Supporting Information

Correlation of Temperature Dependence of Hydride Kinetic Isotope Effects with Donor-Acceptor Distances in Two Solvents of Different Polarities

Mingxuan Bai, Pratap Rijal, Sanaz Salarvand, Yun Lu*

Department of Chemistry, Southern Illinois University Edwardsville, Edwardsville, Illinois 62026, United States

The atom coordinates and electronic energies of the gas-phase TRS's

DAD = 2.8Å
TRS2: product state, electronic energy = -1284.50945516 Hartree

C	4.617787000000	-0.575966000000	-0.807668000000
C	4.884173000000	-0.169950000000	0.516168000000
C	3.380943000000	-0.370061000000	-1.401295000000
H	5.405069000000	-1.069718000000	-1.377615000000
C	3.924174000000	0.465699000000	1.291268000000
H	5.871126000000	-0.358579000000	0.939283000000
C	2.413194000000	0.279241000000	-0.627374000000
H	3.180868000000	-0.697064000000	-2.421132000000
C	2.687181000000	0.694344000000	0.683601000000
H	4.130248000000	0.778254000000	2.314876000000
N	1.113532000000	0.664408000000	-0.889726000000
N	1.543784000000	1.316395000000	1.142974000000
C	0.537253000000	1.188448000000	0.236740000000
C	0.453235000000	0.543239000000	-2.178380000000
C	1.412222000000	1.954360000000	2.441645000000
H	-0.713693000000	0.079193000000	0.846360000000
C	-0.333913000000	2.368997000000	-0.126424000000
H	-0.601549000000	0.291232000000	-2.019910000000
H	0.532158000000	1.487796000000	-2.734864000000
H	0.933938000000	-0.267951000000	-2.737125000000
H	2.199263000000	2.711276000000	2.558047000000
H	0.432602000000	2.443188000000	2.497651000000
H	1.502885000000	1.209973000000	3.245078000000
C	-1.724219000000	2.284921000000	-0.220868000000
C	0.329045000000	3.565096000000	-0.429096000000
C	-2.453811000000	3.398746000000	-0.640344000000
H	-2.243498000000	1.355786000000	0.027863000000
C	-0.407800000000	4.671190000000	-0.841562000000
H	1.417570000000	3.623626000000	-0.351538000000
C	-1.797965000000	4.588146000000	-0.949120000000
H	-3.539422000000	3.333835000000	-0.717775000000
H	0.105465000000	5.603413000000	-1.080273000000
H	-2.370197000000	5.458286000000	-1.272817000000
H	1.486631000000	-1.767092000000	2.465585000000
C	1.263104000000	-2.115068000000	1.454111000000
C	0.046533000000	-1.760153000000	0.876918000000
C	2.189801000000	-2.888049000000	0.757859000000
C	-0.288912000000	-2.218476000000	-0.415739000000
C	-0.918309000000	-0.830335000000	1.519631000000
C	1.866881000000	-3.332394000000	-0.522412000000
H	3.144030000000	-3.152477000000	1.213815000000
C	0.638816000000	-3.017108000000	-1.103645000000
N	-1.518211000000	-1.838288000000	-0.977642000000
C	-2.350689000000	-1.021039000000	1.151336000000
H	2.568284000000	-3.958153000000	-1.076425000000
H	0.400338000000	-3.427566000000	-2.083083000000
C	-2.608621000000	-1.530725000000	-0.136744000000
C	-1.799469000000	-2.211562000000	-2.350271000000
C	-3.407168000000	-0.674822000000	1.991045000000
C	-3.939078000000	-1.687973000000	-0.548069000000
H	-2.579173000000	-1.554420000000	-2.752782000000
H	-0.899961000000	-2.073403000000	-2.961286000000
H	-2.132163000000	-3.259329000000	-2.447975000000
C	-4.728242000000	-0.805316000000	1.566584000000
H	-3.185823000000	-0.295977000000	2.990867000000
C	-4.984306000000	-1.316782000000	0.297153000000
H	-4.175798000000	-2.115442000000	-1.520334000000
H	-5.548696000000	-0.525428000000	2.227074000000
H	-6.012133000000	-1.446774000000	-0.043543000000
H	-0.693151000000	-0.263966000000	2.432451000000

TRS2: reactant state, electronic energy = -1284.50946729 Hartree

C	4.324221000000	-1.342191000000	-1.112924000000
C	4.800045000000	-0.894225000000	0.115873000000
C	3.011630000000	-1.060336000000	-1.527632000000
H	4.981147000000	-1.909841000000	-1.772142000000
C	3.989330000000	-0.139264000000	0.981307000000
H	5.826446000000	-1.115707000000	0.409344000000
C	2.210304000000	-0.320094000000	-0.671660000000
H	2.645428000000	-1.401110000000	-2.496662000000
C	2.696801000000	0.142960000000	0.568647000000
H	4.375658000000	0.226823000000	1.932785000000
N	0.886831000000	0.089312000000	-0.782359000000
N	1.667833000000	0.828479000000	1.194359000000
C	0.560003000000	0.992914000000	0.289858000000
C	0.176536000000	0.141362000000	-2.035746000000
C	1.854992000000	1.703471000000	2.325411000000
H	-0.398594000000	0.652038000000	0.791433000000
C	0.284334940000	2.426479300000	-0.137461280000
H	-0.894997000000	0.296269000000	-1.841659000000
H	0.530996000000	0.959069000000	-2.686308000000
H	0.303201000000	-0.815292000000	-2.562603000000
H	2.390547000000	2.629841000000	2.056194000000
H	0.874844000000	1.983968000000	2.735016000000
H	2.420559000000	1.180397000000	3.109116000000
C	-0.980453950000	2.989113780000	0.026260830000
C	1.313848340000	3.177420470000	-0.717247540000
C	-1.222025430000	4.301464280000	-0.385493340000
H	-1.783864170000	2.398211750000	0.475547250000
C	1.072699910000	4.485499940000	-1.126537780000
H	2.305376580000	2.732326750000	-0.844106400000
C	-0.196239980000	5.047684320000	-0.960359690000
H	-2.211793600000	4.740737990000	-0.255831570000
H	1.874669180000	5.072469950000	-1.575936270000
H	-0.382467860000	6.073473070000	-1.280836400000
H	0.948024000000	-1.489109000000	2.702380000000
C	0.728277000000	-1.992941000000	1.760311000000
C	-0.489414000000	-1.674779000000	1.098084000000
C	1.608829000000	-2.888980000000	1.215572000000
C	-0.823515000000	-2.320826000000	-0.135781000000
C	-1.318522000000	-0.647313000000	1.562961000000
C	1.277739000000	-3.515318000000	-0.008623000000
H	2.552806000000	-3.119208000000	1.708658000000
C	0.090210000000	-3.265150000000	-0.663624000000
N	-2.005779000000	-2.011797000000	-0.761775000000
C	-2.615947000000	-0.478786000000	1.013334000000
H	1.971723000000	-4.238194000000	-0.440472000000
H	-0.131614000000	-3.821730000000	-1.570008000000
C	-2.952284000000	-1.190779000000	-0.169317000000
C	-2.303307000000	-2.584613000000	-2.074525000000
C	-3.568536000000	0.386780000000	1.606688000000
C	-4.253752000000	-1.045333000000	-0.702601000000
H	-2.888887000000	-1.867269000000	-2.656607000000
H	-1.373200000000	-2.762010000000	-2.618704000000
H	-2.860606000000	-3.528188000000	-1.981823000000
C	-4.823381000000	0.529961000000	1.064109000000
H	-3.285902000000	0.927371000000	2.512205000000
C	-5.161100000000	-0.201356000000	-0.093395000000
H	-4.569527000000	-1.612058000000	-1.574872000000
H	-5.557353000000	1.188019000000	1.528585000000
H	-6.163049000000	-0.111441000000	-0.514753000000
H	-1.091156280000	-0.188503470000	2.529398950000

TRS8: product state, electronic energy = -1284.51962522 Hartree

C	-1.870408000000	-1.578971000000	3.343442000000
C	-1.932236000000	-0.206169000000	3.665557000000
C	-1.032194000000	-2.059206000000	2.345883000000
H	-2.497077000000	-2.279735000000	3.895909000000
C	-1.159034000000	0.735469000000	2.999789000000
H	-2.604644000000	0.120675000000	4.459248000000
C	-0.234308000000	-1.114862000000	1.691529000000
H	-0.986243000000	-3.119178000000	2.095794000000
C	-0.299308000000	0.249587000000	2.009748000000
H	-1.209858000000	1.796806000000	3.243447000000
N	0.736645000000	-1.247401000000	0.725355000000
N	0.635081000000	0.883634000000	1.221805000000
C	1.198000000000	-0.006468000000	0.350751000000
C	1.107521000000	-2.518657000000	0.122923000000
C	0.956047000000	2.299307000000	1.311727000000
H	0.658543000000	0.293890000000	-1.196721000000
C	2.695883000000	0.003639000000	0.145463000000
H	1.825211000000	-2.337452000000	-0.683857000000
H	1.569493000000	-3.166506000000	0.881337000000
H	0.211837000000	-3.002760000000	-0.293560000000
H	1.810588000000	2.510999000000	0.659488000000
H	0.094147000000	2.903495000000	0.992312000000
H	1.224279000000	2.540988000000	2.349024000000
C	3.309959000000	0.676297000000	-0.913286000000
C	3.479595000000	-0.634906000000	1.115590000000
C	4.701065000000	0.697867000000	-1.016562000000
H	2.702903000000	1.191660000000	-1.659294000000
C	4.866602000000	-0.611429000000	1.007009000000
H	3.003401000000	-1.142053000000	1.957307000000
C	5.478583000000	0.050177000000	-0.059487000000
H	5.175758000000	1.221473000000	-1.846796000000
H	5.474360000000	-1.110403000000	1.762674000000
H	6.566093000000	0.062897000000	-0.140008000000
H	0.470114000000	3.114326000000	-2.560297000000
C	-0.366531000000	2.958315000000	-1.875371000000
C	-0.766717000000	1.650705000000	-1.596139000000
C	-1.013730000000	4.048870000000	-1.302865000000
C	-1.866306000000	1.406699000000	-0.743302000000
C	-0.024064000000	0.482145000000	-2.120650000000
C	-2.100306000000	3.814302000000	-0.461032000000
H	-0.692004000000	5.065661000000	-1.527066000000
C	-2.531739000000	2.516877000000	-0.191958000000
N	-2.253838000000	0.089925000000	-0.453431000000
C	-0.736851000000	-0.817733000000	-2.130598000000
H	-2.643534000000	4.652252000000	-0.022068000000
H	-3.414719000000	2.386198000000	0.428571000000
C	-1.834978000000	-0.979839000000	-1.258775000000
C	-3.375596000000	-0.125210000000	0.442409000000
C	-0.314238000000	-1.876768000000	-2.935158000000
C	-2.468543000000	-2.234771000000	-1.215855000000
H	-3.283736000000	-1.106569000000	0.918701000000
H	-3.354802000000	0.614464000000	1.247320000000
H	-4.344805000000	-0.064930000000	-0.081523000000
C	-0.932699000000	-3.121428000000	-2.871662000000
H	0.520168000000	-1.712834000000	-3.620840000000
C	-2.011420000000	-3.289435000000	-2.004039000000
H	-3.343629000000	-2.397059000000	-0.591393000000
H	-0.592828000000	-3.942302000000	-3.502804000000
H	-2.528749000000	-4.248513000000	-1.953433000000
H	0.832244000000	0.584975000000	-2.798077000000

TRS8: reactant state, electronic energy = -1284.51962370 Hartree

C	1.442140000000	0.339640000000	3.723053000000
C	1.407255000000	-1.050377000000	3.609342000000
C	0.785779000000	1.161195000000	2.792170000000
H	1.968318000000	0.798141000000	4.560839000000
C	0.716442000000	-1.676395000000	2.558832000000
H	1.906202000000	-1.664506000000	4.359627000000
C	0.105087000000	0.542663000000	1.751449000000
H	0.790487000000	2.246774000000	2.897599000000
C	0.072441000000	-0.863848000000	1.634621000000
H	0.669404000000	-2.763400000000	2.484841000000
N	-0.625432000000	1.074278000000	0.705647000000
N	-0.674379000000	-1.180445000000	0.516710000000
C	-1.252874000000	0.016205000000	-0.045888000000
C	-1.131098000000	2.427256000000	0.703453000000
C	-1.225274000000	-2.493948000000	0.280454000000
H	-0.933159000000	0.102051000000	-1.137670000000
C	-2.770196000000	0.031430000000	-0.085578000000
H	-1.640340000000	2.621316000000	-0.249033000000
H	-1.847394000000	2.600879000000	1.524361000000
H	-0.295617000000	3.137212000000	0.796352000000
H	-1.720051000000	-2.508686000000	-0.698895000000
H	-0.415278000000	-3.238411000000	0.266374000000
H	-1.964586000000	-2.775593000000	1.049385000000
C	-3.455332000000	0.130500000000	-1.294672000000
C	-3.483749000000	-0.059395000000	1.115386000000
C	-4.851574000000	0.137512000000	-1.311754000000
H	-2.895871000000	0.202509000000	-2.231615000000
C	-4.875091000000	-0.051845000000	1.099304000000
H	-2.941777000000	-0.137022000000	2.062757000000
C	-5.559259000000	0.046459000000	-0.115634000000
H	-5.385729000000	0.214648000000	-2.259431000000
H	-5.431788000000	-0.122828000000	2.034554000000
H	-6.649879000000	0.051966000000	-0.126618000000
H	-0.132654000000	-2.180927000000	-3.357908000000
C	0.625076000000	-2.257040000000	-2.575478000000
C	1.043453000000	-1.064014000000	-1.926059000000
C	1.166685000000	-3.469645000000	-2.236477000000
C	2.029299000000	-1.125230000000	-0.899675000000
C	0.470271000000	0.182873000000	-2.246575000000
C	2.145703000000	-3.524746000000	-1.216356000000
H	0.854878000000	-4.381924000000	-2.744625000000
C	2.570000000000	-2.390939000000	-0.558425000000
N	2.446645000000	0.030387000000	-0.278659000000
C	1.053659000000	1.364106000000	-1.747104000000
H	2.588869000000	-4.485248000000	-0.949205000000
H	3.342979000000	-2.482844000000	0.199612000000
C	2.045299000000	1.268678000000	-0.727363000000
C	3.397974000000	-0.069888000000	0.831064000000
C	0.641863000000	2.641189000000	-2.216494000000
C	2.603980000000	2.470062000000	-0.220547000000
H	3.291109000000	0.796324000000	1.485607000000
H	3.148517000000	-0.942199000000	1.441583000000
H	4.429587000000	-0.143572000000	0.456910000000
C	1.196827000000	3.788912000000	-1.713831000000
H	-0.121942000000	2.682845000000	-2.995540000000
C	2.186935000000	3.689294000000	-0.708097000000
H	3.390242000000	2.451176000000	0.528733000000
H	0.889472000000	4.766718000000	-2.084013000000
H	2.645483000000	4.597597000000	-0.314364000000
H	-0.177633000000	0.243471000000	-3.124828000000

DAD = 3.0Å
TRS2: product state, electronic energy = -1284.51304682 Hartree

C	4.647656000000	-0.769183000000	-0.761701000000
C	4.897929000000	-0.433345000000	0.587501000000
C	3.444267000000	-0.470207000000	-1.378808000000
H	5.423225000000	-1.283536000000	-1.329549000000
C	3.956175000000	0.224369000000	1.362670000000
H	5.859873000000	-0.697183000000	1.027703000000
C	2.490688000000	0.199951000000	-0.601833000000
H	3.254701000000	-0.744228000000	-2.416082000000
C	2.750548000000	0.548894000000	0.731083000000
H	4.150258000000	0.482864000000	2.403489000000
N	1.222859000000	0.664456000000	-0.880052000000
N	1.633232000000	1.217589000000	1.182286000000
C	0.648507000000	1.171559000000	0.250455000000
C	0.593353000000	0.622209000000	-2.190056000000
C	1.488602000000	1.793511000000	2.509321000000
H	-0.802641000000	0.042266000000	1.018308000000
C	-0.182903800000	2.384246380000	-0.086479020000
H	-0.483562000000	0.469082000000	-2.063634000000
H	0.777795000000	1.563794000000	-2.726001000000
H	1.013999000000	-0.222841000000	-2.747136000000
H	2.311774000000	2.496303000000	2.692419000000
H	0.535137000000	2.332021000000	2.557439000000
H	1.508089000000	1.001621000000	3.270743000000
C	-1.571736200000	2.331468010000	-0.223914410000
C	0.511971640000	3.577294870000	-0.320626130000
C	-2.267188000000	3.475184420000	-0.618981020000
H	-2.112971620000	1.401709660000	-0.027835490000
C	-0.191900390000	4.713572750000	-0.709038510000
H	1.598581500000	3.611095550000	-0.209313580000
C	-1.579332710000	4.662570900000	-0.860144950000
H	-3.351081030000	3.435611670000	-0.730126370000
H	0.345638040000	5.644178550000	-0.894656460000
H	-2.124960210000	5.556447680000	-1.164607350000
H	1.328419000000	-2.026513000000	2.440308000000
C	1.107900000000	-2.259000000000	1.395499000000
C	-0.087087000000	-1.804353000000	0.846130000000
C	2.015828000000	-2.996942000000	0.635326000000
C	-0.416304000000	-2.113721000000	-0.491753000000
C	-1.041405000000	-0.922094000000	1.577412000000
C	1.692737000000	-3.305876000000	-0.682514000000
H	2.952530000000	-3.341647000000	1.073987000000
C	0.486103000000	-2.882579000000	-1.242713000000
N	-1.616373000000	-1.615889000000	-1.031788000000
C	-2.473975000000	-1.028789000000	1.164007000000
H	2.374503000000	-3.906377000000	-1.286830000000
H	0.244471000000	-3.187561000000	-2.259325000000
C	-2.718662000000	-1.378861000000	-0.177930000000
C	-1.895255000000	-1.859227000000	-2.433628000000
C	-3.538059000000	-0.759418000000	2.020204000000
C	-4.043416000000	-1.455717000000	-0.627035000000
H	-2.636608000000	-1.133028000000	-2.787573000000
H	-0.982518000000	-1.716629000000	-3.022850000000
H	-2.277694000000	-2.877504000000	-2.622413000000
C	-4.854195000000	-0.807306000000	1.561731000000
H	-3.327790000000	-0.506690000000	3.061334000000
C	-5.097367000000	-1.160382000000	0.238152000000
H	-4.271667000000	-1.760860000000	-1.646165000000
H	-5.680392000000	-0.586106000000	2.237224000000
H	-6.120890000000	-1.224651000000	-0.132868000000

H	-0.822078410000	-0.470721700000	2.553616940000

TRS2: reactant state, electronic energy = -1284.51304339 Hartree

C	4.102548499023	-1.902977336038	-1.133336936826
C	4.643386227363	-1.534997389101	0.094214558945
C	2.836699811423	-1.440412797905	-1.533803612697
H	4.671297057263	-2.547734368552	-1.803583280795
C	3.948578463443	-0.683396904673	0.971831077542
H	5.632497355441	-1.895657893021	0.377578763976
C	2.147904641656	-0.607577204660	-0.665573610124
H	2.421853653380	-1.718064626300	-2.503517678365
C	2.702498277566	-0.224669734018	0.574980029783
H	4.389538582803	-0.380275242403	1.921707630348
N	0.885812902035	-0.029780368323	-0.759466584964
N	1.780241942457	0.584830881064	1.218127750553
C	0.722690944968	0.943967158309	0.298489582301
C	0.191878308742	0.140624498751	-2.010891553715
C	2.097210648798	1.417650645758	2.350967701800
H	-0.274059576957	0.784484926701	0.793465193743
C	0.714988388755	2.403296834495	-0.127732957839
H	-0.855737502942	0.414299395191	-1.812529016309
H	0.639517300642	0.928425529521	-2.641285967481
H	0.207344655169	-0.809420586779	-2.563966513349
H	2.730247318981	2.280103254728	2.079685892659
H	1.166767352369	1.802661126425	2.791377471112
H	2.617387542978	0.820504474782	3.112659625874
C	-0.423498185728	3.186082068073	0.055142593889
C	1.857609806352	2.960968419752	-0.714519664342
C	-0.426944620028	4.524759260589	-0.341842133666
H	-1.315005790624	2.745792470688	0.511938095520
C	1.854558280882	4.295295551344	-1.110353672442
H	2.750889091884	2.345212481626	-0.856417776352
C	0.711463037891	5.077660235716	-0.923404143973
H	-1.318214670007	5.135999618853	-0.195200237274
H	2.745135300546	4.731080122624	-1.564939567739
H	0.712081071265	6.123713845571	-1.232339220046
H	0.605633548893	-1.534284478932	2.765243409779
C	0.367504000019	-2.005256097302	1.810858989117
C	-0.806025992858	-1.575936430195	1.125026714533
C	1.176374146386	-2.970232586751	1.276048188372
C	-1.155426224000	-2.170492996568	-0.133315172286
C	-1.563690989487	-0.503990135956	1.593076465826
C	0.822585621470	-3.552821277157	0.034861449743
H	2.084007852685	-3.289510667081	1.787410723423
C	-0.317362253329	-3.189099869978	-0.649014440175
N	-2.284560285211	-1.745562481966	-0.785628639134
C	-2.806701087090	-0.191853116233	0.998274047887
H	1.461148003016	-4.330465400453	-0.387031237715
H	-0.561144050255	-3.712366156197	-1.569334494384
C	-3.164976797601	-0.843674259538	-0.214457200357
C	-2.594392791337	-2.270062575206	-2.117076329017
C	-3.691775844260	0.756482837760	1.574619195904
C	-4.424243999443	-0.558294576720	-0.793132392336
H	-3.076416525388	-1.487031927866	-2.709136536394
H	-1.670128410220	-2.542800711594	-2.629912934062
H	-3.254375603915	-3.147212937783	-2.054137810605
C	-4.902372841874	1.032956805927	0.988782736296
H	-3.391237377766	1.249795643142	2.500791683367
C	-5.265196768110	0.359543860797	-0.197915692499
H	-4.760851544162	-1.072341467640	-1.689759883182
H	-5.585434464676	1.753293498025	1.438247137192
H	-6.236088156490	0.557770544127	-0.653654485920

H	-1.342183282783	-0.113790387454	2.590673666882

TRS8: product state, electronic energy = -1284.52258417 Hartree

C	-1.820435000000	-1.932291000000	3.232024000000
C	-1.868213000000	-0.601321000000	3.705583000000
C	-1.002029000000	-2.304467000000	2.176151000000
H	-2.445106000000	-2.685385000000	3.713317000000
C	-1.100634000000	0.404282000000	3.138039000000
H	-2.527887000000	-0.362051000000	4.540137000000
C	-0.205746000000	-1.296104000000	1.619300000000
H	-0.968248000000	-3.330000000000	1.808450000000
C	-0.256809000000	0.025292000000	2.087106000000
H	-1.143312000000	1.432530000000	3.497353000000
N	0.752622000000	-1.325110000000	0.633385000000
N	0.674700000000	0.733657000000	1.362847000000
C	1.216990000000	-0.058498000000	0.400524000000
C	1.081457000000	-2.514184000000	-0.141338000000
C	0.986298000000	2.140748000000	1.569895000000
H	0.623847000000	0.436159000000	-1.337947000000
C	2.702521000000	-0.032358000000	0.140801000000
H	1.790891000000	-2.241895000000	-0.929424000000
H	1.536228000000	-3.268340000000	0.515668000000
H	0.164845000000	-2.912470000000	-0.600936000000
H	1.894340000000	2.386600000000	1.008034000000
H	0.152717000000	2.767019000000	1.218788000000
H	1.164998000000	2.310149000000	2.639391000000
C	3.282897000000	0.776054000000	-0.840107000000
C	3.514722000000	-0.802849000000	0.983553000000
C	4.668897000000	0.803950000000	-0.993167000000
H	2.650013000000	1.388261000000	-1.485177000000
C	4.896856000000	-0.771479000000	0.824863000000
H	3.066427000000	-1.417278000000	1.766950000000
C	5.474817000000	0.026861000000	-0.163989000000
H	5.117755000000	1.433201000000	-1.762135000000
H	5.527438000000	-1.372239000000	1.481220000000
H	6.558638000000	0.044463000000	-0.283921000000
H	0.397190000000	3.377043000000	-2.373348000000
C	-0.398175000000	3.155842000000	-1.657913000000
C	-0.797183000000	1.830936000000	-1.492821000000
C	-0.995732000000	4.187765000000	-0.936283000000
C	-1.843919000000	1.507340000000	-0.601403000000
C	-0.098599000000	0.712854000000	-2.182932000000
C	-2.037000000000	3.876792000000	-0.066075000000
H	-0.671722000000	5.219328000000	-1.072809000000
C	-2.467692000000	2.559211000000	0.092148000000
N	-2.219190000000	0.165645000000	-0.410988000000
C	-0.821966000000	-0.587012000000	-2.263953000000
H	-2.546284000000	4.668226000000	0.485468000000
H	-3.317482000000	2.371964000000	0.743663000000
C	-1.862238000000	-0.826850000000	-1.341237000000
C	-3.305737000000	-0.123529000000	0.505618000000
C	-0.453337000000	-1.571977000000	-3.178046000000
C	-2.500920000000	-2.078653000000	-1.372159000000
H	-3.208179000000	-1.146263000000	0.883424000000
H	-3.245575000000	0.536480000000	1.375112000000
H	-4.295521000000	-0.006635000000	0.031213000000
C	-1.069675000000	-2.821669000000	-3.182519000000
H	0.337088000000	-1.348585000000	-3.898071000000
C	-2.096294000000	-3.063925000000	-2.273451000000
H	-3.339899000000	-2.294152000000	-0.715171000000
H	-0.768985000000	-3.584804000000	-3.900152000000
H	-2.615436000000	-4.023334000000	-2.275116000000

H	0.715588000000	0.878112000000	-2.899967000000

TRS8: reactant state, electronic energy = -1284.52257955 Hartree

C	-1.052703404686	-1.650731816713	3.479188655842
C	-1.046792939405	-0.298112913263	3.809241236245
C	-0.493887259883	-2.105120622294	2.269537787453
H	-1.474622868789	-2.374948962101	4.176668706073
C	-0.478968739034	0.657792549174	2.946923352526
H	-1.465303044217	0.026336744799	4.762469937071
C	0.055588693954	-1.161565653214	1.414922076337
H	-0.474956244210	-3.167751258467	2.024881345425
C	0.067757928533	0.211136486266	1.752299912410
H	-0.444795429199	1.712377462711	3.223658754494
N	0.646876362285	-1.301198054057	0.167963457311
N	0.678827266500	0.902246540169	0.719167753270
C	1.284552395318	-0.051389785742	-0.197927852504
C	1.174319148419	-2.560420232364	-0.302146719668
C	1.227988066830	2.226529392590	0.887165414008
H	0.971053858086	0.212407209589	-1.244611127407
C	2.801582981486	-0.013210142309	-0.235005800331
H	1.517703830295	-2.443901277792	-1.338883571502
H	2.022168775249	-2.916088453592	0.308675518321
H	0.378261344480	-3.319114138442	-0.289907004472
H	1.593091067981	2.592203617694	-0.081775520624
H	0.439457580011	2.910180973392	1.235056960316
H	2.066886277448	2.246845984251	1.604217012105
C	3.475803968631	0.321533149726	-1.407380266670
C	3.528716488490	-0.307309815423	0.925370801652
C	4.871099571823	0.368680780604	-1.427365510144
H	2.906510448338	0.548628880770	-2.313247635865
C	4.919479810527	-0.262102603119	0.906589368020
H	2.998186283713	-0.570579168211	1.845610516508
C	5.591070867266	0.076970366001	-0.271344331792
H	5.395282073423	0.632315761054	-2.346712859515
H	5.485318987998	-0.491139615089	1.810481081159
H	6.681122002366	0.112613721366	-0.285034964002
H	-0.187780190051	3.116579170068	-2.721345296474
C	-0.832095386466	2.979606704340	-1.850920353536
C	-1.235235422536	1.654612372513	-1.515437179484
C	-1.250135213676	4.049545585804	-1.108584518475
C	-2.070543643391	1.431334090864	-0.376980965802
C	-0.798632729487	0.556857205169	-2.269249210204
C	-2.090289073363	3.824631402333	0.010592307740
H	-0.951488531085	5.063943951288	-1.372010909382
C	-2.491440307206	2.560463171549	0.375742549268
N	-2.463043319933	0.151815054725	-0.067536022520
C	-1.337841665142	-0.713007441196	-2.033885695334
H	-2.440606515554	4.675786753777	0.596413479503
H	-3.158260096038	2.457378310696	1.226269045282
C	-2.158656480052	-0.909450553549	-0.883310845415
C	-3.265496960258	-0.113773316394	1.132802744994
C	-1.044927193904	-1.814086465048	-2.889653836057
C	-2.664319908107	-2.211171538669	-0.626445229533
H	-2.866345778116	-0.997781715023	1.641355315717
H	-3.170409191758	0.710148962974	1.837796230461
H	-4.319623128510	-0.264589603536	0.860699663982
C	-1.552787582782	-3.057171578511	-2.628689957130
H	-0.411709945961	-1.636116325831	-3.760748089326
C	-2.366650923713	-3.245717050256	-1.482650132480
H	-3.303764700702	-2.404085960382	0.230362131133
H	-1.339396492665	-3.897321797092	-3.289296698581
H	-2.777121478078	-4.235188627481	-1.275337263144

H	-0.307055721494	0.759653588907	-3.224661327249

DAD = 3.2Å
TRS2: product state, electronic energy = -1284.51471387 Hartree

C	4.772202000000	-0.771565000000	-0.639171000000
C	4.893120000000	-0.615335000000	0.761711000000
C	3.642014000000	-0.363512000000	-1.325443000000
H	5.593349000000	-1.230592000000	-1.190173000000
C	3.890956000000	-0.036899000000	1.521784000000
H	5.803428000000	-0.959257000000	1.253471000000
C	2.625496000000	0.223858000000	-0.560356000000
H	3.549723000000	-0.495685000000	-2.403066000000
C	2.755079000000	0.393409000000	0.824661000000
H	3.985364000000	0.080754000000	2.601128000000
N	1.394428000000	0.740659000000	-0.896783000000
N	1.601708000000	1.015836000000	1.247071000000
C	0.712332000000	1.093558000000	0.229243000000
C	0.900658000000	0.846960000000	-2.259356000000
C	1.320958000000	1.400884000000	2.620695000000
H	-0.927222000000	-0.063863000000	1.231836000000
C	-0.115528000000	2.328428000000	-0.016345000000
H	-0.189540000000	0.938218000000	-2.238412000000
H	1.337154000000	1.731054000000	-2.744788000000
H	1.182811000000	-0.062960000000	-2.803584000000
H	2.131409000000	2.042447000000	2.989401000000
H	0.376705000000	1.956959000000	2.644688000000
H	1.243931000000	0.505664000000	3.253238000000
C	-1.498728000000	2.281795000000	-0.205843000000
C	0.575976000000	3.543479000000	-0.093839000000
C	-2.192040000000	3.458132000000	-0.494559000000
H	-2.031092000000	1.329498000000	-0.135025000000
C	-0.126275000000	4.711318000000	-0.377397000000
H	1.657754000000	3.571283000000	0.058933000000
C	-1.507572000000	4.668886000000	-0.579364000000
H	-3.271271000000	3.424719000000	-0.645934000000
H	0.407768000000	5.660093000000	-0.441118000000
H	-2.051230000000	5.587962000000	-0.801156000000
H	1.189786000000	-2.362851000000	2.318044000000
C	0.996613000000	-2.408415000000	1.243246000000
C	-0.177059000000	-1.846878000000	0.749921000000
C	1.915309000000	-3.028904000000	0.393221000000
C	-0.471241000000	-1.923877000000	-0.629435000000
C	-1.160499000000	-1.108470000000	1.601657000000
C	1.620574000000	-3.117429000000	-0.962595000000
H	2.834512000000	-3.458224000000	0.792652000000
C	0.434195000000	-2.584154000000	-1.472805000000
N	-1.643969000000	-1.307129000000	-1.109082000000
C	-2.581616000000	-1.144932000000	1.128214000000
H	2.305968000000	-3.629147000000	-1.640146000000
H	0.210334000000	-2.719918000000	-2.529684000000
C	-2.779280000000	-1.238530000000	-0.262175000000
C	-1.894880000000	-1.316323000000	-2.536912000000
C	-3.675477000000	-1.053612000000	1.982623000000
C	-4.086899000000	-1.233414000000	-0.763511000000
H	-2.594687000000	-0.509284000000	-2.787030000000
H	-0.963402000000	-1.130626000000	-3.080797000000
H	-2.318637000000	-2.273136000000	-2.889528000000
C	-4.976152000000	-1.021225000000	1.478709000000
H	-3.502509000000	-1.002658000000	3.059368000000
C	-5.172698000000	-1.114371000000	0.105448000000
H	-4.278959000000	-1.337121000000	-1.829330000000
H	-5.825978000000	-0.937819000000	2.156010000000

H	-6.182702000000	-1.110389000000	-0.305956000000
H	-0.975170000000	-0.827864000000	2.646368000000

TRS2: reactant state, electronic energy = -1284.51472695 Hartree

C	3.870932000000	-2.329835000000	-1.146339000000
C	4.454172000000	-2.036705000000	0.081475000000
C	2.665280000000	-1.720200000000	-1.537534000000
H	4.359280000000	-3.030001000000	-1.824402000000
C	3.864566000000	-1.116867000000	0.968003000000
H	5.396134000000	-2.510899000000	0.358217000000
C	2.078284000000	-0.821902000000	-0.660324000000
H	2.218761000000	-1.939821000000	-2.508129000000
C	2.677367000000	-0.515143000000	0.581774000000
H	4.341138000000	-0.873464000000	1.917901000000
N	0.885701000000	-0.107916000000	-0.742014000000
N	1.855859000000	0.387765000000	1.237801000000
C	0.867366000000	0.897361000000	0.305082000000
C	0.218071000000	0.156324000000	-1.990939000000
C	2.282365000000	1.174360000000	2.367578000000
H	-0.139710750000	0.885143580000	0.792807410000
C	1.077765450000	2.342261220000	-0.117080890000
H	-0.795434000000	0.536879000000	-1.788388000000
H	0.747273000000	0.901752000000	-2.610036000000
H	0.133267000000	-0.780590000000	-2.559823000000
H	3.018924000000	1.949581000000	2.093504000000
H	1.410401000000	1.673628000000	2.812886000000
H	2.726067000000	0.515635000000	3.126941000000
C	0.070437230000	3.285588730000	0.076638340000
C	2.288755950000	2.728995540000	-0.705253820000
C	0.265676420000	4.613185890000	-0.309078640000
H	-0.874799650000	2.979880870000	0.535130120000
C	2.483990310000	4.052026690000	-1.090801980000
H	3.080321480000	1.988852010000	-0.856078310000
C	1.471632000000	4.994973800000	-0.891945870000
H	-0.523691080000	5.349418280000	-0.152754260000
H	3.427960300000	4.353402390000	-1.546616970000
H	1.627429540000	6.031862980000	-1.192439490000
H	0.322810000000	-1.504119000000	2.811204000000
C	0.076137000000	-1.953693000000	1.848730000000
C	-1.053880000000	-1.445417000000	1.139850000000
C	0.824657000000	-2.974051000000	1.330685000000
C	-1.405231000000	-2.005820000000	-0.135323000000
C	-1.771993000000	-0.352478000000	1.613392000000
C	0.461978000000	-3.527631000000	0.078059000000
H	1.694218000000	-3.359278000000	1.862282000000
C	-0.628209000000	-3.079064000000	-0.635134000000
N	-2.485037000000	-1.500656000000	-0.812298000000
C	-2.967436000000	0.050087000000	0.984759000000
H	1.053735000000	-4.348617000000	-0.329557000000
H	-0.882492000000	-3.578950000000	-1.565514000000
C	-3.322270000000	-0.552605000000	-0.255598000000
C	-2.790071000000	-1.988227000000	-2.159631000000
C	-3.813030000000	1.040506000000	1.553023000000
C	-4.539343000000	-0.174233000000	-0.871793000000
H	-3.188240000000	-1.164068000000	-2.758136000000
H	-1.873601000000	-2.329409000000	-2.643977000000
H	-3.519419000000	-2.810153000000	-2.126375000000
C	-4.981376000000	1.403993000000	0.932469000000
H	-3.515034000000	1.494415000000	2.499692000000
C	-5.341613000000	0.780720000000	-0.283316000000
H	-4.874989000000	-0.644835000000	-1.792184000000
H	-5.634485000000	2.156213000000	1.374098000000

H	-6.281087000000	1.050324000000	-0.767476000000
H	-1.564039080000	-0.004266290000	2.629320210000

TRS8: product state, electronic energy = -1284.52352407 Hartree

C	2.212278428460	-2.931534058274	-2.197373664962
C	1.998545273918	-2.023973544927	-3.262318314432
C	1.479771092221	-2.867137967346	-1.023657208811
H	2.975671687915	-3.702189107834	-2.308058872755
C	1.047962478164	-1.019886128394	-3.188326606723
H	2.602266893235	-2.120321409979	-4.165094589738
C	0.499930549843	-1.866809877069	-0.955621891026
H	1.647417053049	-3.561791352842	-0.200700480793
C	0.292285240711	-0.962792230140	-2.008820316912
H	0.893176920255	-0.316492707658	-4.006359819600
N	-0.427572823373	-1.559511300383	0.010263861038
N	-0.752653146986	-0.154363262932	-1.625697071229
C	-1.110878595359	-0.433394838817	-0.349797707529
C	-0.514145454017	-2.245340935004	1.294324173903
C	-1.337211376588	0.909188575140	-2.432473029692
H	-0.758853516031	0.831847394997	1.451775188952
C	-2.567082185423	-0.517180829305	0.030445949410
H	-1.205215313460	-1.698970801190	1.944409299063
H	-0.884426340861	-3.268339846572	1.142174835576
H	0.482489822634	-2.263661780035	1.758913835653
H	-2.356067041075	1.099522580980	-2.075514231876
H	-0.733629066155	1.824143433475	-2.344035921209
H	-1.375845172301	0.575667609422	-3.476036798447
C	-3.272698592423	0.588991935876	0.514457913236
C	-3.232808179429	-1.727400565806	-0.202875216113
C	-4.636063151682	0.482944586362	0.786023199501
H	-2.750370938481	1.535220787910	0.674729602783
C	-4.593891842771	-1.825821225943	0.071468181813
H	-2.692929354160	-2.584607851359	-0.609691933377
C	-5.294649203899	-0.725985995406	0.569307023700
H	-5.183194388677	1.345709551937	1.166826690600
H	-5.111875324680	-2.768033276420	-0.110788041125
H	-6.360573806609	-0.812609601526	0.783047308012
H	-1.246930256704	3.845141700333	1.148392829735
C	-0.468915905437	3.543980942773	0.442615192185
C	0.271377614940	2.397426890824	0.719449984922
C	-0.222342077354	4.316334306759	-0.693516625253
C	1.307443138914	1.996742658372	-0.153556365105
C	-0.023703565488	1.549147084054	1.914612180688
C	0.824327371518	3.950211753542	-1.531725709161
H	-0.813868775234	5.209253754004	-0.894727220235
C	1.589726427803	2.813886916707	-1.261714753472
N	2.011141641503	0.800553757077	0.085926326248
C	1.027923332137	0.560995120739	2.310426596931
H	1.074070098955	4.561666823403	-2.399929489678
H	2.429514800619	2.595170888272	-1.916496848407
C	2.002629533748	0.195540836738	1.358034952813
C	3.066404261785	0.422339753016	-0.833219651209
C	1.018262708622	-0.041231119253	3.565568987250
C	2.938820603055	-0.791605347203	1.710365653333
H	3.191266418173	-0.666186185510	-0.827560743375
H	2.788684597101	0.698286928208	-1.853849022771
H	4.032147767334	0.895745630616	-0.583803646802
C	1.929891716294	-1.042903588192	3.898426937946
H	0.271833159620	0.281991121775	4.294703053010
C	2.888783354435	-1.411608286232	2.960363532919
H	3.736707942906	-1.073346294975	1.027595549833
H	1.904361686748	-1.509061606833	4.883257602164

H	3.632374744556	-2.171679155748	3.203936007998
H	-0.736370966514	1.853718755795	2.693079340600

TRS8: reactant state, electronic energy = -1284.52350503 Hartree

C	-0.628651000000	-1.960987000000	3.393610000000
C	-0.683860000000	-0.635043000000	3.809883000000
C	-0.149651000000	-2.300087000000	2.111887000000
H	-0.935291000000	-2.754933000000	4.075204000000
C	-0.260621000000	0.410216000000	2.965645000000
H	-1.034789000000	-0.399047000000	4.815008000000
C	0.254256000000	-1.270866000000	1.277070000000
H	-0.078602000000	-3.342362000000	1.798633000000
C	0.203601000000	0.077659000000	1.702010000000
H	-0.269560000000	1.445633000000	3.308966000000
N	0.737046000000	-1.291302000000	-0.025943000000
N	0.666969000000	0.871786000000	0.663787000000
C	1.311026000000	0.011605000000	-0.325546000000
C	1.307997000000	-2.481435000000	-0.610651000000
C	1.135808000000	2.220431000000	0.871416000000
H	0.967232000000	0.323941000000	-1.342314000000
C	2.824439000000	0.127298000000	-0.363191000000
H	1.550672000000	-2.285861000000	-1.664136000000
H	2.228217000000	-2.807546000000	-0.094870000000
H	0.569935000000	-3.295919000000	-0.576284000000
H	1.369729000000	2.675124000000	-0.101168000000
H	0.341135000000	2.815885000000	1.344690000000
H	2.042325000000	2.263716000000	1.500265000000
C	3.471418000000	0.581471000000	-1.510635000000
C	3.576994000000	-0.210356000000	0.769452000000
C	4.862032000000	0.704887000000	-1.533513000000
H	2.884044000000	0.842571000000	-2.395315000000
C	4.963216000000	-0.089260000000	0.747616000000
H	3.070922000000	-0.567256000000	1.671562000000
C	5.606412000000	0.369651000000	-0.405223000000
H	5.363427000000	1.061931000000	-2.433872000000
H	5.547654000000	-0.352362000000	1.630163000000
H	6.692893000000	0.464647000000	-0.421000000000
H	-0.795014000000	3.350683000000	-2.580154000000
C	-1.299018000000	3.102186000000	-1.644527000000
C	-1.551538000000	1.726929000000	-1.362333000000
C	-1.683338000000	4.079173000000	-0.769556000000
C	-2.201955000000	1.356505000000	-0.141660000000
C	-1.142405000000	0.726943000000	-2.251409000000
C	-2.334998000000	3.708030000000	0.434189000000
H	-1.499138000000	5.130644000000	-0.988608000000
C	-2.589335000000	2.394223000000	0.749611000000
N	-2.463482000000	0.032121000000	0.105570000000
C	-1.526852000000	-0.598448000000	-2.040690000000
H	-2.653495000000	4.484944000000	1.130859000000
H	-3.111011000000	2.182789000000	1.677442000000
C	-2.165603000000	-0.943207000000	-0.810381000000
C	-3.117385000000	-0.388270000000	1.352751000000
C	-1.249397000000	-1.614919000000	-3.002781000000
C	-2.513205000000	-2.302602000000	-0.584527000000
H	-2.562282000000	-1.228622000000	1.783868000000
H	-3.084895000000	0.411756000000	2.088388000000
H	-4.158760000000	-0.673301000000	1.149182000000
C	-1.600195000000	-2.914312000000	-2.765685000000
H	-0.754992000000	-1.324391000000	-3.931351000000
C	-2.235906000000	-3.249233000000	-1.541081000000
H	-3.007242000000	-2.609506000000	0.332819000000
H	-1.397724000000	-3.690566000000	-3.503411000000

H	-2.519062000000	-4.286065000000	-1.352907000000
H	-0.849781000000	1.046133000000	-3.256080000000

The atom coordinates and electronic energies of the solution-phase TRS's

In Acetonitrile

DAD = 2.8Å

TRS2:product state, electronic energy = -1284.60046995

C	4.550066000000	-0.702143000000	-0.937732000000
C	4.857437000000	-0.331776000000	0.390591000000
C	3.313377000000	-0.435197000000	-1.506163000000
H	5.307084000000	-1.216492000000	-1.531195000000
C	3.938869000000	0.324803000000	1.196426000000
H	5.843907000000	-0.569122000000	0.791132000000
C	2.385483000000	0.235787000000	-0.698591000000
H	3.077366000000	-0.727860000000	-2.529173000000
C	2.698837000000	0.611274000000	0.616027000000
H	4.167536000000	0.611149000000	2.223187000000
N	1.099740000000	0.673739000000	-0.929002000000
N	1.590420000000	1.260692000000	1.112059000000
C	0.573486000000	1.197956000000	0.220199000000
C	0.405363000000	0.585112000000	-2.204158000000
C	1.510824000000	1.867653000000	2.432373000000
H	-0.796012000000	0.101619000000	0.764657000000
C	-0.256684030000	2.419596240000	-0.098724630000
H	-0.652955000000	0.363085000000	-2.027738000000
H	0.505039000000	1.533758000000	-2.750348000000
H	0.852296000000	-0.228694000000	-2.786447000000
H	2.298000000000	2.626945000000	2.526900000000
H	0.527758000000	2.336618000000	2.548615000000
H	1.647348000000	1.097187000000	3.202654000000
C	-1.636771720000	2.366199490000	-0.303485270000
C	0.437690460000	3.625484830000	-0.254864050000
C	-2.323559890000	3.518630880000	-0.687808330000
H	-2.176671500000	1.425329680000	-0.171901000000
C	-0.256967820000	4.771682470000	-0.633990000000
H	1.516872920000	3.662811090000	-0.090102470000
C	-1.635388470000	4.719809420000	-0.852148670000
H	-3.400869460000	3.474722570000	-0.853418790000
H	0.283677920000	5.711043390000	-0.759710250000
H	-2.173869180000	5.621205940000	-1.149292490000
H	1.378279000000	-1.662891000000	2.563328000000
C	1.172015000000	-2.069592000000	1.570172000000
C	-0.017185000000	-1.716888000000	0.938272000000
C	2.099600000000	-2.902772000000	0.941070000000
C	-0.320337000000	-2.230792000000	-0.342653000000
C	-0.989745000000	-0.739044000000	1.502514000000
C	1.808421000000	-3.399184000000	-0.327752000000
H	3.035928000000	-3.160587000000	1.438306000000
C	0.607614000000	-3.080124000000	-0.965416000000
N	-1.525093000000	-1.857508000000	-0.956882000000
C	-2.415821000000	-0.967598000000	1.115529000000
H	2.516872000000	-4.057178000000	-0.834789000000
H	0.396724000000	-3.509862000000	-1.943386000000
C	-2.635770000000	-1.525230000000	-0.163124000000
C	-1.746627000000	-2.227349000000	-2.341968000000
C	-3.497912000000	-0.600934000000	1.911481000000
C	-3.953849000000	-1.702681000000	-0.608773000000
H	-2.499703000000	-1.560773000000	-2.778937000000
H	-0.816441000000	-2.096126000000	-2.906638000000
H	-2.086303000000	-3.271535000000	-2.453827000000

C	-4.808817000000	-0.755926000000	1.453855000000
H	-3.303558000000	-0.174907000000	2.898190000000
C	-5.026424000000	-1.309647000000	0.194668000000
H	-4.154837000000	-2.153005000000	-1.579626000000
H	-5.649207000000	-0.451935000000	2.079323000000
H	-6.043764000000	-1.450714000000	-0.174803000000
H	-0.777515220000	-0.094368840000	2.364762980000

TRS2:reactant state, electronic energy = -1284.60046628

C	4.228005239291	-1.413278708776	-1.182812476193
C	4.724530614512	-0.992530459926	0.044256829409
C	2.915576467918	-1.084018135850	-1.587921817245
H	4.859180733375	-2.000394013207	-1.851979058783
C	3.936574774569	-0.219705020221	0.925858717775
H	5.744719205198	-1.250665971040	0.333636656647
C	2.139496161860	-0.337442950220	-0.717840236463
H	2.524912581220	-1.407280100810	-2.554089897390
C	2.647839943501	0.098047515095	0.530787021084
H	4.332855621977	0.122886857484	1.882730706247
N	0.830619479263	0.103323496967	-0.814867304075
N	1.639915592825	0.789911007352	1.172219266165
C	0.540759864963	1.023658152776	0.259544924090
C	0.090821179769	0.122301029527	-2.051284079561
C	1.826095323437	1.591369661257	2.352514002184
H	-0.420158669410	0.749692597246	0.752773257648
C	0.351279836984	2.483253621714	-0.140605845054
H	-0.955655069276	0.389285536743	-1.845930454439
H	0.501961586354	0.846118534913	-2.777671149621
H	0.107443280256	-0.879558564699	-2.506418116770
H	2.355527766167	2.538657755450	2.144605132354
H	0.845515052757	1.829265254746	2.788364118927
H	2.402895080968	1.023079593834	3.096115831686
C	-0.831207495576	3.150446674843	0.179635569063
C	1.368211268436	3.162870398397	-0.823621829904
C	-1.002392420197	4.490757693770	-0.176553094569
H	-1.623348474502	2.615680451193	0.711533333731
C	1.198471837931	4.499032049710	-1.179158521282
H	2.295754356612	2.640802599182	-1.076152831251
C	0.011659756078	5.164364261692	-0.855441656255
H	-1.929745250284	5.007455934279	0.076764561193
H	1.992411888724	5.026505014905	-1.710848069166
H	-0.119842085058	6.211240866232	-1.134928509436
H	0.925145377218	-1.500768387145	2.720136672554
C	0.686970255188	-2.042951068806	1.803654432062
C	-0.507777421557	-1.688420331864	1.111517114722
C	1.503143307969	-3.029178471209	1.321449804691
C	-0.865644787939	-2.368487276312	-0.097514224269
C	-1.308443006762	-0.632980014029	1.554225321406
C	1.143716887326	-3.698023014240	0.123075317379
H	2.417994097069	-3.305997030751	1.846103486770
C	-0.004108645547	-3.393175491329	-0.571814479522
N	-2.017784661432	-2.025566096048	-0.749393701466
C	-2.583226525009	-0.432779993115	0.984165414400
H	1.788241438124	-4.492962646838	-0.256815554985
H	-0.247028551416	-3.966103458350	-1.462409544869
C	-2.925883429937	-1.148701663267	-0.197286147931
C	-2.323128280719	-2.613302912889	-2.058223742094
C	-3.507249361842	0.489208546157	1.545939068979
C	-4.207690946365	-0.945937474518	-0.768774638574
H	-2.819679180819	-1.861124044505	-2.677533004217
H	-1.396290474383	-2.894110297387	-2.561457655093
H	-2.971215976586	-3.493379853995	-1.945549668334

C	-4.739297485372	0.677602379308	0.972926350087
H	-3.208799885490	1.032268121048	2.444662778769
C	-5.083460510652	-0.054782167595	-0.187867555333
H	-4.523669605905	-1.502109893924	-1.647771092687
H	-5.453573270280	1.377664353188	1.406860658038
H	-6.069643879932	0.080323207660	-0.634910091422
H	-1.071509505593	-0.159033653806	2.510917700194

TRS8:product state, electronic energy = -1284.60536585

C	-1.802911110998	-1.573887938575	3.373708580808
C	-1.883731520855	-0.197586360041	3.682023478944
C	-0.966201988884	-2.053225750540	2.374901844731
H	-2.417624875108	-2.278099905211	3.936060506379
C	-1.130889880751	0.749845705190	3.001852875626
H	-2.558783050958	0.127728591863	4.474714834534
C	-0.190373543156	-1.101632829473	1.703342273405
H	-0.902313785435	-3.114382177690	2.132506162389
C	-0.272551024395	0.264988747233	2.009127382990
H	-1.192629963570	1.813984663006	3.231429136994
N	0.767485010598	-1.227954260900	0.725975782403
N	0.640008966755	0.904493917791	1.202778943952
C	1.205216559387	0.014246123759	0.337968424357
C	1.156914596810	-2.500860188755	0.140024815459
C	0.947080743605	2.323726799959	1.280817469346
H	0.639070723469	0.305784866134	-1.214999997814
C	2.703395845833	0.036905364109	0.121837401901
H	1.831657908565	-2.319067757950	-0.702781558086
H	1.665864818822	-3.113413923773	0.897202217981
H	0.257814698332	-3.023156307222	-0.217075196229
H	1.719648119034	2.563532138150	0.542438746326
H	0.041988582815	2.910012044044	1.067620412018
H	1.312957921597	2.557012297836	2.289809136541
C	3.309087960190	0.724243898075	-0.932580991193
C	3.493142394485	-0.610566288296	1.081456163148
C	4.700295902259	0.751076780957	-1.040763390102
H	2.697883869529	1.246752837215	-1.669897477590
C	4.880398451778	-0.579938145052	0.967206786313
H	3.023899042819	-1.132341798571	1.917957108469
C	5.485925811163	0.095999685789	-0.094357379933
H	5.167817170070	1.286437153616	-1.868274556806
H	5.491717534865	-1.086601102622	1.715592601570
H	6.573654206335	0.113834928434	-0.179697895866
H	0.403984123563	3.112648933299	-2.556572019320
C	-0.438266284786	2.947969473252	-1.880566805751
C	-0.814738973228	1.634283734490	-1.597920755066
C	-1.105376763432	4.029790318350	-1.309935466033
C	-1.908057441905	1.375629582361	-0.739706183317
C	-0.050144621027	0.476569069006	-2.121775322941
C	-2.185862026927	3.779777398125	-0.465027863205
H	-0.793648998475	5.051531175935	-1.529702418731
C	-2.593689322827	2.474941242689	-0.190441971480
N	-2.271476632321	0.054898859172	-0.441548777345
C	-0.748634493054	-0.833808539939	-2.123391882928
H	-2.737733777944	4.608712467429	-0.018166318702
H	-3.463514650885	2.326958450384	0.445309263812
C	-1.842931802279	-1.008948400172	-1.247380848741
C	-3.369975772769	-0.178331985601	0.478851770665
C	-0.313979508417	-1.891070331142	-2.922997161176
C	-2.464345616238	-2.270449612986	-1.200666332655
H	-3.251016935931	-1.156359007633	0.956146262812
H	-3.352609096315	0.568541531536	1.277457209857
H	-4.350042369523	-0.141539922363	-0.027720894536

C	-0.919699317200	-3.144036480355	-2.855684884925
H	0.526728632686	-1.719069521587	-3.599213617445
C	-1.996202717777	-3.322458890435	-1.987777975082
H	-3.328564534200	-2.442960932926	-0.562879684968
H	-0.562303246808	-3.965876330965	-3.477275241528
H	-2.498032018784	-4.289827794560	-1.926108082992
H	0.806047071798	0.589057706148	-2.797679641244

TRS8:reactant state, electronic energy = -1284.60536391

C	-1.276026228049	-1.445510629682	3.509451867197
C	-1.261140256549	-0.079029405159	3.773731584369
C	-0.650367827034	-1.971447820817	2.360847852312
H	-1.769983071264	-2.126686577673	4.204397385097
C	-0.618040603706	0.823926463172	2.903486789099
H	-1.744771471105	0.304091907495	4.673890457561
C	-0.025491739898	-1.081720960227	1.500008037022
H	-0.649237396178	-3.043647359345	2.159043358497
C	-0.006165555606	0.307252748178	1.770623917706
H	-0.591435925790	1.893369794937	3.118146117492
N	0.645101636815	-1.292114584799	0.310673510196
N	0.684140386715	0.930509347694	0.750665431091
C	1.270975202837	-0.063897586854	-0.126394648384
C	1.140872530883	-2.585280756211	-0.092383484804
C	1.218999159837	2.264767010668	0.865643690064
H	0.971433677686	0.149608087160	-1.188168325145
C	2.792565255188	-0.048752331891	-0.154079286921
H	1.543726213656	-2.519024962260	-1.111649491907
H	1.935987460751	-2.954986947237	0.579655276029
H	0.315223518296	-3.312042839282	-0.097980423885
H	1.646478100479	2.569743777543	-0.098325580828
H	0.411194923503	2.967415845804	1.119261594033
H	2.005600171814	2.332948819247	1.638462392354
C	3.477602197069	0.243268406256	-1.332859441845
C	3.509586495490	-0.316473576173	1.018914067992
C	4.874615058951	0.272281483917	-1.344770912067
H	2.913495562265	0.451157394118	-2.246276358465
C	4.902154767959	-0.289256674526	1.007831407935
H	2.969395533006	-0.545295890774	1.942491631836
C	5.585870124840	0.005984092927	-0.175864410319
H	5.406559692720	0.502779763710	-2.269432563434
H	5.459153387156	-0.498390146204	1.922857583986
H	6.677133974487	0.027660709915	-0.183814443184
H	0.154501100850	2.934266843408	-2.713267160668
C	-0.598400149413	2.863617157432	-1.925714472732
C	-1.064150043804	1.567933644280	-1.564131234472
C	-1.089763139082	3.981281310957	-1.305755939854
C	-2.037600650038	1.422932670216	-0.530002077880
C	-0.555318439733	0.419401476200	-2.193074503243
C	-2.062771702230	3.833107753421	-0.286500536859
H	-0.742590919861	4.975510170332	-1.587780931894
C	-2.527681678906	2.596844685062	0.101679570595
N	-2.485592650202	0.169635270290	-0.192128309452
C	-1.181148654211	-0.818832706068	-1.979292546952
H	-2.466728488134	4.721447342577	0.201972855855
H	-3.297283876047	2.545296389006	0.866929164332
C	-2.142949331531	-0.934122334466	-0.932991546930
C	-3.400647112192	-0.009593191952	0.940198638631
C	-0.836450942211	-1.961085328866	-2.755537419121
C	-2.735280162831	-2.202177882886	-0.694256871413
H	-3.126242948104	-0.922288622067	1.478393227924
H	-3.295529935989	0.819686035383	1.640128676502
H	-4.438900415983	-0.076870053785	0.586196841832

C	-1.430706085668	-3.171723148246	-2.517188282025
H	-0.089907289736	-1.838573009407	-3.542631963752
C	-2.383127409554	-3.281266537897	-1.473334360130
H	-3.485456103528	-2.332466626877	0.081394744112
H	-1.175197935380	-4.047022611268	-3.114848345590
H	-2.860174457927	-4.244153215286	-1.282585397894
H	0.077266964217	0.552814066879	-3.074334119603

In Chloroform

DAD = 2.8Å
TRS2:product state, electronic energy = -1284.58886073

C	4.602512000000	-0.644045000000	-0.865787000000
C	4.881232000000	-0.264973000000	0.465447000000
C	3.370291000000	-0.401906000000	-1.453837000000
H	5.378310000000	-1.145640000000	-1.445384000000
C	3.937882000000	0.377252000000	1.253801000000
H	5.865125000000	-0.482806000000	0.882660000000
C	2.417422000000	0.254583000000	-0.664745000000
H	3.157981000000	-0.702892000000	-2.479466000000
C	2.703061000000	0.640700000000	0.652749000000
H	4.147654000000	0.670254000000	2.282723000000
N	1.127207000000	0.670182000000	-0.917450000000
N	1.575446000000	1.274992000000	1.127332000000
C	0.570044000000	1.186589000000	0.221476000000
C	0.462740000000	0.577982000000	-2.207747000000
C	1.463859000000	1.886895000000	2.442351000000
H	-0.763687000000	0.087569000000	0.790634000000
C	-0.283197000000	2.387395000000	-0.114358000000
H	-0.589439000000	0.310739000000	-2.059323000000
H	0.532856000000	1.539502000000	-2.735777000000
H	0.954810000000	-0.205079000000	-2.795443000000
H	2.229958000000	2.666585000000	2.546449000000
H	0.470140000000	2.337624000000	2.542246000000
H	1.606646000000	1.127771000000	3.223216000000
C	-1.661448000000	2.298761000000	-0.320107000000
C	0.382845000000	3.607483000000	-0.283566000000
C	-2.374295000000	3.429955000000	-0.719401000000
H	-2.181470000000	1.348403000000	-0.175481000000
C	-0.337820000000	4.731806000000	-0.677845000000
H	1.460460000000	3.672546000000	-0.116570000000
C	-1.714085000000	4.644245000000	-0.897558000000
H	-3.450078000000	3.359071000000	-0.884739000000
H	0.179731000000	5.682515000000	-0.814030000000
H	-2.272874000000	5.529114000000	-1.206059000000
H	1.423186000000	-1.735025000000	2.509525000000
C	1.203416000000	-2.105876000000	1.505445000000
C	0.003411000000	-1.737646000000	0.903828000000
C	2.122704000000	-2.915181000000	0.836988000000
C	-0.321455000000	-2.215796000000	-0.384807000000
C	-0.958020000000	-0.774825000000	1.509059000000
C	1.810253000000	-3.377017000000	-0.439276000000
H	3.067166000000	-3.185885000000	1.310682000000
C	0.597126000000	-3.046047000000	-1.045527000000
N	-1.536439000000	-1.822512000000	-0.968979000000
C	-2.390798000000	-0.983103000000	1.139923000000
H	2.510115000000	-4.021424000000	-0.974493000000
H	0.366693000000	-3.457503000000	-2.026842000000
C	-2.634795000000	-1.511301000000	-0.145548000000
C	-1.791209000000	-2.178302000000	-2.351602000000
C	-3.457203000000	-0.630344000000	1.963046000000
C	-3.960649000000	-1.677777000000	-0.570058000000

H	-2.553599000000	-1.507284000000	-2.765266000000
H	-0.875806000000	-2.043096000000	-2.939111000000
H	-2.134178000000	-3.221081000000	-2.466993000000
C	-4.775290000000	-0.771789000000	1.525875000000
H	-3.245896000000	-0.230576000000	2.957093000000
C	-5.016903000000	-1.299441000000	0.260256000000
H	-4.181720000000	-2.112408000000	-1.543415000000
H	-5.603660000000	-0.481509000000	2.173062000000
H	-6.041048000000	-1.433428000000	-0.091949000000
H	-0.730675000000	-0.154331000000	2.384876000000

TRS2:reactant state, electronic energy = -1284.58886184

C	4.224717000000	-1.411023000000	-1.204327000000
C	4.735451000000	-0.978648000000	0.013499000000
C	2.905528000000	-1.097569000000	-1.590547000000
H	4.853260000000	-1.993041000000	-1.879895000000
C	3.955094000000	-0.210240000000	0.901798000000
H	5.763173000000	-1.223080000000	0.286459000000
C	2.137316000000	-0.351192000000	-0.713297000000
H	2.506034000000	-1.425724000000	-2.551387000000
C	2.658263000000	0.094205000000	0.522963000000
H	4.365479000000	0.144728000000	1.848034000000
N	0.823969000000	0.087356000000	-0.799912000000
N	1.654244000000	0.788837000000	1.174331000000
C	0.543993000000	1.009850000000	0.273752000000
C	0.093930000000	0.128478000000	-2.041963000000
C	1.874759000000	1.631661000000	2.320966000000
H	-0.412858290000	0.726595930000	0.781499390000
C	0.339807950000	2.464500340000	-0.134149210000
H	-0.947486000000	0.421953000000	-1.847014000000
H	0.527585000000	0.844959000000	-2.761928000000
H	0.090885000000	-0.871712000000	-2.501286000000
H	2.409151000000	2.564104000000	2.066266000000
H	0.908209000000	1.901026000000	2.769685000000
H	2.461007000000	1.084538000000	3.073089000000
C	-0.845491360000	3.126214280000	0.184804140000
C	1.351528660000	3.145965650000	-0.822720340000
C	-1.026023940000	4.463195470000	-0.177573690000
H	-1.634763560000	2.590883800000	0.720538320000
C	1.172330090000	4.478714840000	-1.184145200000
H	2.282334240000	2.628581190000	-1.072889170000
C	-0.017359210000	5.138534750000	-0.861374870000
H	-1.955410510000	4.976240920000	0.074943110000
H	1.962335310000	5.008492320000	-1.719014410000
H	-0.155046570000	6.183265690000	-1.145096260000
H	0.905199000000	-1.465382000000	2.753778000000
C	0.681389000000	-2.005433000000	1.832714000000
C	-0.515099000000	-1.670577000000	1.134854000000
C	1.523811000000	-2.968566000000	1.348674000000
C	-0.853044000000	-2.355418000000	-0.077716000000
C	-1.330913000000	-0.620979000000	1.564212000000
C	1.184798000000	-3.639180000000	0.147074000000
H	2.444246000000	-3.223973000000	1.873634000000
C	0.028860000000	-3.362332000000	-0.547278000000
N	-2.006081000000	-2.029982000000	-0.739806000000
C	-2.603771000000	-0.431704000000	0.978630000000
H	1.851099000000	-4.414868000000	-0.234552000000
H	-0.200125000000	-3.941577000000	-1.437413000000
C	-2.930217000000	-1.158720000000	-0.200011000000
C	-2.292282000000	-2.633342000000	-2.044372000000
C	-3.542908000000	0.481322000000	1.526975000000
C	-4.209960000000	-0.974641000000	-0.779918000000

H	-2.811460000000	-1.902718000000	-2.670988000000
H	-1.356656000000	-2.888050000000	-2.546182000000
H	-2.911259000000	-3.534571000000	-1.930925000000
C	-4.773232000000	0.654388000000	0.943864000000
H	-3.262931000000	1.031872000000	2.427133000000
C	-5.100824000000	-0.088320000000	-0.213011000000
H	-4.516459000000	-1.541891000000	-1.655086000000
H	-5.497897000000	1.348393000000	1.369890000000
H	-6.085215000000	0.031889000000	-0.667841000000
H	-1.110544570000	-0.139171690000	2.520629220000

TRS8:product state, electronic energy = -1284.59556304

C	-1.827955196645	-1.468789618714	3.411131720771
C	-1.898355494112	-0.085121754818	3.684070225422
C	-0.991924745781	-1.980249779482	2.427798720541
H	-2.449740759090	-2.153181214226	3.989724445131
C	-1.135358154651	0.837516693042	2.981699455466
H	-2.572184375195	0.265683900876	4.466692563001
C	-0.204449699027	-1.053843014829	1.735325766064
H	-0.939143714485	-3.048219272110	2.214284034530
C	-0.277067080203	0.320394599295	2.005981619601
H	-1.189402077853	1.907813683284	3.183223549396
N	0.758529148142	-1.212859174094	0.766392184995
N	0.644530894360	0.932828029007	1.188564305432
C	1.206916048742	0.016794726147	0.347328772381
C	1.137508252550	-2.503903094758	0.213878348529
C	0.957065889635	2.351951886022	1.232511851738
H	0.639361676029	0.268242855314	-1.204118673671
C	2.704168713116	0.030491055327	0.128808651539
H	1.835975537513	-2.352889409565	-0.615653986855
H	1.619950394851	-3.111272584448	0.992556991401
H	0.239423256332	-3.018367974515	-0.157425132109
H	1.760858716530	2.564113321456	0.519080161729
H	0.066412738935	2.938407175791	0.964805965919
H	1.288818458061	2.615772280555	2.245842631486
C	3.309128275980	0.695498547359	-0.940508760045
C	3.496441399736	-0.596954398909	1.099479682605
C	4.699741743045	0.718918693984	-1.052891906997
H	2.698488206127	1.204346455809	-1.687934053485
C	4.883078236522	-0.570540737756	0.981123470005
H	3.029315960819	-1.099217315323	1.949033653968
C	5.486495659972	0.082212681335	-0.095595675499
H	5.166387448238	1.236878121861	-1.891727970611
H	5.496251440665	-1.061531920475	1.738191318200
H	6.573773605140	0.096809063262	-0.184271350958
H	0.404806443088	3.048668387709	-2.645325928281
C	-0.429383432327	2.898515229939	-1.956084219226
C	-0.802384937693	1.592461979885	-1.636030758480
C	-1.095209072590	3.994144582361	-1.412514396951
C	-1.896082213398	1.355539144172	-0.772519216849
C	-0.039169358703	0.420453055445	-2.127415344951
C	-2.172097506413	3.765642112272	-0.557346513852
H	-0.788920072345	5.009902204925	-1.664328999604
C	-2.579019287856	2.468555547942	-0.248763485026
N	-2.263140758279	0.042499775716	-0.445413162965
C	-0.739421676928	-0.887985641467	-2.103221814400
H	-2.724622757956	4.606031280221	-0.133627825184
H	-3.449742901780	2.336850425294	0.389190380356
C	-1.838323700891	-1.039756675426	-1.229366592888
C	-3.371888437029	-0.163195282179	0.468747583327
C	-0.306354283121	-1.962454416493	-2.880605514499
C	-2.467277777481	-2.296310124274	-1.163499522108

H	-3.273144720584	-1.137629564767	0.957410618527
H	-3.346242206912	0.590448298063	1.260919958253
H	-4.347676373956	-0.114114305072	-0.044997738721
C	-0.918122623893	-3.210256521763	-2.791828675352
H	0.533800587251	-1.807730373752	-3.561742759106
C	-2.000922198865	-3.365388097375	-1.927492166872
H	-3.340131860415	-2.450666950698	-0.533105353684
H	-0.565411102285	-4.044665413827	-3.398800361464
H	-2.511417519551	-4.327232431410	-1.854297579010
H	0.825893346912	0.512318268857	-2.794918190608

TRS8:reactant state, electronic energy = -1284.59556494

C	-1.333300234158	-1.462812559617	3.491072563763
C	-1.321724345454	-0.096834127647	3.762336110150
C	-0.692753484198	-1.983166688136	2.350408711556
H	-1.832748889856	-2.146647999714	4.179065703748
C	-0.666586479548	0.808970967703	2.907295250887
H	-1.813919488676	0.280111481957	4.660162514181
C	-0.055282754997	-1.088910609557	1.502850070688
H	-0.685867495947	-3.054798672192	2.146479167416
C	-0.038551387423	0.297088993919	1.780534930461
H	-0.637793172939	1.876373158339	3.131041153412
N	0.635610728354	-1.294607030967	0.323536832250
N	0.671793116415	0.925164326542	0.775947315079
C	1.262528365355	-0.064312399944	-0.100838455572
C	1.139270918500	-2.586865827530	-0.073977071364
C	1.211605880758	2.255940244907	0.913454583453
H	0.959294965975	0.155316908648	-1.165307627846
C	2.783281056832	-0.050301268651	-0.131839886366
H	1.574014791302	-2.515777665352	-1.079571984141
H	1.913068270908	-2.963355807242	0.618075534667
H	0.311886111788	-3.310698671314	-0.111404743681
H	1.673134686871	2.562943289256	-0.033812945422
H	0.400789604655	2.963555627079	1.142358877211
H	1.973996846858	2.314882966594	1.710237406623
C	3.469564573091	0.227912784457	-1.312893401762
C	3.498870641325	-0.310490809191	1.043326053564
C	4.866222339569	0.251166064957	-1.325697334375
H	2.908724985905	0.429908182549	-2.229839120071
C	4.890930273898	-0.288942318568	1.031424912155
H	2.957064732375	-0.528943342449	1.968421097833
C	5.575501588123	-0.007230914961	-0.154561332272
H	5.399515150984	0.470930964807	-2.251986918235
H	5.447252757222	-0.492137302413	1.947971858347
H	6.666658752757	0.009926670732	-0.162649384805
H	0.200479133683	2.946522307830	-2.707163503987
C	-0.557338429793	2.872488071839	-1.924530654696
C	-1.031701112568	1.577613927566	-1.573186812905
C	-1.047574873034	3.990740628078	-1.304579311529
C	-2.014698847059	1.433417097930	-0.548650314536
C	-0.522438190177	0.427376195169	-2.201373336540
C	-2.030988765184	3.843750276382	-0.296163878483
H	-0.693033712427	4.983924509080	-1.580618325321
C	-2.504972093700	2.607551227914	0.081227797575
N	-2.471683578858	0.180451303494	-0.217367774700
C	-1.153559817000	-0.810694666794	-1.994170220874
H	-2.436254701116	4.731955009639	0.191324107767
H	-3.283676503626	2.555827476649	0.836974900376
C	-2.124979012718	-0.923957100728	-0.957173083894
C	-3.398998999916	0.002176984520	0.904662407609
C	-0.806190944076	-1.953418883422	-2.767337304655
C	-2.722114365253	-2.190262541670	-0.725198183716

H	-3.126827276926	-0.906029141694	1.451876409908
H	-3.302474571657	0.831523187183	1.605449829997
H	-4.433972698529	-0.067920463043	0.540856206650
C	-1.404702717992	-3.163299784772	-2.535271158319
H	-0.055221718302	-1.834718489709	-3.551153170149
C	-2.366450477862	-3.270821299149	-1.500755910822
H	-3.479118984454	-2.318591341093	0.043854325091
H	-1.146746648807	-4.037961359328	-3.132672063687
H	-2.848684205987	-4.232131759310	-1.315413906036
H	0.121971186709	0.557620920436	-3.074434301656

In Acetonitrile

DAD = 3.2Å

TRS2:product state, electronic energy = -1284.60670490

C	4.754948920265	-0.859816612026	-0.667896605885
C	4.875975873815	-0.711299816357	0.735199550546
C	3.637714168551	-0.420164045574	-1.357213046166
H	5.565900281722	-1.338511182692	-1.218295229670
C	3.885805965975	-0.112305819725	1.495780281854
H	5.776510886440	-1.079939187691	1.228136643258
C	2.633563524960	0.188400250592	-0.590477120619
H	3.538028197880	-0.540833000736	-2.436073716953
C	2.761536809853	0.346215360129	0.796336520319
H	3.972242681280	0.004004250756	2.576220469220
N	1.417382452563	0.731897781668	-0.930937823165
N	1.620907041667	0.984848562083	1.221470531108
C	0.746104084167	1.097611560689	0.197927849679
C	0.948709778877	0.862166061150	-2.301860516462
C	1.351168053935	1.363076088211	2.601184925360
H	-0.964266957042	-0.020450321663	1.146680401255
C	-0.052201327792	2.352855460859	-0.031520565150
H	-0.135866534253	1.001931840587	-2.308340077509
H	1.438800611867	1.726064680729	-2.772059147246
H	1.204171523404	-0.054307440838	-2.848543274875
H	2.147315830528	2.033320073694	2.949030898003
H	0.386001724972	1.878980453526	2.644430550202
H	1.323686492318	0.463586608922	3.230446505878
C	-1.400825377237	2.322650076924	-0.395080522079
C	0.629007358769	3.570352279934	0.078344548542
C	-2.067471564556	3.515794573424	-0.674082701845
H	-1.919339543531	1.363261540265	-0.469861805220
C	-0.046648926987	4.757094146770	-0.198222798085
H	1.681821964348	3.586375841182	0.369118335256
C	-1.391022116994	4.731368850017	-0.575260230474
H	-3.118742742159	3.492648840129	-0.964181002480
H	0.482579608759	5.707881092882	-0.118306766812
H	-1.912984460664	5.665141889068	-0.790797650141
H	1.139183645635	-2.298908125594	2.363543223147
C	0.935299487446	-2.396315455501	1.294261779472
C	-0.226747207394	-1.827362821646	0.780963635942
C	1.837598561866	-3.067723457352	0.463071330233
C	-0.522103124045	-1.945914239628	-0.595721781509
C	-1.191929906672	-1.028686917942	1.598950081952
C	1.546550561132	-3.184804264031	-0.892727388872
H	2.752775393393	-3.495623135971	0.875562919243
C	0.373208950079	-2.640001402180	-1.422556246838
N	-1.690812275903	-1.339109357919	-1.090942933566
C	-2.616182990695	-1.086177868117	1.137632789746
H	2.231510653502	-3.713799146759	-1.558306586842
H	0.159999527883	-2.771477669716	-2.482391985206
C	-2.816979703433	-1.231733725204	-0.251663579940

C	-1.916321367107	-1.323866819802	-2.523741666399
C	-3.709893989502	-0.956601278350	1.987838563407
C	-4.126233327452	-1.233782176036	-0.753196319443
H	-2.605409175626	-0.507035282753	-2.772457536446
H	-0.971959516170	-1.135018866501	-3.044017827963
H	-2.341310916041	-2.272648929154	-2.896074052159
C	-5.013492893421	-0.934437223637	1.482738751420
H	-3.532009727388	-0.856225071978	3.060780133009
C	-5.211724434963	-1.075429845533	0.112629179862
H	-4.312782757914	-1.363442308104	-1.817892008384
H	-5.862155994146	-0.814196379364	2.157559450847
H	-6.222273196661	-1.072792624899	-0.299953303990
H	-0.977779562104	-0.656341343216	2.608907969629

TRS2:reactant state, electronic energy = -1284.60670389

C	3.842398725826	-2.292646299695	-1.247097693345
C	4.451555685851	-2.007376694440	-0.032369022042
C	2.626565462026	-1.672910294390	-1.613160363079
H	4.308077443149	-2.998448269903	-1.937018736200
C	3.880086196734	-1.084948488081	0.872765691025
H	5.394882734166	-2.490511331688	0.228367151809
C	2.056884861835	-0.782993179731	-0.718964719717
H	2.149086342725	-1.891768049194	-2.569662007525
C	2.684923843874	-0.481346139825	0.516786945500
H	4.369788777964	-0.848527699703	1.818515998884
N	0.866782476599	-0.074633376979	-0.768782974747
N	1.878313640505	0.414939595020	1.188173363714
C	0.861173939816	0.924816288558	0.283075824223
C	0.115120302322	0.126408333194	-1.980179222035
C	2.274386081461	1.139224843446	2.365134212724
H	-0.125469368399	0.900000463734	0.794015143834
C	1.043259068098	2.385786445466	-0.110435417304
H	-0.864633459192	0.560500800028	-1.731034089046
H	0.625015783203	0.799495029945	-2.693571849491
H	-0.053701281367	-0.843346518266	-2.471868736892
H	2.994289589458	1.949837345501	2.149719839057
H	1.384424906421	1.580465787201	2.836208318128
H	2.733028746118	0.446160210209	3.084853996278
C	0.030271008045	3.308868140756	0.149903006221
C	2.226449880876	2.813995964550	-0.727273639102
C	0.192877756621	4.652238877988	-0.198142991085
H	-0.891821377996	2.972167935699	0.632202595072
C	2.390371104606	4.153014769224	-1.075253263884
H	3.023610930331	2.093310351740	-0.931321225518
C	1.372030049071	5.074135188803	-0.810309980813
H	-0.603285872818	5.369022858279	0.010373127899
H	3.314032165335	4.482955092419	-1.554109910419
H	1.501589485493	6.123369931482	-1.081854705763
H	0.334914100735	-1.529771149072	2.854770295476
C	0.081962003346	-2.010602162969	1.908368063706
C	-1.028688629250	-1.493361719367	1.174868007340
C	0.790322759337	-3.078752372763	1.433751493798
C	-1.390119008143	-2.076795977096	-0.084675335591
C	-1.730245201473	-0.381125090312	1.631816537300
C	0.413001843298	-3.664359375966	0.196815852517
H	1.635211097661	-3.484091484840	1.991083083997
C	-0.641946987596	-3.192145713175	-0.548006828956
N	-2.445044464352	-1.558942416156	-0.783961947824
C	-2.899072451347	0.038182789364	0.978548657818
H	0.970605178257	-4.525586203049	-0.175968261816
H	-0.898653061125	-3.703858301438	-1.471177891956
C	-3.249149128473	-0.574655106071	-0.260293597448

C	-2.761793377140	-2.061079585269	-2.126630140913
C	-3.719657399615	1.070720491798	1.515399158116
C	-4.438042645101	-0.158401244136	-0.914172301576
H	-3.047384153408	-1.217116981979	-2.761279069959
H	-1.879651995341	-2.523628074745	-2.569464228498
H	-3.583520859805	-2.788373753321	-2.077568013110
C	-4.857749179418	1.463645803128	0.861964313389
H	-3.416089443230	1.528500487098	2.458547855850
C	-5.213120695225	0.832904553680	-0.356199880434
H	-4.761666475438	-0.627027449856	-1.840098737387
H	-5.492815820151	2.248746252293	1.272846624939
H	-6.129243392036	1.133413826687	-0.867226925210
H	-1.514190243730	-0.007345953815	2.636798550074

TRS8:product state, electronic energy = -1284.61122824

C	2.247845464810	-3.309646789782	-1.609803363433
C	1.987787961782	-2.662444832836	-2.842581012839
C	1.532408441424	-3.014324375638	-0.460965843647
H	3.034980507044	-4.063716716864	-1.567389710704
C	1.007853045368	-1.692313895023	-2.967543624678
H	2.580635694176	-2.936287508480	-3.716244526261
C	0.525758189563	-2.046560328153	-0.589634757787
H	1.728367540277	-3.511502360944	0.489213980312
C	0.276700489570	-1.398216090830	-1.808121692916
H	0.809520759097	-1.183826437018	-3.911253778901
N	-0.386980812089	-1.550580703312	0.308009328512
N	-0.770271263690	-0.536627859873	-1.584128890382
C	-1.101307461911	-0.543683638547	-0.272249226179
C	-0.460490080788	-1.969996882092	1.701082221267
C	-1.390759570647	0.291041534145	-2.608006216980
H	-0.689702458615	0.970290713244	1.243155147105
C	-2.547903990667	-0.558596068384	0.154846120248
H	-1.104553859010	-1.275590938290	2.250807802423
H	-0.872888371109	-2.986433008206	1.756783205284
H	0.551702319570	-1.952323508238	2.128452349279
H	-2.266846058222	0.789413642537	-2.179467487857
H	-0.671354550500	1.043344659583	-2.958594559858
H	-1.697465684304	-0.350409105829	-3.443487106659
C	-3.254837457162	0.609157351488	0.456960926171
C	-3.197491138156	-1.799493396671	0.170893004543
C	-4.606824336875	0.537611848930	0.792544153735
H	-2.745046487531	1.574825097620	0.427353311197
C	-4.547667779524	-1.862121715402	0.506509680199
H	-2.652197845120	-2.710355169781	-0.084672392753
C	-5.251978194392	-0.698044621864	0.820694394645
H	-5.154630869574	1.450147592088	1.031604011217
H	-5.052555326280	-2.829210831179	0.518976465407
H	-6.309223384867	-0.756665634814	1.084527910137
H	-1.351273662629	3.983949712146	0.639890179635
C	-0.586166321520	3.618286044713	-0.049011395092
C	0.184396583571	2.524328158064	0.336914359885
C	-0.397799850190	4.240058287901	-1.286106810388
C	1.192491685550	2.030637497108	-0.522315258800
C	-0.047083969152	1.806349897909	1.626678301358
C	0.612005114620	3.774630007834	-2.121719047636
H	-1.019944130822	5.086860840582	-1.578580953666
C	1.409983040335	2.692650977467	-1.742470223040
N	1.935310455994	0.895054284764	-0.152608661218
C	1.091801109183	0.978994651809	2.133590438326
H	0.801249432135	4.259199457869	-3.081341051346
H	2.209131183206	2.378572306564	-2.410303346633
C	2.041612629215	0.515606728502	1.196602818789

C	2.920079528159	0.378977554333	-1.084513053424
C	1.190743259507	0.603070175465	3.470282165427
C	3.063987904931	-0.337540131096	1.645508665914
H	3.081314851314	-0.689310647271	-0.899521181146
H	2.547411874739	0.473804766107	-2.108307674671
H	3.887462166111	0.906289732161	-1.005287815872
C	2.192299088880	-0.267237955038	3.906585619477
H	0.451221762696	0.989264533402	4.175711824274
C	3.123575693911	-0.734204236226	2.983823593515
H	3.830271586198	-0.696270674997	0.961305348440
H	2.245632412544	-0.567139966001	4.953984828625
H	3.924757763891	-1.404614256139	3.300342514003
H	-0.813448144027	2.112122770485	2.351133295421

TRS8:reactant state, electronic energy = -1284.61122491

C	-0.365057142244	-2.502837041937	3.075335702270
C	-0.634839855991	-1.243519491105	3.593765676442
C	0.203584157601	-2.654774660887	1.789287838751
H	-0.579135425278	-3.392776505330	3.669681815769
C	-0.353826259098	-0.073898768129	2.851855274690
H	-1.061097043338	-1.148015637031	4.594031163311
C	0.469942617059	-1.510047301302	1.058511433715
H	0.434831611967	-3.643620948722	1.390034928277
C	0.189035634038	-0.224037697515	1.586504596274
H	-0.548485901456	0.916659755856	3.266583199377
N	0.998192931222	-1.339742706269	-0.215653108582
N	0.543755729764	0.710915837200	0.628854996848
C	1.383995352794	0.054338966478	-0.371179904617
C	1.747787930365	-2.381690513020	-0.872901826183
C	0.716571530173	2.106922426438	0.934229568766
H	1.073034271356	0.399974714626	-1.377997328718
C	2.858765555528	0.424406368115	-0.277384254054
H	2.002805210126	-2.058547458966	-1.891533124551
H	2.681300132285	-2.636539413602	-0.337673681051
H	1.129310235730	-3.288019128540	-0.949041361180
H	0.899780645589	2.660716054764	0.002556785967
H	-0.206268814009	2.500631460115	1.387970498978
H	1.559402456761	2.293050501087	1.625672101331
C	3.451512626455	1.185245718994	-1.285405149649
C	3.621925316485	0.039769465549	0.834036985671
C	4.792194797306	1.566260186915	-1.187943203949
H	2.857082241817	1.482859753369	-2.153601721423
C	4.959813882911	0.416318479009	0.931882899754
H	3.163819762531	-0.558450922938	1.626860155641
C	5.546374122497	1.182088656401	-0.080243912212
H	5.247477619728	2.162741411640	-1.980519580077
H	5.549476487675	0.113406560766	1.798987087611
H	6.594320478423	1.477542078358	-0.003151488585
H	-1.269710041624	3.671798685988	-1.985825899041
C	-1.803527856191	3.212546075792	-1.152033904865
C	-1.831056408611	1.788282757479	-1.081971755372
C	-2.431815018501	3.968030449310	-0.201213223826
C	-2.505448695233	1.137826388451	0.000402644194
C	-1.173034326974	1.011586266678	-2.040097624418
C	-3.107009531953	3.318607645121	0.864236809842
H	-2.419886735094	5.056813938929	-0.254092875764
C	-3.148698945090	1.948614249795	0.975870834146
N	-2.532119588591	-0.231014807745	0.045840100456
C	-1.346425865752	-0.370457220916	-2.059366954375
H	-3.618136404405	3.919690045859	1.618063892574
H	-3.705151380460	1.513251204210	1.800613416663
C	-2.018912634728	-0.995142365016	-0.965181344692

C	-3.143101395898	-0.931610457439	1.183586421067
C	-0.807353803021	-1.169363757601	-3.112674941488
C	-2.161657428394	-2.411106300563	-0.973232984238
H	-2.486941597916	-1.755606503843	1.483059922245
H	-3.232736373199	-0.261448052659	2.036744821926
H	-4.131607612866	-1.315236053332	0.897219535001
C	-0.952722886679	-2.527472844214	-3.094951966709
H	-0.283385600495	-0.659786814590	-3.923348228239
C	-1.640780781172	-3.141175318591	-2.012902256242
H	-2.692118947272	-2.926918897725	-0.177342175351
H	-0.547559920886	-3.143432478938	-3.898190004920
H	-1.765215568726	-4.225404055112	-2.007042162605
H	-0.811594547043	1.520488020285	-2.938694160584

In Chloroform

DAD = 3.2Å

TRS2:product state, electronic energy = -1284.59524385

C	4.779827069492	-0.944814762548	-0.589297350625
C	4.883716795720	-0.794314836837	0.814592925983
C	3.678258943163	-0.492225759426	-1.294441425908
H	5.591639298017	-1.435880793726	-1.127046414380
C	3.892125252567	-0.178969595715	1.559580873223
H	5.772426610497	-1.173441344449	1.320551450147
C	2.673043269867	0.133046245476	-0.543916907707
H	3.593437582590	-0.615571321831	-2.374258824863
C	2.784911427976	0.294420174109	0.843597945957
H	3.967660283566	-0.059430086959	2.640504844145
N	1.469737436023	0.694053114387	-0.902060504257
N	1.648427443632	0.953827004668	1.250142522883
C	0.787557406428	1.075096134985	0.215007837850
C	1.015538552617	0.823396319093	-2.277215104400
C	1.362924393171	1.342259545777	2.623190176224
H	-0.959912059951	-0.017795218276	1.143500569850
C	0.012712766859	2.342005446392	-0.035011298945
H	-0.070414913342	0.953069305765	-2.292348444796
H	1.499093594040	1.693562207007	-2.743044232645
H	1.282942011464	-0.089957535562	-2.822959825218
H	2.166022808181	1.996884801391	2.985460821454
H	0.410606216529	1.883268939563	2.648456833114
H	1.303641684149	0.448515107419	3.258774883234
C	-1.341298081432	2.332215564704	-0.378469642370
C	0.721715891881	3.546994811247	0.032234313712
C	-1.986049115774	3.532309746585	-0.678447959489
H	-1.884010096242	1.384232314489	-0.418703421770
C	0.067955139817	4.740297701987	-0.265685593735
H	1.779220167153	3.549224479748	0.306193894556
C	-1.282105325073	4.734186615534	-0.622170202234
H	-3.042339892354	3.524998119294	-0.950042562006
H	0.618225048572	5.681169204442	-0.219165749825
H	-1.787066691599	5.673218045421	-0.853939493092
H	1.124008123937	-2.379775452493	2.248913095893
C	0.894792596329	-2.433655729122	1.181684546580
C	-0.268258365794	-1.828384737365	0.714892741806
C	1.763489545631	-3.095778980209	0.309699548136
C	-0.601315231164	-1.903546031901	-0.655627675138
C	-1.197530870050	-1.033035336618	1.577056802026
C	1.435509757973	-3.170457960536	-1.040056341072
H	2.679370209810	-3.553464778551	0.686311540291
C	0.258486000157	-2.592026483685	-1.523196458353
N	-1.769424850174	-1.257390561619	-1.103577610260
C	-2.634883287477	-1.054860319737	1.154156205645

H	2.091356383150	-3.697596573169	-1.735502322667
H	0.010818810337	-2.699586996328	-2.578232466170
C	-2.875165479040	-1.161153562233	-0.231155611209
C	-2.034722794114	-1.212637798283	-2.528265265158
C	-3.702864755689	-0.935893465109	2.037552120602
C	-4.196677369456	-1.136889298517	-0.696236004836
H	-2.722742921268	-0.385342747600	-2.743936695617
H	-1.102998684360	-1.023110107604	-3.071505403955
H	-2.478500196708	-2.149638331783	-2.908700361734
C	-5.018263360584	-0.885984620256	1.569406282469
H	-3.496374652911	-0.870445501287	3.107947416903
C	-5.255654035501	-0.989489086759	0.202719837795
H	-4.415606206264	-1.242420338415	-1.757219048762
H	-5.846859770730	-0.776836148581	2.270172580472
H	-6.277167178295	-0.968191325447	-0.180595084814
H	-0.954990335954	-0.695476420943	2.592799697061

TRS2:reactant state, electronic energy = -1284.59524108

C	3.899483112352	-2.246584503791	-1.196779804417
C	4.495326139011	-1.940243537922	0.019805438031
C	2.672142929884	-1.660459185655	-1.570760420688
H	4.388242656201	-2.941123871607	-1.881631695577
C	3.898201172249	-1.028884040556	0.915983302852
H	5.450250775770	-2.396492831574	0.285342291415
C	2.077504021495	-0.778934009402	-0.684328190581
H	2.210387014970	-1.891614519994	-2.531891650489
C	2.690937725384	-0.456526327128	0.550343593194
H	4.380285274755	-0.772754062646	1.860255622294
N	0.871744769605	-0.092117629937	-0.747582775724
N	1.861462316128	0.429196001910	1.214176834432
C	0.845672378017	0.916617800462	0.295393099164
C	0.146294694280	0.108570897717	-1.975130390476
C	2.265151386996	1.197862732431	2.361181252753
H	-0.146033479078	0.883344539057	0.800510840191
C	1.012443644819	2.373742903171	-0.117208198268
H	-0.841849965447	0.536336833808	-1.748140545772
H	0.665908382516	0.787932048272	-2.674776400257
H	-0.006070445263	-0.860964818315	-2.473253366195
H	2.965179662663	2.014202335636	2.107659020896
H	1.377480550692	1.639620765797	2.836391185498
H	2.748789094794	0.535860051181	3.093438555536
C	0.001355550884	3.296042919808	0.150983409641
C	2.183295141900	2.799486064982	-0.758495022320
C	0.152555244766	4.636163302514	-0.212518838178
H	-0.911826360534	2.963251769760	0.652716673804
C	2.335439608491	4.135119521424	-1.122262728077
H	2.979663001771	2.079916008641	-0.969114053094
C	1.319024818170	5.055259466266	-0.848929640973
H	-0.642051100389	5.352455583180	0.002745331436
H	3.249280263977	4.463326736228	-1.620363764724
H	1.440352734888	6.101954717076	-1.133048020776
H	0.348560382425	-1.539979778773	2.838360588966
C	0.104391724587	-2.004112173796	1.881995706570
C	-1.019960803206	-1.498973402952	1.161020887959
C	0.842315304854	-3.039896621802	1.382471246236
C	-1.368320039649	-2.066850563004	-0.110301177950
C	-1.742142455631	-0.407828026719	1.632975031180
C	0.475913132697	-3.611304377172	0.136566381587
H	1.702748932763	-3.430170774386	1.925904393709
C	-0.597959483567	-3.156535937897	-0.592630227829
N	-2.431683057883	-1.554922693903	-0.802400842842
C	-2.923085695696	-0.000905812118	0.988858594994

H	1.056614269808	-4.448736301911	-0.254093573364
H	-0.848986060392	-3.662677637063	-1.520359912234
C	-3.258410303623	-0.595273146928	-0.262390452148
C	-2.737182386111	-2.044086204667	-2.150868675660
C	-3.769217391244	0.998242248103	1.546287247327
C	-4.453317190949	-0.190890314792	-0.910185143997
H	-3.050962529698	-1.201318391132	-2.773718176638
H	-1.842533165115	-2.472307690600	-2.604039230540
H	-3.534639109106	-2.799484163934	-2.115349211200
C	-4.915471641551	1.379798817451	0.899065753303
H	-3.483375801595	1.442801438513	2.501400066802
C	-5.252810962365	0.770894280424	-0.333560491276
H	-4.765437729606	-0.647298653093	-1.846166052163
H	-5.570073595978	2.138734134586	1.327681424348
H	-6.173918110573	1.061937389426	-0.840854773370
H	-1.535087950310	-0.049106302655	2.645320673677

TRS8:product state, electronic energy = -1284.60103861

C	2.229524392924	-3.302142726141	-1.656274361286
C	1.976705443248	-2.633009884604	-2.878002632420
C	1.512252656168	-3.021578128306	-0.504859782148
H	3.012249537322	-4.061208864833	-1.624517695055
C	1.001609625648	-1.656156852722	-2.988834266555
H	2.570108651216	-2.895521244467	-3.754640623925
C	0.510181611345	-2.048060446112	-0.619773560439
H	1.705690559080	-3.534870314964	0.437165458313
C	0.266861370227	-1.378788720688	-1.827944472566
H	0.809665856962	-1.132763664708	-3.925804086301
N	-0.404266397153	-1.564538268740	0.283974307129
N	-0.781250149315	-0.519981255805	-1.593345146768
C	-1.113014193695	-0.544580049242	-0.281192093037
C	-0.463926598492	-1.991483649613	1.675812579381
C	-1.392206402306	0.332506698111	-2.602860359989
H	-0.683271790396	0.957084639051	1.227753382765
C	-2.557751164658	-0.545059678416	0.147047994267
H	-1.138560041387	-1.328471921554	2.227000558882
H	-0.837189785029	-3.023244335525	1.728573187610
H	0.544517847272	-1.933992426842	2.109122034084
H	-2.330636369001	0.736402563798	-2.207776721127
H	-0.712355919670	1.158094381482	-2.855523184147
H	-1.599998169276	-0.271328930212	-3.494720666329
C	-3.252403693262	0.636556683655	0.425556180433
C	-3.222440499339	-1.777339706650	0.184077428955
C	-4.606071464300	0.587721746042	0.756412852557
H	-2.730540847802	1.595670100990	0.380478545802
C	-4.574364216464	-1.817140677197	0.515202026492
H	-2.689684904335	-2.700137891320	-0.053836424655
C	-5.265657374516	-0.639397014513	0.804475675764
H	-5.144603283047	1.510407531055	0.976264015190
H	-5.091912461491	-2.777024205205	0.542961820879
H	-6.324567349630	-0.680582840178	1.064088369496
H	-1.314389575289	3.987876778584	0.614738732717
C	-0.546191535914	3.608621493678	-0.063309914862
C	0.206981082962	2.507828439526	0.336155155332
C	-0.331113776006	4.227994543631	-1.296815894875
C	1.225266088881	2.005018288532	-0.504997372768
C	-0.047721588196	1.794805202152	1.624692241606
C	0.690244229651	3.754995991455	-2.113122797468
H	-0.936883186794	5.083238481082	-1.598118702242
C	1.471402064212	2.666048221624	-1.719582345546
N	1.949733618561	0.861052207690	-0.122298033629
C	1.076664620937	0.960354466120	2.152505519173

H	0.904655819951	4.242786537898	-3.065619252381
H	2.286114830510	2.351447089032	-2.367927782435
C	2.035929224578	0.487210354655	1.231037390523
C	2.951725613028	0.341918615522	-1.032986120126
C	1.153699572906	0.588300270579	3.491449631117
C	3.046972455453	-0.369173621891	1.697418030270
H	3.095567322132	-0.730355078116	-0.855156194074
H	2.606351662730	0.449808061188	-2.064995722062
H	3.922782292281	0.857377716387	-0.925986889391
C	2.142257484868	-0.287585783190	3.944323737428
H	0.411199850289	0.985549580912	4.187460900409
C	3.084723707249	-0.761922772295	3.037392063799
H	3.824871559434	-0.729147662388	1.027408116515
H	2.180945866690	-0.581380146208	4.993870327301
H	3.879758073589	-1.431782539733	3.369654916269
H	-0.829288695540	2.100776137947	2.332609348149

TRS8:reactant state, electronic energy = -1284.60102826

C	-0.399154820335	-2.466940602736	3.101518517733
C	-0.647623930730	-1.202397000821	3.618240022340
C	0.159198462910	-2.630028499313	1.813564531283
H	-0.617490008928	-3.351329076198	3.702098246115
C	-0.354259292596	-0.039746532574	2.872210429178
H	-1.060239037891	-1.098992160706	4.623189537571
C	0.437174522271	-1.491094761021	1.078279755516
H	0.379311870758	-3.622958425224	1.418573691744
C	0.178154361012	-0.200973424453	1.603807624896
H	-0.523701809446	0.954302944671	3.289541621642
N	0.963806353761	-1.332423938686	-0.199920209563
N	0.543450724091	0.727929300821	0.641904227547
C	1.372227962236	0.055163323310	-0.356666734813
C	1.707407679025	-2.386122417869	-0.845959280721
C	0.747971997331	2.119344824787	0.951091519567
H	1.058240714909	0.402357038582	-1.364329245920
C	2.851992580412	0.405473376906	-0.277780463358
H	1.984950495847	-2.067503326346	-1.860101920060
H	2.628533604681	-2.655271465394	-0.297372896438
H	1.075471826873	-3.282015703180	-0.934043727822
H	0.949064671447	2.671909141477	0.022401184341
H	-0.168014781052	2.534310525729	1.400041427334
H	1.592316581689	2.285537011535	1.644920076552
C	3.457250793292	1.119771117535	-1.311588874605
C	3.609950492568	0.044041927290	0.844728330653
C	4.805397365993	1.475915007991	-1.231164287800
H	2.868384791734	1.400893080818	-2.189311951228
C	4.954898524759	0.396382148027	0.925949519278
H	3.141782034950	-0.515623951209	1.659452901488
C	5.554127563767	1.113940355596	-0.113165295437
H	5.270908265584	2.034954404516	-2.044585588308
H	5.540635953488	0.111937198730	1.801713130418
H	6.608132023453	1.389578902884	-0.048832601510
H	-1.230482855620	3.655490592130	-2.041527261640
C	-1.759799565216	3.209268763284	-1.197804826630
C	-1.802339671673	1.786486797199	-1.110468611038
C	-2.371367428199	3.984076006458	-0.251941917346
C	-2.476171496415	1.157062010919	-0.015357690543
C	-1.165962752053	0.989610854012	-2.066762467889
C	-3.045454473146	3.355885805871	0.826220781179
H	-2.348003990497	5.071683096781	-0.319748566874
C	-3.101346240088	1.987883962392	0.954491612558
N	-2.520883817789	-0.211223952134	0.045955907961
C	-1.351000436126	-0.390743696994	-2.065992682555

H	-3.544027634081	3.972131319815	1.576110444871
H	-3.657421783156	1.569911253986	1.788305450878
C	-2.021962107333	-0.993910478735	-0.958559601428
C	-3.133730636788	-0.889762693565	1.196284287619
C	-0.828043502240	-1.209424992153	-3.112241401913
C	-2.180634400647	-2.407878286092	-0.948978922155
H	-2.489892802809	-1.721821154999	1.500098268916
H	-3.197297624461	-0.212006653783	2.045836611595
H	-4.134041653025	-1.255100525932	0.926207269940
C	-0.987856569346	-2.565165323682	-3.076571984977
H	-0.306597393156	-0.718123667547	-3.935925955681
C	-1.675933003403	-3.156993612025	-1.982637728476
H	-2.710612610875	-2.907953910114	-0.143050671975
H	-0.596771621875	-3.195230892206	-3.875720296639
H	-1.814877402668	-4.239266592620	-1.963168109328
H	-0.803434065177	1.483249624260	-2.973442156042

The atom coordinates and electronic energies of the ground state reactants in gas-phase

MA^+

H	1.007756611487	-1.402736777642	2.642416369485
C	0.766316550087	-1.933290074230	1.720173286727
C	-0.485017721917	-1.658710817747	1.089968062752
C	1.629189875149	-2.845619800777	1.181690930331
C	-0.830361515637	-2.325350234195	-0.129281547121
C	-1.392574848147	-0.754336356389	1.641455166489
C	1.263946887929	-3.528642531299	-0.007436572835
H	2.583570029608	-3.061570292892	1.661079560743
C	0.075077044236	-3.284482352230	-0.654257339466
N	-2.020055958650	-2.029052769733	-0.745125616297
C	-2.635818040340	-0.527504779427	1.051317222843
H	1.940868501488	-4.277903173692	-0.420693846624
H	-0.163076243396	-3.858907131227	-1.545087491776
C	-2.954990145203	-1.208065198322	-0.167416207663
C	-2.299812122189	-2.605941447321	-2.067519084075
C	-3.588458013153	0.357027227515	1.641870208491
C	-4.243213535144	-1.013764839754	-0.731738114346
H	-2.916534348494	-1.910754150038	-2.640612050340
H	-1.361790414580	-2.729700028114	-2.612319076658
H	-2.811271369615	-3.573550041493	-1.970892713151
C	-4.813468752612	0.542431028852	1.066015482721
H	-3.313877136683	0.870482412738	2.564516599405
C	-5.135795829240	-0.163428080071	-0.122329745530
H	-4.556265051173	-1.548779355938	-1.623940934695
H	-5.545469231476	1.213155297115	1.515004291527
H	-6.124774699559	-0.036777955415	-0.565364405186
H	-1.132515522777	-0.228523778275	2.563697564248

DMPBIH

C	4.356573245151	-1.066225821603	-1.188279990312
C	4.815652172934	-0.619384931807	0.040283444260
C	3.004891344824	-0.903308382716	-1.561646480711
H	5.047350354738	-1.540093805865	-1.886668142345
C	3.945304813921	0.012037868173	0.955046907293
H	5.866384673371	-0.742891602423	0.305192891273
C	2.149066160025	-0.304039377829	-0.656821659716
H	2.651097635447	-1.234880181109	-2.538324295912
C	2.617668190810	0.152072496406	0.597227160872

H	4.313920771057	0.383612950234	1.911636713523
N	0.791883160444	-0.018871160756	-0.733112419331
N	1.542340777738	0.711592374855	1.275255356530
C	0.438968727766	0.905101593516	0.339933002586
C	0.082020296825	0.012092875805	-1.981803688014
C	1.715443818096	1.602037050291	2.389370107407
H	-0.519193881134	0.603671802007	0.807597826951
C	0.293055393960	2.350362073914	-0.131234617313
H	-0.991745244765	0.142979941508	-1.788135283947
H	0.414998864777	0.829970111408	-2.648832171621
H	0.215125681511	-0.945325633986	-2.505342772817
H	2.192392534676	2.560113749450	2.107711305736
H	0.735686589028	1.824382600070	2.834622671025
H	2.331621729590	1.114812665921	3.158392387629
C	-0.900701687644	3.043036251605	0.062674196001
C	1.364683748219	2.993685253839	-0.765517546214
C	-1.034027661405	4.364957252144	-0.368397796915
H	-1.736988238217	2.541647198697	0.557428737349
C	1.233964273011	4.310860649959	-1.195834786289
H	2.303767563380	2.454960641629	-0.920306836727
C	0.033576945711	4.999085372786	-0.997833701419
H	-1.973061070068	4.898043347437	-0.211577244496
H	2.071431862723	4.806739071787	-1.689017326714
H	-0.065767546503	6.031565704653	-1.336308947619

The atom coordinates and electronic energies of the reactant states in solution

In acetonitrile

DMPBIH, electronic energy = -689.943454936

C	4.358449285183	-1.087878759340	-1.181808399498
C	4.817944764383	-0.640612109754	0.047870290243
C	3.007322967058	-0.911853917602	-1.562324670459
H	5.046681205531	-1.572341695943	-1.876747707603
C	3.949428329015	0.005181334662	0.958886083218
H	5.866930621196	-0.773921452187	0.318361399798
C	2.152738295012	-0.298829549902	-0.662637583706
H	2.651344079989	-1.243354183796	-2.538881602470
C	2.622835624373	0.158759813204	0.595407833826
H	4.316246677344	0.377245720927	1.916638321343
N	0.802652386056	-0.006617950823	-0.742248551642
N	1.553501535591	0.724260060310	1.267114933229
C	0.443632807137	0.916613149517	0.333989487396
C	0.084228108897	0.004138277024	-1.989574435685
C	1.723404214520	1.599701106464	2.397074112976
H	-0.512281741316	0.617092159215	0.800132792568
C	0.294558112729	2.361926202759	-0.136026812065
H	-0.988864583820	0.130803888938	-1.791153717512
H	0.413230225239	0.814376046646	-2.667144916115
H	0.222563098350	-0.957317283617	-2.504417999608
H	2.205149859150	2.558589339792	2.128218097330
H	0.742259837365	1.815887432065	2.841553227635
H	2.339331683642	1.103137471754	3.160392814626
C	-0.904515305132	3.046700833450	0.062794872486
C	1.360549688788	3.014255984630	-0.771508314910
C	-1.046194451885	4.369680399546	-0.365520206749
H	-1.735818707457	2.538139483190	0.558317535172
C	1.221659322076	4.332799660003	-1.199251877588
H	2.305062016031	2.487082969420	-0.932560248560
C	0.016612385832	5.013177561665	-0.996602477112
H	-1.988670388699	4.896481565400	-0.205086277602
H	2.055477942604	4.834835201144	-1.693336921574

H	-0.090063894783	6.046261241240	-1.332542081391

MA^+, electronic energy = -594.653287459

H	0.996818959929	-1.398076474751	2.644276252843
C	0.762986144146	-1.931646383026	1.721581453845
C	-0.485595078881	-1.653526634315	1.087060114928
C	1.622993542046	-2.847468143523	1.184409391734
C	-0.830861766406	-2.317861868717	-0.132554582152
C	-1.389139049553	-0.747857771364	1.642009936595
C	1.258670703455	-3.528493967788	-0.007453241444
H	2.575648576941	-3.068391779679	1.665877739596
C	0.073891036770	-3.280453273259	-0.657712535719
N	-2.016909864971	-2.023283015237	-0.749747572466
C	-2.631233032167	-0.525180803541	1.048531344299
H	1.934577243857	-4.279324836707	-0.419961856058
H	-0.165472628106	-3.847861397399	-1.552885535204
C	-2.948605924690	-1.204180624382	-0.170583735357
C	-2.301062982826	-2.608620791764	-2.067920858039
C	-3.585274957456	0.355010681799	1.643500263365
C	-4.239103874614	-1.012328189272	-0.735168280212
H	-2.922079884669	-1.918611753817	-2.642272668304
H	-1.364849352600	-2.737585868411	-2.614295499583
H	-2.811058089024	-3.574445060157	-1.953753942576
C	-4.811573462462	0.536336997872	1.068860737937
H	-3.304155563920	0.863709157666	2.567046770402
C	-5.132680724379	-0.167406178444	-0.122230229690
H	-4.545736181908	-1.544352373964	-1.631554649480
H	-5.546606504768	1.202931794801	1.520024207782
H	-6.122319741103	-0.042355449905	-0.564651892347
H	-1.129682542642	-0.222971992717	2.564758865306

In chloroform

DMPBIH, electronic energy = -689.943583119

C	4.357889560886	-1.081579331224	-1.183508512932
C	4.817165900441	-0.634498162446	0.045630941930
C	3.006678718102	-0.909615196457	-1.561744807978
H	5.047001945424	-1.562769352959	-1.879556824677
C	3.948081816961	0.006790785032	0.957687037889
H	5.866786509901	-0.764752600548	0.314393566260
C	2.151476551776	-0.301532927647	-0.660323359780
H	2.651735513358	-1.240477627286	-2.538717716235
C	2.621050263343	0.155572354525	0.596374132903
H	4.315789178402	0.379390583608	1.914709177661
N	0.799513618959	-0.010094904131	-0.739645665923
N	1.550220928103	0.720679539781	1.269433562231
C	0.442712474819	0.914119552750	0.335203704533
C	0.084845005834	0.004842714778	-1.988000566910
C	1.722723164440	1.599228542546	2.395381298613
H	-0.514110549691	0.614805974208	0.801598593305
C	0.294112058272	2.359636148627	-0.135056866930
H	-0.988273597576	0.138951067939	-1.793881912630
H	0.419456023041	0.811736595687	-2.666940660719
H	0.215271706851	-0.959126766113	-2.500521149011
H	2.210340759857	2.555066415200	2.125928126032
H	0.742482681522	1.823748389849	2.838066369268
H	2.331654935635	1.101057164786	3.163465331057
C	-0.903662120182	3.046287588342	0.062730831909
C	1.361072193642	3.010171208774	-0.770348796385
C	-1.043727283783	4.368885929866	-0.366010727410
H	-1.736498182253	2.539850037718	0.558129290751
C	1.223690508625	4.328233045361	-1.198443047655
H	2.304333286697	2.480457869215	-0.930121507679

C	0.019884999453	5.010246909284	-0.996715031011
H	-1.985446490805	4.897103368447	-0.206269557308
H	2.058402614044	4.828737874529	-1.692384307205
H	-0.085268694097	6.043247207957	-1.333163945965

MA^+, electronic energy = -594.641935943

H	1.000915106425	-1.398975844015	2.643140775389
C	0.764016545085	-1.931800985581	1.720803659664
C	-0.484208001863	-1.652758722409	1.086504052715
C	1.623172145363	-2.848907286461	1.184833702130
C	-0.830280137479	-2.319041901844	-0.132101966698
C	-1.387987066410	-0.745768996800	1.639035665797
C	1.258102251382	-3.530955644232	-0.005560122309
H	2.575365443115	-3.069840899225	1.666822695548
C	0.073130025013	-3.282474003148	-0.655772438838
N	-2.016915685774	-2.023286241081	-0.749473523435
C	-2.631372287076	-0.523620372325	1.047954763318
H	1.933169301531	-4.283115471125	-0.416825461325
H	-0.166213195443	-3.851799350042	-1.549636957413
C	-2.949915844777	-1.204368517273	-0.170163538001
C	-2.299119973101	-2.604958566986	-2.069275781700
C	-3.585972087690	0.355745838922	1.642701184873
C	-4.240385498297	-1.014067884395	-0.733244642127
H	-2.919092472202	-1.913531819897	-2.643550163679
H	-1.362333394326	-2.732326758264	-2.615565753157
H	-2.809503150980	-3.571660035963	-1.961651335229
C	-4.812875721670	0.535662680706	1.069263624527
H	-3.307194273419	0.866534925665	2.565797537837
C	-5.134435400613	-0.169243850342	-0.120364156286
H	-4.548636207130	-1.547131946164	-1.628361437712
H	-5.547675768758	1.201873656981	1.520959181288
H	-6.124725480923	-0.045611809243	-0.561544205059
H	-1.127444169982	-0.218866195459	2.560464639880

The atom coordinates and electronic energies of the classical TS structures in gas-phase

TS1: electronic energy = -1284.503328128089 Hartree

C	4.990255273445	-0.968491279318	0.164411560275
C	5.075571916526	-0.214577567587	1.339078729962
C	3.858382430721	-0.908645411691	-0.656630020830
H	5.821135353197	-1.614975745369	-0.118521540821
C	4.040925961234	0.640136366296	1.735617374879
H	5.969290948406	-0.288543164806	1.958892569447
C	2.826357606562	-0.068250108709	-0.257332858205
H	3.788570679852	-1.496990484902	-1.571967645631
C	2.921001087904	0.712291652518	0.913821701435
H	4.116867626803	1.229034614901	2.649690710661
N	1.588029131723	0.177583983817	-0.817824695920
N	1.769937840089	1.472423962170	0.994305977624
C	0.839067340186	1.044764664912	0.012048885870
C	1.157806812281	-0.310151309653	-2.106329933598
C	1.412354464255	2.337263433647	2.088270919963
H	-0.015788643011	0.358519424699	0.580636845152
C	0.055348555105	2.134127331902	-0.687318287765
H	0.091692983965	-0.084393404010	-2.237382833640
H	1.720725783177	0.171060497802	-2.922326295804
H	1.303412720572	-1.400390302038	-2.163665379256
H	0.649380271905	3.050887310955	1.750475882423
H	1.021799305411	1.775370870739	2.955156047650
H	2.295358747765	2.904860521571	2.410063659884

C	-1.323991480278	2.273090134728	-0.531133380935
C	0.761191087411	3.025957582154	-1.504061430140
C	-1.999268091949	3.300381632801	-1.194097361904
H	-1.875394713724	1.589160845976	0.115358882013
C	0.085017181699	4.046694828908	-2.164472919552
H	1.842827417898	2.914691570460	-1.614278395643
C	-1.297235121714	4.183422725878	-2.010483621877
H	-3.076881241580	3.410166313443	-1.066648243321
H	0.635273952722	4.741307808618	-2.800341101236
H	-1.825433468887	4.985350435734	-2.527772277090
H	1.669704072506	-2.205797314998	1.303923090822
C	0.969964852632	-2.547243590609	0.537265512887
C	-0.303689674929	-1.942458643145	0.468977187529
C	1.335223197738	-3.534862652187	-0.351018349938
C	-1.225266111161	-2.343288232585	-0.537245160731
C	-0.678906677361	-0.890391480924	1.359854983894
C	0.409902946528	-3.946835364239	-1.329827156575
H	2.319519619124	-3.998616280160	-0.289887980309
C	-0.845144072576	-3.372218772394	-1.427540511323
N	-2.462214269586	-1.730957398046	-0.612719208276
C	-2.062798302973	-0.540107183913	1.461911999799
H	0.676072033808	-4.748116546549	-2.020935961852
H	-1.538309323987	-3.747807921344	-2.176311137593
C	-2.945031485330	-0.954875348654	0.430297175262
C	-3.323038407905	-1.993977965604	-1.760628004292
C	-2.545742410121	0.260931203426	2.519732440134
C	-4.299030112683	-0.561354770694	0.500849164082
H	-3.941617698130	-1.113076478859	-1.956773040098
H	-2.703955727276	-2.161081465156	-2.646779008322
H	-3.970870413133	-2.868380309544	-1.595772280185
C	-3.867914325151	0.646832759906	2.568542613415
H	-1.846685400213	0.570567761771	3.299197111954
C	-4.741492083997	0.225750799852	1.549510121622
H	-5.016459843059	-0.892345520684	-0.246161155791
H	-4.237354916489	1.261324082109	3.389042125496
H	-5.793987980301	0.509369827325	1.588510497770
H	-0.028095162509	-0.688003439956	2.215814120963

TS2: electronic energy = -1284.506184781171 Hartree

C	4.535392394089	-0.719611014705	-1.019172342745
C	4.909387301446	-0.176244388647	0.211874889717
C	3.226767198636	-0.597332317290	-1.501982816772
H	5.276199998766	-1.246961403027	-1.620355239161
C	3.993365339387	0.522345174162	1.008609002559
H	5.937618687035	-0.287221179596	0.556889896206
C	2.317148503055	0.100568173183	-0.715900445285
H	2.943232774956	-1.022606242445	-2.464845952512
C	2.701973609373	0.661781693250	0.517931458939
H	4.289078009216	0.954982046655	1.964628337086
N	0.974738375019	0.395389748809	-0.893301653940
N	1.594249329346	1.297322928088	1.044092001303
C	0.486230160556	1.166794760166	0.181479317575
C	0.223252725174	0.210307619228	-2.110507586573
C	1.593745044633	2.084978728629	2.253765641425
H	-0.399272574935	0.472813393143	0.760670726295
C	-0.258870780526	2.436105274668	-0.178324291619
H	-0.820830279587	-0.035465690204	-1.865532406337
H	0.234231826664	1.116308820251	-2.736809445558
H	0.657072920987	-0.627248938019	-2.671017420018
H	2.298658426958	2.927092261540	2.175186837112
H	0.587945242787	2.491199908852	2.417260877387

H	1.878234934805	1.468480231981	3.120473939256
C	-1.648619625767	2.524377896344	-0.105449005828
C	0.491402688908	3.526370485137	-0.636089213713
C	-2.290862678281	3.703487292793	-0.488241478458
H	-2.234553921076	1.674117775558	0.247767169460
C	-0.152236300273	4.700729722373	-1.014428729454
H	1.580471089448	3.448798514549	-0.692661532918
C	-1.544610210551	4.789273219279	-0.940233528594
H	-3.377634673577	3.772027272076	-0.429641594023
H	0.431704038381	5.551367585726	-1.367965577135
H	-2.047343238087	5.710995636982	-1.235700607280
H	1.349412931125	-1.295233477172	2.618247059136
C	1.170520014253	-1.846054488686	1.692385158010
C	-0.077023965784	-1.692322080087	1.051500080049
C	2.151547348182	-2.645067739190	1.151059432447
C	-0.351740553000	-2.399220030406	-0.152151010666
C	-1.028982610846	-0.727658117264	1.502826727418
C	1.883578481589	-3.329805663634	-0.049183105204
H	3.121186703913	-2.747203576040	1.637871682112
C	0.657962229745	-3.232076301275	-0.683956477877
N	-1.584122988990	-2.256322742116	-0.763101321882
C	-2.387190059711	-0.852166608683	1.043854845246
H	2.649739267961	-3.975212883641	-0.481562261940
H	0.482194802804	-3.825969818685	-1.577601858872
C	-2.642974896248	-1.631704529212	-0.111297599869
C	-1.817529191257	-2.877784529389	-2.060847163104
C	-3.453915986246	-0.206708220415	1.703263438012
C	-3.973248419090	-1.756637505420	-0.563286018792
H	-2.575731088910	-2.307074408366	-2.605641475932
H	-0.897614067182	-2.845939385824	-2.652561909776
H	-2.148463631500	-3.923150260233	-1.962101034364
C	-4.748871237917	-0.324927448647	1.241422330556
H	-3.233848616290	0.387046105926	2.592959590667
C	-4.999737070669	-1.109324358445	0.103381294570
H	-4.216186388783	-2.384205023995	-1.417596303179
H	-5.569711937003	0.169669535929	1.760084253543
H	-6.021855602231	-1.228589613911	-0.257971853443
H	-0.863145390020	-0.262394850434	2.479886110716

TS3: electronic energy = -1284.483220789452 Hartree

C	-5.181262098435	-0.799029871121	-0.946402655378
C	-5.279082861847	0.589563317638	-0.823394213057
C	-4.060522625203	-1.488543979548	-0.473965043166
H	-5.990813199529	-1.355747646408	-1.418782054406
C	-4.258107519817	1.336098522464	-0.227918576331
H	-6.164630456222	1.101606240293	-1.200398522778
C	-3.040730125523	-0.746885884523	0.113505680811
H	-3.993158636986	-2.574221531563	-0.557589938304
C	-3.136044005090	0.653906679470	0.230583310679
H	-4.339703146624	2.418770531411	-0.124125864278
N	-1.850425786792	-1.170985605548	0.715587708191
N	-2.006106331910	1.128715354288	0.901979841073
C	-1.075036552078	0.030926856240	0.875132102839
C	-1.831487620022	-2.368157822678	1.542288119212
C	-2.134629438952	2.139949255101	1.942605107689
H	-0.596153017290	0.147272834465	-0.200061906821
C	0.192092815578	0.074174663844	1.668000081626
H	-2.853981880330	-2.764926299309	1.585976313860
H	-1.175250361319	-3.152578853031	1.132945713557
H	-1.518865797049	-2.135972370358	2.569566616349
H	-3.203567517290	2.299057257300	2.139192318163

H	-1.665011235017	1.800243011538	2.875509262920
H	-1.690324649731	3.104018038979	1.652716553138
C	0.803001049966	1.318204874649	1.908286802570
C	0.921849983586	-1.090900214972	1.953219228614
C	2.063946560793	1.392533477965	2.493606830209
H	0.304445159069	2.241580494703	1.615644512044
C	2.183372566319	-1.012081292792	2.541044714631
H	0.528945044241	-2.073036940519	1.699763642859
C	2.753174167130	0.226855789485	2.827577139402
H	2.509260621553	2.369723595266	2.685699864835
H	2.721969100098	-1.932081160598	2.774360313572
H	3.735144298045	0.284811134092	3.300074175952
H	-1.063843045637	-2.281216912026	-1.920144957682
C	-0.016205613378	-2.363595059650	-1.623240604235
C	0.725539785475	-1.168612480669	-1.457066358402
C	0.572453058661	-3.590867772608	-1.418164928978
C	2.089261708183	-1.220211041739	-1.049461191863
C	0.099995592119	0.097531580599	-1.605268707712
C	1.934948233611	-3.640832835668	-1.062272486644
H	0.005894523795	-4.511935403730	-1.552721627403
C	2.685366805101	-2.493423558059	-0.888739264822
N	2.789137526760	-0.050222838524	-0.832069643010
C	0.875496274357	1.285002126205	-1.505294118578
H	2.421216795785	-4.608943596968	-0.933000535416
H	3.739898157418	-2.593559877442	-0.647229826173
C	2.236871005360	1.187580668352	-1.103957040194
C	4.157958110060	-0.126282822703	-0.325239157164
C	0.287435469966	2.552601724889	-1.733428838161
C	2.988393023791	2.382879810432	-1.012469305397
H	4.373545601075	0.760589296240	0.275016084512
H	4.249013708042	-0.985415393323	0.344023912255
H	4.885408229877	-0.210956501869	-1.146552438641
C	1.026218338797	3.705120361477	-1.599021457235
H	-0.765421118945	2.588446195881	-2.020546602475
C	2.387599651615	3.604114923217	-1.249734427973
H	4.048938494049	2.363044307323	-0.777261863240
H	0.576287868896	4.680980567321	-1.779244696512
H	2.992148636177	4.509166741093	-1.175008106771
H	-0.889658324330	0.147854335726	-2.069659992364

TS8: electronic energy = -1284.516864552883 Hartree

C	-1.858594189750	0.703497704771	-3.555699857344
C	-1.858481960324	-0.697479438688	-3.556944432549
C	-1.051295648215	1.430841460411	-2.675055161933
H	-2.490892445483	1.238781806840	-4.264691681208
C	-1.051066530601	-1.426257504972	-2.677593932382
H	-2.490694673229	-1.231604331903	-4.266886162011
C	-0.241338486428	0.706324210621	-1.804897901631
H	-1.040854574623	2.521208014293	-2.683186931718
C	-0.241224681048	-0.703157606444	-1.806150369907
H	-1.040450554232	-2.516606317320	-2.687662951656
N	0.677749495654	1.118677345290	-0.866128239292
N	0.677933737091	-1.117030321198	-0.868118978931
C	1.260248140196	0.000299652615	-0.224546262529
C	1.111239427590	2.487453588452	-0.695285830923
C	1.111630230381	-2.486041095160	-0.699698339335
H	0.852521874963	-0.000788957793	0.960227010915
C	2.766861487023	0.000301106732	-0.084168438387
H	1.811202696799	2.539841327934	0.147163110832
H	1.620345112894	2.853125226130	-1.601019175777
H	0.248012452691	3.133891345255	-0.474884629829

H	1.811657083326	-2.539800214153	0.142611418269
H	0.248512319510	-3.132991312654	-0.480373295050
H	1.620730659010	-2.850051515835	-1.606103305824
C	3.397086694106	-0.000786119678	1.158777972234
C	3.532237619390	0.001441946861	-1.256790324842
C	4.791198278222	-0.000737919728	1.235597722199
H	2.800953130191	-0.001676236732	2.073296891106
C	4.921206305530	0.001489671457	-1.178825533264
H	3.031855657791	0.002290554249	-2.228958414354
C	5.551136194438	0.000398892377	0.068545525952
H	5.282573434578	-0.001589386139	2.209070286751
H	5.517651898500	0.002378698713	-2.091938246458
H	6.640162633985	0.000438102494	0.128012306519
H	0.482583163191	-2.444008205065	3.061145547416
C	-0.369969472386	-2.457651618642	2.378651628183
C	-0.821007901103	-1.230708801655	1.843671332057
C	-0.990026838029	-3.644189570031	2.055182951773
C	-1.930131823516	-1.206929523463	0.958391452747
C	-0.142576362223	-0.001900355345	2.130174078786
C	-2.086917138862	-3.619614596785	1.173082459594
H	-0.645461381770	-4.587078295833	2.479173336323
C	-2.553663687838	-2.433876539177	0.634802709053
N	-2.378235040721	-0.000618431849	0.443613835485
C	-0.821227334614	1.227287916867	1.845830194155
H	-2.597152756149	-4.549884767758	0.919196285839
H	-3.426721782910	-2.463080946170	-0.011814822076
C	-1.930347193623	1.204865713060	0.960510056184
C	-3.472068685272	0.000134269095	-0.522148376959
C	-0.370408995867	2.453369857955	2.382965857122
C	-2.554097813843	2.432267692015	0.639075457458
H	-3.385049140975	0.874476278898	-1.172235882549
H	-3.384913869540	-0.873064505716	-1.173751456740
H	-4.451855256288	-0.000377963174	-0.019667099570
C	-0.990677734508	3.640363277803	2.061580620985
H	0.482145345912	2.438679658675	3.065435916928
C	-2.087562555059	3.617141811393	1.179436496581
H	-3.427159708726	2.462451513592	-0.007491979828
H	-0.646280947749	4.582567436599	2.487226715414
H	-2.597963523273	4.547765512772	0.927183284841
H	0.602854615812	-0.002535195162	2.929722553153