

Electronic Supplementary Information

Solvent effects on static polarizability, static first hyperpolarizability, and one- and two-photon absorption properties of functionalized triply twisted Möbius annulenes: A DFT Study

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UMA (Acetonitrile)

C	-0.729973000	3.897445000	1.468780000
C	-0.725560000	3.926122000	2.902219000
C	-1.761499000	4.499528000	3.597019000
C	-2.871221000	5.072098000	2.912147000
C	-2.892448000	5.054851000	1.473222000
C	-1.796978000	4.467056000	0.756217000
C	-3.959872000	5.655463000	3.618846000
C	-5.034789000	6.198503000	2.942554000
C	-5.064240000	6.177199000	1.524053000
C	-4.022045000	5.621007000	0.808204000
C	-1.054027000	6.826039000	-3.602757000
C	-0.978144000	6.838195000	-0.792158000
C	-0.607675000	7.960771000	-1.506746000
C	-0.647377000	7.958856000	-2.925159000
C	-1.851063000	4.473777000	-3.583711000
C	-1.796084000	4.469029000	-0.742920000
C	-1.408661000	5.651060000	-1.458544000
C	-1.439430000	5.651841000	-2.897397000
C	0.353026000	3.253023000	0.806393000
C	-2.177627000	3.322142000	-1.456961000
C	-2.204387000	3.342822000	-2.890283000
C	1.277260000	2.627907000	0.296061000
C	2.248676000	1.870093000	-0.276820000
C	3.078620000	1.126137000	-0.789801000
C	4.005078000	0.269548000	-2.891004000
C	3.968117000	0.237811000	-1.458024000
C	4.774015000	-0.669758000	-0.752532000
C	5.616276000	-1.578401000	-1.476841000
C	5.639254000	-1.531943000	-2.915064000
C	4.818487000	-0.585542000	-3.592378000
C	6.436248000	-2.545275000	-0.819951000
C	7.236918000	-3.408182000	-1.542712000
C	7.261884000	-3.352739000	-2.960411000
C	6.477049000	-2.433721000	-3.629074000
C	4.764204000	-0.690544000	0.746472000
C	4.760022000	-0.784946000	3.586350000
C	3.749187000	-1.383511000	2.876185000
C	3.734088000	-1.341892000	1.443086000
C	2.638033000	-1.949598000	0.767467000
C	1.634469000	-2.433226000	0.253171000
C	0.488926000	-2.890062000	-0.317187000
C	-0.575861000	-3.230400000	-0.823031000
C	6.874202000	0.661212000	0.832469000
C	6.860173000	0.539787000	3.641257000
C	5.814009000	-0.098605000	2.918268000
C	5.816542000	-0.046631000	1.479900000
C	7.871116000	1.210960000	2.981573000
C	7.873580000	1.272873000	1.563972000
C	-1.812623000	-3.574190000	-2.911618000
C	-1.800371000	-3.543880000	-1.478261000

C	-2.980520000	-3.788803000	-0.758337000
C	-4.201365000	-4.044922000	-1.467894000
C	-4.194024000	-4.070092000	-2.906881000
C	-2.972118000	-3.833880000	-3.599264000
C	-5.440851000	-4.268740000	-0.795453000
C	-6.601415000	-4.510885000	-1.504306000
C	-6.587094000	-4.542917000	-2.922866000
C	-5.406702000	-4.325332000	-3.606257000
C	-2.860951000	-6.293616000	0.792278000
C	-2.906437000	-6.256817000	3.603246000
C	-2.846266000	-7.459446000	2.926684000
C	-2.820726000	-7.474343000	1.508022000
C	-2.970384000	-3.789450000	0.740847000
C	-2.999121000	-3.775054000	3.581972000
C	-2.946502000	-5.022360000	2.896632000
C	-2.929053000	-5.032121000	1.457534000
C	-3.023194000	-2.591141000	2.887380000
C	-3.005399000	-2.580660000	1.453791000
C	-2.993388000	-1.320434000	0.791590000
C	-2.917542000	-0.206956000	0.281874000
C	-2.747186000	1.014858000	-0.287599000
C	-2.514489000	2.106927000	-0.796174000
H	0.113934000	3.483304000	3.425857000
H	-1.748034000	4.518042000	4.682313000
H	-3.930082000	5.662998000	4.704272000
H	-5.860054000	6.639767000	3.491352000
H	-5.914515000	6.600344000	0.999468000
H	-4.057977000	5.607100000	-0.274621000
H	-1.083444000	6.812932000	-4.688143000
H	-0.939684000	6.850483000	0.290624000
H	-0.281495000	8.852186000	-0.981182000
H	-0.354717000	8.848417000	-3.472887000
H	-1.876625000	4.480483000	-4.668930000
H	-2.508552000	2.444343000	-3.414943000
H	4.841427000	-0.552293000	-4.677134000
H	6.423378000	-2.599969000	0.262082000
H	7.851581000	-4.136614000	-1.024249000
H	7.896644000	-4.036095000	-3.514552000
H	6.485563000	-2.386368000	-4.713875000
H	4.763626000	-0.824212000	4.671179000
H	2.943370000	-1.897905000	3.387147000
H	6.885029000	0.719027000	-0.249429000
H	6.846906000	0.490901000	4.725936000
H	8.667297000	1.807267000	1.052438000
H	-2.970934000	-3.856845000	-4.684555000
H	-5.465271000	-4.242672000	0.287437000
H	-7.533445000	-4.676513000	-0.974092000
H	-5.386266000	-4.343257000	-4.691786000
H	-2.837092000	-6.318057000	-0.290688000
H	-2.921765000	-6.234476000	4.688775000
H	-2.815301000	-8.394856000	3.475332000

H	-2.767232000	-8.422441000	0.983154000
H	-3.015076000	-3.772907000	4.667383000
H	-3.055061000	-1.642718000	3.411335000
H	-0.885560000	-3.386135000	-3.441008000
H	3.375513000	0.984022000	-3.408901000
H	-7.506189000	-4.735662000	-3.466080000
H	8.663462000	1.694855000	3.542810000

TTMA-1 (Acetonitrile)

O	-9.326838000	-0.858514000	-3.584516000
O	-10.150439000	-0.534692000	-1.540327000
N	9.552530000	-2.057253000	2.390227000
N	-9.192144000	-0.824130000	-2.321904000
C	1.546099000	3.867582000	1.340977000
C	1.778361000	3.880348000	2.755848000
C	1.220983000	4.850745000	3.550990000
C	0.390469000	5.863903000	2.992344000
C	0.146700000	5.868372000	1.573939000
C	0.746680000	4.858426000	0.749601000
C	-0.205826000	6.867550000	3.805861000
C	-1.016588000	7.839408000	3.252741000
C	-1.266539000	7.843671000	1.855926000
C	-0.700983000	6.884799000	1.038154000
C	1.790653000	6.673793000	-3.803085000
C	2.285844000	6.627443000	-1.035918000
C	3.001728000	7.473451000	-1.860324000
C	2.752262000	7.501291000	-3.256949000
C	0.050952000	4.921087000	-3.533674000
C	0.523193000	4.870950000	-0.732695000
C	1.280635000	5.762136000	-1.564310000
C	1.037552000	5.787911000	-2.982659000
C	2.121806000	2.813514000	0.576558000
C	-0.427601000	4.019399000	-1.317065000
C	-0.656658000	4.060189000	-2.731767000
C	2.591963000	1.844338000	-0.010932000
C	3.038567000	0.730801000	-0.648658000
C	3.375438000	-0.311399000	-1.201601000
C	3.493615000	-1.548510000	-3.315457000
C	3.676755000	-1.518412000	-1.893818000
C	4.112995000	-2.667347000	-1.215026000
C	4.350774000	-3.875730000	-1.951526000
C	4.158591000	-3.887480000	-3.377828000
C	3.731674000	-2.695928000	-4.030741000
C	4.764659000	-5.085857000	-1.316434000
C	4.982409000	-6.235932000	-2.049801000
C	4.798860000	-6.240065000	-3.456926000
C	4.394486000	-5.088548000	-4.103631000
C	4.331764000	-2.637503000	0.268339000
C	4.734182000	-2.627607000	3.079592000
C	3.467512000	-2.748118000	2.566113000
C	3.240043000	-2.750141000	1.149906000

C	1.902804000	-2.827853000	0.679435000
C	0.724378000	-2.827427000	0.331969000
C	-0.569806000	-2.734575000	-0.063811000
C	-1.733113000	-2.573978000	-0.422250000
C	6.800797000	-2.345047000	-0.043987000
C	7.172568000	-2.345936000	2.739535000
C	5.866316000	-2.490796000	2.219896000
C	5.652217000	-2.496920000	0.793704000
C	8.278587000	-2.201408000	1.897737000
C	8.062811000	-2.202741000	0.481000000
C	-3.242627000	-2.345252000	-2.335863000
C	-3.039919000	-2.317554000	-0.915988000
C	-4.109665000	-2.015318000	-0.053997000
C	-5.393346000	-1.714611000	-0.608506000
C	-5.576147000	-1.744988000	-2.037229000
C	-4.472508000	-2.070979000	-2.877490000
C	-6.514544000	-1.370975000	0.210531000
C	-7.742823000	-1.081820000	-0.337344000
C	-7.895669000	-1.126789000	-1.745070000
C	-6.845615000	-1.447561000	-2.585283000
C	-4.882783000	-4.310459000	1.630040000
C	-4.553341000	-4.226609000	4.421215000
C	-5.100718000	-5.343645000	3.820949000
C	-5.263100000	-5.383793000	2.411934000
C	-3.911617000	-2.007120000	1.431657000
C	-3.573256000	-1.950826000	4.249886000
C	-4.148293000	-3.104838000	3.645210000
C	-4.318477000	-3.137250000	2.216365000
C	-3.172670000	-0.881435000	3.487621000
C	-3.332286000	-0.895123000	2.063148000
C	-2.862402000	0.225694000	1.321580000
C	-2.379963000	1.186798000	0.730911000
C	-1.775279000	2.203710000	0.062693000
C	-1.163545000	3.078075000	-0.542840000
H	2.403663000	3.105477000	3.184364000
H	1.404590000	4.853324000	4.620876000
H	-0.011891000	6.853078000	4.874164000
H	-1.466751000	8.599696000	3.882243000
H	-1.909260000	8.606562000	1.429141000
H	-0.902732000	6.896349000	-0.026362000
H	1.595737000	6.684592000	-4.871266000
H	2.488063000	6.611934000	0.028432000
H	3.762914000	8.121693000	-1.438945000
H	3.321344000	8.171998000	-3.891961000
H	-0.131393000	4.946313000	-4.603492000
H	-1.400710000	3.395175000	-3.155076000
H	3.591541000	-2.708492000	-5.107140000
H	4.905301000	-5.095453000	-0.242173000
H	5.294778000	-7.145650000	-1.547707000
H	4.974931000	-7.150578000	-4.019925000
H	4.247618000	-5.082435000	-5.179504000

H	4.889574000	-2.628633000	4.154047000
H	2.612299000	-2.841541000	3.226260000
H	6.671467000	-2.337514000	-1.119874000
H	7.311230000	-2.344357000	3.816856000
H	8.916069000	-2.086954000	-0.180428000
H	-4.617371000	-2.095159000	-3.952288000
H	-6.390562000	-1.334798000	1.285136000
H	-8.588809000	-0.820510000	0.282896000
H	-6.995060000	-1.469514000	-3.657115000
H	-5.007112000	-4.356837000	0.554588000
H	-4.421037000	-4.188277000	5.498236000
H	-5.405236000	-6.193803000	4.422065000
H	-5.687941000	-6.266962000	1.946521000
H	-3.450302000	-1.929636000	5.328212000
H	-2.727473000	-0.007983000	3.949919000
H	-2.400089000	-2.586582000	-2.972938000
H	3.161083000	-0.644939000	-3.813544000
H	9.730272000	-2.047938000	3.381148000
H	10.340919000	-1.945407000	1.774600000

TTMA-2 (Acetonitrile)

O	10.146107000	-1.764390000	2.884550000
O	10.802287000	-1.548366000	0.766787000
N	9.896706000	-1.725876000	1.639518000
N	-9.247170000	-1.136159000	-1.456320000
C	-0.611779000	4.067189000	-1.197167000
C	-0.961656000	4.091148000	-2.587375000
C	-0.372928000	4.986733000	-3.445156000
C	0.606857000	5.908720000	-2.977937000
C	0.970888000	5.900213000	-1.585486000
C	0.338293000	4.970168000	-0.694229000
C	1.235564000	6.833521000	-3.857810000
C	2.191231000	7.716300000	-3.393956000
C	2.559872000	7.706483000	-2.023742000
C	1.966709000	6.823005000	-1.143032000
C	-0.096072000	6.931253000	3.897940000
C	-0.822501000	6.926545000	1.181748000
C	-1.361326000	7.857523000	2.048325000
C	-0.994847000	7.864341000	3.419151000
C	1.396458000	4.983566000	3.515468000
C	0.688730000	4.970341000	0.763383000
C	0.113797000	5.950649000	1.639844000
C	0.475815000	5.956962000	3.032772000
C	-1.232301000	3.091316000	-0.366773000
C	1.580082000	4.017616000	1.281839000
C	1.929630000	4.040598000	2.672166000
C	-1.753811000	2.186996000	0.277968000
C	-2.260704000	1.139221000	0.978943000
C	-2.655477000	0.150889000	1.589545000
C	-2.729291000	-0.996546000	3.754357000
C	-3.015373000	-0.998121000	2.349349000
C	-3.604499000	-2.123291000	1.751436000

C	-3.892391000	-3.279258000	2.551837000
C	-3.594555000	-3.260520000	3.959805000
C	-3.015321000	-2.091670000	4.531314000
C	-4.458608000	-4.467198000	1.997745000
C	-4.720534000	-5.567609000	2.790533000
C	-4.432200000	-5.541120000	4.179693000
C	-3.880146000	-4.410033000	4.748569000
C	-3.937374000	-2.122977000	0.289211000
C	-4.566456000	-2.184927000	-2.479134000
C	-3.278732000	-2.406410000	-2.061428000
C	-2.936336000	-2.375656000	-0.668309000
C	-1.579590000	-2.569655000	-0.300755000
C	-0.381509000	-2.680304000	-0.050738000
C	0.945046000	-2.714741000	0.229225000
C	2.147002000	-2.672928000	0.477201000
C	-6.335115000	-1.580628000	0.775604000
C	-6.932008000	-1.661781000	-1.965693000
C	-5.607484000	-1.905312000	-1.540869000
C	-5.276676000	-1.875682000	-0.137829000
C	-7.958626000	-1.378460000	-1.049850000
C	-7.618379000	-1.340816000	0.346766000
C	3.845209000	-2.577769000	2.237829000
C	3.513902000	-2.551274000	0.842175000
C	4.524602000	-2.383561000	-0.122177000
C	5.879336000	-2.215399000	0.304400000
C	6.191642000	-2.245204000	1.710561000
C	5.143224000	-2.434212000	2.656705000
C	6.949237000	-2.007015000	-0.622068000
C	8.247570000	-1.847325000	-0.196391000
C	8.526799000	-1.891055000	1.191928000
C	7.531556000	-2.082475000	2.132464000
C	4.914291000	-4.776899000	-1.800135000
C	4.340116000	-4.718766000	-4.551938000
C	4.831471000	-5.871267000	-3.970580000
C	5.117256000	-5.898062000	-2.581044000
C	4.191167000	-2.385225000	-1.583462000
C	3.601225000	-2.355456000	-4.360793000
C	4.116794000	-3.547162000	-3.776009000
C	4.413671000	-3.566116000	-2.367784000
C	3.376765000	-1.236302000	-3.597869000
C	3.665064000	-1.235455000	-2.193631000
C	3.374456000	-0.057979000	-1.448130000
C	3.041236000	0.959927000	-0.849689000
C	2.601364000	2.046942000	-0.163429000
C	2.138019000	2.991868000	0.467295000
C	-10.386474000	-0.919864000	-0.536879000
C	-9.647580000	-1.064606000	-2.876880000
C	-11.616629000	-0.996489000	-1.461234000
C	-11.082903000	-0.508644000	-2.825844000
H	-1.701613000	3.385201000	-2.946738000
H	-0.646277000	4.998435000	-4.495664000

H	0.949752000	6.830216000	-4.905376000
H	2.664742000	8.416823000	-4.073674000
H	3.315615000	8.398611000	-1.667325000
H	2.259640000	6.822968000	-0.099859000
H	0.187514000	6.925346000	4.946095000
H	-1.113513000	6.929369000	0.138076000
H	-2.072414000	8.589744000	1.680319000
H	-1.425380000	8.602444000	4.087593000
H	1.668915000	4.994341000	4.566190000
H	2.624100000	3.295646000	3.043379000
H	-2.796324000	-2.080139000	5.594511000
H	-4.680448000	-4.500056000	0.937753000
H	-5.148904000	-6.461518000	2.349274000
H	-4.644586000	-6.412497000	4.790113000
H	-3.652025000	-4.381597000	5.809830000
H	-4.809188000	-2.213515000	-3.536995000
H	-2.493267000	-2.608181000	-2.781394000
H	-6.118144000	-1.535914000	1.836575000
H	-7.142933000	-1.704368000	-3.027603000
H	-8.383967000	-1.107722000	1.076289000
H	5.385803000	-2.458529000	3.713701000
H	6.729779000	-1.970965000	-1.681342000
H	9.054745000	-1.688368000	-0.897714000
H	7.776887000	-2.105831000	3.186503000
H	5.131416000	-4.813670000	-0.739200000
H	4.113676000	-4.689583000	-5.613461000
H	4.997359000	-6.759236000	-4.571263000
H	5.496403000	-6.808831000	-2.129526000
H	3.381866000	-2.345008000	-5.423856000
H	2.976485000	-0.333341000	-4.044306000
H	3.045235000	-2.713987000	2.955799000
H	-2.279851000	-0.111429000	4.189912000
H	-10.312717000	0.061267000	-0.045399000
H	-10.411293000	-1.687040000	0.244689000
H	-9.614051000	-2.061342000	-3.341649000
H	-8.968808000	-0.412098000	-3.438525000
H	-12.448107000	-0.391828000	-1.089415000
H	-11.961734000	-2.034199000	-1.539385000
H	-11.689042000	-0.855371000	-3.667023000
H	-11.061791000	0.587188000	-2.854128000

TTMA-3 (Acetonitrile)

O	12.699152000	-1.235359000	0.323926000
O	11.858846000	-0.189354000	2.110059000
N	-10.024397000	-1.814796000	-1.163990000
N	9.287672000	0.045718000	3.750074000
N	10.430211000	-2.562689000	-1.623279000
N	11.722257000	-0.856985000	1.042138000
C	-1.774519000	4.107625000	-1.255616000
C	-2.170814000	4.109279000	-2.633545000
C	-1.669869000	5.041554000	-3.508028000
C	-0.736626000	6.024593000	-3.071218000

C	-0.328535000	6.040355000	-1.691170000
C	-0.870775000	5.071708000	-0.781626000
C	-0.196372000	6.986803000	-3.969635000
C	0.715757000	7.928674000	-3.535335000
C	1.127544000	7.943557000	-2.177502000
C	0.619797000	7.025138000	-1.279316000
C	-1.288901000	6.997556000	3.826901000
C	-2.105901000	6.939388000	1.137192000
C	-2.680143000	7.829693000	2.023515000
C	-2.268242000	7.863477000	3.380980000
C	0.325065000	5.161165000	3.389991000
C	-0.473735000	5.096344000	0.663763000
C	-1.087009000	6.033262000	1.561161000
C	-0.678798000	6.066150000	2.940945000
C	-2.296788000	3.089995000	-0.407819000
C	0.501081000	4.210543000	1.149387000
C	0.895301000	4.258643000	2.527016000
C	-2.726493000	2.149961000	0.253399000
C	-3.125308000	1.067526000	0.971457000
C	-3.418338000	0.053075000	1.596389000
C	-3.312785000	-1.089998000	3.761764000
C	-3.658176000	-1.117596000	2.370487000
C	-4.188197000	-2.285482000	1.799378000
C	-4.356682000	-3.456269000	2.612161000
C	-4.001980000	-3.409852000	4.006240000
C	-3.485093000	-2.199868000	4.551155000
C	-4.857701000	-4.684788000	2.084258000
C	-5.006863000	-5.797152000	2.889419000
C	-4.663930000	-5.743398000	4.265292000
C	-4.170913000	-4.573075000	4.808354000
C	-4.581648000	-2.314221000	0.352626000
C	-5.315809000	-2.424318000	-2.389171000
C	-3.997846000	-2.533695000	-2.026763000
C	-3.602317000	-2.479028000	-0.648066000
C	-2.223424000	-2.565708000	-0.336092000
C	-1.011065000	-2.587405000	-0.130529000
C	0.320661000	-2.527356000	0.104635000
C	1.524892000	-2.401918000	0.316893000
C	-6.993871000	-1.983796000	0.941140000
C	-7.694460000	-2.119220000	-1.773883000
C	-6.337651000	-2.241100000	-1.406383000
C	-5.952355000	-2.183635000	-0.017479000
C	-8.703985000	-1.933607000	-0.813556000
C	-8.310105000	-1.862859000	0.567988000
C	3.251709000	-2.181276000	2.033740000
C	2.884663000	-2.183745000	0.646097000
C	3.859646000	-1.948028000	-0.346224000
C	5.203324000	-1.682873000	0.047825000
C	5.553838000	-1.681164000	1.444658000
C	4.545409000	-1.943355000	2.419291000
C	6.235985000	-1.385758000	-0.897313000

C	7.528769000	-1.146256000	-0.502455000
C	7.889419000	-1.173851000	0.884415000
C	6.882170000	-1.414557000	1.830309000
C	4.381966000	-4.313605000	-2.028659000
C	3.738074000	-4.306268000	-4.765646000
C	4.324572000	-5.418657000	-4.194498000
C	4.645493000	-5.420081000	-2.812422000
C	3.491351000	-1.980147000	-1.798533000
C	2.835026000	-2.001939000	-4.560139000
C	3.449868000	-3.151148000	-3.986427000
C	3.781550000	-3.144124000	-2.585828000
C	2.546656000	-0.900032000	-3.793516000
C	2.866681000	-0.874170000	-2.396554000
C	2.507756000	0.279846000	-1.644407000
C	2.115777000	1.270156000	-1.035473000
C	1.616433000	2.321034000	-0.333999000
C	1.104683000	3.228622000	0.313818000
C	-11.140073000	-1.715259000	-0.195730000
C	-10.491667000	-1.785367000	-2.566114000
C	-12.393254000	-1.926784000	-1.065838000
C	-11.974814000	-1.385979000	-2.450390000
C	9.260085000	-0.933599000	1.338455000
C	10.391569000	-1.214658000	0.590007000
C	9.372818000	-0.387536000	2.662019000
C	10.399292000	-1.938400000	-0.629303000
H	-2.874238000	3.356424000	-2.970370000
H	-1.977531000	5.035939000	-4.549037000
H	-0.514541000	6.964319000	-5.007604000
H	1.122197000	8.657160000	-4.228939000
H	1.848815000	8.682558000	-1.844538000
H	0.945515000	7.044406000	-0.246108000
H	-0.969932000	7.012836000	4.864729000
H	-2.431729000	6.920899000	0.103977000
H	-3.454086000	8.508826000	1.681468000
H	-2.727339000	8.569151000	4.065242000
H	0.631841000	5.191442000	4.430837000
H	1.653699000	3.565558000	2.872654000
H	-3.222548000	-2.168153000	5.603992000
H	-5.120398000	-4.739104000	1.034572000
H	-5.387608000	-6.721667000	2.468020000
H	-4.787813000	-6.624734000	4.885670000
H	-3.901108000	-4.523214000	5.858998000
H	-5.599386000	-2.471058000	-3.436073000
H	-3.228273000	-2.664314000	-2.779452000
H	-6.736928000	-1.918115000	1.991962000
H	-7.945559000	-2.180248000	-2.826079000
H	-9.062099000	-1.698883000	1.329599000
H	4.815508000	-1.946587000	3.469892000
H	5.984942000	-1.328515000	-1.948939000
H	8.263625000	-0.883465000	-1.250446000
H	7.117555000	-1.420793000	2.888510000

H	4.627344000	-4.331364000	-0.973425000
H	3.484227000	-4.297224000	-5.821286000
H	4.538876000	-6.294588000	-4.797499000
H	5.100019000	-6.299669000	-2.368799000
H	2.590570000	-2.010578000	-5.617726000
H	2.070576000	-0.030312000	-4.231393000
H	2.481465000	-2.372352000	2.771258000
H	-2.911094000	-0.172703000	4.176885000
H	-11.149164000	-0.728709000	0.289907000
H	-11.048108000	-2.475963000	0.586854000
H	-10.372362000	-2.773072000	-3.035527000
H	-9.910977000	-1.064019000	-3.152576000
H	-13.268333000	-1.415053000	-0.656564000
H	-12.626725000	-2.995930000	-1.131879000
H	-12.576096000	-1.796466000	-3.265863000
H	-12.072105000	-0.294270000	-2.475298000

TTMA-4 (Acetonitrile)

O	13.583494000	-1.813040000	-0.774056000
O	13.009066000	-0.615065000	1.024932000
N	10.673966000	-0.211887000	2.968716000
N	11.033720000	-3.125176000	-2.353650000
N	12.713711000	-1.340855000	0.026387000
N	-11.346779000	-1.456122000	-0.920134000
N	-9.487391000	-0.674202000	-2.138572000
C	-0.696731000	4.227690000	-0.932849000
C	-1.231993000	4.218652000	-2.262898000
C	-0.774135000	5.099977000	-3.210856000
C	0.250511000	6.039137000	-2.900307000
C	0.798804000	6.064639000	-1.569870000
C	0.301648000	5.150068000	-0.582055000
C	0.746330000	6.948235000	-3.876372000
C	1.747238000	7.847402000	-3.564209000
C	2.296474000	7.871366000	-2.256039000
C	1.835155000	7.004336000	-1.284738000
C	0.437419000	7.204895000	3.986425000
C	-0.653593000	7.113802000	1.396648000
C	-1.097744000	8.049910000	2.310131000
C	-0.547295000	8.100247000	3.617033000
C	1.922617000	5.289926000	3.441686000
C	0.844364000	5.189992000	0.814923000
C	0.365823000	6.175587000	1.741693000
C	0.915119000	6.225793000	3.070992000
C	-1.182764000	3.263764000	-0.004636000
C	1.824991000	4.273295000	1.225245000
C	2.362240000	4.340422000	2.552878000
C	-1.588819000	2.370132000	0.731587000
C	-1.964275000	1.335987000	1.529019000
C	-2.239616000	0.361874000	2.222406000
C	-1.976206000	-0.703904000	4.413873000
C	-2.455568000	-0.766029000	3.064050000
C	-3.089992000	-1.926967000	2.594427000

C	-3.230577000	-3.057636000	3.466928000
C	-2.741134000	-2.977230000	4.817987000
C	-2.120926000	-1.774270000	5.261285000
C	-3.834180000	-4.278980000	3.039464000
C	-3.953254000	-5.353172000	3.899601000
C	-3.476564000	-5.265836000	5.233297000
C	-2.882928000	-4.101174000	5.679229000
C	-3.621419000	-1.989113000	1.193321000
C	-4.613158000	-2.163867000	-1.462608000
C	-3.274053000	-2.332084000	-1.220087000
C	-2.748084000	-2.243911000	0.112589000
C	-1.353662000	-2.387375000	0.299254000
C	-0.128409000	-2.458441000	0.392254000
C	1.220017000	-2.451174000	0.492790000
C	2.444921000	-2.373178000	0.573996000
C	-5.950620000	-1.519402000	1.990568000
C	-6.903471000	-1.697168000	-0.644980000
C	-5.526238000	-1.883011000	-0.398839000
C	-5.010111000	-1.798514000	0.946804000
C	-7.822841000	-1.420821000	0.385191000
C	-7.284343000	-1.344807000	1.721742000
C	4.365081000	-2.142231000	2.071713000
C	3.839613000	-2.205203000	0.736967000
C	4.704365000	-2.074923000	-0.371920000
C	6.094647000	-1.862700000	-0.149382000
C	6.605358000	-1.800433000	1.196447000
C	5.703916000	-1.950392000	2.292979000
C	7.024661000	-1.678572000	-1.221851000
C	8.364488000	-1.491455000	-0.991255000
C	8.884014000	-1.461884000	0.344988000
C	7.980679000	-1.590084000	1.411655000
C	4.916955000	-4.541459000	-1.978343000
C	3.967461000	-4.623582000	-4.623761000
C	4.565274000	-5.737157000	-4.066882000
C	5.040199000	-5.693352000	-2.730520000
C	4.167676000	-2.157257000	-1.768822000
C	3.195783000	-2.270735000	-4.433460000
C	3.821107000	-3.422135000	-3.875676000
C	4.310989000	-3.369035000	-2.523253000
C	3.046863000	-1.122365000	-3.695696000
C	3.528520000	-1.049125000	-2.347705000
C	3.314483000	0.154589000	-1.618460000
C	3.045562000	1.187370000	-1.013244000
C	2.681978000	2.287092000	-0.302974000
C	2.290514000	3.239505000	0.364149000
C	10.307415000	-1.277579000	0.622920000
C	11.328746000	-1.654234000	-0.240061000
C	10.606005000	-0.687769000	1.896904000
C	11.154262000	-2.444656000	-1.404008000
C	-9.244906000	-1.267124000	0.231326000
C	-10.000017000	-1.145198000	-0.935437000

C	-11.976206000	-2.236223000	0.174874000
C	-13.683072000	-1.001521000	-0.994721000
C	-13.450081000	-2.335645000	-0.252533000
C	-8.616839000	0.528652000	-2.231864000
C	-9.716204000	-1.291249000	-3.469450000
C	-8.279369000	0.630272000	-3.735818000
C	-9.415533000	-0.142298000	-4.443109000
C	-12.372631000	-0.806178000	-1.779954000
H	-2.005950000	3.499095000	-2.504284000
H	-1.187149000	5.086698000	-4.214667000
H	0.322750000	6.919419000	-4.875816000
H	2.118613000	8.535382000	-4.316358000
H	3.086510000	8.576436000	-2.019533000
H	2.264759000	7.029574000	-0.290373000
H	0.861700000	7.232899000	4.985570000
H	-1.084393000	7.082592000	0.402932000
H	-1.875059000	8.752634000	2.028784000
H	-0.905030000	8.841956000	4.323336000
H	2.336907000	5.334100000	4.444077000
H	3.122648000	3.623333000	2.840220000
H	-1.756893000	-1.716533000	6.282333000
H	-4.199713000	-4.357808000	2.022597000
H	-4.413322000	-6.273183000	3.554363000
H	-3.578253000	-6.117210000	5.897980000
H	-2.511451000	-4.026018000	6.696842000
H	-4.997846000	-2.234706000	-2.475511000
H	-2.586416000	-2.534647000	-2.033680000
H	-5.596120000	-1.443518000	3.012057000
H	-7.257012000	-1.808070000	-1.663705000
H	-7.970041000	-1.134844000	2.537673000
H	6.092969000	-1.906723000	3.304705000
H	6.655993000	-1.667418000	-2.239749000
H	9.019771000	-1.313831000	-1.832489000
H	8.337485000	-1.551819000	2.434611000
H	5.278786000	-4.524411000	-0.957138000
H	3.596050000	-4.648647000	-5.643710000
H	4.670878000	-6.648510000	-4.645747000
H	5.501863000	-6.574230000	-2.296931000
H	2.830967000	-2.315021000	-5.454856000
H	2.562381000	-0.250557000	-4.120003000
H	3.677396000	-2.249993000	2.901953000
H	-1.495446000	0.207457000	4.750594000
H	-9.804017000	-1.301739000	1.160541000
H	-11.898200000	-1.701870000	1.132402000
H	-11.479761000	-3.205015000	0.287900000
H	-14.555764000	-1.023765000	-1.653163000
H	-13.821623000	-0.187203000	-0.273433000
H	-14.117108000	-2.471510000	0.602934000
H	-13.595072000	-3.181206000	-0.935461000
H	-7.710557000	0.430928000	-1.625924000
H	-9.170110000	1.407056000	-1.875767000

H	-10.729023000	-1.682035000	-3.572600000
H	-9.019813000	-2.130011000	-3.622927000
H	-7.316869000	0.144754000	-3.938472000
H	-8.203160000	1.669723000	-4.066861000
H	-10.301202000	0.495161000	-4.553079000
H	-12.445948000	-1.302312000	-2.755947000
H	-12.116212000	0.242846000	-1.953391000
H	-9.129313000	-0.501912000	-5.435514000

UMA (Toluene)

C	-1.927431000	-3.475159000	-1.465206000
C	-1.929849000	-3.510785000	-2.898346000
C	-3.091623000	-3.730789000	-3.595198000
C	-4.327211000	-3.919451000	-2.913223000
C	-4.345204000	-3.888038000	-1.474845000
C	-3.121897000	-3.674236000	-0.755500000
C	-5.542531000	-4.132624000	-3.621330000
C	-6.735791000	-4.303388000	-2.947717000
C	-6.760407000	-4.264694000	-1.529915000
C	-5.597673000	-4.062790000	-0.812618000
C	-3.185371000	-6.125826000	3.614347000
C	-3.118594000	-6.174762000	0.805460000
C	-3.132300000	-7.353370000	1.525114000
C	-3.168761000	-7.332408000	2.943018000
C	-3.175704000	-3.642294000	3.583313000
C	-3.124999000	-3.668781000	0.743479000
C	-3.140497000	-4.909102000	1.465270000
C	-3.169167000	-4.893516000	2.903735000
C	-0.696820000	-3.205246000	-0.803201000
C	-3.115718000	-2.456534000	1.450733000
C	-3.145432000	-2.461705000	2.884000000
C	0.378268000	-2.903236000	-0.296115000
C	1.540162000	-2.489540000	0.272998000
C	2.563220000	-2.044796000	0.782637000
C	3.703618000	-1.516055000	2.885099000
C	3.685003000	-1.480011000	1.452078000
C	4.739938000	-0.875646000	0.750792000
C	5.821032000	-0.274586000	1.478751000
C	5.821359000	-0.320792000	2.916870000
C	4.740885000	-0.958650000	3.590068000
C	6.905655000	0.384790000	0.825573000
C	7.932816000	0.955739000	1.550941000
C	7.932844000	0.899479000	2.968331000
C	6.896361000	0.274838000	3.633400000
C	4.744811000	-0.858697000	-0.748081000
C	4.778818000	-0.785131000	-3.587473000
C	4.001039000	0.100911000	-2.884817000
C	3.969285000	0.075861000	-1.451749000
C	3.116762000	0.999241000	-0.783960000
C	2.316513000	1.776105000	-0.273858000
C	1.376176000	2.573922000	0.295518000

C	0.477733000	3.236684000	0.803127000
C	6.335467000	-2.794888000	-0.817862000
C	6.368316000	-2.693260000	-3.625954000
C	5.567693000	-1.759010000	-2.911741000
C	5.549324000	-1.800030000	-1.473646000
C	7.121344000	-3.638854000	-2.958412000
C	7.100238000	-3.689065000	-1.540919000
C	-0.573688000	3.953630000	2.897326000
C	-0.578525000	3.924394000	1.464071000
C	-1.621462000	4.537485000	0.752515000
C	-2.691981000	5.169308000	1.469769000
C	-2.670100000	5.186576000	2.908308000
C	-1.584564000	4.569132000	3.592354000
C	-3.797861000	5.780117000	0.805133000
C	-4.816441000	6.378530000	1.520362000
C	-4.785985000	6.399926000	2.938398000
C	-3.733879000	5.814181000	3.614275000
C	-0.719179000	6.876749000	-0.797141000
C	-0.793162000	6.866137000	-3.606308000
C	-0.347267000	7.984161000	-2.929491000
C	-0.308650000	7.985083000	-1.511498000
C	-1.621126000	4.538578000	-0.746445000
C	-1.672439000	4.543177000	-3.586345000
C	-1.220324000	5.706696000	-2.901262000
C	-1.191039000	5.705401000	-1.462770000
C	-2.066626000	3.426661000	-2.892214000
C	-2.043041000	3.405391000	-1.459027000
C	-2.426556000	2.204216000	-0.799137000
C	-2.702622000	1.122059000	-0.292358000
C	-2.923877000	-0.091407000	0.276385000
C	-3.047906000	-1.200064000	0.785878000
H	-0.991478000	-3.357308000	-3.418917000
H	-3.082224000	-3.757470000	-4.680604000
H	-5.513587000	-4.155238000	-4.706805000
H	-7.656995000	-4.463785000	-3.498187000
H	-7.702308000	-4.392658000	-1.006495000
H	-5.629294000	-4.030187000	0.269862000
H	-3.208184000	-6.098642000	4.699861000
H	-3.086349000	-6.203083000	-0.277125000
H	-3.112652000	-8.304689000	1.003459000
H	-3.180035000	-8.266288000	3.495379000
H	-3.199448000	-3.635119000	4.668802000
H	-3.141033000	-1.509847000	3.402684000
H	4.746007000	-0.993142000	4.675294000
H	6.913816000	0.437943000	-0.256517000
H	8.746507000	1.454152000	1.034222000
H	8.746993000	1.351456000	3.525316000
H	6.884264000	0.230943000	4.718536000
H	4.797049000	-0.756418000	-4.672704000
H	3.394057000	0.836217000	-3.400541000
H	6.323790000	-2.845601000	0.264309000

H	6.373485000	-2.649583000	-4.711156000
H	7.688874000	-4.438794000	-1.022338000
H	-1.570388000	4.586876000	4.677897000
H	-3.834082000	5.765447000	-0.277608000
H	-5.649291000	6.834618000	0.995158000
H	-3.703680000	5.820728000	4.699929000
H	-0.680985000	6.886913000	0.285593000
H	-0.821905000	6.853373000	-4.691948000
H	-0.022471000	8.862441000	-3.477670000
H	0.049049000	8.864289000	-0.985614000
H	-1.695511000	4.549401000	-4.671868000
H	-2.401143000	2.537912000	-3.414992000
H	0.247120000	3.475386000	3.419468000
H	2.876876000	-1.993018000	3.398967000
H	-5.592780000	6.874371000	3.487344000
H	7.727515000	-4.347259000	-3.513466000

TTMA-1 (Toluene)

O	-9.312179000	-0.901099000	-3.601586000
O	-10.145384000	-0.576134000	-1.559039000
N	9.571712000	-2.069812000	2.385619000
N	-9.187225000	-0.861792000	-2.339509000
C	1.531574000	3.875829000	1.342361000
C	1.763539000	3.890750000	2.757078000
C	1.206650000	4.861438000	3.551609000
C	0.375775000	5.873950000	2.993074000
C	0.131442000	5.876330000	1.575149000
C	0.731706000	4.866108000	0.751262000
C	-0.220638000	6.878183000	3.805164000
C	-1.032467000	7.848605000	3.251917000
C	-1.283349000	7.850511000	1.855728000
C	-0.717521000	6.891164000	1.039212000
C	1.756277000	6.689403000	-3.801902000
C	2.254195000	6.647061000	-1.036589000
C	2.961883000	7.499203000	-1.861249000
C	2.710972000	7.525237000	-3.257201000
C	0.032183000	4.921668000	-3.530559000
C	0.506363000	4.876684000	-0.730596000
C	1.255861000	5.773433000	-1.563477000
C	1.011626000	5.797147000	-2.981277000
C	2.108952000	2.821652000	0.580307000
C	-0.437936000	4.017141000	-1.313099000
C	-0.667317000	4.055723000	-2.727587000
C	2.581376000	1.852032000	-0.003506000
C	3.031440000	0.739129000	-0.638966000
C	3.373064000	-0.301193000	-1.191342000
C	3.495514000	-1.531176000	-3.307824000
C	3.679631000	-1.504647000	-1.886396000
C	4.123417000	-2.653996000	-1.213804000
C	4.367242000	-3.857985000	-1.955700000
C	4.174559000	-3.865318000	-3.381579000

C	3.739901000	-2.673563000	-4.028347000
C	4.787816000	-5.068368000	-1.326171000
C	5.011967000	-6.214024000	-2.063989000
C	4.828439000	-6.213633000	-3.470666000
C	4.417266000	-5.061861000	-4.111923000
C	4.343469000	-2.629707000	0.269201000
C	4.750855000	-2.629736000	3.078981000
C	3.483504000	-2.745985000	2.566467000
C	3.253736000	-2.743677000	1.151268000
C	1.915214000	-2.821315000	0.683506000
C	0.736840000	-2.822629000	0.338956000
C	-0.558087000	-2.733814000	-0.054636000
C	-1.721829000	-2.578162000	-0.412000000
C	6.812157000	-2.339119000	-0.044623000
C	7.189948000	-2.353305000	2.736372000
C	5.881286000	-2.492732000	2.218713000
C	5.665571000	-2.492817000	0.793972000
C	8.292680000	-2.208146000	1.893942000
C	8.075418000	-2.201966000	0.479191000
C	-3.227204000	-2.356090000	-2.328690000
C	-3.028258000	-2.327162000	-0.908192000
C	-4.102827000	-2.029455000	-0.051279000
C	-5.386273000	-1.734233000	-0.610701000
C	-5.564690000	-1.766211000	-2.039752000
C	-4.456105000	-2.087731000	-2.874843000
C	-6.511729000	-1.394393000	0.203523000
C	-7.739750000	-1.111053000	-0.349077000
C	-7.887744000	-1.158209000	-1.756392000
C	-6.834088000	-1.474558000	-2.592030000
C	-4.883617000	-4.319096000	1.637385000
C	-4.564947000	-4.227560000	4.427965000
C	-5.111657000	-5.345547000	3.829629000
C	-5.268441000	-5.389531000	2.420536000
C	-3.910122000	-2.017242000	1.434897000
C	-3.580779000	-1.953707000	4.253153000
C	-4.155404000	-3.108745000	3.650670000
C	-4.320381000	-3.144737000	2.221691000
C	-3.176849000	-0.887340000	3.489039000
C	-3.331953000	-0.903736000	2.064236000
C	-2.861184000	0.215947000	1.322549000
C	-2.378743000	1.177130000	0.733024000
C	-1.776188000	2.195210000	0.065591000
C	-1.168200000	3.072020000	-0.539074000
H	2.388398000	3.114979000	3.184649000
H	1.390172000	4.864695000	4.621760000
H	-0.026292000	6.864823000	4.873635000
H	-1.483227000	8.609091000	3.881047000
H	-1.927752000	8.611644000	1.428053000
H	-0.920250000	6.899819000	-0.025061000
H	1.560316000	6.698115000	-4.870130000
H	2.457327000	6.631953000	0.027511000

H	3.718217000	8.153503000	-1.440176000
H	3.273704000	8.200779000	-3.893049000
H	-0.150864000	4.944629000	-4.600538000
H	-1.406013000	3.383344000	-3.148661000
H	3.598387000	-2.682561000	-5.104852000
H	4.927183000	-5.081021000	-0.251846000
H	5.328683000	-7.124160000	-1.565104000
H	5.009036000	-7.120984000	-4.037662000
H	4.269304000	-5.052214000	-5.187852000
H	4.907613000	-2.633854000	4.153393000
H	2.627971000	-2.838887000	3.226176000
H	6.679712000	-2.325548000	-1.119951000
H	7.329618000	-2.356143000	3.813863000
H	8.927798000	-2.083863000	-0.183448000
H	-4.597409000	-2.112468000	-3.950442000
H	-6.390059000	-1.356339000	1.278407000
H	-8.590784000	-0.852052000	0.265484000
H	-6.982895000	-1.496618000	-3.664174000
H	-5.002533000	-4.367923000	0.561468000
H	-4.436180000	-4.186122000	5.505524000
H	-5.419518000	-6.193552000	4.432347000
H	-5.692235000	-6.273659000	1.955709000
H	-3.460724000	-1.929926000	5.331974000
H	-2.731079000	-0.012737000	3.948621000
H	-2.379961000	-2.592898000	-2.961412000
H	3.156016000	-0.627031000	-3.800172000
H	9.750141000	-2.063085000	3.375706000
H	10.357101000	-1.955505000	1.767744000

TTMA-2 (Toluene)

O	10.134041000	-1.805580000	2.899231000
O	10.798212000	-1.594604000	0.781105000
N	9.893723000	-1.765531000	1.653885000
N	-9.260206000	-1.138582000	-1.457942000
C	-0.591432000	4.070410000	-1.201013000
C	-0.937359000	4.094661000	-2.592035000
C	-0.348557000	4.990967000	-3.448468000
C	0.628547000	5.914561000	-2.979705000
C	0.989452000	5.905747000	-1.586837000
C	0.356191000	4.974868000	-0.696855000
C	1.257882000	6.840499000	-3.857369000
C	2.211434000	7.724138000	-3.391769000
C	2.577253000	7.713770000	-2.021259000
C	1.983350000	6.829256000	-1.142553000
C	-0.073745000	6.942443000	3.892192000
C	-0.796399000	6.938443000	1.176429000
C	-1.331310000	7.873179000	2.040897000
C	-0.966642000	7.879826000	3.411759000
C	1.408245000	4.985899000	3.513406000
C	0.704966000	4.974493000	0.760979000
C	0.134044000	5.958230000	1.636237000

C	0.493941000	5.964135000	3.029330000
C	-1.214353000	3.094603000	-0.373254000
C	1.590199000	4.017136000	1.280640000
C	1.937017000	4.039772000	2.671427000
C	-1.739014000	2.190547000	0.268291000
C	-2.250566000	1.144447000	0.967522000
C	-2.650790000	0.159031000	1.578202000
C	-2.730189000	-0.978923000	3.746484000
C	-3.016539000	-0.985020000	2.341686000
C	-3.612919000	-2.109797000	1.750973000
C	-3.907309000	-3.259770000	2.557788000
C	-3.609559000	-3.235685000	3.965296000
C	-3.022822000	-2.067442000	4.529605000
C	-4.479963000	-4.447328000	2.010289000
C	-4.748516000	-5.541850000	2.808519000
C	-4.460694000	-5.509899000	4.197218000
C	-3.902195000	-4.379137000	4.759635000
C	-3.946087000	-2.116086000	0.289099000
C	-4.578070000	-2.190164000	-2.477428000
C	-3.289983000	-2.408314000	-2.059408000
C	-2.946499000	-2.371717000	-0.667364000
C	-1.588872000	-2.565359000	-0.301197000
C	-0.391275000	-2.676735000	-0.053622000
C	0.935377000	-2.713802000	0.224719000
C	2.137102000	-2.675582000	0.471641000
C	-6.343591000	-1.572070000	0.773713000
C	-6.944121000	-1.666946000	-1.964597000
C	-5.617867000	-1.907649000	-1.540209000
C	-5.286734000	-1.871287000	-0.138716000
C	-7.967851000	-1.379522000	-1.050128000
C	-7.627526000	-1.334623000	0.344622000
C	3.832375000	-2.585932000	2.234554000
C	3.503503000	-2.558657000	0.838230000
C	4.518045000	-2.395910000	-0.122336000
C	5.872972000	-2.234135000	0.307913000
C	6.182236000	-2.265189000	1.714572000
C	5.129653000	-2.448443000	2.656979000
C	6.946286000	-2.031122000	-0.615342000
C	8.244779000	-1.878196000	-0.186336000
C	8.520323000	-1.923386000	1.201801000
C	7.522515000	-2.109168000	2.139198000
C	4.909218000	-4.784191000	-1.808151000
C	4.343144000	-4.716309000	-4.559810000
C	4.832000000	-5.871136000	-3.981731000
C	5.113642000	-5.902764000	-2.591890000
C	4.188586000	-2.392603000	-1.584375000
C	3.605116000	-2.353141000	-4.362081000
C	4.118446000	-3.547307000	-3.780970000
C	4.411499000	-3.570972000	-2.372398000
C	3.380040000	-1.236907000	-3.595696000
C	3.665152000	-1.240009000	-2.190951000

C	3.375905000	-0.063796000	-1.443922000
C	3.043943000	0.953999000	-0.845564000
C	2.606211000	2.041959000	-0.160286000
C	2.145373000	2.988741000	0.468453000
C	-10.396637000	-0.921435000	-0.539030000
C	-9.658527000	-1.067262000	-2.876763000
C	-11.628174000	-0.997353000	-1.462270000
C	-11.094231000	-0.511005000	-2.827499000
H	-1.674674000	3.386092000	-2.951729000
H	-0.619087000	5.001967000	-4.499962000
H	0.974386000	6.836774000	-4.905801000
H	2.685851000	8.425232000	-4.070537000
H	3.332163000	8.405889000	-1.662713000
H	2.274259000	6.827661000	-0.098898000
H	0.208378000	6.935869000	4.940964000
H	-1.085901000	6.940338000	0.132416000
H	-2.038439000	8.608393000	1.670852000
H	-1.394146000	8.620892000	4.079152000
H	1.679004000	4.995615000	4.564807000
H	2.626316000	3.290120000	3.042857000
H	-2.802811000	-2.051848000	5.592783000
H	-4.700166000	-4.484067000	0.950153000
H	-5.181083000	-6.435840000	2.371213000
H	-4.677716000	-6.377019000	4.812377000
H	-3.673293000	-4.346419000	5.820847000
H	-4.821493000	-2.222935000	-3.535171000
H	-2.503532000	-2.611384000	-2.777828000
H	-6.124308000	-1.521424000	1.833838000
H	-7.155802000	-1.715015000	-3.026265000
H	-8.392271000	-1.096691000	1.073663000
H	5.369442000	-2.472681000	3.714983000
H	6.728101000	-1.993745000	-1.674901000
H	9.056662000	-1.722975000	-0.883313000
H	7.768722000	-2.132812000	3.193242000
H	5.122146000	-4.823979000	-0.746510000
H	4.119155000	-4.683226000	-5.621961000
H	4.998700000	-6.757215000	-4.585240000
H	5.490447000	-6.815446000	-2.141991000
H	3.387547000	-2.339094000	-5.425697000
H	2.980528000	-0.331644000	-4.038166000
H	3.028431000	-2.716912000	2.949239000
H	-2.273961000	-0.093992000	4.175356000
H	-10.323700000	0.059534000	-0.045635000
H	-10.422481000	-1.688730000	0.243074000
H	-9.624644000	-2.063439000	-3.344195000
H	-8.979603000	-0.414108000	-3.438330000
H	-12.460033000	-0.392456000	-1.090962000
H	-11.974042000	-2.035009000	-1.539842000
H	-11.701128000	-0.857299000	-3.668630000
H	-11.072858000	0.584925000	-2.856508000

TTMA-3 (Toluene)

O	12.703034000	-1.243943000	0.356379000
O	11.846903000	-0.210076000	2.143717000
N	-10.034584000	-1.812236000	-1.161336000
N	9.256563000	0.010942000	3.764721000
N	10.438242000	-2.535504000	-1.632884000
N	11.725518000	-0.868548000	1.070346000
C	-1.759976000	4.107347000	-1.255885000
C	-2.154275000	4.108794000	-2.634203000
C	-1.655510000	5.042203000	-3.508189000
C	-0.725597000	6.027885000	-3.071152000
C	-0.318815000	6.043949000	-1.691110000
C	-0.859297000	5.073912000	-0.781910000
C	-0.187089000	6.991761000	-3.968290000
C	0.722287000	7.935588000	-3.533507000
C	1.133046000	7.950547000	-2.175830000
C	0.626900000	7.030595000	-1.278767000
C	-1.268316000	7.008205000	3.823148000
C	-2.085971000	6.948893000	1.135050000
C	-2.655955000	7.843183000	2.019628000
C	-2.243655000	7.877719000	3.376506000
C	0.337012000	5.163755000	3.388624000
C	-0.461927000	5.098762000	0.663224000
C	-1.071023000	6.039212000	1.559759000
C	-0.662653000	6.072636000	2.939079000
C	-2.282360000	3.088969000	-0.409897000
C	0.508880000	4.209210000	1.149247000
C	0.902698000	4.257853000	2.526724000
C	-2.713387000	2.148282000	0.248573000
C	-3.115597000	1.066413000	0.964763000
C	-3.413162000	0.053605000	1.589195000
C	-3.312522000	-1.084475000	3.756350000
C	-3.657979000	-1.114116000	2.365260000
C	-4.193983000	-2.281475000	1.799370000
C	-4.368111000	-3.448507000	2.616504000
C	-4.013723000	-3.399291000	4.010165000
C	-3.490566000	-2.190027000	4.549957000
C	-4.874488000	-4.676401000	2.093079000
C	-5.029314000	-5.785164000	2.901687000
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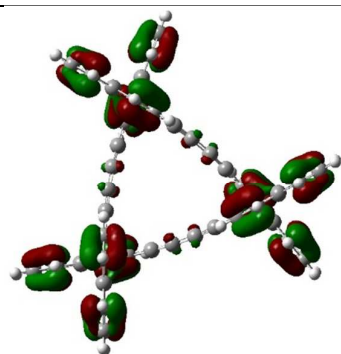
TTMA-4 (Toluene)

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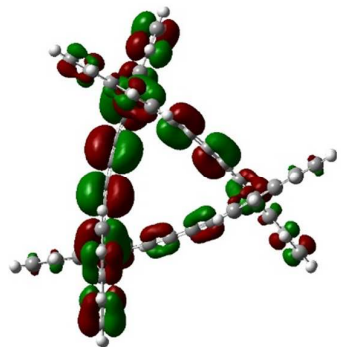
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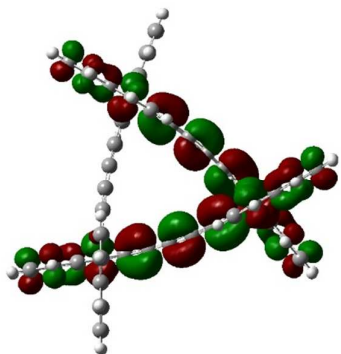
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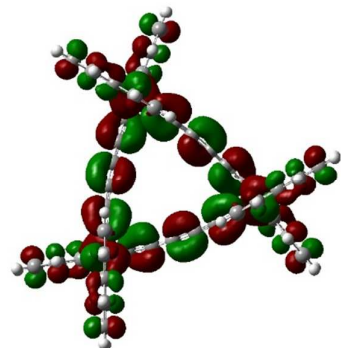
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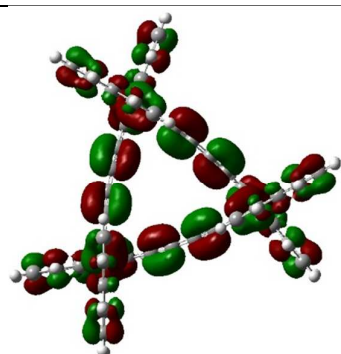
HOMO-1



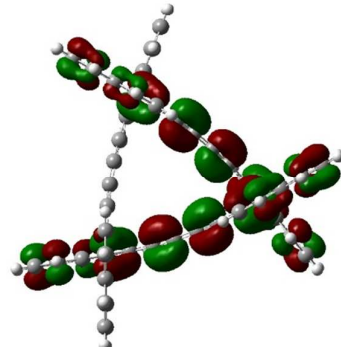
LUMO



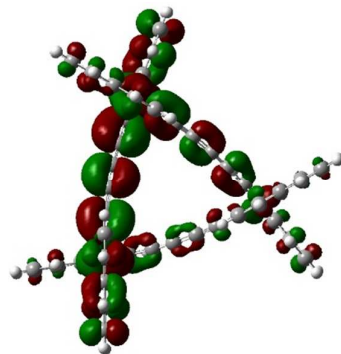
LUMO+2



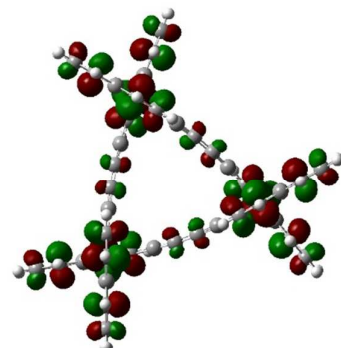
HOMO-2



HOMO



LUMO+1



LUMO+3

Figure S1 Orbital involved in $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions for UMA in Toluene.

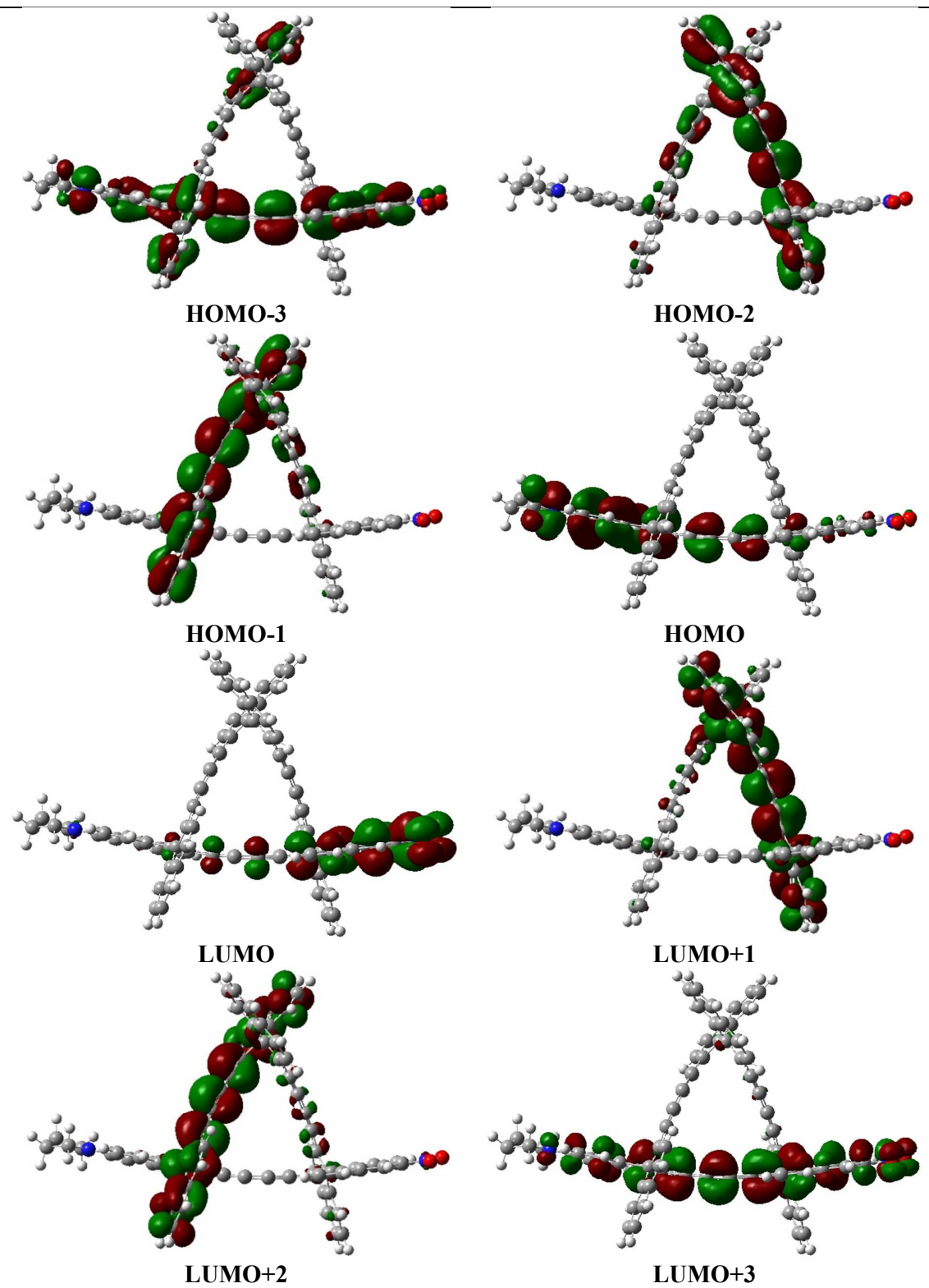


Figure S2 Orbital involved in $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions for TTMA-2 in Toluene.

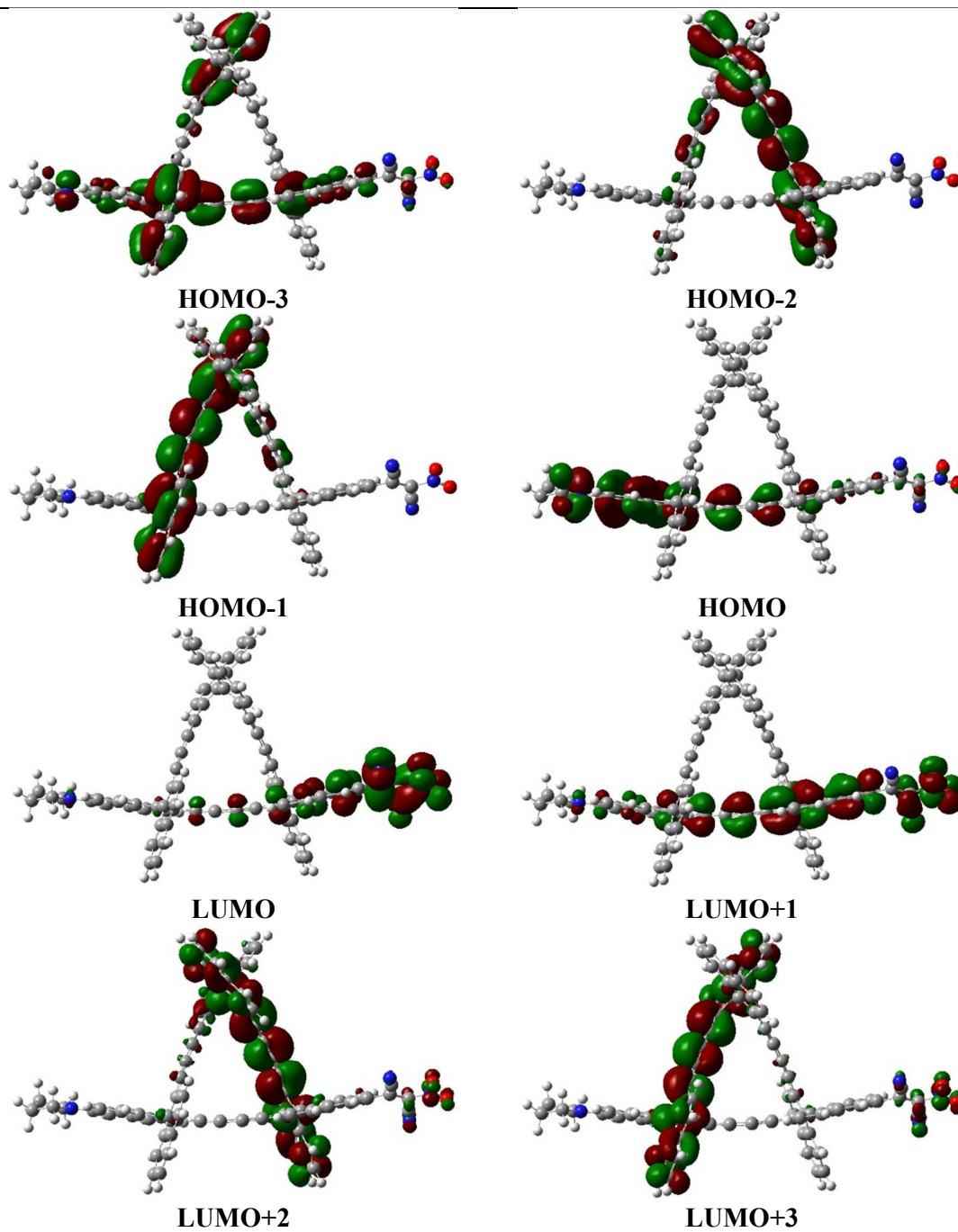


Figure S3 Orbital involved in $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions for TTMA-3 in Toluene.

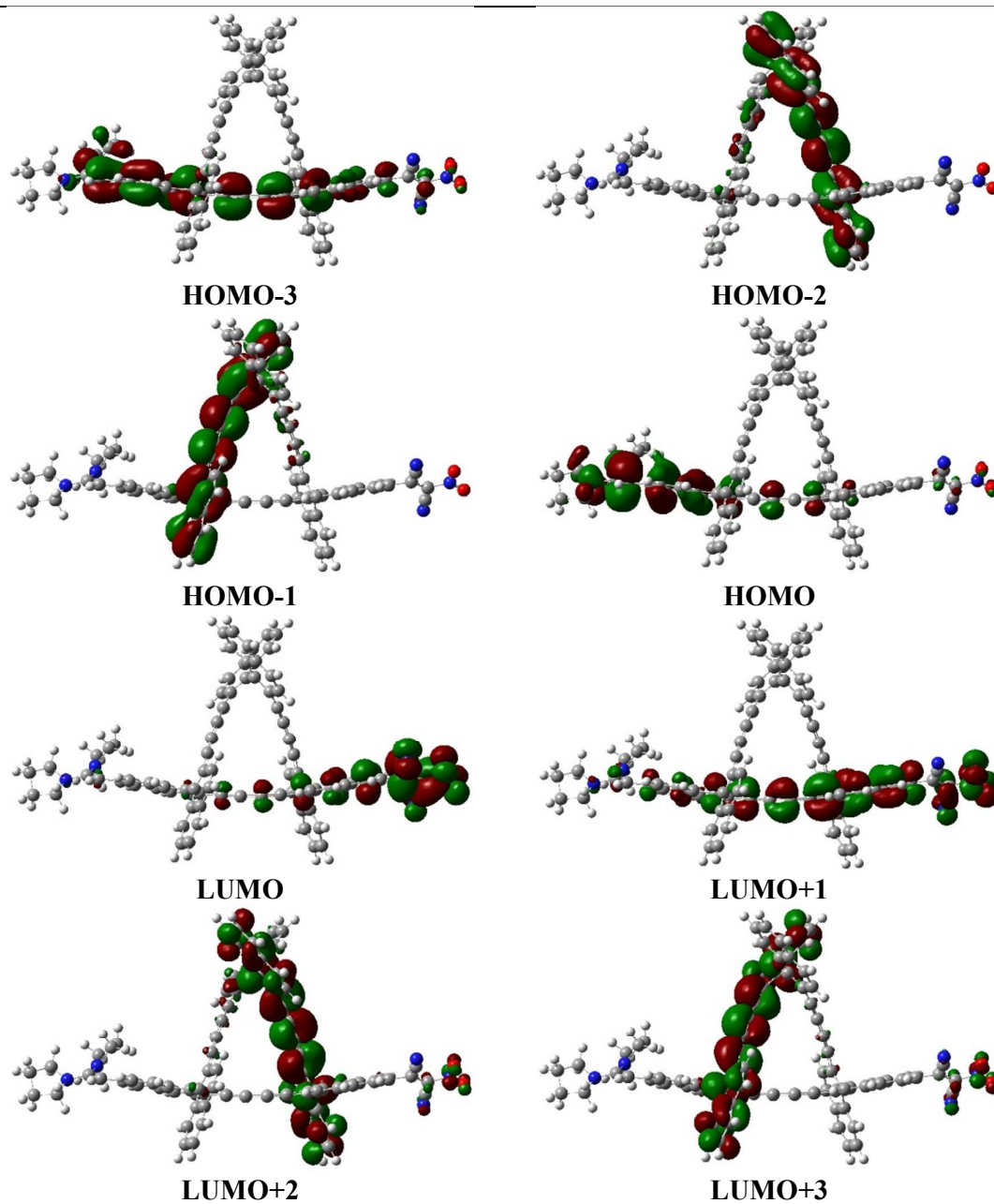


Figure S4 Orbital involved in $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions for TTMA-4 in Toluene.

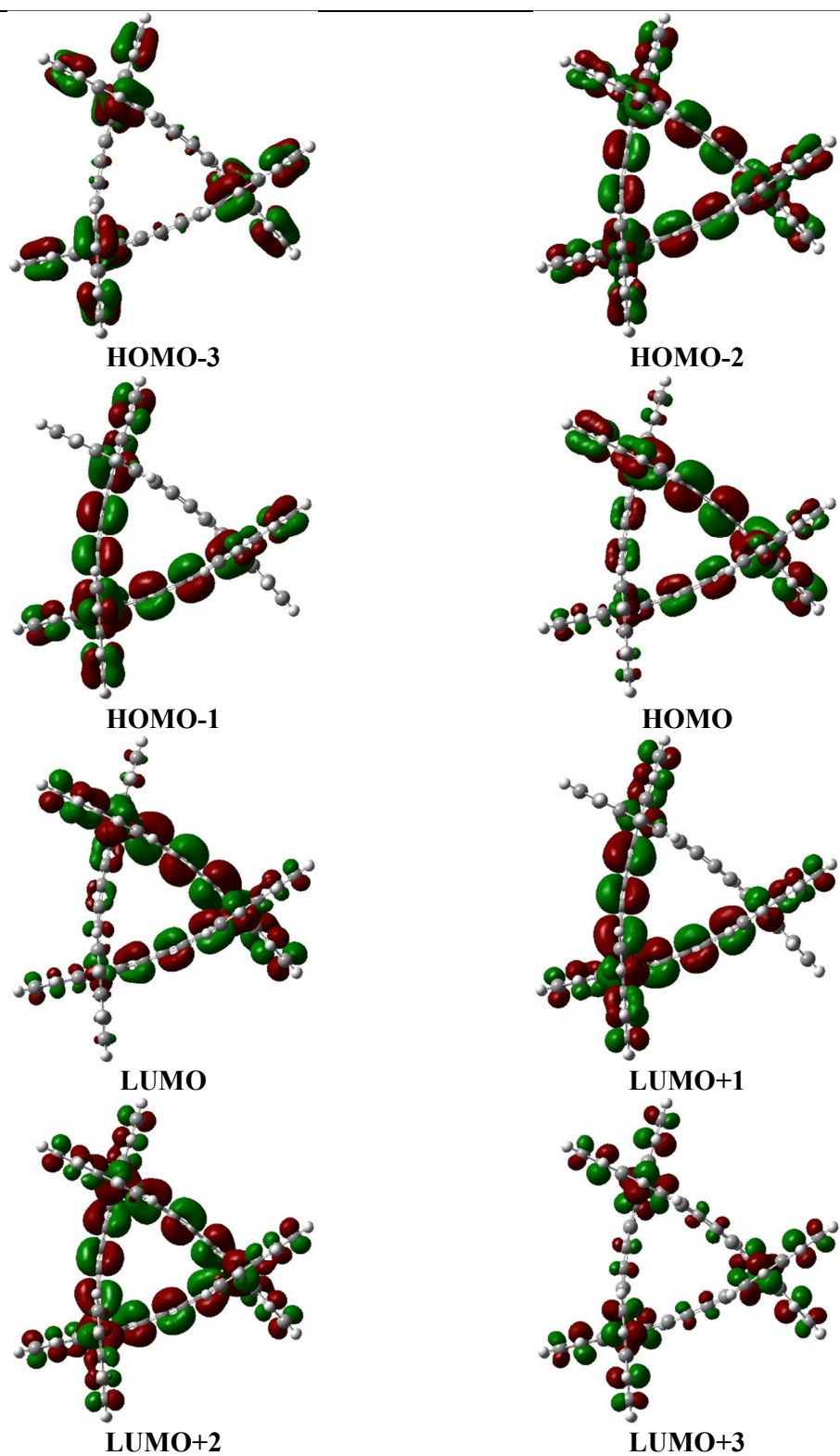


Figure S5 Orbital involved in $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions for UMA in Acetonitrile.

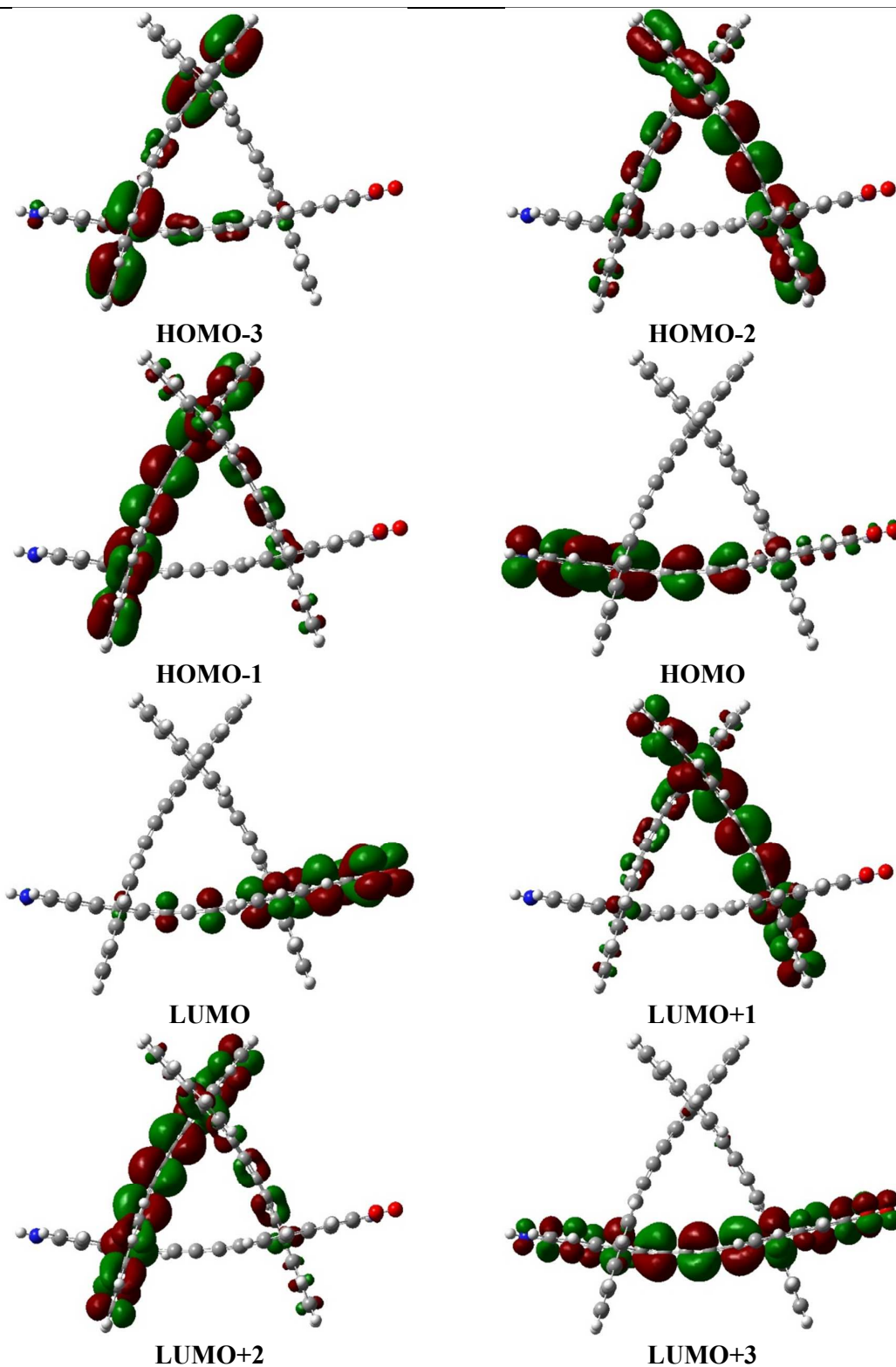


Figure S6 Orbital involved in $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions for TTMA-1 in Acetonitrile.

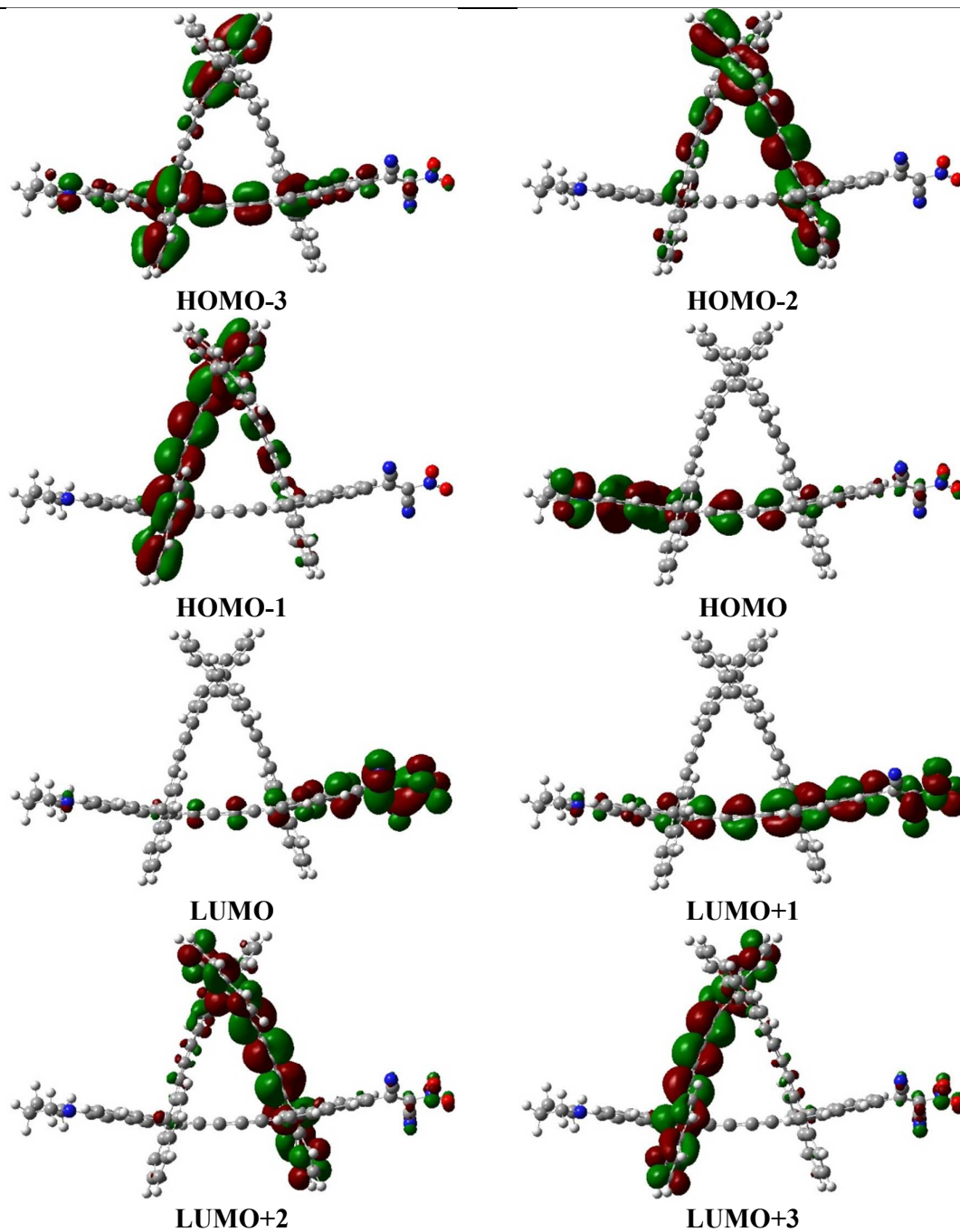


Figure S7 Orbital involved in $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions for TTMA-2 in Acetonitrile.

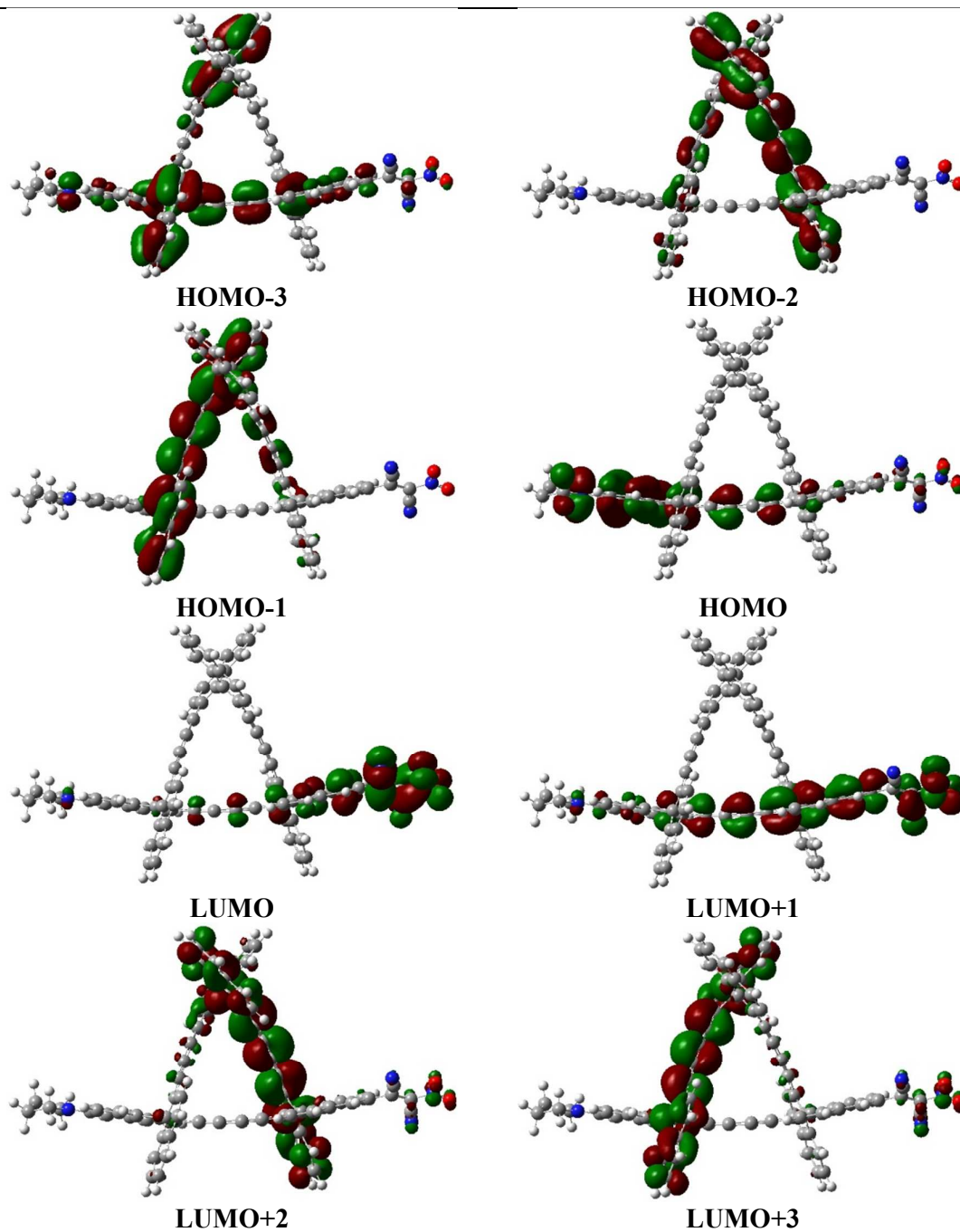


Figure S8 Orbital involved in $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions for TTMA-3 in Acetonitrile.

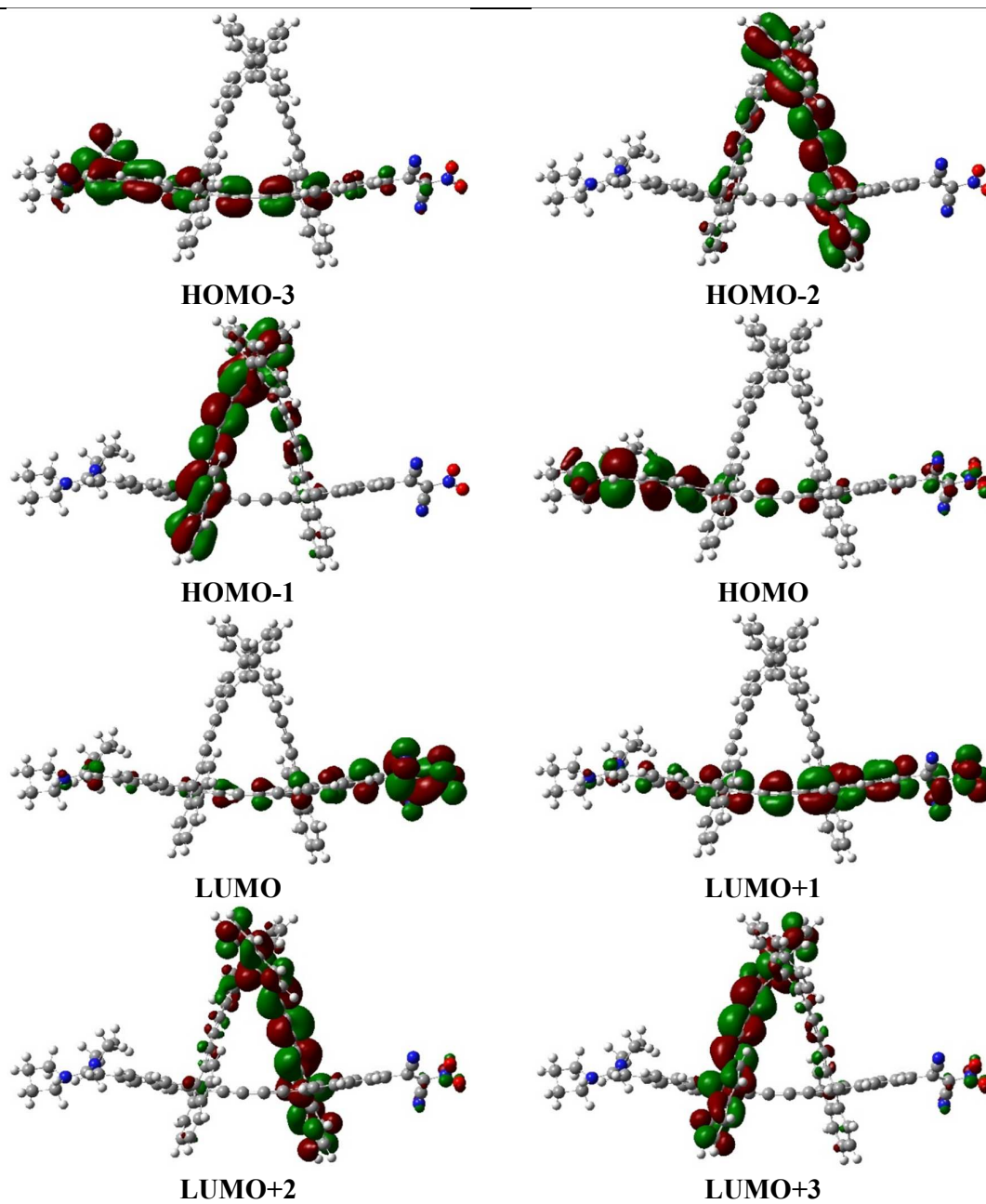


Figure S9 Orbital involved in $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions for TTMA-4 in Acetonitrile.

Table S1 TP tensor elements for the first two excited states of the five molecules in toluene solvent.

System	Ex. St.	S_{xx}	S_{yy}	S_{zz}	S_{xy}	S_{xz}	S_{yz}
UMA	1	0.0	0.0	0.0	0.1	0.1	-0.1
	2	-1.3	1.5	0.0	-2.1	-0.8	-0.1
TTMA-1	1	-657.8	-1.4	-19.3	53.1	-138.2	9.9
	2	233.9	16.1	10.4	-13.6	43.7	-7.1
TTMA-2	1	833.7	-2.4	3.1	-24.5	104.0	-4.5
	2	267.7	17.6	5.4	-10.3	28.3	2.1
TTMA-3	1	-2228.3	-4.6	-10.3	-109.3	-207.2	-9.8
	2	114.0	-5.9	10.2	26.7	18.8	0.7
TTMA-4	1	-3050.9	0.4	3.0	6.3	-79.0	1.8
	2	178.8	-7.2	7.8	15.6	18.7	-2.0

Table S2 TP tensor elements for the first two excited states of the five molecules in acetonitrile solvent.

System	Ex. St.	S_{xx}	S_{yy}	S_{zz}	S_{xy}	S_{xz}	S_{yz}
UMA	1	0.1	0.0	0.0	-0.1	-0.1	0.0
	2	-0.7	0.8	0.0	-2.5	-0.8	0.1
TTMA-1	1	750.5	2.4	23.7	-61.8	158.4	-12.2
	2	222.2	17.6	15.6	-14.8	41.4	-5.9
TTMA-2	1	-938.0	2.2	-5.1	25.2	-118.0	4.4
	2	271.3	18.6	10.5	-8.9	28.7	1.3
TTMA-3	1	2445.8	5.3	14.1	121.8	235.1	11.3
	2	112.3	-7.0	9.9	27.7	18.0	1.0
TTMA-4	1	-3738.0	0.4	1.2	27.9	-114.1	2.3
	2	200.9	-8.7	7.9	14.8	18.6	-2.0

ST 1. Components of dipole moment (μ_x , μ_y , and μ_z) and first hyperpolarizability (β_x , β_y , and β_z) of all the molecules in vacuum phase.

System	μ_x	μ_y	μ_z	β_x	β_y	β_z
UMA	0.005079	-0.00063	0.000184	-6.47933	0.736234	-0.87083
TTMA-1	3.948859	-0.30922	1.154515	19659.99	-960.597	4205.62
TTMA-2	-4.37476	0.112822	-0.88803	-26255.5	1335.674	-3484.53
TTMA-3	-5.77069	-0.13944	-0.7138	-82489.9	-3304.28	-8134.14
TTMA-4	-6.22723	0.247883	-0.85215	-112588	672.2101	-3310.17

ST 2. Components of dipole moment (μ_x , μ_y , and μ_z) and first hyperpolarizability (β_x , β_y , and β_z) of all the molecules in Toluene.

System	μ_x	μ_y	μ_z	β_x	β_y	β_z
UMA	0.002138	0.002771	0.004095	-10.29665505	5.04513127	-1.53424565
TTMA-1	4.223958	-0.347864	1.218946	26585.39355	-1438.452435	5568.011955
TTMA-2	-4.807736	0.102555	-0.960065	-38346.64225	1782.78512	-4987.159214
TTMA-3	-6.34366	-0.168049	-0.73889	-128448.3758	-5657.262097	-12445.51147
TTMA-4	-6.942844	0.298384	-1.002426	-181700.766	862.0769142	-5586.967486

ST 3. Components of dipole moment (μ_x , μ_y , and μ_z) and first hyperpolarizability (β_x , β_y , and β_z) of all the molecules in Acetonitrile.

System	μ_x	μ_y	μ_z	β_x	β_y	β_z
UMA	0.002746	0.002968	0.009169	-8.14689148	3.18066608	-1.68170724
TTMA-1	4.8276951	-0.429895	1.377934	33225.93446	-2064.073917	6995.985947
TTMA-2	-5.244174	0.071912	-1.031192	-42643.24501	1781.842211	-5516.363067
TTMA-3	-6.934614	-0.210940	-0.743242	-151761.5422	-6965.813012	-14907.38291
TTMA-4	-8.025339	0.281474	-1.034378	-271439.3062	2141.722373	-8073.304728