000	1	-3.050494000	1.637985000	-0.552339000
1	-3.060721000	-1.578818000	0.580760000	1	-4.139061000	-1.090277000	0.424077000
1	-4.161130000	1.129397000	-0.436150000	6	-0.546868000	0.773830000	-0.275807000
6	-0.569112000	-0.691058000	0.346991000	1	-0.734158000	1.814071000	-0.557163000
1	-0.767572000	-1.724106000	0.643154000				

D5-π-A E(RB3LYP) = -1331.78737769 a. u.				D6-π-A E(RB3LYP) = -1110.31136848 a. u.			
7	-4.082982000	2.248285000	0.033468000	6	3.761386000	2.462707000	0.060986000
6	-3.143697000	1.174787000	-0.042479000	6	3.227925000	1.291174000	-0.710932000
6	-5.179088000	1.985530000	0.950890000	6	4.189625000	0.304153000	-0.784872000
6	-3.608522000	-0.153146000	0.140352000	6	5.071929000	1.828113000	0.691573000
6	-5.891636000	0.710267000	0.531084000	7	5.363622000	0.582538000	-0.107150000
7	-4.945019000	-0.383341000	0.408849000	6	1.902539000	0.955099000	-0.486614000
6	-1.792648000	1.408289000	-0.329840000	6	3.848852000	-1.030082000	-0.828340000
6	-2.714765000	-1.248520000	-0.012076000	6	5.745317000	-0.712200000	0.567220000
6	-5.454982000	-1.735932000	0.537583000	6	2.536271000	-1.410157000	-0.597460000
6	-1.349544000	-1.007084000	-0.219816000	6	1.487748000	-0.426766000	-0.518136000
6	-0.841194000	0.330607000	-0.317501000	6	4.907221000	-1.851779000	-0.153375000
7	-3.229840000	-2.577715000	0.062020000	1	4.901053000	1.540630000	1.748052000
1	-5.884521000	2.829855000	0.909625000	1	5.477920000	-0.645086000	1.640555000
6	-4.629121000	-2.691105000	-0.308602000	1	5.927627000	2.517034000	0.660144000
1	-4.796365000	-2.470002000	-1.386752000	1	6.828920000	-0.880836000	0.495674000
1	-6.427275000	0.878158000	-0.424215000	6	2.607984000	-2.824697000	-0.024984000
1	-6.502166000	-1.752678000	0.193082000	1	1.802622000	-3.055841000	0.687753000
1	-4.828422000	1.889683000	2.002471000	6	4.020733000	-2.839990000	0.669569000
1	-4.957684000	-3.726034000	-0.125648000	1	3.910599000	-2.464530000	1.701196000
1	-6.644592000	0.444053000	1.292422000	1	4.438776000	-3.856363000	0.730437000
1	-5.443420000	-2.066534000	1.594642000	6	1.288303000	2.150001000	0.243170000
7	-0.454420000	-2.086589000	-0.290938000	1	0.509565000	1.860471000	0.962891000
1	0.169417000	-2.033431000	-1.091089000	1	0.828415000	2.864142000	-0.463263000
6	-0.966186000	-3.421372000	-0.020115000	6	2.529355000	2.804311000	0.954955000
1	-0.287503000	-4.159295000	-0.470483000	1	2.390967000	3.884361000	1.114465000
1	-0.972834000	-3.594760000	1.069706000	1	2.652643000	2.336965000	1.946739000
6	-2.384615000	-3.590266000	-0.552168000	1	4.043255000	3.321347000	-0.572155000
1	-2.378529000	-3.510181000	-1.662488000	1	5.563990000	-2.397613000	-0.852191000
1	-2.784141000	-4.583838000	-0.290687000	1	2.564477000	-3.585594000	-0.824393000
7	-1.356585000	2.722383000	-0.568785000	6	-4.751183000	-0.558267000	0.057247000
1	-0.594606000	2.768912000	-1.237107000	6	-5.978045000	0.059454000	0.020623000
6	-2.369808000	3.740075000	-0.807474000	6	-6.111944000	1.446330000	-0.296855000
1	-2.804578000	3.677096000	-1.825092000	7	-6.180608000	2.580459000	-0.558727000
1	-1.907659000	4.733256000	-0.694677000	6	-7.184096000	-0.748427000	0.322958000
6	-3.482599000	3.562967000	0.211139000	8	-7.174234000	-1.930530000	0.605640000
1	-3.069897000	3.697549000	1.234507000	8	-8.322898000	-0.021688000	0.251438000
1	-4.261823000	4.326407000	0.057858000	1	-9.045013000	-0.639921000	0.464184000
6	5.430695000	0.544230000	0.033098000	6	-1.016223000	-0.111870000	-0.376036000
6	6.679224000	-0.028361000	0.149309000	1	-0.964517000	0.942086000	-0.662590000
6	6.847795000	-1.443720000	0.238890000	1	-4.777235000	-1.621938000	0.314672000
7	6.942767000	-2.604332000	0.307558000	6	-2.313071000	-0.658218000	-0.130776000
6	7.861326000	0.858540000	0.177370000	6	-3.488391000	0.045072000	-0.201230000
8	7.826123000	2.072902000	0.104305000	1	-2.363048000	-1.721690000	0.135197000
8	9.023981000	0.171831000	0.295425000	1	-3.464919000	1.108004000	-0.462085000
1	9.725008000	0.847793000	0.303853000	6	0.129049000	-0.858100000	-0.293409000

6	1.707306000	-0.078231000	-0.196746000	1	0.002148000	-1.924030000	-0.072455000
1	1.675175000	-1.163220000	-0.113258000				
1	5.431931000	1.637280000	-0.029899000				
6	2.988852000	0.538162000	-0.136007000				
6	4.184929000	-0.131375000	-0.012198000				
1	3.021575000	1.633868000	-0.200055000				
1	4.182831000	-1.224131000	0.053687000				
6	0.554545000	0.672515000	-0.301715000				
1	0.744198000	1.750358000	-0.301318000				
D7- π -A E(RB3LYP) = -1126.33329613 a. u.				D8- π -A E(RB3LYP) = -1142.35569667 a. u.			
6	3.768061000	2.434472000	0.098517000	7	3.720152000	2.352337000	0.061404000
6	3.227316000	1.287351000	-0.705469000	6	3.215834000	1.261161000	-0.665201000
6	4.193594000	0.315120000	-0.815398000	6	4.198250000	0.320564000	-0.852177000
6	5.057185000	1.761726000	0.738945000	6	5.010019000	1.839853000	0.650969000
7	5.379234000	0.567447000	-0.131225000	7	5.371082000	0.608287000	-0.143101000
6	1.893294000	0.959863000	-0.497883000	6	1.874672000	0.945577000	-0.502967000
6	3.840781000	-1.011630000	-0.786188000	6	3.845493000	-1.001093000	-0.781647000
6	5.753567000	-0.766703000	0.460500000	6	5.713912000	-0.704041000	0.521204000
6	2.531114000	-1.410891000	-0.593125000	6	2.535103000	-1.425536000	-0.613614000
6	1.486025000	-0.422515000	-0.524734000	6	1.488716000	-0.442313000	-0.536820000
7	4.852402000	-1.787218000	-0.190760000	7	4.853837000	-1.748299000	-0.148713000
1	4.843226000	1.407743000	1.767301000	1	4.879494000	1.582980000	1.727989000
1	5.603389000	-0.752754000	1.564019000	1	5.499281000	-0.653847000	1.614045000
1	5.913548000	2.448945000	0.782195000	1	5.801852000	2.596125000	0.561248000
1	6.807313000	-0.997970000	0.251346000	1	6.778535000	-0.934763000	0.379499000
6	2.657011000	-2.813089000	-0.004417000	6	2.676347000	-2.823071000	-0.017351000
1	1.890728000	-3.062822000	0.743822000	1	1.898246000	-3.087614000	0.713490000
6	4.093040000	-2.764808000	0.636285000	6	4.092363000	-2.737625000	0.663198000
1	4.028263000	-2.401876000	1.682433000	1	3.990603000	-2.368408000	1.704072000
1	4.576312000	-3.752595000	0.643683000	1	4.599129000	-3.713163000	0.691106000
6	1.285383000	2.153028000	0.240941000	6	1.305529000	2.145624000	0.252152000
1	0.495679000	1.864520000	0.949212000	1	0.536761000	1.880570000	0.991644000
1	0.843538000	2.888130000	-0.455609000	1	0.868398000	2.897477000	-0.427976000
6	2.526980000	2.777512000	0.980099000	6	2.586450000	2.739924000	0.943874000
1	2.402721000	3.856981000	1.154631000	1	2.524365000	3.830909000	1.066277000
1	2.630056000	2.293242000	1.966019000	1	2.721779000	2.285815000	1.946590000
1	4.078720000	3.300925000	-0.510179000	1	2.685728000	-3.606964000	-0.794507000
1	2.625926000	-3.589470000	-0.788364000	6	-4.749057000	-0.564454000	0.053980000
6	-4.753031000	-0.562213000	0.057573000	6	-5.969761000	0.062951000	0.021369000
6	-5.978951000	0.055917000	0.019391000	6	-6.094241000	1.450773000	-0.296766000
6	-6.112984000	1.441132000	-0.305690000	7	-6.155747000	2.585188000	-0.558548000
7	-6.182149000	2.573760000	-0.573520000	6	-7.182343000	-0.735512000	0.330044000
6	-7.185517000	-0.749940000	0.328631000	8	-7.179155000	-1.916822000	0.614479000
8	-7.174887000	-1.930135000	0.618188000	8	-8.314531000	0.000534000	0.261514000
8	-8.323461000	-0.022880000	0.254460000	1	-9.042160000	-0.610141000	0.477626000

1	-9.046353000	-0.638666000	0.471793000	6	-1.012130000	-0.138168000	-0.392925000
6	-1.018466000	-0.116041000	-0.384332000	1	-0.955471000	0.914952000	-0.682535000
1	-0.967487000	0.935975000	-0.678086000	1	-4.781678000	-1.627459000	0.313131000
1	-4.778822000	-1.624336000	0.321200000	6	-2.312015000	-0.679393000	-0.142012000
6	-2.315149000	-0.662633000	-0.133363000	6	-3.481912000	0.030505000	-0.211075000
6	-3.489960000	0.039896000	-0.206748000	1	-2.365967000	-1.741753000	0.126952000
1	-2.363832000	-1.724404000	0.139271000	1	-3.452947000	1.092446000	-0.475385000
1	-3.467093000	1.101168000	-0.474289000	6	0.130179000	-0.885497000	-0.313053000
6	0.127292000	-0.859240000	-0.298971000	1	0.009810000	-1.950821000	-0.085593000
1	0.005039000	-1.924430000	-0.070437000				
D9-π-A E(RB3LYP) = -1158.37982254 a. u.				D10-π-A E(RB3LYP) = -1174.40750304 a. u.			
7	3.765923000	2.349600000	0.043302000	7	3.694622000	2.394863000	-0.005096000
6	3.247078000	1.262899000	-0.695441000	6	3.276967000	1.291865000	-0.810221000
6	4.215577000	0.291368000	-0.841237000	6	4.237530000	0.308223000	-0.781296000
6	5.012206000	1.795937000	0.682682000	6	4.791334000	1.816562000	0.848859000
7	5.362922000	0.546513000	-0.087232000	7	5.265538000	0.589028000	0.114759000
6	1.909253000	0.960675000	-0.534997000	6	1.951522000	0.935272000	-0.612334000
6	3.857879000	-1.024296000	-0.826017000	6	3.928569000	-1.030707000	-0.829764000
6	5.641557000	-0.769341000	0.600381000	6	5.498391000	-0.716331000	0.830925000
6	2.545947000	-1.407537000	-0.583866000	6	2.610680000	-1.409309000	-0.623904000
6	1.492095000	-0.427576000	-0.551805000	6	1.529155000	-0.449375000	-0.657631000
7	4.826687000	-1.798896000	-0.148907000	7	4.861876000	-1.768317000	-0.038941000
1	4.833629000	1.546374000	1.754241000	1	4.423431000	1.534770000	1.864618000
1	5.342773000	-0.720901000	1.674759000	1	5.037842000	-0.679938000	1.847331000
1	5.834300000	2.522230000	0.621363000	1	5.611452000	2.539192000	0.958098000
1	6.710405000	-1.013655000	0.539238000	1	6.574523000	-0.909590000	0.937177000
7	2.630526000	-2.697846000	-0.008170000	7	2.640217000	-2.664698000	0.007933000
1	1.902241000	-2.904232000	0.672147000	1	1.908908000	-2.795000000	0.703771000
6	4.015458000	-2.808027000	0.575323000	6	4.035930000	-2.848081000	0.552734000
1	4.019267000	-2.601126000	1.669791000	1	4.045566000	-2.804163000	1.661211000
1	4.405593000	-3.823311000	0.410973000	1	4.419733000	-3.831584000	0.242543000
6	1.340631000	2.169514000	0.204047000	7	1.333592000	2.013843000	0.041066000
1	0.566734000	1.913052000	0.941187000	1	0.623979000	1.738181000	0.717631000
1	0.909051000	2.915461000	-0.485738000	6	2.432997000	2.878438000	0.604747000
6	2.620590000	2.763923000	0.899054000	1	2.250968000	3.926442000	0.323527000
1	2.566367000	3.857700000	0.998091000	1	2.467921000	2.815530000	1.711974000
1	2.736015000	2.331349000	1.913693000	6	-4.694861000	-0.568369000	0.002247000
6	-4.741755000	-0.560856000	0.038307000	6	-5.918742000	0.056953000	0.057867000
6	-5.966935000	0.062113000	0.029516000	6	-6.048330000	1.469176000	-0.115083000
6	-6.097467000	1.459101000	-0.240830000	7	-6.111868000	2.624909000	-0.257006000
7	-6.162745000	2.601810000	-0.463486000	6	-7.121937000	-0.769786000	0.309957000
6	-7.173739000	-0.751103000	0.313063000	8	-7.114926000	-1.974188000	0.476986000
8	-7.165958000	-1.941599000	0.558549000	8	-8.257811000	-0.034483000	0.337436000
8	-8.310669000	-0.019178000	0.270811000	1	-8.978003000	-0.668255000	0.506164000
1	-9.033610000	-0.641720000	0.467582000	6	-0.966969000	-0.112035000	-0.459430000

6	-1.008435000	-0.113554000	-0.396862000	1	-0.906422000	0.963316000	-0.654513000
1	-0.951758000	0.948340000	-0.651701000	1	-4.724183000	-1.651981000	0.155390000
1	-4.770405000	-1.632210000	0.261314000	6	-2.262156000	-0.666635000	-0.246239000
6	-2.304631000	-0.662891000	-0.164842000	6	-3.434983000	0.048111000	-0.226811000
6	-3.478889000	0.045926000	-0.208102000	1	-2.318436000	-1.750050000	-0.079141000
1	-2.357690000	-1.734024000	0.068161000	1	-3.407794000	1.130438000	-0.389095000
1	-3.453066000	1.116273000	-0.436388000	6	0.176418000	-0.876872000	-0.464569000
6	0.137738000	-0.863779000	-0.339985000	1	0.035479000	-1.957944000	-0.341374000
1	0.005023000	-1.936617000	-0.152473000				
D11-π-A E(RB3LYP) = -1777.79373916 a. u.				D12-π-A E(RB3LYP) = -1774.15158672 a. u.			
6	0.679966000	-0.681171000	0.076549000	6	1.011942000	-1.049631000	0.009422000
6	2.074002000	-0.801103000	-0.041288000	6	2.366894000	-1.171607000	-0.361228000
6	0.082369000	0.625941000	0.003115000	6	0.484857000	0.285714000	0.239147000
6	2.315824000	1.578570000	-0.337922000	6	2.783880000	1.162332000	0.083499000
6	0.935636000	1.768302000	-0.210498000	6	1.438102000	1.384934000	0.375123000
6	2.922111000	0.308306000	-0.237427000	6	3.279285000	-0.100951000	-0.334985000
1	2.510706000	-1.797713000	0.023533000	1	2.717529000	-2.159228000	-0.668553000
1	2.944530000	2.446689000	-0.548256000	6	4.675156000	-0.228035000	-0.704843000
6	4.363747000	0.201857000	-0.427892000	1	5.152527000	0.677837000	-1.084905000
1	4.804169000	1.014410000	-1.007839000	6	5.478879000	-1.358775000	-0.701871000
6	5.241123000	-0.772394000	-0.027756000	7	6.627310000	-1.514783000	-1.469900000
7	6.565244000	-0.855129000	-0.482409000	6	7.230503000	-2.735502000	-1.176604000
6	7.031642000	-2.221018000	-0.259033000	6	6.474393000	-3.351758000	-0.239630000
6	6.267732000	-2.592982000	1.003892000	7	5.392160000	-2.518302000	0.065185000
7	5.018266000	-1.837051000	0.862459000	1	6.599833000	-4.315674000	0.241515000
1	6.075020000	-3.672996000	1.095788000	1	8.132790000	-3.063013000	-1.681869000
1	6.758517000	-2.887654000	-1.104508000	6	0.998611000	2.686484000	0.869572000
1	6.823964000	-2.260412000	1.903947000	1	0.256716000	2.686385000	1.669669000
1	8.123747000	-2.255880000	-0.128879000	6	1.490768000	3.934862000	0.529098000
6	0.357070000	3.103054000	-0.421639000	7	1.346288000	5.084154000	1.301185000
1	-0.554175000	3.134500000	-1.017592000	6	1.889942000	6.177599000	0.629725000
6	0.857405000	4.327769000	-0.067926000	6	2.386133000	5.730896000	-0.546233000
7	0.319816000	5.541719000	-0.520225000	7	2.153044000	4.353290000	-0.623223000
6	1.315522000	6.588385000	-0.315193000	1	2.893557000	6.264023000	-1.342857000
6	2.021580000	6.080065000	0.933060000	1	1.890575000	7.171692000	1.063743000
7	1.947628000	4.625668000	0.768170000	6	0.249943000	-2.284811000	0.034912000
1	3.065594000	6.419720000	1.014324000	1	0.614144000	-3.059761000	-0.643860000
1	2.019005000	6.658874000	-1.172183000	6	-0.771426000	-2.713413000	0.874057000
1	1.477105000	6.401926000	1.844847000	7	-1.579463000	-3.813511000	0.613627000
1	0.841071000	7.571167000	-0.173585000	6	-2.489740000	-3.989057000	1.651908000
6	-0.116688000	-1.865793000	0.408947000	6	-2.267326000	-3.010263000	2.559079000
1	-0.929659000	-1.693980000	1.113659000	7	-1.211514000	-2.223218000	2.092906000
6	0.053888000	-3.167507000	0.023737000	1	-3.227884000	-4.783472000	1.637028000
7	-0.652967000	-4.240130000	0.588335000	1	-2.770241000	-2.788808000	3.493746000
6	0.055669000	-5.473670000	0.266456000	6	4.645692000	-2.612048000	1.309873000

6	0.650006000	-5.125107000	-1.090167000	1	3.591798000	-2.880543000	1.147277000
7	0.911365000	-3.687837000	-0.963756000	1	5.122426000	-3.369680000	1.946999000
1	1.573102000	-5.679733000	-1.319139000	1	4.669063000	-1.638257000	1.824508000
1	0.853150000	-5.694540000	1.008432000	6	7.054950000	-0.571914000	-2.476890000
1	-0.085738000	-5.322265000	-1.896712000	1	7.481873000	0.342201000	-2.028304000
1	-0.631229000	-6.332531000	0.229430000	1	7.820320000	-1.042085000	-3.109047000
6	2.159644000	3.872501000	1.997386000	1	6.196597000	-0.277586000	-3.102993000
1	1.331015000	4.020167000	2.719570000	6	-1.533481000	-4.575921000	-0.614119000
1	2.261794000	2.801463000	1.790086000	1	-0.625133000	-5.200362000	-0.671443000
1	3.094049000	4.221377000	2.463488000	1	-2.414781000	-5.228683000	-0.662936000
6	-0.472400000	5.593032000	-1.732407000	1	-1.539268000	-3.895931000	-1.481468000
1	-1.400787000	5.014963000	-1.615136000	6	-0.514898000	-1.243619000	2.903897000
1	-0.755841000	6.638358000	-1.923453000	1	-0.794940000	-1.397845000	3.955277000
1	0.070456000	5.200707000	-2.616216000	1	0.571281000	-1.378698000	2.794989000
6	4.338683000	-1.587459000	2.129597000	6	0.748613000	5.100603000	2.614694000
1	3.365009000	-1.111850000	1.969574000	1	-0.342971000	4.939157000	2.570369000
1	4.167763000	-2.551620000	2.632868000	1	1.186615000	4.305668000	3.241194000
1	4.947106000	-0.945460000	2.798672000	1	0.939275000	6.075003000	3.084328000
6	6.957988000	-0.210539000	-1.719946000	6	2.179311000	3.604965000	-1.866799000
1	6.345467000	-0.537291000	-2.584672000	1	2.938412000	2.808271000	-1.854853000
1	6.873260000	0.882570000	-1.632477000	1	1.200790000	3.127810000	-2.037686000
1	8.013389000	-0.446153000	-1.920178000	1	2.389158000	4.302321000	-2.689380000
6	-1.239820000	-4.126673000	1.908315000	1	-0.763594000	-0.215046000	2.602604000
1	-2.022397000	-3.354597000	1.921880000	6	-5.725615000	0.591385000	-0.671584000
1	-1.716826000	-5.083840000	2.164666000	6	-6.964074000	0.026608000	-0.936087000
1	-0.492243000	-3.877179000	2.689246000	6	-7.107861000	-1.378300000	-1.138516000
6	1.056775000	-2.996919000	-2.239294000	7	-7.174837000	-2.533710000	-1.292653000
1	0.104275000	-2.975042000	-2.806786000	6	-8.141390000	0.905345000	-0.998102000
1	1.405332000	-1.968276000	-2.094250000	8	-8.131555000	2.113900000	-0.834679000
1	1.808612000	-3.530224000	-2.841346000	8	-9.290578000	0.228302000	-1.263641000
6	-6.191192000	0.286552000	0.138220000	1	-9.986056000	0.909323000	-1.279793000
6	-7.386630000	-0.373255000	-0.051469000	6	-2.044609000	-0.061877000	-0.153907000
6	-7.432184000	-1.720053000	-0.524684000	1	-2.013029000	-1.136786000	-0.319270000
7	-7.428231000	-2.820935000	-0.910460000	1	-5.742066000	1.676758000	-0.527037000
6	-8.643239000	0.344106000	0.250123000	6	-3.302426000	0.569179000	-0.283868000
8	-8.714951000	1.488586000	0.657881000	6	-4.491161000	-0.080623000	-0.571797000
8	-9.743176000	-0.415237000	0.023041000	1	-3.341328000	1.656000000	-0.129201000
1	-10.501129000	0.151782000	0.251937000	1	-4.476757000	-1.165094000	-0.721818000
6	-2.420700000	0.064506000	-0.071892000	6	-0.892112000	0.653207000	0.137100000
1	-2.287969000	-0.950366000	-0.451105000	1	-1.052152000	1.732721000	0.228029000
1	-6.287597000	1.312503000	0.508135000	1	3.500682000	1.970287000	0.248408000
6	-3.754551000	0.517983000	0.138813000				
6	-4.888994000	-0.225801000	-0.092612000				
1	-3.880030000	1.540265000	0.519075000				
1	-4.791093000	-1.249945000	-0.466914000				
6	-1.333696000	0.876560000	0.150494000				
1	-1.573045000	1.900899000	0.457964000				

D13-π-A E(RB3LYP) = -1433.64341007 a. u.				D14-π-A E(RB3LYP) = -1431.21430809 a. u.			
6	-0.055538000	-0.314225000	-0.238629000	6	-0.039740000	0.317832000	-0.056022000
6	0.947335000	-1.301887000	-0.299800000	6	-1.041066000	1.303416000	-0.188604000
6	0.316015000	1.043612000	-0.211576000	6	-0.410279000	-1.023771000	0.144327000
6	2.641358000	0.412708000	-0.337644000	6	-2.738093000	-0.381775000	0.114474000
6	1.667525000	1.433120000	-0.255620000	6	-1.768017000	-1.407532000	0.203063000
6	2.314315000	-0.958878000	-0.342461000	6	-2.410881000	0.979688000	-0.078389000
1	0.655636000	-2.352101000	-0.361490000	1	-0.744543000	2.329128000	-0.419215000
1	3.691429000	0.698298000	-0.430324000	6	-3.477295000	1.965554000	-0.219536000
6	3.387346000	-1.943393000	-0.500351000	1	-4.407537000	1.603509000	-0.661568000
1	4.275121000	-1.567822000	-1.010912000	6	-3.447362000	3.316342000	0.072315000
6	3.421828000	-3.264375000	-0.150828000	7	-4.332171000	4.259185000	-0.445037000
7	4.432728000	-4.151763000	-0.552934000	6	-4.060805000	5.512721000	0.101724000
6	3.897926000	-5.507475000	-0.456103000	6	-3.016387000	5.375023000	0.948082000
6	2.962939000	-5.372132000	0.737349000	7	-2.621420000	4.029875000	0.942222000
7	2.493309000	-3.985462000	0.627500000	1	-2.502062000	6.112299000	1.554982000
1	2.122563000	-6.083057000	0.716712000	1	-4.624640000	6.394087000	-0.184780000
1	3.339756000	-5.793381000	-1.372995000	6	-2.107059000	-2.804298000	0.446825000
1	3.522369000	-5.520589000	1.683304000	1	-1.378661000	-3.376138000	1.024790000
1	4.699458000	-6.243809000	-0.294180000	6	-3.258387000	-3.486906000	0.103517000
6	1.995647000	2.859392000	-0.307050000	7	-3.683070000	-4.673593000	0.695417000
1	1.214138000	3.488544000	-0.735060000	6	-4.841823000	-5.126893000	0.067383000
6	3.140794000	3.511407000	0.057759000	6	-5.158074000	-4.241097000	-0.903026000
7	3.397033000	4.858445000	-0.240394000	7	-4.197062000	-3.219884000	-0.894710000
6	4.841012000	5.063951000	-0.171963000	1	-5.988172000	-4.230322000	-1.601048000
6	5.226605000	4.086075000	0.928871000	1	-5.349367000	-6.029664000	0.390267000
7	4.254100000	3.000409000	0.754761000	6	-1.888239000	3.418633000	2.037812000
1	6.260007000	3.716197000	0.842396000	1	-0.926529000	2.995203000	1.712408000
1	5.337174000	4.804432000	-1.131474000	1	-1.706145000	4.181767000	2.806772000
1	5.107919000	4.560497000	1.924236000	1	-2.483036000	2.599481000	2.474271000
1	5.086027000	6.108173000	0.073864000	6	-5.318301000	3.963856000	-1.455762000
6	4.037495000	2.213770000	1.964722000	1	-6.158716000	3.372503000	-1.050699000
1	3.581940000	2.821326000	2.772943000	1	-5.715923000	4.905496000	-1.858054000
1	3.391811000	1.350990000	1.766345000	1	-4.858061000	3.385584000	-2.274659000
1	5.009832000	1.836783000	2.318103000	6	-3.034058000	-5.280156000	1.832834000
6	2.678419000	5.520325000	-1.310825000	1	-2.066260000	-5.736300000	1.559036000
1	1.607885000	5.596830000	-1.069882000	1	-2.845145000	-4.520222000	2.609497000
1	3.067776000	6.543334000	-1.417134000	1	-3.685501000	-6.062912000	2.244484000
1	2.778351000	4.994026000	-2.281958000	6	-3.918651000	-2.390900000	-2.054810000
6	2.041716000	-3.423217000	1.896326000	1	-4.049605000	-1.319080000	-1.843478000
1	1.605822000	-2.427693000	1.755972000	1	-2.876304000	-2.541712000	-2.381136000
1	1.263650000	-4.079689000	2.316099000	1	-4.597115000	-2.685305000	-2.867198000
1	2.870026000	-3.349317000	2.630220000	6	6.235131000	0.410670000	-0.214640000
6	5.258500000	-3.843334000	-1.703263000	6	7.453787000	-0.216541000	-0.126059000
1	4.662608000	-3.659954000	-2.620573000	6	7.562306000	-1.619161000	0.126442000
1	5.874840000	-2.952848000	-1.510326000	7	7.613109000	-2.765324000	0.334027000

1	5.941417000	-4.686353000	-1.883564000	6	8.680760000	0.598222000	-0.299079000
6	-6.329872000	-0.429738000	-0.054047000	8	8.695207000	1.794182000	-0.515279000
6	-7.543699000	0.207595000	0.011769000	8	9.809591000	-0.139567000	-0.189660000
6	-7.644203000	1.631923000	0.079123000	1	10.546353000	0.484575000	-0.318155000
7	-7.688284000	2.795651000	0.133138000	6	2.475062000	-0.020923000	-0.056854000
6	-8.775987000	-0.619312000	0.012103000	1	2.395964000	-1.094813000	0.136737000
8	-8.796034000	-1.833053000	-0.041171000	1	6.282780000	1.486609000	-0.410696000
8	-9.899291000	0.130765000	0.079240000	6	3.792289000	0.523671000	-0.183511000
1	-10.640760000	-0.501049000	0.073302000	6	4.953615000	-0.195601000	-0.078168000
6	-2.568471000	0.016047000	-0.148279000	1	3.867363000	1.600674000	-0.379805000
1	-2.488729000	1.106274000	-0.101585000	1	4.905743000	-1.271603000	0.117193000
1	-6.382797000	-1.522057000	-0.101883000	6	1.350396000	0.742156000	-0.166434000
6	-3.887713000	-0.541228000	-0.133541000	1	1.493712000	1.812493000	-0.359893000
6	-5.044982000	0.187153000	-0.065225000	1	-3.790387000	-0.640239000	0.256278000
1	-3.965490000	-1.634613000	-0.180980000	1	0.354736000	-1.797222000	0.232322000
1	-4.993068000	1.279516000	-0.017293000				
6	-1.446050000	-0.753397000	-0.216188000				
1	-1.587947000	-1.840098000	-0.258168000				
1	-0.449924000	1.819631000	-0.160528000				
D15- π -A E(RB3LYP) = -972.769311022 a. u.				D16- π -A E(RB3LYP) = -1200.18219790 a. u.			
6	2.731609000	-2.124559000	-0.042692000	6	2.221202000	-1.220532000	-0.078703000
6	1.817388000	-1.053125000	-0.066562000	6	1.130035000	-0.313362000	-0.119306000
6	2.321270000	0.281487000	-0.113451000	6	1.453915000	1.091250000	-0.143995000
6	3.686520000	0.480143000	-0.154658000	6	2.758641000	1.519968000	-0.129437000
6	4.591690000	-0.616393000	-0.124145000	6	3.842331000	0.596728000	-0.050957000
6	4.119314000	-1.924133000	-0.061530000	6	3.564970000	-0.753420000	-0.024536000
7	4.438813000	1.656036000	-0.245840000	7	3.302486000	2.807541000	-0.236002000
6	5.815183000	1.317104000	0.101589000	6	4.739603000	2.727711000	0.017525000
7	5.883073000	-0.114862000	-0.180563000	7	5.039511000	1.293567000	0.027235000
1	6.539846000	1.883007000	-0.510054000	7	4.482021000	-1.846871000	0.122105000
1	6.036796000	1.529112000	1.181620000	6	3.677638000	-2.990029000	-0.299714000
1	4.802222000	-2.773533000	-0.019903000	7	2.275623000	-2.619736000	-0.017333000
1	2.344912000	-3.144967000	0.004973000	1	5.320862000	3.242675000	-0.774052000
1	1.637950000	1.130362000	-0.109730000	1	5.008851000	3.200422000	0.990021000
6	7.036871000	-0.861170000	0.268168000	1	3.963158000	-3.903759000	0.242380000
1	7.068180000	-0.980833000	1.371078000	1	3.813158000	-3.164445000	-1.389256000
1	7.038073000	-1.859875000	-0.191619000	6	6.261935000	0.824782000	-0.603108000
1	7.954856000	-0.345640000	-0.052367000	1	7.142449000	1.232824000	-0.081597000
6	3.918491000	2.928455000	0.204722000	1	6.293378000	-0.271622000	-0.552283000
1	2.957717000	3.135273000	-0.288565000	1	6.318445000	1.124798000	-1.669151000
1	3.765592000	2.968551000	1.303812000	6	2.588921000	3.979167000	0.220257000
1	4.615338000	3.731246000	-0.080263000	1	1.585320000	4.005779000	-0.228756000
6	-4.432069000	-0.536350000	0.021986000	1	2.479073000	4.018421000	1.324948000
6	-5.576804000	0.223600000	0.011136000	1	3.118655000	4.885909000	-0.109777000
6	-5.530580000	1.650566000	-0.051697000	6	1.265962000	-3.521587000	-0.538784000

7	-5.451906000	2.812777000	-0.103178000	1	0.913415000	-3.236890000	-1.549663000
6	-6.885670000	-0.470746000	0.067195000	1	1.701130000	-4.530116000	-0.599881000
8	-7.029767000	-1.676315000	0.122960000	1	0.395758000	-3.590247000	0.131117000
8	-7.928154000	0.391523000	0.049675000	6	4.990165000	-1.967186000	1.501890000
1	-8.729095000	-0.161493000	0.089410000	1	4.185683000	-2.135147000	2.244428000
6	-0.646746000	-0.476211000	-0.052245000	1	5.709283000	-2.799033000	1.553744000
1	-0.463279000	0.601244000	-0.107810000	1	5.518898000	-1.041269000	1.770248000
1	-4.595587000	-1.617547000	0.072787000	1	0.644517000	1.816183000	-0.207180000
6	-2.011406000	-0.897294000	-0.007670000	6	-5.130039000	-0.386935000	0.003228000
6	-3.093371000	-0.055286000	-0.025412000	6	-6.350600000	0.249701000	0.041804000
1	-2.197334000	-1.977361000	0.045062000	6	-7.577047000	-0.577755000	0.047510000
1	-2.932793000	1.026373000	-0.077258000	8	-7.598002000	-1.793898000	0.020302000
6	0.400848000	-1.353217000	-0.029282000	8	-8.706511000	0.169037000	0.087019000
1	0.154895000	-2.420480000	0.022101000	1	-9.441926000	-0.469506000	0.087188000
				6	-1.372136000	0.043366000	-0.061809000
				1	-1.292574000	1.133506000	-0.033000000
				1	-5.183075000	-1.480208000	-0.020333000
				6	-2.686180000	-0.504480000	-0.048456000
				6	-3.850037000	0.226404000	-0.008453000
				1	-2.770200000	-1.598727000	-0.071807000
				1	-3.796994000	1.319616000	0.014963000
				6	-0.245952000	-0.741540000	-0.102833000
				1	-0.427786000	-1.815684000	-0.113106000
				6	-6.452091000	1.674083000	0.075976000
				7	-6.492611000	2.839414000	0.103088000
D17-π-A E(RB3LYP) = -1200.21148450 a. u.				D18-π-A E(RB3LYP) = -1278.80566731 a. u.			
6	2.795798000	-1.290474000	0.052876000	6	1.170186000	1.103066000	0.026255000
6	1.452202000	-0.897505000	0.022316000	6	2.487962000	1.560977000	-0.032673000
6	3.795735000	-0.274109000	0.039220000	6	0.833577000	-0.258611000	0.051393000
6	1.070024000	0.461177000	0.007023000	6	3.536367000	0.604363000	-0.159608000
6	3.425459000	1.086320000	0.112097000	6	1.892154000	-1.218384000	0.109229000
6	2.067445000	1.464980000	0.084025000	6	3.221165000	-0.784504000	-0.079075000
7	5.186459000	-0.584073000	0.026793000	7	2.725006000	2.959453000	-0.098792000
6	5.461077000	-1.944090000	0.489694000	6	4.063859000	3.327079000	-0.546627000
1	5.293718000	-1.989708000	1.578518000	1	4.246755000	4.381868000	-0.294980000
1	6.518369000	-2.177532000	0.297502000	1	4.121774000	3.237434000	-1.646613000
7	1.700771000	2.835611000	0.129559000	7	4.253766000	-1.754864000	-0.234425000
1	1.116223000	3.046468000	0.935658000	6	3.732736000	-3.019677000	-0.745185000
6	2.788132000	3.797218000	-0.028824000	1	4.557455000	-3.743459000	-0.829775000
1	2.443206000	4.780409000	0.322197000	1	3.333220000	-2.845963000	-1.758662000
1	3.029891000	3.891397000	-1.101530000	7	4.881001000	1.020810000	-0.294939000
7	3.169622000	-2.638468000	0.110706000	6	5.111541000	2.411332000	0.092572000
6	4.551769000	-2.966349000	-0.192537000	1	5.052370000	2.495690000	1.192081000
1	4.765751000	-3.976706000	0.191675000	1	6.131390000	2.692278000	-0.208378000
1	4.752934000	-2.984176000	-1.286408000	7	1.574988000	-2.583210000	0.333527000

7	4.437831000	2.055339000	0.202901000	6	2.641288000	-3.569257000	0.158100000
1	5.273092000	1.658557000	0.632544000	1	3.085606000	-3.832583000	1.141542000
6	4.047348000	3.359472000	0.721244000	1	2.211046000	-4.502292000	-0.250260000
1	3.833990000	3.341982000	1.811018000	1	0.373511000	1.843008000	-0.054442000
1	4.870630000	4.071654000	0.550756000	6	5.575560000	0.632919000	-1.527755000
1	0.673016000	-1.651650000	-0.052496000	1	5.250098000	1.230359000	-2.403685000
6	5.877323000	-0.246746000	-1.227493000	1	6.659161000	0.777931000	-1.391853000
1	6.964718000	-0.341147000	-1.076224000	1	5.386055000	-0.427224000	-1.730329000
1	5.581453000	-0.898982000	-2.073582000	6	5.207847000	-1.873771000	0.868464000
1	5.653936000	0.793201000	-1.500217000	1	6.055923000	-2.501053000	0.549179000
6	2.180223000	-3.664382000	-0.147721000	1	5.590653000	-0.874904000	1.116382000
1	2.646276000	-4.649026000	-0.000721000	1	4.770846000	-2.319715000	1.785962000
1	1.338574000	-3.588076000	0.558820000	6	0.790693000	-2.905363000	1.528946000
1	1.766181000	-3.627172000	-1.176702000	1	-0.016392000	-2.184081000	1.692788000
6	-5.197061000	0.415581000	-0.153389000	1	0.338545000	-3.903279000	1.408155000
6	-6.400791000	-0.226597000	0.009181000	1	1.428036000	-2.927794000	2.438480000
6	-6.474588000	-1.588371000	0.436431000	6	2.237051000	3.753687000	1.027080000
7	-6.494649000	-2.700402000	0.786442000	1	2.869253000	3.660736000	1.936740000
6	-7.646530000	0.527490000	-0.270094000	1	2.201140000	4.816015000	0.738341000
8	-7.689443000	1.685885000	-0.635630000	1	1.218998000	3.445185000	1.297447000
8	-8.757076000	-0.219661000	-0.072490000	6	-5.429083000	-0.343500000	-0.253543000
1	-9.508601000	0.363808000	-0.281474000	6	-6.650658000	0.261883000	-0.085004000
6	-1.430329000	0.095512000	0.077108000	6	-6.766637000	1.592274000	0.424040000
1	-1.332421000	-0.939741000	0.419270000	7	-6.821290000	2.679156000	0.842551000
1	-5.269667000	1.456295000	-0.484999000	6	-7.871311000	-0.499398000	-0.445069000
6	-2.756216000	0.589253000	-0.127862000	8	-7.877858000	-1.633182000	-0.882896000
6	-3.903223000	-0.136514000	0.064807000	8	-9.003149000	0.210411000	-0.232372000
1	-2.851911000	1.629549000	-0.463332000	1	-9.735739000	-0.374124000	-0.498000000
1	-3.832484000	-1.177262000	0.396899000	6	-1.677866000	0.039575000	0.102559000
6	-0.318083000	0.863954000	-0.119712000	1	-1.611506000	1.053619000	0.509811000
1	-0.469238000	1.907095000	-0.417370000	1	-5.469389000	-1.362892000	-0.650452000
				6	-2.986656000	-0.467540000	-0.170292000
				6	-4.154064000	0.221208000	0.033769000
				1	-3.050420000	-1.487099000	-0.570738000
				1	-4.115699000	1.241027000	0.429901000
				6	-0.543160000	-0.691467000	-0.108925000
				1	-0.664240000	-1.717283000	-0.473858000

Table 3 Cartesian coordinates (in Angstrom unit) of D1- π -A / TiO₂ – D18- π -A / TiO₂ systems, optimized at B3LYP level DFT with LANL2DZ basis set for Ti atom and cc-pVDZ for non-metal atoms.

D1- π -A / TiO ₂ E(RB3LYP) = -3146.44469513 a. u.				D2- π -A / TiO ₂ E(RB3LYP) = -3162.47794169 a. u.			
22	-7.995403000	-0.216806000	-1.070796000	22	-8.006982000	-0.250072000	0.982554000
22	-7.377797000	2.579932000	-0.693857000	22	-7.357426000	-2.639153000	-0.506184000

22	-4.756751000	1.065211000	-0.789460000	22	-4.752073000	-1.294768000	0.254810000
22	-8.306471000	1.038585000	1.506275000	22	-8.266468000	-0.328141000	-1.888046000
22	-1.564093000	0.151344000	-0.404360000	22	-1.561939000	-0.295402000	0.341099000
22	-5.948251000	-1.854853000	-1.398429000	22	-5.980094000	1.108417000	1.995726000
22	-3.238802000	-2.414775000	-0.766242000	22	-3.267298000	1.886791000	1.701827000
22	-5.761925000	-0.613689000	1.569851000	22	-5.737110000	1.207667000	-1.216516000
22	-2.766773000	-1.823957000	2.189792000	22	-2.744153000	2.572929000	-1.224574000
8	-8.284941000	1.535982000	-1.801550000	8	-8.291337000	-2.149011000	0.917705000
8	-7.786274000	-1.676309000	-2.034385000	8	-7.826517000	0.679596000	2.467551000
8	-5.620243000	2.693079000	-1.097443000	8	-5.605564000	-2.906030000	-0.154482000
8	-7.175753000	0.117814000	2.563351000	8	-7.128010000	0.949741000	-2.449355000
8	-8.318791000	2.791925000	0.891567000	8	-8.272044000	-2.178474000	-2.054229000
8	-9.213028000	-0.002994000	0.392269000	8	-9.200032000	0.157505000	-0.459579000
8	-1.897846000	-1.356682000	-1.383803000	8	-1.926942000	0.670871000	1.850966000
8	-5.884102000	-0.057725000	-1.895257000	8	-5.907136000	-0.732835000	1.705762000
8	-4.655058000	-3.066214000	-1.799430000	8	-4.705754000	2.048120000	2.886316000
8	-4.447311000	-1.112400000	-0.208353000	8	-4.454716000	0.929573000	0.633135000
8	-2.795955000	-3.117947000	0.782773000	8	-2.807134000	3.169012000	0.590627000
8	-3.060821000	1.159101000	-1.119955000	8	-3.061368000	-1.512682000	0.548298000
8	-4.637847000	1.011782000	1.206567000	8	-4.602960000	-0.419227000	-1.537526000
8	-2.069747000	-0.238355000	1.237665000	8	-2.047753000	0.737053000	-1.001815000
8	-6.807415000	-1.573889000	0.252015000	8	-6.812019000	1.533849000	0.361569000
8	-1.891123000	-2.256782000	3.479353000	8	-1.852770000	3.502647000	-2.203673000
8	-4.655837000	-1.469188000	2.578050000	8	-4.623507000	2.406385000	-1.759454000
8	-6.902616000	0.925972000	0.180720000	8	-6.884483000	-0.770953000	-0.609764000
8	-0.448089000	1.868653000	-0.543091000	8	-0.433071000	-1.914662000	-0.216062000
8	0.446795000	-0.109147000	-0.421683000	8	0.443610000	-0.059183000	0.501818000
6	0.630382000	1.171301000	-0.478298000	6	0.640354000	-1.251482000	0.035147000
1	-3.704468000	0.915709000	1.500257000	1	-3.665938000	-0.207861000	-1.747644000
6	12.233301000	2.298497000	0.697505000	6	12.134565000	2.614947000	-0.210160000
6	11.391746000	1.089154000	0.306546000	6	11.341981000	1.321571000	-0.042708000
6	13.383518000	2.436105000	-0.303889000	6	13.230404000	2.404548000	-1.257827000
6	12.105899000	-0.078013000	-0.110974000	6	12.062520000	0.099353000	-0.144066000
6	14.256362000	1.192301000	-0.270157000	6	14.156650000	1.285285000	-0.818349000
7	13.473709000	-0.044600000	-0.268985000	7	13.417893000	0.097421000	-0.402062000
6	9.997106000	1.086093000	0.352923000	6	9.962119000	1.309136000	0.183835000
6	11.387073000	-1.280517000	-0.343173000	6	11.378401000	-1.147592000	0.035325000
6	14.195429000	-1.218550000	-0.749506000	6	14.214297000	-1.116837000	-0.348804000
6	9.990610000	-1.270671000	-0.349151000	6	9.997719000	-1.163577000	0.264168000
6	9.252742000	-0.083995000	-0.033349000	6	9.256449000	0.063149000	0.276399000
6	12.101691000	-2.600424000	-0.591401000	7	12.152229000	-2.321861000	-0.045629000
1	14.003367000	3.316671000	-0.070686000	1	13.817582000	3.325877000	-1.398838000
6	13.581608000	-2.500457000	-0.214716000	6	13.507653000	-2.187727000	0.460698000
1	13.681425000	-2.508989000	0.884853000	1	13.534508000	-1.927793000	1.540750000
1	14.909381000	1.207752000	0.624144000	1	14.804933000	1.626978000	0.013528000
1	15.241259000	-1.127857000	-0.415690000	1	15.190124000	-0.877147000	0.112608000
1	12.968452000	2.585207000	-1.315553000	1	12.768405000	2.156098000	-2.228873000
1	14.138910000	-3.369365000	-0.598455000	1	14.037170000	-3.141865000	0.332644000

1	14.926624000	1.174685000	-1.147728000	1	14.831934000	0.995593000	-1.643282000
1	14.212542000	-1.227932000	-1.859422000	1	14.415087000	-1.490773000	-1.371443000
6	9.365864000	-2.575305000	-0.808766000	6	9.333625000	-2.491842000	0.584335000
1	8.271451000	-2.570134000	-0.779532000	1	8.536406000	-2.332981000	1.324577000
6	9.892311000	-3.799474000	-0.032514000	6	10.329653000	-3.529919000	1.099893000
1	9.367082000	-3.869271000	0.933399000	1	10.706796000	-3.239998000	2.095898000
1	9.626431000	-4.707640000	-0.596578000	1	9.839659000	-4.510664000	1.203616000
6	11.415361000	-3.727871000	0.208096000	6	11.488333000	-3.614987000	0.114454000
1	11.615826000	-3.542212000	1.276437000	1	12.241151000	-4.348448000	0.436627000
1	11.896452000	-4.689086000	-0.036509000	1	11.106755000	-3.954902000	-0.867246000
6	9.269952000	2.323620000	0.855931000	6	9.198694000	2.626524000	0.280762000
1	8.417128000	2.015229000	1.478448000	1	8.494911000	2.588619000	1.126726000
6	10.150010000	3.306082000	1.629643000	6	10.079685000	3.867645000	0.442071000
1	10.411981000	2.883544000	2.616220000	1	10.470684000	3.920314000	1.474213000
1	9.585530000	4.232298000	1.820242000	1	9.469019000	4.771345000	0.289354000
6	11.423038000	3.586365000	0.840760000	6	11.248064000	3.817468000	-0.533290000
1	11.158870000	3.974995000	-0.160429000	1	10.867908000	3.732964000	-1.568292000
1	12.040774000	4.357651000	1.329158000	1	11.848589000	4.740798000	-0.486736000
1	12.685232000	2.079516000	1.686672000	1	12.640437000	2.827288000	0.754044000
1	12.033126000	-2.850345000	-1.669077000	1	8.840080000	-2.902512000	-0.315037000
1	9.626127000	-2.701513000	-1.876257000	1	8.573421000	2.745547000	-0.623015000
1	8.834887000	2.858289000	-0.008339000	6	3.077800000	-0.997644000	0.091715000
6	3.068466000	0.943870000	-0.366659000	6	1.967022000	-1.782936000	-0.182703000
6	1.952015000	1.760158000	-0.465591000	6	2.091319000	-3.115355000	-0.685975000
6	2.062384000	3.183471000	-0.546012000	7	2.243645000	-4.196449000	-1.093257000
7	2.202404000	4.338455000	-0.609828000	6	6.844589000	-0.813451000	0.082061000
6	6.834089000	0.819698000	-0.173438000	1	7.091031000	-1.800176000	-0.308236000
1	7.071429000	1.879305000	-0.249802000	1	2.859524000	0.005779000	0.469483000
1	2.860404000	-0.128687000	-0.307001000	6	5.465414000	-0.509779000	0.226146000
6	5.457386000	0.470022000	-0.218618000	6	4.428133000	-1.371084000	-0.071978000
6	4.414908000	1.366727000	-0.331009000	1	5.208599000	0.488311000	0.603335000
1	5.208843000	-0.597118000	-0.156106000	1	4.652564000	-2.373899000	-0.448480000
1	4.629392000	2.438272000	-0.389821000	6	7.818365000	0.119593000	0.369834000
6	7.811407000	-0.147955000	-0.086227000	1	7.413486000	1.087456000	0.672696000
1	7.406646000	-1.162572000	-0.084970000				
D3- π -A / TiO ₂ E(RB3LYP) = -3178.50657262 a. u.				D4- π -A / TiO ₂ E(RB3LYP) = -3194.55062502 a. u.			
22	-7.977524000	-0.273694000	-1.107084000	22	-7.986867000	-0.268834000	-1.072593000
22	-7.365434000	2.539006000	-0.863480000	22	-7.346865000	2.542210000	-0.889015000
22	-4.743070000	1.023331000	-0.839544000	22	-4.738055000	1.003091000	-0.855836000
22	-8.329313000	1.111278000	1.397057000	22	-8.305697000	1.168205000	1.406343000
22	-1.556360000	0.134075000	-0.356205000	22	-1.555295000	0.094977000	-0.378946000
22	-5.925335000	-1.924159000	-1.318141000	22	-5.951135000	-1.941363000	-1.267588000
22	-3.226311000	-2.448392000	-0.614026000	22	-3.251432000	-2.476413000	-0.573922000
22	-5.786011000	-0.533690000	1.585268000	22	-5.776114000	-0.496155000	1.606749000
22	-2.801286000	-1.708310000	2.315258000	22	-2.796542000	-1.683742000	2.337024000

8	-8.255047000	1.439461000	-1.930997000	8	-8.255242000	1.430511000	-1.927882000
8	-7.753469000	-1.780029000	-1.991845000	8	-7.783847000	-1.793961000	-1.929524000
8	-5.602009000	2.633155000	-1.244079000	8	-5.586093000	2.613017000	-1.285051000
8	-7.215852000	0.246618000	2.517705000	8	-7.191363000	0.315528000	2.535208000
8	-8.331940000	2.831165000	0.693938000	8	-8.298247000	2.874127000	0.670068000
8	-9.218573000	0.013648000	0.323457000	8	-9.213925000	0.058128000	0.361695000
8	-1.876788000	-1.423197000	-1.263612000	8	-1.898751000	-1.477203000	-1.254045000
8	-5.853177000	-0.155146000	-1.905155000	8	-5.867898000	-0.185309000	-1.890002000
8	-4.625757000	-3.152907000	-1.636092000	8	-4.665333000	-3.187771000	-1.571637000
8	-4.444822000	-1.120459000	-0.142617000	8	-4.454972000	-1.128393000	-0.119257000
8	-2.808605000	-3.072140000	0.975740000	8	-2.826909000	-3.073117000	1.024653000
8	-3.042815000	1.101643000	-1.147990000	8	-3.040323000	1.059980000	-1.179466000
8	-4.656387000	1.072504000	1.158456000	8	-4.635260000	1.090935000	1.140221000
8	-2.088902000	-0.173502000	1.295256000	8	-2.078999000	-0.176062000	1.282343000
8	-6.811628000	-1.560370000	0.301743000	8	-6.821737000	-1.538185000	0.351802000
8	-1.947202000	-2.075029000	3.639501000	8	-1.935442000	-2.032227000	3.661914000
8	-4.696816000	-1.335665000	2.653914000	8	-4.686093000	-1.287183000	2.682701000
8	-6.904696000	0.932345000	0.101695000	8	-6.893411000	0.950678000	0.103822000
8	-0.443155000	1.844113000	-0.556767000	8	-0.431592000	1.790567000	-0.616355000
8	0.451425000	-0.125201000	-0.337567000	8	0.447311000	-0.182955000	-0.373820000
6	0.636720000	1.152565000	-0.449456000	6	0.644590000	1.092026000	-0.506879000
1	-3.727882000	0.991803000	1.471613000	1	-3.704956000	1.006869000	1.447295000
7	12.174900000	2.264082000	0.524928000	7	12.255000000	-2.393707000	-0.535800000
6	11.390330000	1.117985000	0.249607000	6	11.434573000	-1.268283000	-0.263448000
6	13.409091000	2.347665000	-0.236875000	6	13.539552000	-2.375262000	0.142413000
6	12.088434000	-0.075938000	-0.098604000	6	12.094942000	-0.020068000	0.001434000
6	14.250884000	1.116088000	0.034958000	6	14.294985000	-1.119425000	-0.248405000
7	13.465921000	-0.086796000	-0.175038000	7	13.472173000	0.053956000	-0.014975000
6	9.988825000	1.122061000	0.323679000	6	10.043032000	-1.325327000	-0.291629000
6	11.356135000	-1.272943000	-0.354557000	6	11.334947000	1.133433000	0.298277000
6	14.224329000	-1.305518000	-0.408611000	6	14.173708000	1.308051000	0.200833000
6	9.965976000	-1.299007000	-0.201952000	6	9.930170000	1.064431000	0.334093000
6	9.255754000	-0.080528000	0.069288000	6	9.256727000	-0.153965000	-0.007725000
7	12.104946000	-2.396055000	-0.762221000	7	12.020578000	2.343533000	0.599167000
1	13.960306000	3.244073000	0.084097000	1	14.114382000	-3.259807000	-0.170387000
6	13.386907000	-2.534183000	-0.091629000	6	13.274528000	2.489519000	-0.120672000
1	13.282486000	-2.647758000	1.008547000	1	13.116992000	2.557697000	-1.219259000
1	14.645038000	1.147464000	1.069452000	1	14.601164000	-1.177379000	-1.311114000
1	15.124045000	-1.289480000	0.232846000	1	15.062695000	1.332500000	-0.453075000
1	13.218617000	2.445579000	-1.327890000	1	13.429358000	-2.421150000	1.248448000
1	13.901806000	-3.426859000	-0.473452000	1	13.763965000	3.420156000	0.204371000
1	15.117128000	1.097279000	-0.649632000	1	15.212045000	-1.033754000	0.359140000
1	14.566409000	-1.346824000	-1.460570000	1	14.528187000	1.378577000	1.247253000
6	9.236529000	-2.628708000	-0.339657000	7	9.210977000	2.192289000	0.725263000
1	8.463445000	-2.713259000	0.438916000	1	8.310426000	1.976573000	1.141255000
6	10.173539000	-3.832493000	-0.224475000	6	9.927265000	3.273801000	1.384291000
1	10.515395000	-3.952486000	0.818376000	1	9.286313000	4.168065000	1.393038000
1	9.642850000	-4.756075000	-0.504826000	1	10.191629000	3.028161000	2.431596000

6	11.377756000	-3.606597000	-1.131121000	6	11.199458000	3.546372000	0.600870000
1	12.079202000	-4.452390000	-1.095030000	1	10.934777000	3.872028000	-0.427699000
1	11.032621000	-3.516612000	-2.178798000	1	11.772766000	4.358708000	1.075040000
6	9.289334000	2.392417000	0.774674000	6	9.353626000	-2.622990000	-0.687450000
1	8.445882000	2.135381000	1.431750000	1	8.544690000	-2.415040000	-1.403940000
6	10.230073000	3.353585000	1.500102000	6	10.313227000	-3.637420000	-1.311736000
1	10.504417000	2.948820000	2.488722000	1	10.557246000	-3.342033000	-2.345892000
1	9.735006000	4.322900000	1.663559000	1	9.844450000	-4.632449000	-1.353623000
6	11.489798000	3.541492000	0.674626000	6	11.600523000	-3.695626000	-0.507953000
1	11.228904000	3.979286000	-0.314987000	1	11.381347000	-4.014522000	0.536259000
1	12.187657000	4.241056000	1.162991000	1	12.300025000	-4.432730000	-0.933510000
1	8.702556000	-2.675869000	-1.306403000	1	8.867106000	-3.073051000	0.198229000
1	8.852430000	2.915611000	-0.095527000	6	3.080615000	0.847659000	-0.382256000
6	3.073766000	0.929872000	-0.309040000	6	1.967479000	1.667835000	-0.526170000
6	1.956192000	1.741410000	-0.450074000	6	2.091668000	3.083153000	-0.683617000
6	2.067483000	3.159926000	-0.589215000	7	2.245938000	4.231583000	-0.808081000
7	2.209198000	4.311257000	-0.699925000	6	6.841251000	0.705202000	-0.182895000
6	6.836523000	0.814211000	-0.090607000	1	7.094397000	1.757448000	-0.325638000
1	7.073275000	1.870244000	-0.207466000	1	2.863150000	-0.218045000	-0.262871000
1	2.865224000	-0.139350000	-0.206633000	6	5.467211000	0.362557000	-0.209969000
6	5.462174000	0.462245000	-0.128986000	6	4.426856000	1.259819000	-0.371301000
6	4.418254000	1.353748000	-0.282462000	1	5.211508000	-0.697852000	-0.087737000
1	5.213526000	-0.601756000	-0.026184000	1	4.650399000	2.324560000	-0.490841000
1	4.633346000	2.422056000	-0.383449000	6	7.827882000	-0.260028000	-0.063666000
6	7.815820000	-0.149729000	0.037537000	1	7.441459000	-1.282229000	-0.041820000
1	7.411655000	-1.163863000	0.065130000				
D5- π -A / TiO ₂ E(RB3LYP) = -3210.58509080 a. u.				D6- π -A / TiO ₂ E(RB3LYP) = -2989.10636372 a. u.			
22	-8.005442000	0.032298000	-0.961188000	22	-7.274145000	-0.086826000	-0.911025000
22	-7.372665000	2.647055000	0.089327000	22	-6.600819000	2.652957000	-0.287862000
22	-4.755614000	1.223916000	-0.466525000	22	-4.008616000	1.132948000	-0.663528000
22	-8.232029000	0.595283000	1.857406000	22	-7.443969000	0.906293000	1.790541000
22	-1.548091000	0.269207000	-0.421132000	22	-0.815568000	0.155825000	-0.530361000
22	-5.971413000	-1.455461000	-1.752736000	22	-5.267021000	-1.700537000	-1.503058000
22	-3.242022000	-2.132148000	-1.364869000	22	-2.538908000	-2.347188000	-1.064521000
22	-5.687317000	-0.999622000	1.423757000	22	-4.922170000	-0.766474000	1.562824000
22	-2.673190000	-2.301116000	1.627904000	22	-1.917968000	-2.060523000	1.909009000
8	-8.317006000	1.910110000	-1.217484000	8	-7.573844000	1.733368000	-1.447971000
8	-7.830456000	-1.137956000	-2.265898000	8	-7.130425000	-1.442623000	-2.026239000
8	-5.631004000	2.872351000	-0.326699000	8	-4.862530000	2.790341000	-0.763995000
8	-7.069184000	-0.553105000	2.613872000	8	-6.276001000	-0.126184000	2.692844000
8	-8.262478000	2.446874000	1.706849000	8	-7.461617000	2.712296000	1.354996000
8	-9.176025000	-0.138540000	0.546145000	8	-8.416797000	-0.010130000	0.623719000
8	-1.922185000	-0.946103000	-1.740507000	8	-1.214138000	-1.242953000	-1.637203000
8	-5.924310000	0.408082000	-1.784412000	8	-5.201156000	0.137055000	-1.819231000
8	-4.690523000	-2.515315000	-2.485576000	8	-4.012064000	-2.877440000	-2.086702000

8	-4.433983000	-1.021348000	-0.460708000	8	-3.700001000	-1.096942000	-0.319535000
8	-2.750016000	-3.200193000	-0.057555000	8	-2.032127000	-3.206279000	0.382893000
8	-3.075115000	1.412642000	-0.817624000	8	-2.328111000	1.244153000	-1.065160000
8	-4.574390000	0.673548000	1.448191000	8	-3.794484000	0.876873000	1.308630000
8	-2.010031000	-0.523037000	1.086376000	8	-1.244248000	-0.393343000	1.087035000
8	-6.776298000	-1.607507000	-0.058910000	8	-6.042354000	-1.578781000	0.207714000
8	-1.757689000	-3.039755000	2.739331000	8	-0.986400000	-2.627780000	3.103694000
8	-4.550388000	-2.072749000	2.149898000	8	-3.780354000	-1.728859000	2.424435000
8	-6.872518000	0.829699000	0.503772000	8	-6.106620000	0.915229000	0.392639000
8	-0.448800000	1.973840000	-0.182684000	8	0.320110000	1.869791000	-0.546795000
8	0.449873000	0.030940000	-0.559493000	8	1.191911000	-0.118295000	-0.673976000
6	0.638116000	1.294007000	-0.322218000	6	1.388445000	1.158605000	-0.607827000
1	-3.631557000	0.510782000	1.676098000	1	-2.849736000	0.744924000	1.546241000
7	11.974087000	-2.591339000	0.035698000	6	12.652881000	2.140534000	0.799206000
6	11.289357000	-1.341561000	-0.038235000	6	12.025241000	1.296974000	-0.272129000
6	13.011927000	-2.614961000	1.053581000	6	12.799185000	0.173582000	-0.494889000
6	11.999615000	-0.150743000	0.273593000	6	13.740067000	1.134936000	1.369151000
6	14.006256000	-1.498479000	0.782993000	7	13.897512000	0.055548000	0.328027000
7	13.319299000	-0.223228000	0.660134000	6	10.646390000	1.190603000	-0.246217000
6	9.955231000	-1.267816000	-0.451460000	6	12.242797000	-1.024652000	-0.892532000
6	11.372074000	1.119958000	0.122889000	6	13.973057000	-1.406558000	0.692746000
6	14.084705000	0.982632000	0.928178000	6	10.867712000	-1.175856000	-0.868507000
6	10.013511000	1.186062000	-0.205053000	6	10.003807000	-0.041286000	-0.648535000
6	9.245692000	-0.011384000	-0.425590000	6	13.047024000	-2.168522000	-0.347830000
7	12.143289000	2.302546000	0.320844000	1	13.392345000	0.668343000	2.311739000
1	13.530050000	-3.585068000	1.007915000	1	13.595577000	-1.531944000	1.726603000
6	13.565438000	2.132299000	0.081278000	1	14.703155000	1.625754000	1.566023000
1	13.789336000	1.933961000	-0.990709000	1	15.013405000	-1.758626000	0.663857000
1	14.581965000	-1.721655000	-0.136080000	6	10.615184000	-2.665593000	-0.646556000
1	15.140987000	0.789965000	0.680501000	1	9.697971000	-2.880021000	-0.078684000
1	12.592952000	-2.503891000	2.077991000	6	11.904003000	-3.116020000	0.137656000
1	14.082641000	3.062333000	0.363393000	1	11.731587000	-2.963739000	1.216603000
1	14.722752000	-1.433604000	1.618872000	1	12.125834000	-4.183039000	-0.014435000
1	14.032647000	1.251612000	2.000654000	6	10.159937000	2.292380000	0.695179000
7	9.375120000	2.429459000	-0.275414000	1	9.259542000	2.010548000	1.259028000
1	8.791751000	2.540367000	-1.099023000	1	9.921766000	3.219300000	0.143454000
6	10.124684000	3.617459000	0.105333000	6	11.395861000	2.518824000	1.642311000
1	9.659285000	4.495781000	-0.363091000	1	11.428145000	3.544817000	2.038311000
1	10.066646000	3.751082000	1.199001000	1	11.309274000	1.834889000	2.503536000
6	11.589459000	3.497149000	-0.299536000	1	13.160085000	3.041461000	0.414518000
1	11.668509000	3.463650000	-1.408920000	1	13.681958000	-2.666753000	-1.099847000
1	12.163050000	4.370201000	0.051344000	1	10.540149000	-3.207166000	-1.606024000
7	9.285031000	-2.437583000	-0.825810000	6	3.826131000	0.900508000	-0.641792000
1	8.583531000	-2.289758000	-1.543222000	6	2.719271000	1.732026000	-0.599928000
6	10.072355000	-3.643867000	-1.038206000	6	2.845069000	3.154986000	-0.536302000
1	10.600030000	-3.636505000	-2.012194000	7	2.997436000	4.308923000	-0.484375000
1	9.398368000	-4.514227000	-1.021046000	6	7.594821000	0.726980000	-0.639114000
6	11.098075000	-3.755148000	0.076772000	1	7.858681000	1.787588000	-0.628472000

1	10.574465000	-3.846194000	1.052637000	1	3.606669000	-0.170636000	-0.682696000
1	11.711572000	-4.658871000	-0.063383000	6	6.213707000	0.395348000	-0.656753000
6	3.077496000	1.061024000	-0.363867000	6	5.179683000	1.306741000	-0.630468000
6	1.952885000	1.871632000	-0.226083000	1	5.956647000	-0.670899000	-0.690025000
6	2.065257000	3.275737000	0.015593000	1	5.405047000	2.377012000	-0.593063000
7	2.211362000	4.415886000	0.208563000	6	8.580645000	-0.231328000	-0.662782000
6	6.839163000	0.918900000	-0.383988000	1	8.243830000	-1.270836000	-0.745563000
1	7.091525000	1.961765000	-0.199527000				
1	2.868484000	0.001875000	-0.542507000				
6	5.469455000	0.579459000	-0.436094000				
6	4.418612000	1.472583000	-0.293069000				
1	5.217394000	-0.475082000	-0.608771000				
1	4.635798000	2.530539000	-0.116091000				
6	7.822232000	-0.053727000	-0.504350000				
1	7.412354000	-1.063382000	-0.604570000				
D7- π -A / TiO ₂ E(RB3LYP) = -3005.12792810 a. u.				D8- π -A / TiO ₂ E(RB3LYP) = -3021.14996993 a. u.			
22	-7.274689000	-0.092244000	-0.905478000	22	-7.276102000	-0.082785000	-0.899961000
22	-6.604365000	2.649062000	-0.287856000	22	-6.595235000	2.658337000	-0.291058000
22	-4.011563000	1.130865000	-0.666276000	22	-4.008489000	1.130598000	-0.669300000
22	-7.440643000	0.904734000	1.795346000	22	-7.434532000	0.922372000	1.798149000
22	-0.817732000	0.158025000	-0.539730000	22	-0.818951000	0.145171000	-0.545013000
22	-5.268029000	-1.707540000	-1.495258000	22	-5.275211000	-1.705192000	-1.490777000
22	-2.537786000	-2.348954000	-1.063298000	22	-2.547486000	-2.357437000	-1.060907000
22	-4.916822000	-0.765236000	1.566767000	22	-4.917358000	-0.757667000	1.569492000
22	-1.909787000	-2.054218000	1.907969000	22	-1.915216000	-2.058370000	1.908960000
8	-7.578383000	1.726114000	-1.444616000	8	-7.573823000	1.735464000	-1.443656000
8	-7.131860000	-1.452235000	-2.015906000	8	-7.138789000	-1.444570000	-2.008846000
8	-4.867080000	2.786865000	-0.768272000	8	-4.857622000	2.788870000	-0.774147000
8	-6.269079000	-0.123823000	2.697575000	8	-6.265265000	-0.108514000	2.700743000
8	-7.461608000	2.709970000	1.356432000	8	-7.449786000	2.726383000	1.354171000
8	-8.413929000	-0.015238000	0.631795000	8	-8.412674000	0.002650000	0.638536000
8	-1.215580000	-1.243870000	-1.641829000	8	-1.221793000	-1.257653000	-1.643053000
8	-5.205823000	0.130412000	-1.815810000	8	-5.205864000	0.131696000	-1.815254000
8	-4.012996000	-2.884203000	-2.079337000	8	-4.026021000	-2.888391000	-2.074085000
8	-3.697808000	-1.097866000	-0.318540000	8	-3.701448000	-1.100646000	-0.316951000
8	-2.025882000	-3.203580000	0.384873000	8	-2.036871000	-3.210645000	0.388488000
8	-2.331635000	1.243318000	-1.072334000	8	-2.327792000	1.235249000	-1.077037000
8	-3.792678000	0.879770000	1.305803000	8	-3.787330000	0.882027000	1.302893000
8	-1.239729000	-0.387961000	1.079938000	8	-1.239498000	-0.396157000	1.076121000
8	-6.037920000	-1.583472000	0.216862000	8	-6.043300000	-1.573658000	0.222221000
8	-0.974077000	-2.617221000	3.101354000	8	-0.979764000	-2.621705000	3.102270000
8	-3.770900000	-1.723455000	2.427669000	8	-3.773964000	-1.718637000	2.430762000
8	-6.106377000	0.912903000	0.394653000	8	-6.102036000	0.922339000	0.395198000
8	0.318469000	1.874111000	-0.558564000	8	0.325987000	1.857799000	-0.564834000
8	1.191613000	-0.113271000	-0.689789000	8	1.191416000	-0.133009000	-0.698463000

6	1.385972000	1.163150000	-0.622267000	6	1.389410000	1.142066000	-0.630256000
1	-2.847334000	0.751304000	1.542487000	1	-2.842182000	0.750829000	1.538719000
6	12.644524000	2.094147000	0.861174000	7	12.577598000	2.043566000	0.818196000
6	12.023521000	1.294052000	-0.247545000	6	11.997435000	1.274873000	-0.203593000
6	12.808811000	0.193472000	-0.506818000	6	12.821276000	0.225495000	-0.532211000
6	13.701800000	1.049265000	1.423294000	6	13.674655000	1.166429000	1.366655000
7	13.910962000	0.037880000	0.318217000	7	13.915813000	0.103506000	0.322204000
6	10.639349000	1.202208000	-0.245785000	6	10.614652000	1.197845000	-0.246228000
6	12.233267000	-1.006907000	-0.850170000	6	12.249805000	-0.981033000	-0.842902000
6	13.976114000	-1.444728000	0.580240000	6	13.953932000	-1.371325000	0.648338000
6	10.862106000	-1.166658000	-0.878359000	6	10.877712000	-1.166897000	-0.902964000
6	10.004341000	-0.027146000	-0.660335000	6	10.009427000	-0.040868000	-0.673712000
7	13.006414000	-2.084223000	-0.382551000	7	13.026381000	-2.037867000	-0.338549000
1	13.301714000	0.525269000	2.313817000	1	13.365976000	0.698980000	2.329934000
1	13.689155000	-1.659351000	1.634218000	1	13.613539000	-1.544801000	1.695111000
1	14.654921000	1.520775000	1.699024000	1	14.589699000	1.750836000	1.532939000
1	14.993759000	-1.821105000	0.407395000	1	14.975948000	-1.758025000	0.538146000
6	10.660188000	-2.661724000	-0.651072000	6	10.700207000	-2.664937000	-0.674764000
1	9.769824000	-2.915638000	-0.057779000	1	9.799131000	-2.936142000	-0.105737000
6	11.985443000	-3.054837000	0.101065000	6	12.008765000	-3.023401000	0.122879000
1	11.847798000	-2.940944000	1.195472000	1	11.835240000	-2.900326000	1.211105000
1	12.283606000	-4.093155000	-0.103046000	1	12.335170000	-4.057092000	-0.060381000
6	10.153807000	2.289988000	0.713076000	6	10.158387000	2.272443000	0.739304000
1	9.240052000	2.010402000	1.256330000	1	9.265373000	1.995617000	1.317075000
1	9.941719000	3.237353000	0.185781000	1	9.947429000	3.233196000	0.238170000
6	11.375973000	2.468369000	1.689478000	6	11.417747000	2.426746000	1.668846000
1	11.418033000	3.482175000	2.114944000	1	11.522723000	3.449389000	2.058355000
1	11.261734000	1.762066000	2.529118000	1	11.341688000	1.733059000	2.530530000
1	13.178595000	2.995922000	0.516612000	1	10.679657000	-3.227862000	-1.623872000
1	10.597121000	-3.213309000	-1.604855000	6	3.826893000	0.879165000	-0.671369000
6	3.823873000	0.907582000	-0.659877000	6	2.724561000	1.712762000	-0.624036000
6	2.717764000	1.738084000	-0.615198000	6	2.853300000	3.135411000	-0.555130000
6	2.842139000	3.161120000	-0.548639000	7	3.006366000	4.288925000	-0.498726000
7	2.992108000	4.315206000	-0.494443000	6	7.598040000	0.703891000	-0.671067000
6	7.593930000	0.736332000	-0.656591000	1	7.862881000	1.764505000	-0.653979000
1	7.858159000	1.796829000	-0.642769000	1	3.605206000	-0.191320000	-0.716073000
1	3.605061000	-0.163573000	-0.703190000	6	6.214244000	0.371363000	-0.690727000
6	6.211533000	0.403831000	-0.676133000	6	5.183733000	1.283323000	-0.660450000
6	5.178529000	1.314650000	-0.647952000	1	5.957363000	-0.694616000	-0.728749000
1	5.955141000	-0.662406000	-0.712628000	1	5.410455000	2.353185000	-0.619544000
1	5.403374000	2.384924000	-0.607842000	6	8.584430000	-0.249342000	-0.701208000
6	8.579231000	-0.220248000	-0.682618000	1	8.258612000	-1.292078000	-0.787535000
1	8.245155000	-1.260664000	-0.769181000				
D9- π -A / TiO ₂ E(RB3LYP) = -3037.17503132 a. u.				D10- π -A / TiO ₂ E(RB3LYP) = -3053.20335896 a. u.			
22	-7.275661000	-0.074274000	-0.882701000	22	-7.262293000	-0.051628000	-0.860726000

22	-6.600393000	2.654230000	-0.214635000	22	-6.582085000	2.658602000	-0.128354000
22	-4.009855000	1.145299000	-0.644028000	22	-3.994870000	1.160876000	-0.615393000
22	-7.420526000	0.867570000	1.838723000	22	-7.386278000	0.820255000	1.884990000
22	-0.814275000	0.171311000	-0.560523000	22	-0.798023000	0.187896000	-0.579744000
22	-5.272614000	-1.674526000	-1.522916000	22	-5.264922000	-1.636381000	-1.554073000
22	-2.539170000	-2.324180000	-1.123820000	22	-2.527625000	-2.293043000	-1.192373000
22	-4.898524000	-0.796499000	1.555702000	22	-4.866081000	-0.835348000	1.541480000
22	-1.889012000	-2.091456000	1.848040000	22	-1.853798000	-2.135369000	1.779195000
8	-7.583364000	1.754930000	-1.382393000	8	-7.574215000	1.789302000	-1.311337000
8	-7.141266000	-1.409840000	-2.023217000	8	-7.137509000	-1.359565000	-2.033836000
8	-4.867197000	2.803070000	-0.705037000	8	-4.853205000	2.820067000	-0.628074000
8	-6.242126000	-0.179383000	2.710456000	8	-6.201290000	-0.247669000	2.721546000
8	-7.445213000	2.681368000	1.437378000	8	-7.414263000	2.643820000	1.530361000
8	-8.403276000	-0.028541000	0.664490000	8	-8.378136000	-0.045884000	0.695983000
8	-1.222059000	-1.207750000	-1.689268000	8	-1.216207000	-1.163307000	-1.740435000
8	-5.212919000	0.168866000	-1.805824000	8	-5.208589000	0.213661000	-1.791716000
8	-4.021726000	-2.838291000	-2.140604000	8	-4.018061000	-2.783109000	-2.210093000
8	-3.694638000	-1.089618000	-0.344439000	8	-3.678069000	-1.078410000	-0.373768000
8	-2.016481000	-3.209066000	0.302556000	8	-1.993611000	-3.213566000	0.207409000
8	-2.333856000	1.266904000	-1.060536000	8	-2.323033000	1.294404000	-1.042490000
8	-3.775966000	0.853305000	1.320898000	8	-3.746088000	0.821020000	1.340110000
8	-1.226580000	-0.408477000	1.050820000	8	-1.198414000	-0.433484000	1.019682000
8	-6.030652000	-1.586051000	0.197375000	8	-6.008877000	-1.592055000	0.173538000
8	-0.943923000	-2.678907000	3.022524000	8	-0.899394000	-2.751803000	2.931481000
8	-3.746545000	-1.772601000	2.388138000	8	-3.707563000	-1.831159000	2.340882000
8	-6.097136000	0.904775000	0.428389000	8	-6.074101000	0.893433000	0.466286000
8	0.318718000	1.886007000	-0.552434000	8	0.331363000	1.901035000	-0.526859000
8	1.190659000	-0.098235000	-0.728177000	8	1.201690000	-0.075819000	-0.776087000
6	1.387721000	1.177396000	-0.635004000	6	1.401504000	1.196867000	-0.640799000
1	-2.828663000	0.718227000	1.546381000	1	-2.797043000	0.680198000	1.554563000
7	12.624428000	2.029379000	0.769363000	7	12.542675000	2.089699000	0.706870000
6	12.021662000	1.254660000	-0.244683000	6	12.035528000	1.280689000	-0.355733000
6	12.812303000	0.156285000	-0.525745000	6	12.782207000	0.126819000	-0.451219000
6	13.658637000	1.113549000	1.367675000	6	13.385741000	1.137950000	1.511714000
7	13.870755000	0.007913000	0.362993000	7	13.709558000	0.005932000	0.571954000
6	10.644936000	1.202632000	-0.279550000	6	10.654285000	1.166010000	-0.346535000
6	12.237117000	-1.032724000	-0.866350000	6	12.253078000	-1.086450000	-0.832334000
6	13.832489000	-1.455573000	0.736758000	6	13.618057000	-1.436913000	0.996620000
6	10.857962000	-1.184495000	-0.824712000	6	10.873486000	-1.219313000	-0.815609000
6	9.994763000	-0.037344000	-0.667441000	6	9.994369000	-0.066849000	-0.742084000
7	12.958977000	-2.112000000	-0.307989000	7	12.930549000	-2.139307000	-0.143745000
1	13.302981000	0.685944000	2.332913000	1	12.841236000	0.745426000	2.403117000
1	13.410575000	-1.585691000	1.761434000	1	13.041671000	-1.514126000	1.948936000
1	14.599856000	1.651840000	1.543661000	1	14.306262000	1.633413000	1.848447000
1	14.843156000	-1.883483000	0.709969000	1	14.620927000	-1.856026000	1.153993000
7	10.632434000	-2.546637000	-0.547104000	7	10.589145000	-2.541982000	-0.456828000
1	9.802982000	-2.740179000	0.009468000	1	9.774208000	-2.650538000	0.142964000
6	11.900357000	-3.080679000	0.068637000	6	11.860277000	-3.136400000	0.098223000

1	11.813553000	-3.161695000	1.174817000	1	11.755218000	-3.372516000	1.175322000
1	12.116757000	-4.079111000	-0.338719000	1	12.089388000	-4.067746000	-0.440727000
6	10.205206000	2.313482000	0.670761000	7	10.163068000	2.181093000	0.481511000
1	9.309841000	2.064985000	1.257755000	1	9.342114000	1.923635000	1.026087000
1	10.003711000	3.259781000	0.139673000	6	11.325777000	2.709736000	1.283000000
6	11.468895000	2.478918000	1.594111000	1	11.372760000	3.803447000	1.174635000
1	11.596935000	3.516026000	1.935334000	1	11.213431000	2.469370000	2.358947000
1	11.373353000	1.830560000	2.488427000	6	3.837264000	0.936684000	-0.714534000
6	3.824732000	0.918367000	-0.683035000	6	2.730047000	1.767134000	-0.613659000
6	2.717877000	1.750067000	-0.619789000	6	2.860552000	3.182617000	-0.462296000
6	2.845203000	3.170781000	-0.522557000	7	3.018761000	4.330324000	-0.337401000
7	2.999038000	4.322991000	-0.442703000	6	7.600338000	0.735548000	-0.715179000
6	7.591036000	0.734026000	-0.670114000	1	7.878446000	1.791212000	-0.640134000
1	7.861495000	1.792577000	-0.633905000	1	3.613445000	-0.129324000	-0.818683000
1	3.603504000	-0.151210000	-0.748158000	6	6.221305000	0.419747000	-0.763848000
6	6.211154000	0.408037000	-0.704823000	6	5.189344000	1.335426000	-0.684917000
6	5.177901000	1.321645000	-0.662571000	1	5.954756000	-0.640481000	-0.861783000
1	5.950313000	-0.656358000	-0.762652000	1	5.421005000	2.400450000	-0.585816000
1	5.405688000	2.390333000	-0.601623000	6	8.582636000	-0.234318000	-0.791233000
6	8.577382000	-0.226553000	-0.704168000	1	8.233127000	-1.262821000	-0.944537000
1	8.235548000	-1.263111000	-0.814389000				
D11-π-A / TiO ₂ E(RB3LYP) = -3656.59209089 a. u.				D12-π-A / TiO ₂ E(RB3LYP) = -3652.95515032 a. u.			
6	8.563530000	-0.826532000	0.070087000	6	-8.819475000	-1.155531000	-0.047686000
6	9.957735000	-0.719570000	-0.028310000	6	-10.080660000	-0.982570000	0.552890000
6	7.760760000	0.372369000	-0.018173000	6	-8.073071000	0.051632000	-0.410100000
6	9.818743000	1.672803000	-0.331155000	6	-10.095107000	1.386400000	0.046005000
6	8.426241000	1.642929000	-0.226989000	6	-8.809101000	1.323276000	-0.482799000
6	10.619571000	0.514058000	-0.215332000	6	-10.746088000	0.258444000	0.622584000
1	10.549031000	-1.631674000	0.048102000	1	-10.568161000	-1.868468000	0.964434000
1	10.306098000	2.627116000	-0.542008000	6	-12.044269000	0.435965000	1.225528000
6	12.056551000	0.643403000	-0.382803000	1	-12.272044000	1.442140000	1.583954000
1	12.369931000	1.531740000	-0.933165000	6	-13.030667000	-0.514530000	1.478084000
6	13.076459000	-0.194910000	0.000904000	7	-13.992603000	-0.407110000	2.470799000
7	14.390146000	-0.065510000	-0.458429000	6	-14.861747000	-1.492090000	2.406906000
6	15.077428000	-1.335752000	-0.237903000	6	-14.453022000	-2.283697000	1.387906000
6	14.374811000	-1.842753000	1.013917000	7	-13.329998000	-1.691154000	0.803655000
7	13.022211000	-1.288646000	0.876363000	1	-14.857168000	-3.220255000	1.019482000
1	14.352566000	-2.940671000	1.087921000	1	-15.681158000	-1.610930000	3.107580000
1	14.928300000	-2.028917000	-1.092252000	6	-8.207217000	2.469300000	-1.140188000
1	14.865510000	-1.441925000	1.923688000	1	-7.590853000	2.268209000	-2.017732000
1	16.158373000	-1.187937000	-0.096084000	6	-8.403120000	3.815695000	-0.857805000
6	7.646286000	2.862065000	-0.458273000	7	-8.183098000	4.853142000	-1.753788000
1	6.741956000	2.741081000	-1.052453000	6	-8.399118000	6.076279000	-1.124061000
6	7.951133000	4.161707000	-0.137639000	6	-8.765130000	5.819315000	0.152859000
7	7.236421000	5.259195000	-0.626813000	7	-8.772186000	4.432744000	0.331248000

6	8.039403000	6.461960000	-0.430387000	1	-9.023870000	6.495654000	0.960162000
6	8.810363000	6.097718000	0.829875000	1	-8.287640000	7.018081000	-1.650337000
7	8.970821000	4.645844000	0.695647000	6	-8.342339000	-2.511756000	-0.161703000
1	9.786268000	6.600697000	0.906782000	1	-8.785912000	-3.211989000	0.550378000
1	8.726776000	6.637124000	-1.284821000	6	-7.508779000	-3.125961000	-1.097514000
1	8.216882000	6.344511000	1.733881000	7	-6.893030000	-4.350862000	-0.893099000
1	7.404748000	7.352124000	-0.306829000	6	-6.152722000	-4.702063000	-2.016717000
6	7.962477000	-2.118019000	0.398734000	6	-6.293144000	-3.706851000	-2.923605000
1	7.121126000	-2.076173000	1.089023000	7	-7.131304000	-2.738458000	-2.369276000
6	8.354242000	-3.382098000	0.038847000	1	-5.576451000	-5.619812000	-2.058802000
7	7.829070000	-4.542920000	0.617759000	1	-5.867936000	-3.590811000	-3.914185000
6	8.716843000	-5.657890000	0.305240000	6	-12.873839000	-2.001989000	-0.542693000
6	9.261734000	-5.229772000	-1.049380000	1	-11.924358000	-2.556641000	-0.546984000
7	9.291189000	-3.767472000	-0.933609000	1	-13.647936000	-2.597507000	-1.046075000
1	10.263052000	-5.632417000	-1.265570000	1	-12.720199000	-1.063280000	-1.096018000
1	9.531914000	-5.752423000	1.054215000	6	-14.011069000	0.642174000	3.466507000
1	8.574898000	-5.544759000	-1.861110000	1	-14.360117000	1.599675000	3.043450000
1	8.166925000	-6.610060000	0.268610000	1	-14.686274000	0.351465000	4.282250000
6	9.296085000	3.961712000	1.940925000	1	-12.996459000	0.791395000	3.869069000
1	8.446357000	3.976766000	2.652760000	6	-6.941191000	-5.086229000	0.353730000
1	9.584483000	2.920931000	1.755949000	1	-7.932203000	-5.542746000	0.516386000
1	10.150508000	4.475723000	2.407087000	1	-6.184612000	-5.880913000	0.328026000
6	6.445971000	5.157992000	-1.837785000	1	-6.726947000	-4.411359000	1.197432000
1	5.616525000	4.448265000	-1.703580000	6	-7.702898000	-1.638872000	-3.122974000
1	6.005891000	6.142231000	-2.053105000	1	-7.640550000	-1.878246000	-4.193659000
1	7.043941000	4.832515000	-2.712447000	1	-8.757382000	-1.510513000	-2.840478000
6	12.305904000	-1.170564000	2.143255000	6	-7.817934000	4.660619000	-3.138819000
1	11.274596000	-0.837571000	1.986133000	1	-6.777293000	4.307160000	-3.240788000
1	12.275108000	-2.160644000	2.623335000	1	-8.482824000	3.915100000	-3.604613000
1	12.812176000	-0.462874000	2.830195000	1	-7.917375000	5.615402000	-3.671978000
6	14.680442000	0.652487000	-1.684666000	6	-8.745069000	3.789811000	1.633062000
1	14.127644000	0.247666000	-2.555838000	1	-9.639666000	3.173521000	1.808731000
1	14.427824000	1.717732000	-1.580653000	1	-7.866689000	3.129011000	1.703753000
1	15.759739000	0.585780000	-1.883547000	1	-8.674391000	4.567948000	2.404829000
6	7.217680000	-4.511786000	1.931783000	1	-7.176558000	-0.693335000	-2.923930000
1	6.319167000	-3.878325000	1.929585000	6	-1.900013000	-0.939740000	-0.186311000
1	6.901071000	-5.531044000	2.195867000	6	-0.771996000	-1.765166000	-0.001062000
1	7.907004000	-4.135359000	2.714728000	6	-0.918968000	-3.150898000	0.310234000
6	9.350382000	-3.070232000	-2.213127000	7	-1.109182000	-4.275463000	0.555332000
1	8.412729000	-3.192810000	-2.791519000	6	-5.646480000	-0.795639000	-0.244798000
1	9.542039000	-2.000597000	-2.073013000	1	-5.885783000	-1.825973000	0.012076000
1	10.180181000	-3.491657000	-2.800850000	1	-1.674298000	0.103557000	-0.427288000
6	1.632493000	-0.901397000	0.038227000	6	-4.297837000	-0.444976000	-0.305905000
6	0.529180000	-1.730036000	-0.167063000	6	-3.229900000	-1.328901000	-0.092339000
6	0.677216000	-3.082958000	-0.602766000	1	-4.048985000	0.594675000	-0.557311000
7	0.851177000	-4.180526000	-0.954672000	1	-3.456248000	-2.371654000	0.152394000
6	5.381218000	-0.594200000	-0.093069000	6	-6.666955000	0.140589000	-0.467895000
1	5.672300000	-1.590870000	-0.427666000	1	-6.301914000	1.158740000	-0.639244000

1	1.395110000	0.113755000	0.370586000	1	-10.666043000	2.312023000	-0.056560000
6	4.004922000	-0.331775000	0.079340000	22	9.200394000	-0.140279000	-0.863142000
6	2.981468000	-1.242333000	-0.143806000	22	8.527659000	-2.678276000	0.337068000
1	3.723893000	0.674397000	0.416726000	22	5.928329000	-1.246535000	-0.293107000
1	3.229358000	-2.254644000	-0.478010000	22	9.426585000	-0.546146000	1.982104000
6	6.333128000	0.393839000	0.098984000	22	2.727409000	-0.242357000	-0.284422000
1	5.923654000	1.379241000	0.346473000	22	7.187419000	1.330667000	-1.730500000
22	-9.452770000	-0.319903000	1.040022000	22	4.468426000	2.066881000	-1.371673000
22	-8.777169000	-2.753197000	-0.360714000	22	6.906154000	1.060835000	1.464883000
22	-6.185311000	-1.338891000	0.325469000	22	3.912579000	2.418061000	1.607482000
22	-9.733938000	-0.513239000	-1.823107000	8	9.482375000	-2.034682000	-1.012722000
22	-3.005994000	-0.290309000	0.340700000	8	9.044427000	0.958326000	-2.230296000
22	-7.441158000	1.111863000	1.977819000	8	6.785522000	-2.902345000	-0.059797000
22	-4.740771000	1.914098000	1.629249000	8	8.286292000	0.661306000	2.677640000
22	-7.222901000	1.085611000	-1.235718000	8	9.426792000	-2.403661000	1.941268000
22	-4.250072000	2.491130000	-1.326355000	8	10.380901000	0.096047000	0.630318000
8	-9.708868000	-2.223623000	1.051555000	8	3.134235000	0.889187000	-1.680910000
8	-9.278649000	0.674556000	2.483092000	8	7.116121000	-0.528691000	-1.659926000
8	-7.021113000	-2.979971000	-0.014027000	8	5.919189000	2.363371000	-2.520538000
8	-8.620797000	0.758372000	-2.445959000	8	5.653480000	0.991187000	-0.410701000
8	-9.711824000	-2.368498000	-1.919004000	8	3.999156000	3.218430000	-0.126176000
8	-10.664822000	0.013032000	-0.407066000	8	4.252249000	-1.431918000	-0.634414000
8	-3.382710000	0.728498000	1.818007000	8	5.764943000	-0.588908000	1.589818000
8	-7.345356000	-0.737818000	1.762282000	8	3.228587000	0.626074000	1.175688000
8	-6.172604000	2.102790000	2.819814000	8	8.002772000	1.569198000	-0.050903000
8	-5.924621000	0.897453000	0.610460000	8	3.015718000	3.237228000	2.679207000
8	-4.309336000	3.158719000	0.463828000	8	5.791592000	2.193333000	2.132264000
8	-4.493818000	-1.522425000	0.615871000	8	8.060730000	-0.833391000	0.649014000
8	-6.065829000	-0.535578000	-1.502545000	8	1.629677000	-1.905279000	0.042806000
8	-3.529370000	0.677694000	-1.039873000	8	0.759883000	0.029293000	-0.428707000
8	-8.290945000	1.461449000	0.335921000	6	0.536535000	-1.224456000	-0.126203000
8	-3.381739000	3.396432000	-2.349372000	1	4.824348000	-0.390276000	1.802096000
8	-6.132766000	2.278423000	-1.835940000				
8	-8.336137000	-0.883220000	-0.541580000				
8	-1.868979000	-1.911829000	-0.144941000				
8	-1.017273000	-0.007059000	0.462896000				
6	-0.796629000	-1.220340000	0.050945000				
1	-5.133209000	-0.315286000	-1.724896000				
D13-π-A / TiO ₂ E(RB3LYP) = -3312.43670112 a. u.				D14-π-A / TiO ₂ E(RB3LYP) = -3310.00932341 a. u.			
6	8.141313000	0.124201000	0.155599000	6	-8.659254000	-0.034394000	-0.048410000
6	8.765100000	1.384046000	0.265074000	6	-9.472649000	1.111547000	-0.191244000
6	8.932786000	-1.041115000	0.128412000	6	-9.255655000	-1.294016000	0.147475000
6	10.919152000	0.307977000	0.353275000	6	-11.434915000	-0.257435000	0.094260000
6	10.335073000	-0.972812000	0.221556000	6	-10.659667000	-1.437992000	0.190874000
6	10.166784000	1.501430000	0.358362000	6	-10.878694000	1.029577000	-0.093933000

1	8.145421000	2.280627000	0.326323000	1	-8.999599000	2.069066000	-0.419272000
1	12.001032000	0.375918000	0.486133000	6	-11.759409000	2.180692000	-0.241955000
6	10.857963000	2.774125000	0.569066000	1	-12.739512000	1.980316000	-0.678780000
1	11.804524000	2.692599000	1.104766000	6	-11.494471000	3.510625000	0.035007000
6	10.469645000	4.044825000	0.244555000	7	-12.194079000	4.586390000	-0.502115000
7	11.121603000	5.199081000	0.701269000	6	-11.711431000	5.779579000	0.033514000
6	10.180586000	6.312022000	0.602753000	6	-10.714927000	5.470999000	0.892733000
6	9.376650000	5.912381000	-0.626458000	7	-10.565455000	4.077445000	0.906535000
7	9.381896000	4.445184000	-0.557158000	1	-10.084148000	6.113430000	1.497516000
1	8.350152000	6.310014000	-0.625257000	1	-12.109510000	6.742590000	-0.267885000
1	9.532751000	6.379398000	1.502378000	6	-11.238262000	-2.752667000	0.429104000
1	9.884581000	6.260008000	-1.548668000	1	-10.622165000	-3.446180000	1.004305000
1	10.705738000	7.271172000	0.480819000	6	-12.494056000	-3.219569000	0.085179000
6	11.107228000	-2.214207000	0.271816000	7	-13.125999000	-4.306376000	0.680703000
1	10.557432000	-3.074748000	0.654837000	6	-14.346172000	-4.546675000	0.051742000
6	12.418806000	-2.446394000	-0.042340000	6	-14.495570000	-3.623190000	-0.923762000
7	13.089102000	-3.639094000	0.260004000	7	-13.365140000	-2.793883000	-0.917454000
6	14.523197000	-3.363140000	0.251482000	1	-15.308237000	-3.466387000	-1.624695000
6	14.611115000	-2.286735000	-0.821128000	1	-15.008114000	-5.342405000	0.376408000
7	13.329052000	-1.583898000	-0.683379000	6	-9.952960000	3.359191000	2.011260000
1	15.460847000	-1.600646000	-0.682947000	1	-9.066548000	2.787295000	1.698871000
1	14.870816000	-2.980543000	1.234538000	1	-9.661236000	4.084460000	2.782901000
1	14.695356000	-2.749142000	-1.825363000	1	-10.677221000	2.646912000	2.438860000
1	15.103380000	-4.265039000	0.005397000	6	-13.208326000	4.456865000	-1.520907000
6	12.916529000	-0.884579000	-1.896379000	1	-14.145158000	4.034146000	-1.116891000
1	12.721286000	-1.589691000	-2.729544000	1	-13.425128000	5.447911000	-1.941874000
1	12.014839000	-0.286604000	-1.723300000	1	-12.851673000	3.791596000	-2.324953000
1	13.724376000	-0.201071000	-2.200364000	6	-12.599997000	-5.013977000	1.824192000
6	12.583188000	-4.525893000	1.289004000	1	-11.731307000	-5.640226000	1.555172000
1	11.609305000	-4.944731000	0.995759000	1	-12.277814000	-4.295913000	2.596542000
1	13.283056000	-5.365979000	1.405487000	1	-13.383842000	-5.662339000	2.238326000
1	12.462648000	-4.018980000	2.267818000	6	-12.942721000	-2.025489000	-2.075744000
6	9.180445000	3.803094000	-1.852576000	1	-12.910966000	-0.944389000	-1.872675000
1	9.087623000	2.716349000	-1.746965000	1	-11.930925000	-2.338531000	-2.381175000
1	8.245875000	4.183656000	-2.293200000	1	-13.643707000	-2.217723000	-2.899463000
1	10.011825000	4.022726000	-2.552760000	6	-2.472865000	-0.988757000	-0.130698000
6	11.970343000	5.144416000	1.875013000	6	-1.363896000	-1.808296000	-0.013993000
1	11.441304000	4.751057000	2.766712000	6	-1.480868000	-3.207717000	0.257211000
1	12.849205000	4.509736000	1.688552000	7	-1.622127000	-4.342794000	0.478244000
1	12.334569000	6.158582000	2.094301000	6	-6.241723000	-0.803736000	-0.020368000
6	2.183542000	-1.768985000	-0.239744000	1	-6.503494000	-1.847170000	0.176460000
6	1.233150000	-2.765758000	-0.350737000	1	-2.258698000	0.064616000	-0.335009000
6	1.591658000	-4.147885000	-0.437444000	6	-4.858820000	-0.484029000	-0.133749000
7	1.929876000	-5.260264000	-0.508257000	6	-3.825614000	-1.385055000	-0.008663000
6	5.876562000	-1.002334000	-0.025178000	1	-4.605110000	0.564410000	-0.334517000
1	6.304203000	-2.007736000	-0.074873000	1	-4.047772000	-2.437303000	0.193515000
1	1.791767000	-0.748826000	-0.184478000	6	-7.221250000	0.143229000	-0.144823000
6	4.455765000	-0.892364000	-0.080661000	1	-6.892129000	1.171456000	-0.339140000

6	3.588025000	-1.952681000	-0.192366000	1	-12.517364000	-0.330201000	0.225199000
1	4.032068000	0.118354000	-0.028913000	1	-8.635410000	-2.186646000	0.243889000
1	3.983782000	-2.971496000	-0.245741000	22	8.595024000	-0.132013000	-1.114411000
6	6.689557000	0.090194000	0.086264000	22	7.957484000	-2.743752000	-0.056335000
1	6.200639000	1.070911000	0.129476000	22	5.348875000	-1.272231000	-0.506742000
1	8.461721000	-2.021488000	0.038596000	22	8.917398000	-0.717404000	1.690765000
22	-7.755354000	1.903911000	-1.060961000	22	2.168450000	-0.256956000	-0.342261000
22	-5.573421000	3.654650000	-0.340832000	22	6.559140000	1.396358000	-1.823151000
22	-4.448462000	0.860364000	-0.643243000	22	3.860474000	2.124450000	-1.335093000
22	-7.411808000	2.811259000	1.655431000	22	6.387572000	0.926754000	1.360760000
22	-2.539375000	-1.872410000	-0.395980000	22	3.408127000	2.284842000	1.677972000
22	-7.137765000	-0.607633000	-1.603517000	8	8.863569000	-2.013680000	-1.392481000
22	-5.408823000	-2.793365000	-1.065320000	8	8.389624000	1.047402000	-2.406512000
22	-6.442364000	-0.060650000	1.494568000	8	6.195060000	-2.934053000	-0.408919000
22	-4.886219000	-2.925916000	1.941220000	8	7.802776000	0.446920000	2.494905000
8	-6.846472000	3.521625000	-1.564645000	8	8.909810000	-2.568108000	1.526572000
8	-8.420531000	0.740157000	-2.201598000	8	9.822773000	0.008865000	0.348945000
8	-4.094092000	2.692504000	-0.737848000	8	2.505054000	0.959624000	-1.664099000
8	-7.169528000	1.286342000	2.581011000	8	6.474915000	-0.467404000	-1.861066000
8	-6.293033000	4.243908000	1.263952000	8	5.274298000	2.485470000	-2.504285000
8	-8.683007000	2.678344000	0.425810000	8	5.060964000	0.987111000	-0.479328000
8	-3.658317000	-2.733015000	-1.551580000	8	3.436553000	3.191992000	-0.004546000
8	-5.941279000	0.800967000	-1.873006000	8	3.648630000	-1.425308000	-0.793802000
8	-6.846116000	-2.310340000	-2.160480000	8	5.246960000	-0.726249000	1.414882000
8	-5.590621000	-1.084638000	-0.341305000	8	2.688024000	0.520327000	1.150027000
8	-5.608869000	-3.766175000	0.382610000	8	7.429326000	1.521517000	-0.159307000
8	-3.034171000	-0.085300000	-0.967955000	8	2.546958000	3.031503000	2.825755000
8	-4.531090000	0.540477000	1.329705000	8	5.296325000	2.015821000	2.132320000
8	-3.288477000	-2.029338000	1.188539000	8	7.503499000	-0.920404000	0.386497000
8	-7.757722000	-0.021080000	0.073374000	8	1.035555000	-1.946900000	-0.047514000
8	-4.567712000	-3.929779000	3.167049000	8	0.155676000	0.006411000	-0.418788000
8	-6.174847000	-1.513883000	2.380348000	6	-0.035402000	-1.246528000	-0.161455000
8	-6.283868000	1.986245000	0.316567000	1	4.317098000	-0.552866000	1.682750000
8	-0.589626000	-1.198913000	-0.316192000				
8	-1.102594000	-3.305377000	-0.486582000				
6	-0.176720000	-2.417266000	-0.383839000				
1	-3.882705000	-0.147240000	1.600598000				
D15-π-A / TiO ₂ E(RB3LYP) = -2851.56326617 a. u.				D16-π-A / TiO ₂ E(RB3LYP) = -3078.97922332 a. u.			
6	10.494750000	2.643327000	0.252435000	6	10.596044000	-1.103910000	-0.203496000
6	9.958895000	1.343468000	0.133203000	6	9.674667000	-0.016459000	-0.185265000
6	10.852726000	0.229714000	0.076270000	6	10.236878000	1.308536000	-0.059406000
6	12.209890000	0.458324000	0.160890000	6	11.591748000	1.497975000	0.026957000
6	12.728638000	1.780769000	0.273126000	6	12.501123000	0.391966000	0.042829000
6	11.873010000	2.880395000	0.313758000	6	11.996186000	-0.887053000	-0.063489000
7	13.289290000	-0.427047000	0.177922000	7	12.353422000	2.669664000	0.063211000

6	14.502092000	0.349490000	-0.054195000	6	13.745592000	2.323341000	0.327305000
7	14.104498000	1.700414000	0.334371000	7	13.784006000	0.866148000	0.211222000
1	15.343445000	-0.014938000	0.561730000	7	12.701656000	-2.135781000	0.010579000
1	14.822874000	0.315152000	-1.128275000	6	11.736500000	-3.073668000	-0.555442000
1	12.258816000	3.897989000	0.382613000	7	10.408313000	-2.479909000	-0.294969000
1	9.809310000	3.493001000	0.284707000	1	14.430368000	2.792049000	-0.408969000
1	10.467351000	-0.783095000	-0.036905000	1	14.068915000	2.654785000	1.340802000
6	14.989516000	2.811136000	0.065398000	1	11.823452000	-4.067850000	-0.093401000
1	15.038385000	3.066487000	-1.012695000	1	11.898329000	-3.171901000	-1.650022000
1	14.654467000	3.698700000	0.620788000	6	14.977468000	0.211244000	-0.290776000
1	16.004339000	2.563592000	0.411373000	1	15.828105000	0.382651000	0.388898000
6	13.203638000	-1.755330000	-0.389296000	1	14.789229000	-0.867305000	-0.367555000
1	12.347495000	-2.291978000	0.044452000	1	15.254821000	0.588354000	-1.294909000
1	13.091764000	-1.746907000	-1.493522000	6	11.832457000	3.918080000	0.573434000
1	14.111724000	-2.321993000	-0.134111000	1	10.881317000	4.158123000	0.076029000
6	4.189783000	-1.042084000	-0.268708000	1	11.659509000	3.899687000	1.669790000
6	3.330839000	-2.122203000	-0.379398000	1	12.536234000	4.732324000	0.343797000
6	3.815376000	-3.464931000	-0.466220000	6	9.259954000	-3.158215000	-0.863854000
7	4.258987000	-4.539835000	-0.537378000	1	8.947449000	-2.729879000	-1.835407000
6	7.798676000	0.040772000	-0.049124000	1	9.525924000	-4.212976000	-1.024781000
1	8.305757000	-0.927526000	-0.094865000	1	8.398559000	-3.145226000	-0.178583000
1	3.707707000	-0.061327000	-0.213908000	6	13.087994000	-2.473111000	1.395439000
6	6.378442000	0.031605000	-0.107696000	1	12.219148000	-2.556131000	2.076994000
6	5.601762000	-1.100742000	-0.220343000	1	13.640938000	-3.424743000	1.396305000
1	5.869828000	1.002505000	-0.057752000	1	13.756013000	-1.690715000	1.782950000
1	6.084919000	-2.081320000	-0.272570000	1	9.567348000	2.166238000	-0.065540000
6	8.525911000	1.198177000	0.062842000	6	3.513309000	0.960124000	-0.278719000
1	7.960309000	2.136283000	0.107630000	6	2.398138000	1.789726000	-0.214997000
22	-6.047427000	1.702383000	-1.056766000	6	7.273224000	0.766927000	-0.187833000
22	-4.029389000	3.648868000	-0.363206000	1	7.533972000	1.821398000	-0.066388000
22	-2.657315000	0.965997000	-0.658358000	1	3.294842000	-0.105225000	-0.399657000
22	-5.768264000	2.654459000	1.652173000	6	5.899188000	0.447265000	-0.264445000
22	-0.503191000	-1.578084000	-0.410165000	6	4.859498000	1.359660000	-0.199597000
22	-5.209656000	-0.747068000	-1.586164000	1	5.637005000	-0.612020000	-0.382666000
22	-3.282392000	-2.760861000	-1.049419000	1	5.086088000	2.423673000	-0.079956000
22	-4.541797000	-0.117762000	1.501105000	6	8.257643000	-0.200379000	-0.255207000
22	-2.726155000	-2.825259000	1.953242000	1	7.894304000	-1.221511000	-0.362741000
8	-5.294155000	3.393123000	-1.576376000	6	2.521855000	3.204312000	-0.052228000
8	-6.614768000	0.474296000	-2.182608000	7	2.675710000	4.351967000	0.080099000
8	-2.472242000	2.822877000	-0.766804000	22	-7.564216000	0.015407000	-1.045329000
8	-5.380634000	1.164674000	2.585605000	22	-6.920364000	2.694217000	-0.179637000
8	-4.787662000	4.180653000	1.244047000	22	-4.311946000	1.202191000	-0.569273000
8	-7.031103000	2.398320000	0.433467000	22	-7.844238000	0.791146000	1.717812000
8	-1.550235000	-2.544748000	-1.551883000	22	-1.120784000	0.215944000	-0.382940000
8	-4.150352000	0.764295000	-1.874844000	22	-5.534776000	-1.554277000	-1.674962000
8	-4.767190000	-2.419597000	-2.135072000	22	-2.823274000	-2.231475000	-1.180267000
8	-3.614633000	-1.069756000	-0.335484000	22	-5.312218000	-0.862004000	1.463224000
8	-3.381513000	-3.738316000	0.406096000	22	-2.320528000	-2.180477000	1.828515000

8	-1.165241000	0.152819000	-0.990603000	8	-7.845807000	1.871863000	-1.448269000
8	-2.694452000	0.654353000	1.317308000	8	-7.377103000	-1.253739000	-2.252317000
8	-1.224302000	-1.791914000	1.181494000	8	-5.166881000	2.866124000	-0.573105000
8	-5.867420000	-0.209587000	0.092123000	8	-6.712630000	-0.309846000	2.584577000
8	-2.307443000	-3.787544000	3.182676000	8	-7.847189000	2.626299000	1.427577000
8	-4.135522000	-1.534196000	2.393920000	8	-8.768628000	-0.028630000	0.444193000
8	-4.580150000	1.926949000	0.309639000	8	-1.480051000	-1.091729000	-1.614397000
8	1.373464000	-0.728173000	-0.343165000	8	-5.462719000	0.301988000	-1.845904000
8	1.054053000	-2.872832000	-0.508407000	8	-4.253777000	-2.681369000	-2.298917000
6	1.897920000	-1.904127000	-0.409937000	8	-4.017786000	-1.041438000	-0.387986000
1	-1.984231000	0.029713000	1.586129000	8	-2.373157000	-3.203194000	0.214414000
				8	-2.621096000	1.343600000	-0.896982000
				8	-4.178286000	0.795526000	1.384663000
				8	-1.620964000	-0.456341000	1.168894000
				8	-6.376001000	-1.568397000	0.007424000
				8	-1.437448000	-2.843326000	3.011565000
				8	-4.204113000	-1.890093000	2.292117000
				8	-6.452971000	0.907202000	0.381080000
				8	-0.002325000	1.921771000	-0.233379000
				8	0.879437000	-0.051330000	-0.466898000
				6	1.076687000	1.221252000	-0.305631000
				1	-3.243033000	0.641572000	1.646588000
D17- π -A / TiO ₂ E(RB3LYP) = -3079.00642696 a. u.				D18- π -A / TiO ₂ E(RB3LYP) = -3157.60069130 a. u.			
6	11.605700000	1.284590000	0.205018000	6	-9.897609000	1.329548000	-0.045176000
6	10.230029000	1.109308000	0.028589000	6	-11.266269000	1.539166000	0.109090000
6	12.448606000	0.133259000	0.123710000	6	-9.324583000	0.049359000	-0.145760000
6	9.665556000	-0.156629000	-0.250768000	6	-12.118737000	0.401259000	0.257791000
6	11.909585000	-1.118257000	-0.247582000	6	-10.199314000	-1.084374000	-0.194574000
6	10.519969000	-1.277090000	-0.427291000	6	-11.568391000	-0.905051000	0.094026000
7	13.851243000	0.215552000	0.333120000	7	-11.745993000	2.866310000	0.252287000
6	14.370473000	1.574572000	0.178038000	6	-13.093465000	2.971107000	0.801068000
1	14.357491000	1.840810000	-0.891711000	1	-13.477557000	3.983818000	0.611865000
1	15.414574000	1.595685000	0.521579000	1	-13.057575000	2.832506000	1.896895000
7	9.982634000	-2.539126000	-0.773704000	7	-12.399534000	-2.051280000	0.251787000
1	9.453338000	-2.511922000	-1.641790000	6	-11.631274000	-3.221798000	0.667608000
6	10.896113000	-3.676691000	-0.707787000	1	-12.307159000	-4.085257000	0.758913000
1	10.464577000	-4.508801000	-1.281825000	1	-11.207051000	-3.020977000	1.665786000
1	10.984997000	-4.005248000	0.341832000	7	-13.497954000	0.567894000	0.489419000
7	12.165722000	2.542478000	0.447108000	6	-14.003402000	1.905823000	0.185201000
6	13.527959000	2.588797000	0.950355000	1	-14.040299000	2.040243000	-0.910215000
1	13.925303000	3.604498000	0.795444000	1	-15.032282000	1.983358000	0.564947000
1	13.583513000	2.378706000	2.040928000	7	-9.665657000	-2.354636000	-0.511836000
7	12.782834000	-2.201930000	-0.429747000	6	-10.518213000	-3.527952000	-0.320675000
1	13.711839000	-1.872882000	-0.690848000	1	-10.965780000	-3.835279000	-1.289194000
6	12.286413000	-3.313784000	-1.230576000	1	-9.897563000	-4.376762000	0.020285000

1	12.216372000	-3.065790000	-2.310472000	1	-9.242632000	2.198276000	0.022404000
1	12.977270000	-4.165123000	-1.124015000	6	-14.056920000	-0.011017000	1.716370000
1	9.558738000	1.951766000	0.172026000	1	-13.817955000	0.596761000	2.612296000
6	14.339294000	-0.461940000	1.545033000	1	-15.152375000	-0.072564000	1.620095000
1	15.438515000	-0.522112000	1.505480000	1	-13.658718000	-1.022229000	1.854440000
1	14.048041000	0.062694000	2.476679000	6	-13.382313000	-2.294225000	-0.805302000
1	13.936537000	-1.482505000	1.583653000	1	-14.084338000	-3.076896000	-0.475520000
6	11.300896000	3.655831000	0.781548000	1	-13.951365000	-1.371970000	-0.982543000
1	11.914140000	4.562859000	0.876757000	1	-12.928473000	-2.614845000	-1.765626000
1	10.564350000	3.836375000	-0.017491000	6	-8.892048000	-2.489698000	-1.749952000
1	10.746249000	3.511050000	1.731485000	1	-8.273492000	-1.607397000	-1.941713000
6	3.491707000	0.789812000	-0.514280000	1	-8.227489000	-3.365495000	-1.672926000
6	2.390890000	1.626020000	-0.599105000	1	-9.558491000	-2.643893000	-2.624449000
6	2.526546000	3.045774000	-0.703372000	6	-11.481636000	3.779883000	-0.858034000
7	2.685990000	4.196811000	-0.787922000	1	-12.149937000	3.614108000	-1.730421000
6	7.259368000	0.601520000	-0.416709000	1	-11.610122000	4.818930000	-0.516433000
1	7.526416000	1.658553000	-0.510257000	1	-10.446802000	3.667005000	-1.205863000
1	3.265284000	-0.277567000	-0.433086000	6	-3.148665000	1.012192000	-0.037322000
6	5.875639000	0.275617000	-0.418566000	6	-2.035618000	1.819112000	-0.205567000
6	4.847921000	1.188218000	-0.519351000	6	-2.146448000	3.185444000	-0.612514000
1	5.614150000	-0.786481000	-0.332830000	7	-2.285472000	4.293531000	-0.944588000
1	5.080062000	2.254526000	-0.601733000	6	-6.910583000	0.802172000	-0.239070000
6	8.237151000	-0.355383000	-0.318656000	1	-7.165651000	1.818392000	-0.554793000
1	7.913065000	-1.400378000	-0.269447000	1	-2.939446000	-0.016375000	0.271644000
22	-7.605620000	-0.145248000	-0.990135000	6	-5.534201000	0.502604000	-0.049383000
22	-6.923353000	2.640882000	-0.651746000	6	-4.496419000	1.391179000	-0.231157000
22	-4.337466000	1.068841000	-0.778823000	1	-5.285764000	-0.520428000	0.259723000
22	-7.844292000	1.140784000	1.580188000	1	-4.713132000	2.418852000	-0.538687000
22	-1.158856000	0.090726000	-0.444290000	6	-7.895368000	-0.137000000	-0.061580000
22	-5.601210000	-1.833041000	-1.332600000	1	-7.576421000	-1.148492000	0.211631000
22	-2.892295000	-2.443303000	-0.746879000	22	7.906740000	0.188100000	1.116858000
22	-5.333963000	-0.564280000	1.617106000	22	7.298432000	2.683290000	-0.204594000
22	-2.353150000	-1.830812000	2.193400000	22	4.674334000	1.290482000	0.386197000
8	-7.871931000	1.605636000	-1.732745000	22	8.240942000	0.479444000	-1.732791000
8	-7.445298000	-1.620789000	-1.938676000	22	1.483821000	0.296508000	0.317596000
8	-5.171133000	2.711376000	-1.088148000	22	5.856309000	-1.245121000	1.967966000
8	-6.713870000	0.207644000	2.626900000	22	3.149997000	-1.989270000	1.549057000
8	-7.830776000	2.887950000	0.947647000	22	5.693165000	-1.096614000	-1.246452000
8	-8.791569000	0.107515000	0.492751000	22	2.699589000	-2.446850000	-1.433974000
8	-1.540232000	-1.419653000	-1.400342000	8	7.688327000	-0.855551000	2.519021000
8	-5.509144000	-0.041742000	-1.849968000	8	5.537674000	2.925534000	0.122392000
8	-4.341573000	-3.075732000	-1.744987000	8	7.115820000	-0.748617000	-2.418793000
8	-4.061117000	-1.109328000	-0.180874000	8	1.806191000	-0.783364000	1.756259000
8	-2.435352000	-3.138709000	0.801266000	8	5.792315000	0.614632000	1.816952000
8	-2.645840000	1.122918000	-1.141540000	8	4.558523000	-2.246700000	2.751434000
8	-4.183152000	1.033499000	1.214748000	8	4.362838000	-0.955843000	0.586469000
8	-1.639607000	-0.270011000	1.211023000	8	2.715824000	-3.180344000	0.331344000
8	-6.421412000	-1.517442000	0.329925000	8	2.975704000	1.490338000	0.652271000

8	-1.462954000	-2.268567000	3.470967000	8	4.569983000	0.554727000	-1.470315000
8	-4.226327000	-1.431670000	2.613359000	8	1.998982000	-0.630626000	-1.088524000
8	-6.467368000	0.985408000	0.231119000	8	6.725453000	-1.547211000	0.328046000
8	-0.007398000	1.783144000	-0.626208000	8	1.830900000	-3.295289000	-2.502851000
8	0.848996000	-0.211262000	-0.495743000	8	4.591404000	-2.245813000	-1.908055000
6	1.055870000	1.063255000	-0.574294000	8	6.826786000	0.828522000	-0.460761000
1	-3.246910000	0.922425000	1.493308000	8	0.363756000	1.956668000	-0.143528000
				1	3.638641000	0.364084000	-1.720983000
				8	8.194498000	2.084913000	1.202127000
				8	8.252228000	2.337314000	-1.758087000
				8	9.135721000	-0.114685000	-0.320728000
				8	-0.530178000	0.051491000	0.403360000
				6	-0.712482000	1.273876000	0.021188000