

# ORIGINS OF THE DIASTERESELECTIVITY IN HYDROGEN BONDING DIRECTED DIELS-ALDER REACTIONS OF CHIRAL DIENES WITH ACHIRAL DIENOPHILES: A COMPUTATIONAL STUDY

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## CARTESIAN COORDINATES (Å) AND ABSOLUTE ENERGIES (au)

### REACTANTS

#### Maleic anhydride (MA)

B3LYP/6-31+G\*

C,0.668614,-1.258963,0.000006\C,-0.668611,-1.258967,-0.000005\H,-1.362744,-2.089813,-0.000005\C,-1.131986,0.158169,0.000004\C,1.131989,0.158176,0.000009\H,1.362748,-2.08981,0.000011\O,2.246372,0.600606,-0.000018\O,-2.246367,0.600605,-0.000012\O,-0.00001,0.972431,0.000019\\Version=AM64L-G03RevE.01\State=1-A\HF=-379.306312\RMSD=9.790e-09\RMSF=5.036e-05\ZeroPoint=0.0556758\Thermal=0.0626284\Dipole=0.0000302,-1.7360812,0.0000235

Zero-point correction=	0.055676 (Hartree/Particle)
Thermal correction to Energy=	0.062628
Thermal correction to Enthalpy=	0.063746
Thermal correction to Gibbs Free Energy=	0.019948
Sum of electronic and zero-point Energies=	-379.250636
Sum of electronic and thermal Energies=	-379.243684
Sum of electronic and thermal Enthalpies=	-379.242566
Sum of electronic and thermal Free Energies=	-379.286364

B3LYP/6-31+G\* ( $\epsilon=2.2706$ )

HF = -379.310153

BMK/6-31+G\*

C,0.795536968,-0.6696875755,-0.0575493617\C,0.7978340924,0.6668898027,-0.0579869585\H,1.6239494715,1.3673127475,-0.1181305564\C,-0.6297481113,1.1241771275,0.0456217224\C,-0.633606074,-1.1219900369,0.0463473176\H,1.6192373943,-1.3729885603,-0.1172520154\O,-1.0779286218,-2.2273947224,0.0788515982\O,-1.0702173481,2.2311560182,0.0774177775\O,-1.4260577709,0.0025251991,0.1036804763\\Version=AM64L-G09RevA.02\State=1-A\HF=-379.118932\RMSD=3.614e-09\RMSF=8.560e-05\Dipole=1.7736415,-0.0032704,-0.1288547

Zero-point correction=	0.056756 (Hartree/Particle)
Thermal correction to Energy=	0.063629
Thermal correction to Enthalpy=	0.064747
Thermal correction to Gibbs Free Energy=	0.021065
Sum of electronic and zero-point Energies=	-379.062176
Sum of electronic and thermal Energies=	-379.055303
Sum of electronic and thermal Enthalpies=	-379.054185
Sum of electronic and thermal Free Energies=	-379.097867

## N-Methyl Maleimide (NMM)

B3LYP/6-31+G\*

C,-0.004492,-1.628437,0.667882\C,0.009888,-1.62867,-0.669636\H,0.019618,-2.462505,-1.360459\C,0.01111,-0.204063,-1.149941\C,-0.013564,-0.202872,1.145325\H,-0.009616,-2.46239,1.358615\O,-0.02699,0.205533,2.290927\N,-0.003474,0.594402,-0.001342\O,0.02235,0.196951,-2.297829\C,-0.007502,2.048462,0.006501\H,-0.90375,2.423545,0.509282\H,0.002228,2.384592,-1.031826\H,0.876194,2.428451,0.527501\\Version=AM64L-G03RevE.01\State=1-A\HF=-398.762127\RMSD=4.287e-09\RMSF=2.813e-06\ZeroPoint=0.0963692\Thermal=0.1059524\Dipole=0.0244461,-0.4627376,-0.000002

Zero-point correction=	0.096369 (Hartree/Particle)
Thermal correction to Energy=	0.105952
Thermal correction to Enthalpy=	0.107070
Thermal correction to Gibbs Free Energy=	0.056621
Sum of electronic and zero-point Energies=	-398.665758
Sum of electronic and thermal Energies=	-398.656175
Sum of electronic and thermal Enthalpies=	-398.655057
Sum of electronic and thermal Free Energies=	-398.705506

B3LYP/6-31+G\* ( $\epsilon=2.2706$ )

HF = -398.762548

BMK/6-31+G\*

C,-0.0045752959,-1.6310560897,0.6679720676\C,0.0098566553,-1.6340647601,-0.6694436214\H,0.0196096007,-2.4678423497,-1.3638437438\C,0.0111386711,-0.1974197257,-1.1502785791\C,-0.0135696249,-0.1935216252,1.1400601493\H,-0.0098336802,-2.4626441308,1.3649540263\O,-0.0269290274,0.2177389872,2.2753523467\N,-0.0033660195,0.5957147101,-0.0049070867\O,0.0223376781,0.2016721438,-2.2895005582\C,-0.0074491315,2.0442991338,0.0082124631\H,-0.9061053151,2.4152341918,0.5143398637\H,0.0027992149,2.3847969759,-1.0314361009\H,0.8780862744,2.4200925384,0.5335187734\\Version=AM64L-G09RevA.02\State=1-A\HF=-398.5436434\RMSD=6.763e-09\RMSF=1.582e-05\Dipole=0.0014958,-0.5020857,-0.0126265

Zero-point correction=	0.098036 (Hartree/Particle)
Thermal correction to Energy=	0.107373
Thermal correction to Enthalpy=	0.108491
Thermal correction to Gibbs Free Energy=	0.059256
Sum of electronic and zero-point Energies=	-398.445607
Sum of electronic and thermal Energies=	-398.436271
Sum of electronic and thermal Enthalpies=	-398.435153
Sum of electronic and thermal Free Energies=	-398.484388

## N-Phenyl Maleimide (NPM)

### B3LYP/6-31+G\*

C,0.6781201949,0,-3.2765846331\C,-0.6546342046,0,-3.2814246766\H,-1.3507300739,0,-4.11066886  
23\C,-1.1415595546,0,-1.8667930503\C,1.1547670114,0,-1.858447674\H,1.3802169157,0,-4.1007545  
384\O,2.3180263388,0,-1.5095675485\N,0.0036159316,0,-1.0272 112824\O,-2.307297121 3,0,-1.5263  
204728\C,-0.0015455642,0,0.4131583763\C,-0.011642 2764,0,3.2318821236\C,-1.2166744562,0,1.12  
10829793\C,1.2084856649,0,1.1297656493\C,1.1917181506,0,2.5257680089\C,-1.2099144204,0,2.51  
71663856\H,-2.1574156636,0,05917713631\H,2.1529872858,0,0.6072255887\H,2.1392893368,0,3.05  
84024231\H,-2.1612776897,0,3.0429973064\H,-0.0155358056,0,4.318552534\\Version=AM64L-G03R  
evE.01 \State=1-A'\HF=-590.4988505

Zero-point correction=	0.149356 (Hartree/Particle)
Thermal correction to Energy=	0.158315
Thermal correction to Enthalpy=	0.159259
Thermal correction to Gibbs Free Energy=	0.114821
Sum of electronic and zero-point Energies=	-590.349495
Sum of electronic and thermal Energies=	-590.340535
Sum of electronic and thermal Enthalpies=	-590.339591
Sum of electronic and thermal Free Energies=	-590.384029

### B3LYP/6-31+G\* ( $\epsilon=2.2706$ )

HF = -590.496133

## 1

### B3LYP/6-31+G\*

C,2.948094,-1.768917,0.171453\C,1.600215,-1.294458,0.082769\C,1.340628,0.123393,-0.071605\C,2.49  
5461,0.977988,-0.150265\C,3.773784,0.483989,-0.067712\C,4.011722,-0.909624,0.10004\C,0.529602,-2.  
189269,0.137704\C,-0.794153,-1.753859,0.038054\C,-1.074198,-0.34085,-0.110981\C,-0.000437,0.5896  
87,-0.15266\C,-1.873363,-2.693952,0.075312\C,-3.175221,-2.283526,-0.034666\C,-3.463556,-0.896882,-  
0.183924\C,-2.457867,0.037216,-0.217402\C,-0.265655,2.090516,-0.342278\C,-0.605451,2.448832,-1.79  
2512\O,-1.317009,2.610228,0.479367\C,-1.023733,2.611227,1.867187\H,-4.497749,-0.57219,-0.26879\  
H,-2.709997,1.084976,-0.304437\H,-3.986341,-3.006658,-0.007709\H,0.731966,-3.252757,0.25224\H,-1.  
631225,-3.748327,0.190536\H,3.106814,-2.8383,0.293018\H,2.375423,2.045538,-0.288331\H,4.616774,  
1.16735,-0.133208\H,5.030451,-1.282387,0.166027\H,0.639319,2.641682,-0.064764\H,-0.76772,3.5288  
07,-1.878989\H,-1.50711,1.931233,-2.132395\H,0.22054,2.161683,-2.452487\H,-0.112861,3.19348,2.07  
9193\H,-0.893262,1.592387,2.257858\H,-1.874193,3.082599,2.366226\\Version=AM64L-G03RevE.01\S  
tate=1-A'\HF=-732.6920449\RMSD=3.808e-09\RMSF=4.939e-06\ZeroPoint=0.2837057\Thermal=0.3044  
419\Dipole=0.3657727,-0.1177432,0.1532281

Zero-point correction=	0.283706 (Hartree/Particle)
Thermal correction to Energy=	0.304442
Thermal correction to Enthalpy=	0.305560

Thermal correction to Gibbs Free Energy= 0.230859  
Sum of electronic and zero-point Energies= -732.408339  
Sum of electronic and thermal Energies= -732.387603  
Sum of electronic and thermal Enthalpies= -732.386485  
Sum of electronic and thermal Free Energies= -732.461186

### B3LYP/6-31+G\* ( $\epsilon=2.2706$ )

HF = -732.676003

### BMK/6-31+G\*

C,2.9590063927,-1.7665957326,0.1730273753\C,1.6054227234,-1.286184954,0.0914187098\C,1.34825  
99594,0.1318820345,-0.0717653864\C,2.5086734177,0.9888100065,-0.1742338517\C,3.7864613242,0.  
4904815574,-0.1014832529\C,4.0237569426,-0.9099302342,0.0812527808\C,0.5322308975,-2.181546  
4323,0.1614461015\C,-0.7929150783,-1.740491763,0.0597618501\C,-1.0706456449,-0.3277222791,-0.  
1004603101\C,0.0064288856,0.6019075099,-0.144718885\C,-1.8787152658,-2.6832112276,0.1046586  
727\C,-3.1795297129,-2.2698053081,-0.0126061238\C,-3.4663605838,-0.876383176,-0.1795114419\C,  
-2.4591105228,0.056754505,-0.219108895\C,-0.259525761,2.1100878556,-0.3275995757\C,-0.579041  
9052,2.4595438264,-1.7906340285\O,-1.3118371107,2.6154110252,0.4668064417\C,-1.0743577001,2.  
5492539374,1.85013217\H,-4.5014655204,-0.5514780804,-0.2741894125\H,-2.7061692631,1.1065579  
315,-0.3258659694\H,-3.9950763417,-2.9905330937,0.0191101741\H,0.7333876103,-3.2466855443,0.  
2844052619\H,-1.6360251983,-3.7385764341,0.2287986003\H,3.1146842505,-2.8376073009,0.302685  
0291\H,2.3886434201,2.0563966336,-0.3272498671\H,4.6333155109,1.1695576128,-0.1880404416\H,  
5.0444847795,-1.2837156631,0.1392217375\H,0.6454119199,2.6584012689,-0.0332854706\H,-0.7597  
82938,3.5381857529,-1.8794800697\H,-1.4692841002,1.9200902646,-2.1354191646\H,0.2644880329,  
2.1805001334,-2.4349810688\H,-0.1269290779,3.0514011445,2.1124728747\H,-1.0342978766,1.5076  
836734,2.2060663931\H,-1.9038944653,3.06841555,2.3412380426\\Version=AM64L-G09RevA.02\Stat  
e=1-A\HF=-732.1917817\RMSD=3.461e-09\RMSF=6.404e-06\Dipole=0.3538689,-0.1247149,0.1644906

Zero-point correction= 0.286241 (Hartree/Particle)  
Thermal correction to Energy= 0.306721  
Thermal correction to Enthalpy= 0.307839  
Thermal correction to Gibbs Free Energy= 0.233943  
Sum of electronic and zero-point Energies= -731.905540  
Sum of electronic and thermal Energies= -731.885061  
Sum of electronic and thermal Enthalpies= -731.883943  
Sum of electronic and thermal Free Energies= -731.957839

## 2

### B3LYP/6-31+G\*

H,-4.260674,-2.504298,0.126386\C,-3.395666,-1.847616,0.081058\H,-1.968342,-3.442173,0.096144\C,-2  
.128534,-2.36659,0.063996\C,-2.501226,0.415721,-0.026032\C,-0.979364,-1.514334,0.009131\C,-3.5764  
87,-0.43566,0.036663\C,-1.149836,-0.077317,-0.039734\C,0.307648,-2.057925,0.010132\H,-4.583218,-0  
.025199,0.047056\C,-0.150703,2.291186,-0.127609\H,-2.6715,1.481408,-0.09106\C,1.444971,-1.248095,

-0.016213\H,0.427163,-3.139473,0.042002\C,2.752066,-1.831987,0.003848\C,1.296482,0.193123,-0.05697\H,2.477129,2.042596,-0.050284\C,-0.005498,0.766392,-0.086698\C,3.87921,-1.05465,0.000864\H,2.827113,-2.91704,0.026845\H,4.866,-1.509566,0.019107\C,3.749869,0.362928,-0.020545\H,4.643055,0.982615,-0.013012\C,2.513813,0.959964,-0.047709\H,0.805384,2.723566,-0.431925\C,-0.516715,2.903295,1.227209\O,-1.13242,2.752675,-1.074632\H,0.263062,2.677714,1.962824\H,-1.465521,2.511878,1.605464\H,-0.601726,3.991065,1.127645\H,-0.93875,2.35491,-1.938495\\Version=AM64L-G03RevE.01\State=1-A\HF=-693.3860103\RMSD=4.211e-09\RMSF=1.167e-05\ZeroPoint=0.2553404\Thermal=0.2742342\Dipole=0.4237133,-0.3642145,-0.0505333

Zero-point correction=	0.255340 (Hartree/Particle)
Thermal correction to Energy=	0.274234
Thermal correction to Enthalpy=	0.275352
Thermal correction to Gibbs Free Energy=	0.205114
Sum of electronic and zero-point Energies=	-693.130670
Sum of electronic and thermal Energies=	-693.111776
Sum of electronic and thermal Enthalpies=	-693.110658
Sum of electronic and thermal Free Energies=	-693.180897

### B3LYP/6-31+G\* ( $\epsilon=2.2706$ )

HF = -693.374774

### BMK/6-31+G\*

H,-4.2697734181,-2.5049663863,0.1354460708\C,-3.4019801498,-1.8493703262,0.0863551191\H,-1.9746574799,-3.4489379019,0.079788894\C,-2.1356368267,-2.3711449784,0.0556588458\C,-2.5068037448,0.4229850436,-0.0120060297\C,-0.980947611,-1.5151581733,-0.0016188284\C,-3.5821122379,-0.4284668261,0.0557779012\C,-1.1502947086,-0.0771959589,-0.0435375069\C,0.3078969749,-2.0630736584,-0.0066174087\H,-4.5904627843,-0.0179790343,0.0820475425\C,-0.1536833705,2.2972283074,-0.1540616545\H,-2.6724887119,1.4928743484,-0.059982932\C,1.4464492721,-1.249138687,-0.0240248792\H,0.4269592999,-3.1471945198,0.0162984157\C,2.7602767112,-1.8353710744,-0.0017863489\C,1.2983689093,0.1925425221,-0.057387547\H,2.4776986959,2.0518978762,-0.0170733514\C,-0.0046092648,0.7667980532,-0.0958644428\C,3.8863875636,-1.0552118456,0.0104695209\H,2.8345626068,-2.9226774408,0.0114313821\H,4.875899916,-1.5084440422,0.0305386586\C,3.7554847157,0.3706167344,0.0041371675\H,4.6498595396,0.9911457555,0.0294999081\C,2.5188701989,0.9673968781,-0.028848038\H,0.8027762817,2.7264016858,-0.4697949165\C,-0.5093245312,2.905329246,1.2123735075\O,-1.1392077568,2.7377635247,-1.0771223818\H,0.2748996792,2.6676427382,1.9423578651\H,-1.4612257165,2.5081437112,1.5843237112\H,-0.5923392875,3.9954965853,1.1178206298\H,-0.9640577645,2.3391808434,-1.9391428741\\Version=AM64L-G09RevA.02\State=1-A\HF=-692.9162894\RMSD=8.889e-09\RMSF=3.704e-06\Dipole=0.4242873,-0.344793,-0.0720262

Zero-point correction=	0.257589 (Hartree/Particle)
Thermal correction to Energy=	0.276361
Thermal correction to Enthalpy=	0.277479
Thermal correction to Gibbs Free Energy=	0.207471
Sum of electronic and zero-point Energies=	-692.658700
Sum of electronic and thermal Energies=	-692.639928
Sum of electronic and thermal Enthalpies=	-692.638810



Sum of electronic and thermal Free Energies= -692.708818

### 3

#### B3LYP/6-31+G\*

H,-4.903787,-1.600414,0.085107\C,-3.910028,-1.165636,0.016923\H,-2.885151,-3.018833,0.316574\C,-2.794554,-1.948281,0.145379\C,-2.510727,0.800372,-0.298113\C,-1.478124,-1.391895,0.055148\C,-3.756815,0.230534,-0.212629\C,-1.301523,0.030896,-0.166166\C,-0.359564,-2.216983,0.178814\H,-4.639186,0.855882,-0.323566\C,0.184758,2.095366,-0.450402\H,-2.461799,1.866552,-0.479757\C,0.93591,-1.706863,0.078688\H,-0.500605,-3.282658,0.350064\C,2.065431,-2.579471,0.193038\C,1.132782,-0.288812,-0.144532\H,2.713125,1.190914,-0.436737\C,0.011411,0.583158,-0.247316\C,3.345565,-2.105585,0.087631\H,1.878028,-3.637437,0.364013\H,4.194711,-2.778404,0.174527\C,3.557156,-0.717311,-0.143855\H,4.571483,-0.337297,-0.237649\C,2.497784,0.148892,-0.253755\H,-0.815766,2.529135,-0.445007\C,0.753826,2.465111,-1.840249\C,0.903195,2.839774,0.707933\H,0.154589,2.004727,-2.634406\H,1.789757,2.147308,-1.98735\H,0.71729,3.553233,-1.978777\C,0.243308,2.638249,2.077522\H,0.888253,3.909817,0.455309\H,1.959756,2.561966,0.776241\H,-0.811814,2.940127,2.060987\H,0.749187,3.237121,2.844351\H,0.283184,1.589165,2.391724\\Version=AM64L-G03RevE.01\State=1-A\HF=-696.7937954\RMS D=6.009e-09\RMSF=2.369e-06\ZeroPoint=0.3078359\Thermal=0.3290354\Dipole=0.0011528,0.1232428,-0.0079218

Zero-point correction=	0.307836 (Hartree/Particle)
Thermal correction to Energy=	0.329035
Thermal correction to Enthalpy=	0.330153
Thermal correction to Gibbs Free Energy=	0.254324
Sum of electronic and zero-point Energies=	-696.485959
Sum of electronic and thermal Energies=	-696.464760
Sum of electronic and thermal Enthalpies=	-696.463642
Sum of electronic and thermal Free Energies=	-696.539472

#### B3LYP/6-31+G\* ( $\epsilon=2.2706$ )

HF = -696.775239

#### BMK/6-31+G\*

H,-4.9140304812,-1.5976063617,0.093479227\C,-3.9181226798,-1.1636746851,0.0229664175\H,-2.8887610312,-3.0156156716,0.3437791804\C,-2.8020765974,-1.944622012,0.1606792583\C,-2.5201858774,0.8103615534,-0.3136830369\C,-1.4803438001,-1.3837110597,0.0644368496\C,-3.7654835262,0.237933954,-0.2237034317\C,-1.3055312327,0.0376781659,-0.1702439355\C,-0.360090283,-2.2104541092,0.1962699102\H,-4.650428306,0.8607133394,-0.3449357921\C,0.1839208292,2.1063586978,-0.4559585374\H,-2.4727008442,1.8755783084,-0.511984549\C,0.9369666667,-1.6971480321,0.0876935593\H,-0.5001502816,-3.2765276026,0.3799965908\C,2.0718321799,-2.5729504535,0.2101123233\C,1.1323924034,-0.2805532076,-0.1490104812\H,2.7168008116,1.202879986,-0.4660006661\C,0.0086440698,0.5913184684,-0.2557148944\C,3.3516778058,-2.0985064511,0.0974687394\H,1.8826323745,-3.6308558365,0.3927516196\H,4.2039633814,-2.7693149048,0.1909163475\C,3.5629180303,-0.7047813483,-0.1514546114\H,4.5791749797,-0.3267103806,-0.2525056696\C,2.5033152321,0.1610806528,-0.2680



431066\H,-0.8168309984,2.5431977184,-0.4402759996\C,0.7553616458,2.4758000407,-1.8498976017  
\C,0.9142418404,2.8332915428,0.7106384802\H,0.1382731433,2.032125702,-2.6426494135\H,1.7844  
026501,2.1318742103,-2.0007281053\H,0.7422169592,3.5678129146,-1.9757127303\C,0.2443149454,  
2.5928795267,2.0767787056\H,0.8949425261,3.9093167694,0.478192441\H,1.9707162338,2.5475487  
43,0.7724475211\H,-0.8171259753,2.8787341385,2.0496378864\H,0.7347502523,3.1845655177,2.861  
1487092\H,0.2994499539,1.5344031662,2.3628157959\\Version=AM64L-G09RevA.02\State=1-A\HF=-  
696.2915451\RMSD=3.260e-09\RMSF=5.463e-06\Dipole=0.0003163,0.1212786,-0.0053457

Zero-point correction=	0.309933 (Hartree/Particle)
Thermal correction to Energy=	0.330984
Thermal correction to Enthalpy=	0.332101
Thermal correction to Gibbs Free Energy=	0.256612
Sum of electronic and zero-point Energies=	-695.981613
Sum of electronic and thermal Energies=	-695.960562
Sum of electronic and thermal Enthalpies=	-695.959444
Sum of electronic and thermal Free Energies=	-696.034933

#### 4

#### B3LYP/6-31+G\*

H,0,4.930356,-1.848443,0.566163\C,0,3.927399,-1.498222,0.33637\H,0,4.33641,0.5376,0.851677\C,0,3.5  
98212,-0.17742,0.494583\C,0,1.673924,-1.993629,-0.431883\C,0,2.282666,0.301995,0.197123\C,0,2.946  
015,-2.416876,-0.134378\C,0,1.277512,-0.621426,-0.283068\C,0,1.955736,1.651804,0.356607\H,0,3.208  
52,-3.464499,-0.259365\C,0,-1.060725,-1.129732,-1.124439\H,0,0.955301,-2.725344,-0.78386\C,0,0.672  
903,2.130145,0.075839\H,0,2.717176,2.345744,0.70848\C,0,0.354015,3.515976,0.245092\C,0,-0.347213  
,1.213435,-0.390071\H,0,-2.457549,1.10094,-0.931603\C,0,-0.029647,-0.155539,-0.58322\C,0,-0.903002,  
3.991743,-0.018745\H,0,1.138955,4.185103,0.591332\H,0,-1.132026,5.046269,0.112496\C,0,-1.918639,  
3.094755,-0.459644\H,0,-2.920254,3.472251,-0.650022\C,0,-1.652064,1.759933,-0.63457\H,0,-1.808979  
, -0.609105,-1.729019\C,0,-1.814399,-1.947368,-0.056194\H,0,-0.575376,-1.83309,-1.809682\O,0,-2.6651  
1,-1.036697,0.644351\H,0,-1.086209,-2.364824,0.658059\C,0,-2.622108,-3.087555,-0.68527\H,0,-3.3274  
68,-2.692678,-1.42622\H,0,-3.194069,-3.63606,0.071122\H,0,-1.959963,-3.805583,-1.184709\C,0,-3.026  
568,-1.438102,1.953381\H,0,-3.615118,-0.621947,2.380496\H,0,-2.135289,-1.602996,2.578372\H,0,-3.6  
37644,-2.353277,1.956391\\Version=AM64L-G03RevE.01\State=1-A\HF=-772.0101755\RMSD=7.224e-  
09\RMSF=3.380e-06\ZeroPoint=0.312085\Thermal=0.3346231\Dipole=0.375065,-0.4323737,-0.0219

Zero-point correction=	0.312085 (Hartree/Particle)
Thermal correction to Energy=	0.334623
Thermal correction to Enthalpy=	0.335741
Thermal correction to Gibbs Free Energy=	0.255969
Sum of electronic and zero-point Energies=	-771.698091
Sum of electronic and thermal Energies=	-771.675552
Sum of electronic and thermal Enthalpies=	-771.674434
Sum of electronic and thermal Free Energies=	-771.754207

#### B3LYP/6-31+G\* ( $\epsilon=2.2706$ )

HF = -771.991321

### BMK/6-31+G\*

H,4.9453376694,-1.8495728683,0.5680032477\C,3.9411273576,-1.4980096146,0.3373502882\H,4.358  
470547,0.5463885255,0.8262468369\C,3.616592075,-0.1736758168,0.4807785143\C,1.6764297097,-2.  
0041966342,-0.4163006327\C,2.2935756047,0.3059782402,0.18426255\C,2.9490409257,-2.426201862  
4,-0.1170764233\C,1.2852883411,-0.6212503597,-0.2827641371\C,1.969674151,1.6611892138,0.3355  
233153\H,3.2097087733,-3.4780373711,-0.2248714826\C,-1.0566967542,-1.1317172749,-1.130940658  
4\H,0.9496782142,-2.7388563073,-0.7529156981\C,0.6791846579,2.1344585672,0.0661593976\H,2.7  
36597202,2.3593691779,0.6738444659\C,0.3571386039,3.5273328554,0.2333651073\C,-0.344586826  
6,1.2133102121,-0.3837744986\H,-2.4735750753,1.0811358528,-0.8765124603\C,-0.0237824268,-0.15  
56980244,-0.5837487662\C,-0.9067498664,3.9954047903,-0.0130917219\H,1.1478044908,4.20085611  
38,0.5641944621\H,-1.1402421478,5.0512486056,0.1149711909\C,-1.9331176774,3.0862959847,-0.43  
10693339\H,-2.9420290099,3.4593851864,-0.6004925045\C,-1.6646099834,1.7514571999,-0.6059775  
682\H,-1.8093171965,-0.6081129794,-1.7311821983\C,-1.8072788704,-1.938284395,-0.0469098254\H  
,-0.5709019256,-1.837930388,-1.8149621751\O,-2.6367773548,-1.0278330012,0.6414719571\H,-1.071  
4093059,-2.3589988079,0.6631753375\C,-2.6274251526,-3.079800621,-0.6755560272\H,-3.325698687  
5,-2.6719285073,-1.4194923965\H,-3.2072687582,-3.6197229038,0.083657921\H,-1.9672512805,-3.80  
3782087,-1.1724709929\C,-3.0442614025,-1.4442870602,1.9176674471\H,-3.627681633,-0.625109533  
5,2.3504594691\H,-2.1732075854,-1.6465946981,2.563436184\H,-3.6760984026,-2.3469284096,1.877  
5138092\\Version=AM64L-G09RevA.02\State=1-A\HF=-771.4791899\RMSD=4.606e-09\RMSF=6.446e-  
06\Dipole=-0.1136325,-0.5337737,0.2693452

Zero-point correction=	0.316124 (Hartree/Particle)
Thermal correction to Energy=	0.338096
Thermal correction to Enthalpy=	0.339214
Thermal correction to Gibbs Free Energy=	0.261294
Sum of electronic and zero-point Energies=	-771.163066
Sum of electronic and thermal Energies=	-771.141094
Sum of electronic and thermal Enthalpies=	-771.139976
Sum of electronic and thermal Free Energies=	-771.217896

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### B3LYP/6-31+G\*

C,-1.3320370855,0.6050379682,2.6339475194\C,-1.4024187829,0.4103723486,4.1200087599\H,-0.531  
8604012,-0.1380086267,4.4969789277\H,-2.3057550779,-0.1469771669,4.4055140793\H,-1.45127516  
81,1.3745872466,4.6453570732\C,-0.3364596717,0.1691091474,1.8397634928\H,-2.1634375814,1.146  
7430171,2.1777750099\C,-0.2893108108,0.3685643403,0.3974410589\H,0.5005765916,-0.371801547  
3,2.285658785\C,0.704211678,-0.0558329339,-0.4049100868\H,-1.1291301882,0.9097629098,-0.0446  
186676\H,1.5478904956,-0.6049599205,0.0186222967\C,0.7675154316,0.1745581985,-1.8928155158  
\H,-0.1461519116,0.7041526596,-2.2148106534\O,0.8592684832,-1.0628788707,-2.6145045777\C,1.9  
956975763,0.9906623069,-2.2960287986\H,1.9734248742,1.9769699939,-1.8200503136\H,2.0218997  
595,1.1197601504,-3.3835081515\H,2.9132700099,0.4759910695,-1.9884285217\C,-0.3201833719,-1.  
8491084826,-2.5849266042\H,-1.1756430052,-1.2978100387,-3.007969492\H,-0.5770046315,-2.17010

37227,-1.5656665242\H,-0.1230872122,-2.7297900467,-3.2018290958\\Version=IA32L-G03RevD.01\State=1-A\HF=-388.4791433

Zero-point correction=	0.202959 (Hartree/Particle)
Thermal correction to Energy=	0.214349
Thermal correction to Enthalpy=	0.215293
Thermal correction to Gibbs Free Energy=	0.165584
Sum of electronic and zero-point Energies=	-388.276184
Sum of electronic and thermal Energies=	-388.264794
Sum of electronic and thermal Enthalpies=	-388.263850
Sum of electronic and thermal Free Energies=	-388.313559

B3LYP/6-31+G\* ( $\epsilon=2.2706$ )

HF = -388.466560

BMK/6-31+G\*

C,-1.3217713223,0.6305271566,2.636268078\C,-1.3911231683,0.4220347255,4.129421835\H,-0.5479186801,-0.1826257725,4.4869657656\H,-2.3248944234,-0.0865494447,4.4122097899\H,-1.3761610165,1.3848834919,4.6616494814\C,-0.3485095599,0.154399796,1.8372980487\H,-2.1281809977,1.2181167951,2.1879581066\C,-0.3038469341,0.3700422181,0.3866718521\H,0.4660330376,-0.4321995041,2.2712419039\C,0.6738321652,-0.0859102394,-0.4174046093\H,-1.1260559553,0.9478929387,-0.04677773\H,1.4998599805,-0.6709342856,-0.0005983858\C,0.7473314839,0.1624351203,-1.9113770684\H,-0.171538328,0.6886916957,-2.2334445495\O,0.8643758616,-1.0481214802,-2.6336712685\C,1.9763787883,1.0062826362,-2.2783770229\H,1.9204736886,1.9912069235,-1.7986019129\H,2.0288038038,1.1340405288,-3.366893928\H,2.8916167256,0.5010524817,-1.9423162775\C,-0.2813661808,-1.8592180207,-2.5932750714\H,-1.1604265797,-1.3214076268,-2.9904129023\H,-0.5089926597,-2.1960834621,-1.5697156405\H,-0.0779197292,-2.729558672,-3.2258204944\\Version=EM64L-G09RevA.02\State=1-A\HF=-388.1985605\RMSD=3.614e-09\RMSF=9.442e-06\ZeroPoint=0.2055294\Thermal=0.2166976\Dipole=-0.5154262,0.1702338,0.4750904

Zero-point correction=	0.205529 (Hartree/Particle)
Thermal correction to Energy=	0.216698
Thermal correction to Enthalpy=	0.217642
Thermal correction to Gibbs Free Energy=	0.168605
Sum of electronic and zero-point Energies=	-387.993031
Sum of electronic and thermal Energies=	-387.981863
Sum of electronic and thermal Enthalpies=	-387.980919
Sum of electronic and thermal Free Energies=	-388.029956

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B3LYP/6-31+G\*

C,0.3569729762,-0.1143393113,-0.1393062215\H,1.3369430872,0.1908452433,-0.5136799588\C,-0.7179730523,0.6369644756,-0.4457882285\H,-1.7071108184,0.3473776679,-0.0850058849\C,0.3233471585,-1.3218109662,0.674251355\H,-0.6541050752,-1.6318180345,1.0488951036\C,1.4070911768,-2.0585933485,0.9822603528\H,2.3800370783,-1.7381723535,0.6035183822\C,1.3975468306,-3.3046655493,1.8175390224\H,2.0401510407,-3.1943781518,2.7023204294\H,1.7872759254,-4.1638567124,1.2536133328\H,0.3869344719,-3.5532897685,2.1602328511\C,-0.6746740067,1.8782486569,-1.2934987862\H,0.3675656867,2.0732682105,-1.593026897\O,-1.4837521227,1.7127015167,-2.4767101731\H,-1.2170265449,0.8871984884,-2.9123177072\C,-1.2272175793,3.1082235831,-0.5769580292\H,-0.6193904417,3.3453187294,0.3029204166\H,-2.2594641564,2.9310315667,-0.2535946224\H,-1.2221516345,3.9697460576,-1.2536647372\\Version=IA32L-G03RevD.01\State=1-A\HF=-349.1739102

Zero-point correction=	0.174744 (Hartree/Particle)
Thermal correction to Energy=	0.184675
Thermal correction to Enthalpy=	0.185619
Thermal correction to Gibbs Free Energy=	0.139734
Sum of electronic and zero-point Energies=	-348.999166
Sum of electronic and thermal Energies=	-348.989235
Sum of electronic and thermal Enthalpies=	-348.988291
Sum of electronic and thermal Free Energies=	-349.034176

B3LYP/6-31+G\* ( $\epsilon=2.2706$ )

HF = -349.171402

BMK/6-31+G\*

C,0.3570780605,-0.1155279831,-0.1540109816\H,1.3409574645,0.1953320251,-0.518678629\C,-0.7233268571,0.6235815001,-0.4694679905\H,-1.7161384203,0.3270395781,-0.1172098123\C,0.318735367,-1.3292026722,0.6688849496\H,-0.6626612273,-1.6454305608,1.0329100059\C,1.409390886,-2.0510622781,0.9883513341\H,2.3841439283,-1.7203339952,0.6181909065\C,1.3995971428,-3.3012470707,1.833228799\H,2.0292535965,-3.1761924529,2.7267747897\H,1.8044805041,-4.1574501292,1.2731499422\H,0.3828769883,-3.553363083,2.160369064\C,-0.6794545682,1.8763726981,-1.3165105472\H,0.3642202602,2.065422051,-1.6227430833\O,-1.5019779461,1.7337946488,-2.4682985435\H,-1.252435081,0.922547961,-2.9290517611\C,-1.2118206451,3.1012453041,-0.5623786489\H,-0.5885167478,3.3117442655,0.315461039\H,-2.2427111248,2.9166800607,-0.2320578378\H,-1.2106925806,3.9760511326,-1.2249159947\\Version=AM64L-G09RevA.02\State=1-A\HF=-348.9239179\RMSE=1.453e-09\RMSEF=1.437e-05\ZeroPoint=0.1770009\Thermal=0.1900741\Dipole=0.6016305,-0.6039626,0.3504366

Zero-point correction=	0.177001 (Hartree/Particle)
Thermal correction to Energy=	0.190074
Thermal correction to Enthalpy=	0.191192
Thermal correction to Gibbs Free Energy=	0.133563
Sum of electronic and zero-point Energies=	-348.746917
Sum of electronic and thermal Energies=	-348.733844
Sum of electronic and thermal Enthalpies=	-348.732726
Sum of electronic and thermal Free Energies=	-348.790355

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**B3LYP/6-31+G\***

C,-1.472391,3.361441,2.602294\C,-0.732875,2.266129,2.233581\C,0.470442,2.406051,1.469986\C,0.861924,3.738608,1.064379\C,0.063609,4.854246,1.474247\C,-1.066422,4.676089,2.228635\C,1.275373,1.304672,1.095599\C,2.,3.914282,0.269661\C,2.782093,2.829161,-0.139774\C,2.425146,1.496879,0.291535\C,3.27,0.4141,-0.116304\H,3.017097,-0.590324,0.207618\C,4.375613,0.626689,-0.902225\C,4.718273,1.941448,-1.334163\C,3.942613,3.007804,-0.958681\H,-2.386304,3.227327,3.175576\H,-1.078882,1.271326,2.482767\H,0.374486,5.850801,1.16804\H,-1.663444,5.531779,2.533685\H,2.282457,4.919431,-0.038401\H,4.99935,-0.213229,-1.198424\H,5.596706,2.092606,-1.956157\H,4.198589,4.016266,-1.276461\C,0.185891,-0.922624,0.755879\C,1.112532,-0.426568,2.937266\C,0.181715,-2.247802,1.562377\H,0.603346,-1.034824,-0.257646\C,0.969273,-1.958576,2.856742\H,0.354431,0.02324,3.59169\H,-0.856123,-2.522237,1.775268\H,0.626275,-3.067969,0.988988\H,0.489986,-2.364947,3.752769\H,1.977371,-2.387292,2.806459\N,0.983803,-0.023612,1.535534\O,2.328853,0.017346,3.504948\O,-1.146402,-0.39769,0.598076\C,-1.875384,-0.988204,-0.463082\H,-2.823341,-0.449195,-0.534436\H,-2.085919,-2.054027,-0.281025\H,-1.335251,-0.893722,-1.418676\H,3.05449,-0.243875,2.91186\\Version=AM64L-G03RevE.01\State=1-A\HF=-940.6821248

Zero-point correction=	0.340329 (Hartree/Particle)
Thermal correction to Energy=	0.357952
Thermal correction to Enthalpy=	0.358896
Thermal correction to Gibbs Free Energy=	0.294811
Sum of electronic and zero-point Energies=	-940.341796
Sum of electronic and thermal Energies=	-940.324173
Sum of electronic and thermal Enthalpies=	-940.323229
Sum of electronic and thermal Free Energies=	-940.387314

**B3LYP/6-31+G\* ( $\epsilon=2.2706$ )**

HF = -940.6904099

## TRANSITION STATES

### TS1N-A

#### B3LYP/6-31+G\*

N,-2.468121,0.272834,-1.363897\C,-2.138042,-1.073339,-1.529395\C,-0.642452,-1.140657,-1.597935\C,-0.163681,0.18368,-1.587444\C,-1.328591,1.089656,-1.458341\O,-2.943866,-1.987753,-1.589408\O,-1.354117,2.313272,-1.435742\C,-3.819212,0.761996,-1.158311\C,-0.180141,-2.042485,0.287011\C,1.249485,-1.923405,0.16821\C,1.802839,-0.614046,0.258303\C,0.883312,0.483078,0.51424\C,-0.318075,0.18545,1.272207\C,-0.854179,-1.131475,1.168434\C,2.074063,-3.028049,-0.136689\C,3.435449,-2.856302,-0.317074\C,3.992648,-1.563546,-0.237353\C,3.194184,-0.462154,0.023057\C,-2.059868,-1.466189,1.826025\C,-2.713947,-0.531905,2.607861\C,-2.197504,0.777026,2.711867\C,-1.039021,1.135451,2.044642\C,1.359923,1.933152,0.475461\C,2.141001,2.338945,1.742522\O,2.161146,2.144167,-0.693097\C,2.052285,3.455647,-1.23618\H,5.059925,-1.425894,-0.39067\H,3.635308,0.525511,0.035726\H,4.072137,-3.712216,-0.525287\H,-0.619933,-3.029318,0.155073\H,1.626971,-4.017012,-0.210576\H,-2.459922,-2.470418,1.712089\H,-0.683535,2.155355,2.134765\H,-2.715584,1.515385,3.318474\H,-3.625846,-0.800906,3.134301\H,0.4685,2.565226,0.38515\H,2.444517,3.389743,1.673789\H,3.039339,1.727524,1.86275\H,1.530357,2.222083,2.643394\H,2.40489,4.221209,-0.529359\H,1.01556,3.672007,-1.525718\H,2.692856,3.476241,-2.121808\H,-0.187933,-1.950844,-2.154661\H,0.756746,0.543279,-2.023914\H,-4.139257,0.591655,-0.124281\H,-4.50138,0.237992,-1.832562\H,-3.825021,1.832894,-1.37014\\Version=AM64L-G03RevE.01\State=1-A\HF=-1131.422047\RMSD=9.716e-09\RMSF=4.502e-06\ZeroPoint=0.3816593\Thermal=0.404182\Dipole=0.7565819,0.7199451,-0.1666752\

Zero-point correction=	0.381659 (Hartree/Particle)
Thermal correction to Energy=	0.412557
Thermal correction to Enthalpy=	0.413675
Thermal correction to Gibbs Free Energy=	0.316501
Sum of electronic and zero-point Energies=	-1131.040388
Sum of electronic and thermal Energies=	-1131.009490
Sum of electronic and thermal Enthalpies=	-1131.008372
Sum of electronic and thermal Free Energies=	-1131.105546

#### B3LYP/6-31+G\* ( $\epsilon=2.2706$ )

HF = -1131.398698

#### BMK/6-31+G\*

N,-2.2682485499,0.1365172921,-1.2070339071\C,-1.8950159357,-1.1920363556,-1.3901921139\C,-0.3975834298,-1.2016930927,-1.5201214331\C,0.0328688299,0.1299614673,-1.5034897348\C,-1.1757820578,0.9940662672,-1.339662081\O,-2.6647670384,-2.1278635296,-1.4108223843\O,-1.2421431758,2.2072570669,-1.3076285517\C,-3.6254064366,0.5620493868,-0.9476566933\C,0.0901283278,-2.0880457755,0.467894516\C,1.5056527783,-1.8783928415,0.3324960555\C,1.9812034603,-0.5352141333,0.386600594\C,0.9967585806,0.5158024541,0.5972248275\C,-0.2121211305,0.1797496403,1.3238894111\C,-0.6708245762,-1.1711372855,1.2615287455\C,2.3977373765,-2.9452237171,0.0472480592\C,3.7459961317,-2.6961880801,-0.1412682794\C,4.2291552697,-1.3642755876,-0.0876006245\C,3.368179



2641,-0.3046544813,0.148834649\C,-1.908654084,-1.5383611689,1.8588292995\C,-2.6584082929,-0.6012243996,2.5438812609\C,-2.2135326115,0.7456584134,2.6104349431\C,-1.0338732612,1.1332981414,1.9996490372\C,1.3999534507,1.9920628285,0.5301382628\C,2.1365938224,2.4442981126,1.8149532179\O,2.1993555501,2.2221769263,-0.6134971206\C,2.0228412956,3.5033912112,-1.175066509\H,5.2891008361,-1.1688452548,-0.2424124995\H,3.7490624166,0.7105706955,0.144440412\H,4.4337044119,-3.5180250893,-0.3333635231\H,-0.299315664,-3.0993048029,0.3387977857\H,2.0079931389,-3.96197235,0.00007327\H,-2.2482587363,-2.5693973983,1.7699583531\H,-0.7346968675,2.1759356444,2.0527736652\H,-2.8106715991,1.4853590107,3.1412736548\H,-3.5924415016,-0.8902657108,3.0228039753\H,0.4771284368,2.5768753677,0.4177445055\H,2.4094966594,3.5049449609,1.7356237177\H,3.0501785572,1.8572295141,1.9632164042\H,1.5005867596,2.3165313413,2.6997429568\H,2.3001768669,4.3000710679,-0.4650766162\H,0.9788827501,3.6447254808,-1.4947742618\H,2.6867186835,3.5620580172,-2.0439457575\H,0.0937859033,-2.0258408222,-2.025352342\H,0.9427913936,0.5371358095,-1.927664799\H,-3.9559124443,0.1936982068,0.0318576085\H,-4.2938985187,0.1690768392,-1.7223822322\H,-3.6373095497,1.6560364426,-0.9576493842\\Version=EM64L-G09RevA.02\State=1-A\HF=-1130.7148225\RMSD=7.607e-09\RMSF=1.046e-05\ZeroPoint=0.3867555\Thermal=0.4084209\Dipole=0.6684039,0.3201515,0.6487575

Zero-point correction=	0.386756 (Hartree/Particle)
Thermal correction to Energy=	0.408421
Thermal correction to Enthalpy=	0.409365
Thermal correction to Gibbs Free Energy=	0.338276
Sum of electronic and zero-point Energies=	-1130.328067
Sum of electronic and thermal Energies=	-1130.306402
Sum of electronic and thermal Enthalpies=	-1130.305457
Sum of electronic and thermal Free Energies=	-1130.376546

## **TS1N-B**

B3LYP/6-31+G\*

N,-2.723219,0.244459,-1.162304\C,-1.622169,-0.331051,-1.832883\C,-0.497678,0.609253,-1.675338\C,-0.94469,1.722866,-0.932494\C,-2.418886,1.516165,-0.69216\O,-1.666997,-1.40151,-2.423495\O,-3.211319,2.284793,-0.173052\C,-4.027464,-0.380438,-1.03509\C,-0.193141,1.670957,0.947497\C,1.213907,1.718205,0.620726\C,1.799073,0.533902,0.088386\C,0.95773,-0.646069,-0.033567\C,-0.150149,-0.775727,0.893575\C,-0.70807,0.41908,1.442287\C,1.962771,2.909506,0.709306\C,3.29049,2.934449,0.316488\C,3.887385,1.764516,-0.194565\C,3.16032,0.592019,-0.316714\C,-1.795748,0.35943,2.340197\C,-2.3207,-0.860365,2.72671\C,-1.789718,-2.049361,2.184729\C,-0.745874,-2.010033,1.278018\C,1.498802,-1.897581,-0.752141\C,1.747356,-1.741407,-2.254506\O,2.744185,-2.340796,-0.181918\C,2.673058,-2.879286,1.128833\H,4.93327,1.777453,-0.490423\H,3.646206,-0.303067,-0.681236\H,3.871454,3.848364,0.408446\H,-0.63754,2.576409,1.357872\H,1.487927,3.804071,1.10667\H,-2.211014,1.287318,2.724656\H,-0.373291,-2.947083,0.883837\H,-2.203631,-3.010007,2.480328\H,-3.140467,-0.903353,3.438801\H,0.767983,-2.705348,-0.641153\H,2.27297,-2.635131,-2.606402\H,2.361852,-0.867735,-2.490159\H,0.795483,-1.669468,-2.785742\H,2.000179,-3.74943,1.167445\H,2.340417,-2.13603,1.866359\H,3.685696,-3.203715,1.381817\H,0.342334,0.594207,-2.352054\H,-0.609152,2.735578,-1.128129\H,-4.216623,-0.667619,0.004941\H,-4.033176,-1.26881,-1.669242\H,-4.804938,0.318116,-1.356554\\Version=IA32L-G03 RevD.01\State=1-A\HF=-1131.4167997\RMSD=8.931e-09\RMSF=2.764e-06\ZeroPoint=0.3818584\Thermal=0.4042884\Dipole=0.5466433,0.902291,0.1440412\



Zero-point correction=	0.381858 (Hartree/Particle)
Thermal correction to Energy=	0.412649
Thermal correction to Enthalpy=	0.413767
Thermal correction to Gibbs Free Energy=	0.316601
Sum of electronic and zero-point Energies=	-1131.034941
Sum of electronic and thermal Energies=	-1131.004150
Sum of electronic and thermal Enthalpies=	-1131.003032
Sum of electronic and thermal Free Energies=	-1131.100198

### B3LYP/6-31+G\* ( $\epsilon=2.2706$ )

HF = -1131.394501

### BMK/6-31+G\*

N,-2.7004233903,0.0701458511,-0.9877061512\C,-1.6233636025,-0.504731203,-1.6751937956\C,-0.53  
89046199,0.5152103439,-1.691088903\C,-0.9999974095,1.6553525356,-1.018441801\C,-2.442478145  
3,1.3899121804,-0.649930293\O,-1.6324378579,-1.6255390418,-2.1426134252\O,-3.2349656352,2.145  
4510127,-0.1322231062\C,-3.9380271087,-0.6120590088,-0.6812776674\C,-0.164423078,1.730130350  
6,0.9009023274\C,1.2194023793,1.7817028405,0.4950353971\C,1.8019704663,0.5811946252,-0.0070  
09019\C,0.9757675293,-0.6165584387,-0.0463349966\C,-0.1124927737,-0.7192099983,0.9055005856  
\C,-0.6649584033,0.4917771676,1.4319506018\C,1.9496212995,2.9966417081,0.4833707982\C,3.2559  
636451,3.0234117015,0.0243775553\C,3.854545614,1.8322865565,-0.4559126792\C,3.1463514597,0.  
6414085882,-0.4839245169\C,-1.7641724736,0.4575204542,2.3309075836\C,-2.2978712026,-0.75095  
64197,2.7372725653\C,-1.7705807085,-1.9605773846,2.2153687929\C,-0.7228158756,-1.9483424953,  
1.3120814277\C,1.5159474535,-1.8911469911,-0.7385186827\C,1.7334944522,-1.7638292636,-2.2553  
260976\O,2.756187019,-2.2985750421,-0.1816651684\C,2.7131100107,-2.7275380375,1.1561709612\  
H,4.8857916605,1.8498497425,-0.8045638241\H,3.6301173429,-0.2636755495,-0.8331949477\H,3.824  
2201676,3.9518149994,0.0397553215\H,-0.6254175635,2.6518783204,1.2606866836\H,1.4733836545  
,3.9027609167,0.8578959098\H,-2.1762437227,1.3995166056,2.6897638046\H,-0.3610692343,-2.8972  
950196,0.9311021434\H,-2.1963554637,-2.9133088449,2.5262902088\H,-3.1238756756,-0.776484573  
1,3.4459138074\H,0.7860801618,-2.6988471177,-0.5955718333\H,2.2859152671,-2.6503117544,-2.59  
00236688\H,2.3137406445,-0.8722523865,-2.5194628624\H,0.7661782136,-1.7404677921,-2.7679865  
332\H,2.0140722178,-3.5716442879,1.2817452006\H,2.4202981823,-1.916110767,1.841034544\H,3.7  
242275122,-3.0620219441,1.409956735\H,0.277540119,0.463247983,-2.3986591452\H,-0.6997046851  
,2.6733482768,-1.2479501473\H,-3.880892559,-1.6127469731,-1.1198586776\H,-4.78549696,-0.06107  
10421,-1.1054841179\H,-4.067464504,-0.6860526441,0.4063302457\\Version=EM64L-G09RevA.02\Sta  
te=1-A\HF=-1130.7099115\RMSD=7.039e-09\RMSF=4.063e-06\Dipole=0.6432386,0.059592,0.7253253

Zero-point correction=	0.387568 (Hartree/Particle)
Thermal correction to Energy=	0.417383
Thermal correction to Enthalpy=	0.418500
Thermal correction to Gibbs Free Energy=	0.325341
Sum of electronic and zero-point Energies=	-1130.322344
Sum of electronic and thermal Energies=	-1130.292529
Sum of electronic and thermal Enthalpies=	-1130.291411
Sum of electronic and thermal Free Energies=	-1130.384571

## **TS10-A**

### **B3LYP/6-31+G\***

H,0.241736,3.576604,3.233957\C,0.620143,2.698328,2.717494\H,-1.20595,2.38241,1.653278\C,-0.2064  
99,2.014102,1.841488\C,2.433821,1.167578,2.264768\C,0.249917,0.84555,1.178997\C,1.947245,2.2764  
59,2.935757\C,1.594354,0.433759,1.400259\C,-0.533863,0.075217,0.224537\H,2.58692,2.824168,3.622  
737\H,3.120932,-0.960755,0.734473\H,3.461021,0.840303,2.409646\C,-0.209279,-1.334466,0.076479\  
C,-1.927249,0.532854,-0.198618\C,-1.123546,-2.329179,-0.358659\C,1.141244,-1.724141,0.304547\H,2.  
58207,-3.333701,0.269638\C,2.077119,-0.675335,0.614818\C,-0.720706,-3.645382,-0.506238\H,-2.1553  
83,-2.075072,-0.571357\H,-1.443453,-4.393525,-0.820493\C,0.616309,-4.020998,-0.266597\H,0.921728,  
-5.055694,-0.394705\C,1.540807,-3.064723,0.112289\H,-2.181493,-0.00748,-1.118787\O,-1.894825,1.93  
0013,-0.509201\C,-2.999354,0.237538,0.871387\H,-3.983682,0.557292,0.511951\H,-2.782724,0.768181  
,1.802425\H,-3.054742,-0.831718,1.097445\C,-2.835259,2.323977,-1.503324\H,-3.871576,2.164926,-1.1  
72152\H,-2.662074,1.780955,-2.441871\H,-2.680096,3.393569,-1.666108\C,0.83868,0.781114,-1.54661  
6\C,2.143123,0.350429,-1.216961\H,2.942584,1.008813,-0.899843\C,2.477618,-0.747386,-2.165749\C,0.  
.350807,-0.078489,-2.631535\H,0.421061,1.767512,-1.408576\O,-0.686532,-0.06369,-3.249381\O,1.336  
037,-1.04386,-2.904179\O,3.511008,-1.344054,-2.325422\\Version=AM64L-G03RevE.01\State=1-A\HF=  
-1111.967515 \RMSD=8.323e-10\RMSF=7.975e-06\ZeroPoint=0.340889\Thermal=0.3614363\Dipole=-0  
.8020897,0.7275144,1.8500154

Zero-point correction=	0.340889 (Hartree/Particle)
Thermal correction to Energy=	0.369210
Thermal correction to Enthalpy=	0.370327
Thermal correction to Gibbs Free Energy=	0.279530
Sum of electronic and zero-point Energies=	-1111.626626
Sum of electronic and thermal Energies=	-1111.598305
Sum of electronic and thermal Enthalpies=	-1111.597188
Sum of electronic and thermal Free Energies=	-1111.687985

### **B3LYP/6-31+G\* ( $\epsilon=2.2706$ )**

HF = -1111.949408

### **BMK/6-31+G\***

H,0.2533977879,3.6362858268,3.1944554443\C,0.6278337243,2.7442075451,2.6952538548\H,-1.2054  
330279,2.4079516425,1.6425417296\C,-0.2032547668,2.0425154752,1.8372933831\C,2.4443132513,1  
.193243963,2.2840286716\C,0.2524418047,0.8512326867,1.2001898206\C,1.962376576,2.322064498  
2,2.9228756196\C,1.5954496334,0.434046904,1.4362909422\C,-0.5305234072,0.0745385136,0.25202  
86189\H,2.6043293074,2.8889201873,3.5949807324\H,3.1265010942,-0.980493862,0.7969321394\H,  
3.4708076157,0.8607548523,2.4378464432\C,-0.2046310815,-1.330697504,0.0891619766\C,-1.921298  
5326,0.5373833018,-0.1906099157\C,-1.116828208,-2.3128575471,-0.4010926144\C,1.14497225,-1.72  
83783425,0.3273890089\H,2.5983614427,-3.3356787727,0.2287769869\C,2.076093049,-0.701605036  
1,0.6953871873\C,-0.7059006472,-3.6186560182,-0.6033882198\H,-2.1491005057,-2.0487560247,-0.6  
120125286\H,-1.4211356363,-4.3566272099,-0.9620531884\C,0.6392025091,-4.0019808015,-0.367313  
3987\H,0.9508731478,-5.0286103587,-0.549648741\C,1.5552413417,-3.0649539559,0.0718648872\H,-  
2.167418309,-0.0148051488,-1.1086467924\O,-1.8849230001,1.9141428025,-0.5084096423\C,-2.9956

423235,0.2415985527,0.8842252026\H,-3.9835267977,0.5549289473,0.5218324939\H,-2.7740719317,  
0.7821268667,1.8118079687\H,-3.0375678748,-0.8306966574,1.1128659136\C,-2.7988544779,2.2899  
223838,-1.5148225716\H,-3.8423041852,2.1329308188,-1.1964470324\H,-2.6084035894,1.725629980  
1,-2.4407094571\H,-2.6439841986,3.358349383,-1.6975937276\C,0.8217951335,0.7906230227,-1.516  
2160927\C,2.1265750487,0.3715718925,-1.2261299017\H,2.9454110066,0.9952303441,-0.885825424  
2\C,2.4088770683,-0.7907718986,-2.1203793991\C,0.2979934879,-0.1268342247,-2.555016097\H,0.37  
8482272,1.769076745,-1.3768156195\O,-0.7555277373,-0.1277398322,-3.1311366146\O,1.252224252  
2,-1.094347167,-2.804151574\O,3.4147764336,-1.422783774,-2.2676124725\\Version=AM64L-G09Rev  
A.02\State=1-A\HF=-1111.2902943\RMSD=5.885e-09\RMSF=7.299e-06\Dipole=-0.707069,0.7916925,1.  
6673668

Zero-point correction=	0.345137 (Hartree/Particle)
Thermal correction to Energy=	0.372819
Thermal correction to Enthalpy=	0.373937
Thermal correction to Gibbs Free Energy=	0.285285
Sum of electronic and zero-point Energies=	-1110.945158
Sum of electronic and thermal Energies=	-1110.917475
Sum of electronic and thermal Enthalpies=	-1110.916357
Sum of electronic and thermal Free Energies=	-1111.005009

## **TS10-B**

### **B3LYP/6-31+G\***

H,1.1415608364,4.6244634533,0.7680788143\C,1.3497233488,3.5594812439,0.7068012244\H,-0.6176  
620108,3.0821474889,0.015433091\C,0.3511896618,2.6909601659,0.2985797738\C,2.9133123694,1.7  
267354148,0.9123751161\C,0.6082033734,1.3010375284,0.173477313\C,2.6352377712,3.0785442499  
,1.0289149466\C,1.9222582642,0.8322101884,0.4580383824\C,-0.3853637188,0.3176851848,-0.21775  
12865\H,3.4096198359,3.7694133403,1.3514924404\H,3.1554439835,-0.9520616464,0.5723165314\H  
,3.9061582445,1.3461189347,1.1421155538\C,0.0926342292,-0.8432865296,-0.9421421882\C,-1.8625  
251841,0.7041925096,-0.3449886782\C,-0.6798444334,-1.5752830827,-1.8818737294\C,1.418785183  
5,-1.2928661841,-0.6731339367\H,2.9297164295,-2.7844755858,-1.0722223148\C,2.1533233898,-0.58  
96464092,0.3490735572\C,-0.1486531055,-2.6750171638,-2.5311792995\H,-1.6860326649,-1.2583523  
96,-2.1290142821\H,-0.7488862221,-3.2039581266,-3.2665540833\C,1.1596370335,-3.117544501,-2.2  
469144481\H,1.5608111419,-3.9898433089,-2.7553468147\C,1.9269531561,-2.4428489461,-1.314936  
9184\H,-2.4204221258,-0.1976812629,-0.6207640466\O,-1.9274381281,1.6325569991,-1.4465127184  
\C,-2.5381332955,1.258607371,0.9187378768\H,-3.5017335752,1.7032224425,0.6476747167\H,-1.943  
7974051,2.0241754603,1.4234536145\H,-2.745253568,0.4442124287,1.6181844513\C,-3.1700514297,  
1.6508296292,-2.1320591712\H,-3.9940387892,1.9990320176,-1.4931213416\H,-3.4244433451,0.6545  
619934,-2.5253428156\H,-3.0523415023,2.3453939317,-2.9675520096\C,1.1663279596,-1.171260336,  
2.0550978153\C,-0.1852912868,-0.7754698541,1.9857878968\H,-0.6149998696,0.1069262529,2.4329  
741807\C,-0.9948048014,-1.9707547687,1.7447548919\C,1.1701353666,-2.6594722181,1.925903502\  
H,1.8936943073,-0.7214131726,2.7209121083\O,2.0819219705,-3.4376551082,2.0358898264\O,-0.118  
3578435,-3.0693379483,1.6171775364\O,-2.1885735519,-2.1242796804,1.6551649213\\Version=AM6  
4L-G03RevE.01\State=1-A\HF=-1111.9617943\RMSD=9.641e-09\RMSF=2.491e-06\ZeroPoint=0.340973  
7\Thermal=0.3615141\Dipole=0.1940002,1.9828105,-0.7127613

Zero-point correction=	0.340974 (Hartree/Particle)
------------------------	-----------------------------

Thermal correction to Energy=	0.369281
Thermal correction to Enthalpy=	0.370399
Thermal correction to Gibbs Free Energy=	0.279174
Sum of electronic and zero-point Energies=	-1111.620821
Sum of electronic and thermal Energies=	-1111.592513
Sum of electronic and thermal Enthalpies=	-1111.591395
Sum of electronic and thermal Free Energies=	-1111.682621

### B3LYP/6-31+G\* ( $\epsilon=2.2706$ )

HF = -1111.944286

### BMK/6-31+G\*

H,-4.3784666509,2.6368756897,-0.0135004454\C,-3.3141709864,2.4531904751,-0.1504232051\H,-3.5047084209,0.3379400735,0.1436487482\C,-2.8244663709,1.1614926333,-0.0471869644\C,-1.1009383871,3.299886741,-0.669662689\C,-1.4408689292,0.891612723,-0.2624717037\C,-2.4472179529,3.5356517004,-0.4466493231\C,-0.5877427413,1.9782920541,-0.6160343031\C,-0.8402181526,-0.4216847498,-0.1246841702\H,-2.8437522127,4.5471993148,-0.5147412495\H,1.4804096936,2.5174516925,-1.0504548487\H,-0.4270823637,4.1200807714,-0.9167651787\C,0.3258310753,-0.708114466,-0.9340751173\C,-1.6386375023,-1.600041232,0.4557600675\C,0.7137078281,-2.0206035787,-1.3389936028\C,1.1646882308,0.3856374493,-1.3090560669\H,3.0064541187,0.9994823972,-2.2753690604\C,0.8114184422,1.688452032,-0.812509179\C,1.8592298768,-2.2173919023,-2.0882847462\H,0.0900067456,-2.8745025714,-1.0917877912\H,2.1237145026,-3.2230021337,-2.4101073566\C,2.6968034095,-1.1261384152,-2.4353328233\H,3.6034285402,-1.3003228104,-3.0117135462\C,2.3627065646,0.1543819167,-2.0363647371\H,-0.9557537347,-2.4585988604,0.5214444051\O,-2.6534537077,-1.8898427528,-0.4959342903\C,-2.2064851999,-1.400585566,1.8778096881\H,-2.9320811818,-2.1967443387,2.0872476587\H,-2.7097964875,-0.4373996389,2.0108651608\H,-1.3989175049,-1.4946772695,2.61221482\C,-3.0798052946,-3.2290271999,-0.5068185814\H,-3.5743037127,-3.5166328835,0.4346680968\H,-2.2329687206,-3.9139144046,-0.6836043871\H,-3.7962108038,-3.3267682191,-1.3287819917\C,1.2965148621,1.4305535633,1.2399867671\C,0.5122980591,0.4022162256,1.7749936765\H,-0.403023215,0.4992953813,2.3421272243\C,1.3670696458,-0.7974779018,1.8812586745\C,2.6764027405,0.8635390674,1.0919875758\H,1.1805430085,2.4895854904,1.4456762596\O,3.6924468782,1.4049584499,0.7653229523\O,2.6192445341,-0.4773915442,1.3772612418\O,1.1320964779,-1.8967664032,2.3013753408\\Version=EM64L-G09RevA.02\State=1-A\HF=-1111.2833478\RMSD=6.815e-09\RMSF=6.380e-06\ZeroPoint=0.3462543\Thermal=0.3735862\Dipole=-1.7993973,0.4940327,-0.5994233

Zero-point correction=	0.346254 (Hartree/Particle)
Thermal correction to Energy=	0.373586
Thermal correction to Enthalpy=	0.374704
Thermal correction to Gibbs Free Energy=	0.286736
Sum of electronic and zero-point Energies=	-1110.937093
Sum of electronic and thermal Energies=	-1110.909762
Sum of electronic and thermal Enthalpies=	-1110.908644
Sum of electronic and thermal Free Energies=	-1110.996611

## **TS2N-A**

### **B3LYP/6-31+G\***

C,1.142066,1.349118,1.888677\C,0.290501,0.436887,1.206181\C,0.582867,-0.953294,1.317012\C,1.692944,-1.39388,2.07214\C,2.482485,-0.483865,2.750388\C,2.199349,0.895442,2.657306\C,-0.821824,0.831289,0.364332\C,-1.918027,-0.110204,0.214412\C,-1.618373,-1.496773,0.354429\C,-0.233867,-1.854041,0.550515\C,-3.238391,0.253994,-0.154372\C,-4.221736,-0.710402,-0.303311\C,-3.922875,-2.077734,-0.134089\C,-2.627829,-2.464769,0.167602\C,-0.99285,2.328901,0.07715\O,-1.567467,2.582562,-1.206903\C,-1.829635,3.057529,1.138768\C,0.442001,-1.392478,-1.389745\C,0.054558,-0.073561,-1.693522\C,1.255059,0.769346,-1.762803\N,2.347243,-0.052142,-1.448313\C,1.942883,-1.382927,-1.292898\O,2.698991,-2.321417,-1.111956\O,1.327782,1.966763,-2.03214\C,3.722777,0.3988,-1.330826\H,-0.034259,-2.271765,-1.807469\H,-0.856212,0.224166,-2.191232\H,3.750097,1.455114,-1.604392\H,4.36435,-0.178222,-2.003098\H,4.080275,0.271331,-0.303963\H,-4.703362,-2.824604,-0.253083\H,-2.377493,-3.518221,0.27363\H,-5.23234,-0.407686,-0.564985\H,-3.478817,1.292357,-0.340828\H,0.009778,-2.913423,0.608463\H,0.957286,2.416084,1.840667\H,1.910944,-2.4576,2.117726\H,3.319875,-0.827986,3.351458\H,2.817502,1.610909,3.193434\H,0.007851,2.770152,0.078334\H,-1.413185,2.90268,2.139877\H,-2.865715,2.710228,1.14935\H,-1.82899,4.130024,0.917649\H,-0.825221,2.593937,-1.839443\\Version=AM64L-G03RevE.01\State=1-A\HF=-1092.1196106\RMSD=6.823e-09\RMSF=2.166e-06\ZeroPoint=0.3539323\Thermal=0.3747354\Dipole=0.321291,0.8508938,-0.083657

Zero-point correction=	0.353932 (Hartree/Particle)
Thermal correction to Energy=	0.382635
Thermal correction to Enthalpy=	0.383753
Thermal correction to Gibbs Free Energy=	0.292258
Sum of electronic and zero-point Energies=	-1091.765678
Sum of electronic and thermal Energies=	-1091.736975
Sum of electronic and thermal Enthalpies=	-1091.735857
Sum of electronic and thermal Free Energies=	-1091.827352

### **B3LYP/6-31+G\* ( $\epsilon=2.2706$ )**

HF = -1092.101341

### **BMK/6-31+G\***

C,1.2083322545,1.3584376391,1.7835950191\C,0.3092541172,0.4333583356,1.1656730661\C,0.5942634826,-0.9599043757,1.2944689474\C,1.7603061394,-1.3943142587,1.9837148626\C,2.5975576005,-0.4756179485,2.5871583209\C,2.309420665,0.9118666618,2.4921654559\C,-0.8207392001,0.8224710752,0.3480895707\C,-1.9239991208,-0.1141357315,0.2123985415\C,-1.6374794613,-1.502250793,0.3780115423\C,-0.2651662995,-1.8741748721,0.6035693305\C,-3.2412452262,0.2590279995,-0.1843235658\C,-4.2292506276,-0.7008037035,-0.3357901967\C,-3.9423769884,-2.0764347971,-0.1444182695\C,-2.6567469425,-2.4708489278,0.1841295827\C,-1.0010917243,2.3233184604,0.0531943796\O,-1.5838646239,2.5623194903,-1.2113794676\C,-1.8389797406,3.0315572386,1.1356684027\C,0.4103320125,-1.3870088457,-1.4329704093\C,0.0251782766,-0.0690047316,-1.6965814501\C,1.2414806161,0.7819501411,-1.6886779539\N,2.310447072,-0.0451047053,-1.3540463306\C,1.9074180437,-1.3776260784,-1.2646886269\O,2.6536051555,-2.3109919135,-1.0710724702\O,1.3202884715,1.9786404989,-1.9108365425\C,3.6623298428,0.4042128019,-1.1029861387\H,-0.0813209725,-2.2784272254,-1.807592363



3\H,-0.8816058983,0.2589551211,-2.1895327317\H,3.7106081997,1.4678642842,-1.3549120365\H,4.3  
656940689,-0.1625686448,-1.7233700185\H,3.9171255217,0.2581727615,-0.0448902998\H,-4.729603  
2792,-2.8179586769,-0.2694358792\H,-2.4127354555,-3.5259983823,0.3079573557\H,-5.2346429071,  
-0.3942246614,-0.6196304621\H,-3.4671627329,1.2999240893,-0.3903842928\H,-0.0163870922,-2.93  
58314125,0.6471025997\H,1.0208602726,2.4270491064,1.7315552028\H,1.977483699,-2.4604698154  
,2.0291494371\H,3.4758355057,-0.8122507255,3.1352210908\H,2.9628105386,1.6335942145,2.97968  
67487\H,-0.0027014436,2.772479883,0.0498972119\H,-1.3979416962,2.8731138041,2.1284968644\H,  
-2.8678157082,2.6561905677,1.1561085504\H,-1.8632529678,4.1068860937,0.919866447\H,-0.85352  
54476,2.6051799587,-1.8492300243\\Version=AM64L-G09RevA.02\State=1-A\HF=-1091.4427618\RMS  
D=7.213e-09\RMSF=2.341e-06\Dipole=-0.2576318,-0.2006017,0.7455707

Zero-point correction=	0.359110 (Hartree/Particle)
Thermal correction to Energy=	0.387018
Thermal correction to Enthalpy=	0.388136
Thermal correction to Gibbs Free Energy=	0.299607
Sum of electronic and zero-point Energies=	-1091.083652
Sum of electronic and thermal Energies=	-1091.055744
Sum of electronic and thermal Enthalpies=	-1091.054626
Sum of electronic and thermal Free Energies=	-1091.143155

## **TS2N-B**

B3LYP/6-31+G\*

C,3.330952,0.231556,-0.417928\C,2.018155,-0.018682,0.063959\C,1.729127,-1.326561,0.546156\C,2.72  
5879,-2.324262,0.550008\C,4.007312,-2.039704,0.109289\C,4.305082,-0.752594,-0.381206\C,0.939069,  
0.955998,0.036848\C,-0.147949,0.785537,0.975776\C,-0.424439,-0.535208,1.441631\C,0.354556,-1.610  
745,0.88362\C,-0.980457,1.844069,1.437119\C,-1.992942,1.597808,2.346592\C,-2.253761,0.288148,2.8  
04189\C,-1.49107,-0.767391,2.338286\C,1.217516,2.311747,-0.632685\O,0.059586,3.029742,-1.026831  
\C,2.008317,3.259899,0.285279\C,-0.356364,-1.711094,-1.043987\C,-0.176391,-0.468218,-1.688289\C,-  
1.487894,0.185365,-1.80037\N,-2.432181,-0.676867,-1.227922\C,-1.837479,-1.873356,-0.82632\O,-2.43  
5268,-2.834111,-0.374507\O,-1.765656,1.279374,-2.289909\C,-3.843386,-0.371832,-1.064391\H,0.2121  
75,-2.6004,-1.291038\H,0.632713,-0.199262,-2.352559\H,-4.447955,-1.179683,-1.485555\H,-4.044559,0.  
.562406,-1.591171\H,-4.089274,-0.259069,-0.003254\H,-3.055143,0.109676,3.516497\H,-1.695491,-1.7  
84596,2.662371\H,-2.599967,2.424808,2.705983\H,-0.822198,2.846512,1.063066\H,0.123527,-2.61607  
3,1.232165\H,3.597474,1.206755,-0.807735\H,2.476563,-3.318581,0.914203\H,4.778686,-2.804646,0.1  
36261\H,5.30775,-0.527374,-0.734913\H,1.826872,2.10738,-1.525178\H,2.951227,2.81904,0.620405\H,  
1.419548,3.518491,1.170217\H,2.222768,4.182083,-0.265062\H,-0.501745,2.487694,-1.620739\\Versio  
n=AM64L-G03RevE.01\State=1-A\HF=-1092.1218625\RMSD=3.219e-09\RMSF=5.037e-06\ZeroPoint=0.  
3540037\Thermal=0.3745716\Dipole=0.8388393,0.6511897,-0.698003

Zero-point correction=	0.354004 (Hartree/Particle)
Thermal correction to Energy=	0.382440
Thermal correction to Enthalpy=	0.383558
Thermal correction to Gibbs Free Energy=	0.292854
Sum of electronic and zero-point Energies=	-1091.767859
Sum of electronic and thermal Energies=	-1091.739423

Sum of electronic and thermal Enthalpies= -1091.738305  
Sum of electronic and thermal Free Energies= -1091.829008

### B3LYP/6-31+G\* ( $\epsilon=2.2706$ )

HF = -1092.103493

### BMK/6-31+G\*

C,3.3485525231,0.239766648,-0.4283988057\C,2.0286965172,-0.0141100263,0.0541220665\C,1.74116  
62121,-1.3232254001,0.5392218516\C,2.7416318658,-2.3280580066,0.5355034476\C,4.0211651489,-2  
.0429584252,0.089558365\C,4.3213454094,-0.746510586,-0.397032536\C,0.9501503278,0.962456313  
5,0.0220420925\C,-0.1663207117,0.7813776513,0.9218649608\C,-0.4391170965,-0.5399463207,1.398  
1075086\C,0.3719506368,-1.6141666018,0.8904060015\C,-1.0474253486,1.83523727,1.3262028081\C  
,-2.10205988,1.5786485521,2.1834103172\C,-2.3630454729,0.2626414197,2.6489801399\C,-1.554568  
255,-0.7831640631,2.243755646\C,1.2411310236,2.3244709295,-0.6415059429\O,0.108492542,3.0467  
01715,-1.0435618155\C,2.0186930675,3.2481338934,0.3215041715\C,-0.3373966024,-1.7359806737,-  
1.0724783256\C,-0.1686427039,-0.5032726937,-1.7219775722\C,-1.4821027776,0.1812712374,-1.751  
344558\N,-2.4009347858,-0.6620713739,-1.1295260924\C,-1.8142289057,-1.869989414,-0.773388964  
6\O,-2.4001849244,-2.8102591316,-0.2867072636\O,-1.7631185687,1.2768425459,-2.2103728633\C,-3  
.7794422142,-0.3235880027,-0.8489698012\H,0.2333692054,-2.6341585895,-1.2875795592\H,0.63308  
75185,-0.2123624099,-2.3902020694\H,-4.4451740303,-1.0768816936,-1.285290839\H,-3.9772224375  
,0.6576049216,-1.2901733658\H,-3.940650047,-0.2856345567,0.2365275294\H,-3.201161457,0.07875  
38647,3.3193243167\H,-1.7552061013,-1.8028584422,2.5695601191\H,-2.7447054029,2.3989263557,  
2.4992977249\H,-0.8827963389,2.8388498784,0.9505414936\H,0.135627879,-2.6232643042,1.233038  
907\H,3.6165282338,1.2197800397,-0.8114236931\H,2.4899057003,-3.3234111792,0.9014569254\H,4  
.7939022848,-2.8094474538,0.1095692349\H,5.3255833306,-0.5205098327,-0.7513828151\H,1.86935  
07821,2.1243656115,-1.5236315736\H,2.9532283771,2.7888617617,0.6629551683\H,1.4033137486,3.  
4748068319,1.200523241\H,2.2445894845,4.1875713695,-0.1980503632\H,-0.4626727563,2.5125393  
707,-1.6261042171\Version=AM64L-G09RevA.02\State=1-A\HF=-1091.4441125\RMSD=4.788e-09\RM  
SF=8.940e-06\Dipole=1.0427374,-0.4921135,0.480766

Zero-point correction= 0.358524 (Hartree/Particle)  
Thermal correction to Energy= 0.386237  
Thermal correction to Enthalpy= 0.387355  
Thermal correction to Gibbs Free Energy= 0.299268  
Sum of electronic and zero-point Energies= -1091.085589  
Sum of electronic and thermal Energies= -1091.057875  
Sum of electronic and thermal Enthalpies= -1091.056757  
Sum of electronic and thermal Free Energies= -1091.144844

### **TS20-A**

### B3LYP/6-31+G\*

C,-1.053836,0.448671,-1.700484\C,0.213414,0.594531,-2.306947\H,0.557539,-0.017897,-3.132848\C,0.4  
43232,2.069384,-2.403953\C,-1.569632,1.77081,-1.384909\H,-1.716135,-0.399324,-1.78703\O,-2.62523  
9,2.1046,-0.889353\O,-0.597199,2.718804,-1.738053\O,1.337286,2.677807,-2.929051\H,3.12367,3.6213



12,1.341081\C,2.374004,2.848412,1.196324\H,3.410034,1.920561,-0.443864\C,2.540114,1.896206,0.207005\C,0.252073,1.852792,1.828088\C,1.581124,0.875306,0.034493\C,1.222471,2.822246,2.00906\C,0.411924,0.838239,0.846045\C,1.665407,-0.095475,-1.028402\H,1.08997,3.574575,2.781772\C,-1.915259,-0.102676,1.298438\H,-0.622309,1.868752,2.46818\C,1.100957,-1.402871,-0.773351\H,2.548675,-0.049259,-1.663563\C,1.593753,-2.571572,-1.388684\C,-0.080702,-1.452586,0.020957\H,-1.691925,-2.749122,0.680124\C,-0.564427,-0.201243,0.579564\C,0.948267,-3.783748,-1.205866\H,2.493454,-2.512057,-1.997276\H,1.345553,-4.688069,-1.659001\C,-0.235115,-3.838235,-0.442087\H,-0.753662,-4.785264,-0.318068\C,-0.754803,-2.694504,0.142162\H,-2.136253,0.961615,1.419685\C,-1.900937,-0.74695,2.69289\O,-2.983937,-0.681789,0.544998\H,-1.10078,-0.328142,3.311991\H,-1.751816,-1.828207,2.637157\H,-2.862274,-0.556927,3.181179\H,-3.335681,0.021295,-0.029407\\Version=AM64L-G03RevE.01\State=1-A\HF=-1072.6641487\RMSD=7.571e-09\RMSF=3.473e-06\ZeroPoint=0.3130617\Thermal=0.3319687\Dipole=0.892932,-1.5673851,0.7219119

Zero-point correction=	0.313062 (Hartree/Particle)
Thermal correction to Energy=	0.339276
Thermal correction to Enthalpy=	0.340394
Thermal correction to Gibbs Free Energy=	0.254474
Sum of electronic and zero-point Energies=	-1072.351087
Sum of electronic and thermal Energies=	-1072.324873
Sum of electronic and thermal Enthalpies=	-1072.323755
Sum of electronic and thermal Free Energies=	-1072.409675

B3LYP/6-31+G\* ( $\epsilon=2.2706$ )

HF = -1072.649888

BMK/6-31+G\*

C,-1.0422541401,0.4334370468,-1.6610804084\C,0.1897239769,0.5871459438,-2.30799475\H,0.5752975978,-0.0353742451,-3.1080591199\C,0.4583874668,2.0598282456,-2.3339766287\C,-1.5143408881,1.7755784889,-1.2835561465\H,-1.7282834209,-0.400762662,-1.7319644413\O,-2.5430735693,2.1076071707,-0.7514516876\O,-0.5428862395,2.6928121744,-1.6218126106\O,1.3544526308,2.6690399925,-2.8390918001\H,3.0600567424,3.7104589001,1.2570304589\C,2.334740634,2.9080933942,1.1365447899\H,3.4171167231,1.9437182125,-0.4556773744\C,2.5399835113,1.9230583282,0.1892305063\C,0.223831804,1.8833716321,1.7900071081\C,1.6050292567,0.8622523539,0.0468640435\C,1.1696036838,2.8806131403,1.945284347\C,0.4199234533,0.8338775359,0.8410627901\C,1.7400181676,-0.1422234188,-0.9696976729\H,1.0115843571,3.6581721146,2.690419302\C,-1.9123054026,-0.11242734,1.2841231896\H,-0.6618257488,1.8981682401,2.418803112\C,1.1275609044,-1.4287301,-0.753723558\H,2.614229256,-0.0885450699,-1.6207960076\C,1.5996096237,-2.6063034608,-1.390129991\C,-0.0720265979,-1.4630215595,0.0175231917\H,-1.7336282183,-2.7246003701,0.633614583\C,-0.5508807702,-0.2085981756,0.5738171916\C,0.917027579,-3.8015104877,-1.2405646577\H,2.5124609136,-2.5576284789,-1.9836070541\H,1.2945262902,-4.7098321597,-1.7070655119\C,-0.2850320152,-3.8395487331,-0.4887369559\H,-0.8294325942,-4.7770731988,-0.3889925947\C,-0.7845719623,-2.6937552083,0.1088518128\H,-2.1397800888,0.9527203524,1.4004433081\C,-1.8802593559,-0.7572930087,2.6841912488\O,-2.957399524,-0.6972994001,0.5323126408\H,-1.0872246654,-0.3119124476,3.2979775977\H,-1.6983800385,-1.8359233416,2.6228631477\H,-2.8487820696,-0.5927252627,3.1719887257\H,-3.3517972628,0.005135862,-0.005978124\\Version=AM64L-G09RevA.02\State=1-A\HF=-1072.0175133\RMSD=8.557e-09\RMSF=1.045e-05\Dipole=0.7165743,-1.4821351,0.5691734

Zero-point correction=	0.317651 (Hartree/Particle)
Thermal correction to Energy=	0.343253
Thermal correction to Enthalpy=	0.344371
Thermal correction to Gibbs Free Energy=	0.260232
Sum of electronic and zero-point Energies=	-1071.699862
Sum of electronic and thermal Energies=	-1071.674260
Sum of electronic and thermal Enthalpies=	-1071.673142
Sum of electronic and thermal Free Energies=	-1071.757281

## **TS20-B**

### **B3LYP/6-31+G\***

C,0.972322,0.76375,1.718819\C,2.093562,0.836443,0.854353\H,2.997788,0.257091,1.007597\C,2.27383  
7,2.292827,0.550907\C,0.418331,2.100792,1.848214\H,0.770736,0.003485,2.4593\O,-0.537803,2.51138  
2,2.473642\O,1.184879,2.981315,1.069392\O,3.157073,2.848745,-0.04583\H,2.703585,-4.403719,-0.106  
012\C,1.995689,-3.584246,-0.016319\H,3.23017,-2.181947,-1.083266\C,2.286401,-2.347176,-0.568231\  
C,-0.133331,-2.737929,0.785381\C,1.357544,-1.291341,-0.483189\C,0.778889,-3.773867,0.667932\C,0.1  
19433,-1.471437,0.194275\C,1.66779,0.050031,-0.932522\H,0.551441,-4.740719,1.108805\C,-2.033114,  
-0.480015,1.168545\H,-1.055527,-2.920722,1.323913\C,0.55902,0.852107,-1.399808\H,2.615339,0.187  
643,-1.451851\C,0.712492,1.840305,-2.393968\C,-0.691637,0.687569,-0.733409\H,-2.703729,1.48348,-  
0.566935\C,-0.782023,-0.333535,0.287821\C,-0.360781,2.634775,-2.757684\H,1.680167,1.964159,-2.87  
31\H,-0.245553,3.380673,-3.539377\C,-1.599085,2.487623,-2.099981\H,-2.434426,3.125641,-2.375611\  
C,-1.761852,1.552592,-1.093704\H,-1.733885,-1.051147,2.059083\C,-3.154149,-1.252817,0.451597\O,-2  
.612216,0.745702,1.584728\H,-2.827078,-2.242065,0.120107\H,-3.504047,-0.698185,-0.423646\H,-3.99  
468,-1.368965,1.143622\H,-1.961573,1.294701,2.06741\\Version=AM64L-G03RevE.01\State=1-A\HF=-  
1072.6653662\RMSD=4.230e-09\RMSF=3.425e-06\Thermal=0.\Dipole=0.3047291,-2.4555891,-0.72344  
13

Zero-point correction=	0.313273 (Hartree/Particle)
Thermal correction to Energy=	0.339157
Thermal correction to Enthalpy=	0.340275
Thermal correction to Gibbs Free Energy=	0.255355
Sum of electronic and zero-point Energies=	-1072.352093
Sum of electronic and thermal Energies=	-1072.326209
Sum of electronic and thermal Enthalpies=	-1072.325092
Sum of electronic and thermal Free Energies=	-1072.410011

### **B3LYP/6-31+G\* ( $\epsilon=2.2706$ )**

HF = -1072.651519

### **BMK/6-31+G\***

C,0.9867317232,0.7623831658,1.7110825484\C,2.1053120925,0.819758791,0.8583080892\H,3.009623  
4365,0.2306312632,0.9765750928\C,2.2496752796,2.267603936,0.4780551141\C,0.4006660375,2.106  
8268084,1.7513096826\H,0.7598067661,0.0229698337,2.4687272919\O,-0.5673938554,2.5244679502

,2.336669057\O,1.149748149,2.9428316573,0.9455633189\O,3.1153540276,2.8087077021,-0.1439691622\H,2.7234052796,-4.4100274784,-0.0414437205\C,2.0107348773,-3.5902785808,0.0296988205\H,3.231402549,-2.2057773091,-1.0827681397\C,2.2912943215,-2.3665678107,-0.5553240143\C,-0.1293957641,-2.7404491544,0.8219492614\C,1.349684144,-1.3092703575,-0.4931363434\C,0.7897713304,-3.7727027012,0.7253233919\C,0.1162086257,-1.4795853469,0.1992368638\C,1.6546312217,0.0167135624,-0.9806923393\H,0.5696451166,-4.7320913084,1.1900832956\C,-2.0447378488,-0.4984615295,1.1677449189\H,-1.0522248022,-2.9163471151,1.3662022647\C,0.5538219135,0.8486816886,-1.4014367\H,2.6083006367,0.1620134524,-1.4921744391\C,0.720530098,1.8774701445,-2.3639993299\C,-0.6949453087,0.6887606548,-0.7233359645\H,-2.7041734694,1.508289168,-0.5242052479\C,-0.7909646927,-0.3458005005,0.2830676825\C,-0.3397175034,2.7049928352,-2.686717491\H,1.6891552836,1.9974194196,-2.8471271643\H,-0.2170206512,3.4804052903,-3.4406198954\C,-1.5843443941,2.5528256353,-2.0240140575\H,-2.4116378867,3.214685666,-2.273937232\C,-1.759600942,1.5860487314,-1.0503114774\H,-1.7418512971,-1.0771031701,2.0547487574\C,-3.14794202,-1.2786787592,0.4199304461\O,-2.6310493999,0.7054854637,1.5817046734\H,-2.7986512984,-2.2616693197,0.084629888\H,-3.478066283,-0.7107020029,-0.4582062663\H,-4.0034918355,-1.4078764864,1.0941770978\H,-1.9882946567,1.2764151109,2.0396314277\Version=AM64L-G09RevA.02\State=1-A\HF=-1072.0177598\RMSD=2.637e-09\RMSF=8.671e-06\Dipole=0.3708099,-2.3634137,-0.563763

Zero-point correction=	0.317363 (Hartree/Particle)
Thermal correction to Energy=	0.342727
Thermal correction to Enthalpy=	0.343845
Thermal correction to Gibbs Free Energy=	0.260295
Sum of electronic and zero-point Energies=	-1071.700397
Sum of electronic and thermal Energies=	-1071.675033
Sum of electronic and thermal Enthalpies=	-1071.673915
Sum of electronic and thermal Free Energies=	-1071.757465

## **TS3N-A**

### **B3LYP/6-31+G\***

C,-0.709109,-0.787022,-2.165771\C,-0.242191,0.469731,-1.730379\H,-0.832505,1.367847,-1.635658\C,1.208312,0.542583,-1.975212\C,0.468057,-1.493903,-2.784612\H,-1.681907,-0.938212,-2.62017\O,0.482443,-2.566757,-3.366001\N,1.579651,-0.691573,-2.55258\O,1.989152,1.459212,-1.757615\C,2.938526,-1.060917,-2.904113\H,3.297413,-1.86667,-2.254731\H,3.56584,-0.17692,-2.775691\H,2.973864,-1.400442,-3.943121\H,2.906133,-4.037781,0.525226\C,2.275366,-3.15384,0.568703\H,0.640132,-4.062337,-0.49152\C,1.008543,-3.173733,0.014467\C,1.956854,-0.842671,1.244482\C,0.171517,-2.039082,0.099355\C,2.749512,-1.974879,1.181253\C,0.630184,-0.845434,0.730591\C,-1.114253,-1.986194,-0.54661\H,3.749425,-1.951674,1.606981\C,0.297875,1.618971,1.314784\H,2.362902,0.046171,1.711787\C,-2.124136,-1.16337,0.073865\H,-1.448615,-2.890682,-1.051952\C,-3.499697,-1.451891,-0.043596\C,-1.687803,0.024686,0.730223\H,-2.400233,1.781051,1.795312\C,-0.262074,0.30039,0.77461\C,-4.446365,-0.609533,0.514407\H,-3.805992,-2.3578,-0.562274\H,-5.503816,-0.849972,0.443575\C,-4.029444,0.55935,1.181741\H,-4.767834,1.218947,1.630194\C,-2.684617,0.876582,1.275082\H,1.336553,1.651709,0.970926\C,0.326056,1.617596,2.86641\C,-0.343318,2.939297,0.795016\H,0.872589,0.760248,3.270831\H,-0.686388,1.588302,3.282993\H,0.812729,2.531145,3.228675\C,0.710932,4.023165,0.531412\H,-1.065921,3.320603,1.527772\H,-0.910284,2.763689,-0.124241\H,1.30338,4.233265,1.431473\H,0.23655,4.963136,0.22401\H,1.397012,3.708614,-0.262308\Version=AM64L-G03RevE.01\State=1-A\HF=-1095.5230193\RMSD=5.021e-09\RMSF=2.621e-06\Thermal=0.\Dipole=-0.6283218,0.0833687,1.0260907

Zero-point correction=	0.406127 (Hartree/Particle)
Thermal correction to Energy=	0.437221
Thermal correction to Enthalpy=	0.438339
Thermal correction to Gibbs Free Energy=	0.341618
Sum of electronic and zero-point Energies=	-1095.116892
Sum of electronic and thermal Energies=	-1095.085798
Sum of electronic and thermal Enthalpies=	-1095.084680
Sum of electronic and thermal Free Energies=	-1095.181401

### B3LYP/6-31+G\* ( $\epsilon=2.2706$ )

HF = -1095.497753

### BMK/6-31+G\*

C,-0.7252329144,-0.7571016769,-2.1902908709\C,-0.2693765849,0.4872990091,-1.7366231944\H,-0.8486291859,1.3935359631,-1.6226091951\C,1.206791305,0.5304632925,-1.8924242826\C,0.4807734376,-1.4868672276,-2.7372481377\H,-1.6970403632,-0.9407422498,-2.6382446754\O,0.5169818281,-2.5598547913,-3.2990997369\N,1.5850470517,-0.7016574109,-2.4439482182\O,1.9823283853,1.423152708,-1.6121930078\C,2.9503192746,-1.1083162914,-2.6903279848\H,3.2014892351,-1.9781921326,-2.0698925302\H,3.5977536426,-0.2655281836,-2.4300658316\H,3.078763532,-1.3718997883,-3.7466702999\H,2.9545511179,-3.9968147505,0.3507608964\C,2.3079793893,-3.1245407235,0.4315892963\H,0.6422801965,-4.0540294597,-0.5698172982\C,1.0194354349,-3.1644172448,-0.0673555766\C,1.9824446122,-0.8180051941,1.1495007062\C,0.1606960902,-2.0406037445,0.0699095563\C,2.7907713985,-1.9349946518,1.0376591349\C,0.6264863784,-0.8433109321,0.6953642455\C,-1.1429101042,-2.0058278763,-0.5342024601\H,3.8107243828,-1.8987187077,1.4170555467\C,0.2952626751,1.6182141109,1.2945355423\H,2.3895063381,0.0786591836,1.6064206304\C,-2.1427249801,-1.1659167051,0.0757696718\H,-1.4779269938,-2.9016920907,-1.0601140515\C,-3.5288085053,-1.4379406429,-0.0472349513\C,-1.6969251954,0.0205663177,0.7324835572\H,-2.3799281516,1.7820893822,1.8135968757\C,-0.2708121649,0.2940303933,0.7722331531\C,-4.4652168768,-0.5846310208,0.5128489903\H,-3.8441442991,-2.3424509776,-0.5673881407\H,-5.5273203021,-0.8121446031,0.4412208938\C,-4.034751825,0.5826015486,1.1919610881\H,-4.7690561662,1.2449405117,1.647213722\C,-2.6861355997,0.8857205293,1.2860965141\H,1.3227271848,1.6628240127,0.9146586183\C,0.3652312514,1.6051411754,2.8481560406\C,-0.3785709416,2.934952314,0.7974902297\H,0.9523373766,0.7576529464,3.223368865\H,-0.640298485,1.5359166477,3.2837939265\H,0.8305353771,2.5345169474,3.2050267158\C,0.6803046838,4.0089344641,0.4790707079\H,-1.0609599833,3.322928364,1.5669994865\H,-0.9902597172,2.7525263415,-0.0944101581\H,1.3086915116,4.2116109586,1.3588604211\H,0.2062800053,4.9536183502,0.1806451922\H,1.3315362433,3.6673046056,-0.3361286228\\Version=AM64L-G09RevA.02\State=1-A\HF=-1094.8140851\RMSD=6.661e-09\RMSF=5.144e-06\Dipole=-0.6216439,0.091012,0.9369929

Zero-point correction=	0.411596 (Hartree/Particle)
Thermal correction to Energy=	0.441758
Thermal correction to Enthalpy=	0.442876
Thermal correction to Gibbs Free Energy=	0.349465
Sum of electronic and zero-point Energies=	-1094.402489
Sum of electronic and thermal Energies=	-1094.372327
Sum of electronic and thermal Enthalpies=	-1094.371209
Sum of electronic and thermal Free Energies=	-1094.464620

## **TS3N-B**

### **B3LYP/6-31+G\***

C,-1.185382,0.235609,-1.626884\C,-1.547896,-1.119325,-1.732084\H,-1.355984,-1.728493,-2.60777\C,-2.879394,-1.269058,-1.047224\C,-2.212003,0.93456,-0.831653\H,-0.541437,0.775615,-2.303566\O,-2.289135,2.117365,-0.529172\N,-3.164545,-0.03945,-0.46278\O,-3.588371,-2.26048,-0.984611\C,-4.321547,0.216497,0.375602\H,-4.416032,1.297842,0.491461\H,-4.196504,-0.249683,1.359067\H,-5.217742,-0.192246,-0.099027\H,-2.299939,-2.277621,3.682165\C,-1.698724,-1.756614,2.94177\H,-1.789087,-3.350127,1.500665\C,-1.405395,-2.3601,1.732868\C,-0.454888,0.219609,2.273068\C,-0.593538,-1.701698,0.781923\C,-1.216165,-0.457621,3.208579\C,-0.102131,-0.386755,1.035663\C,-0.316605,-2.266379,-0.510956\H,-1.444649,0.018861,4.158517\C,1.071342,1.732738,0.223911\H,-0.105422,1.216585,2.513341\C,0.94346,-1.920751,-1.119237\H,-0.71758,-3.257744,-0.714368\C,1.604535,-2.792629,-2.010207\C,1.463044,-0.61731,-0.861861\H,3.136307,0.699673,-1.306476\C,0.703545,0.260262,0.015435\C,2.794884,-2.418719,-2.609386\H,1.176238,-3.774291,-2.201202\H,3.313126,-3.104008,-3.27481\C,3.33795,-1.146727,-2.339743\H,4.282016,-0.854492,-2.792283\C,2.682433,-0.263139,-1.49867\H,0.2435,2.166664,0.793028\C,1.149237,2.595598,-1.055071\C,2.343262,1.873792,1.119537\H,0.146278,2.782468,-1.44693\H,1.75458,2.152209,-1.849616\H,1.584504,3.571997,-0.81533\C,2.41495,3.212661,1.86614\H,3.246638,1.752223,0.509329\H,2.362982,1.058324,1.853123\H,2.442355,4.067276,1.180607\H,3.317229,3.260308,2.487489\H,1.548702,3.346722,2.526629\\Version=AM64L-G03RevE.01\State=1-A\HF=-1095.5229048\RM SD=7.212e-09\RMSF=1.710e-06\Thermal=0.\Dipole=1.2457819,-0.1417601,0.2554238

Zero-point correction=	0.406033 (Hartree/Particle)
Thermal correction to Energy=	0.437241
Thermal correction to Enthalpy=	0.438359
Thermal correction to Gibbs Free Energy=	0.341273
Sum of electronic and zero-point Energies=	-1095.116872
Sum of electronic and thermal Energies=	-1095.085664
Sum of electronic and thermal Enthalpies=	-1095.084546
Sum of electronic and thermal Free Energies=	-1095.181631

### **B3LYP/6-31+G\* ( $\epsilon=2.2706$ )**

HF = -1095.497972

### **BMK/6-31+G\***

C,-1.1649595138,0.2392238202,-1.6522062896\C,-1.5422969977,-1.1013913912,-1.7716450307\H,-1.3488855657,-1.7332214197,-2.6326270813\C,-2.8417412992,-1.2596662204,-1.0173445616\C,-2.1421709932,0.9217669196,-0.7638223285\H,-0.5085689202,0.7958054371,-2.3076386255\O,-2.171093687,2.0807542341,-0.4009517351\N,-3.0803484901,-0.0487426543,-0.3853726157\O,-3.5464419961,-2.2418465642,-0.9326590675\C,-4.1671139614,0.1787124248,0.5406845228\H,-4.1223168189,1.2282787554,0.8467018429\H,-4.0578275187,-0.4729998136,1.4170669121\H,-5.1273008966,-0.0316586725,0.0549958498\H,-2.4854933659,-2.2171538835,3.5747375659\C,-1.8359710143,-1.7172882384,2.8581426661\H,-1.8754566249,-3.3350788032,1.4371354947\C,-1.4876011981,-2.3461341299,1.6774942312\C,-0.530570384,0.2415109163,2.2280617571\C,-0.6107400054,-1.7115572572,0.7557590117\C,-1.34820



25112,-0.4120178698,3.1322892871\C,-0.119673813,-0.3943337712,1.0146265595\C,-0.2941189348,-  
2.2953803557,-0.5162507367\H,-1.6223638149,0.0832661793,4.0623357791\C,1.0630054314,1.72562  
68323,0.2096999274\H,-0.1788982647,1.2413784204,2.4658464727\C,0.9596545291,-1.9345932359,-  
1.1263707299\H,-0.7112294938,-3.2789694113,-0.739101528\C,1.6219989505,-2.7993239427,-2.0353  
144316\C,1.4786264602,-0.6306404152,-0.8597408118\H,3.1561823539,0.6970866188,-1.283365487\  
C,0.7148945918,0.2444199659,0.0160156971\C,2.810928256,-2.4158255826,-2.6315801971\H,1.19185  
89832,-3.7806171306,-2.2357201669\H,3.3301036832,-3.0922827182,-3.3083418326\C,3.3595258227,  
-1.1412157036,-2.3437388139\H,4.3065067449,-0.8457035314,-2.7924213482\C,2.7045174624,-0.266  
0805699,-1.492855429\H,0.2181933878,2.1647417206,0.7532036904\C,1.1534599979,2.562579808,-1.  
093006916\C,2.3189111854,1.8813698249,1.1277635659\H,0.143937136,2.7801274072,-1.460604169  
7\H,1.7180771545,2.0713007054,-1.8922598239\H,1.6380059132,3.5248567847,-0.8828468561\C,2.3  
627676814,3.2424479144,1.8494770513\H,3.2368496663,1.749774753,0.5374311394\H,2.315574602  
7,1.0791794605,1.8798082158\H,2.3998212855,4.0803879889,1.1412102365\H,3.2481454929,3.31053  
34653,2.4955342329\H,1.4728413107,3.3785909293,2.4807649045\\Version=AM64L-G09RevA.02\Stat  
e=1-A\HF=-1094.8136626\RMSD=2.906e-09\RMSF=3.203e-06\Dipole=1.1764988,-0.1242232,0.190975

Zero-point correction=	0.410655 (Hartree/Particle)
Thermal correction to Energy=	0.441151
Thermal correction to Enthalpy=	0.442269
Thermal correction to Gibbs Free Energy=	0.347406
Sum of electronic and zero-point Energies=	-1094.403008
Sum of electronic and thermal Energies=	-1094.372512
Sum of electronic and thermal Enthalpies=	-1094.371394
Sum of electronic and thermal Free Energies=	-1094.466256

## **TS4N-A**

### **B3LYP/6-31+G\***

H,5.59566,-0.109377,-0.352086\C,4.515016,0.004974,-0.340276\H,4.163604,-1.851947,0.687719\C,3.71  
5905,-0.97144,0.231843\C,2.542862,1.308485,-0.889982\C,2.31136,-0.843225,0.223467\C,3.920278,1.1  
54728,-0.897118\C,1.697771,0.30327,-0.354584\C,1.443433,-1.766673,0.914431\H,4.545329,1.929305,-  
1.333955\C,-0.412895,1.717597,-0.68951\H,2.117609,2.212164,-1.311499\C,0.115651,-1.950807,0.3899  
27\H,1.907104,-2.624869,1.398195\C,-0.599516,-3.158456,0.552282\C,-0.515061,-0.813355,-0.194891\  
H,-2.376696,-0.086752,-1.040146\C,0.24924,0.414173,-0.279752\C,-1.910261,-3.256223,0.121599\H,-0.  
104558,-4.005891,1.019463\H,-2.450195,-4.193959,0.225142\C,-2.548297,-2.131563,-0.444375\H,-3.58  
1004,-2.207705,-0.77545\C,-1.875701,-0.930617,-0.585146\H,-1.418263,1.77447,-0.261374\C,-0.512558  
,2.019631,-2.204206\H,0.145556,2.542762,-0.233808\O,-1.500904,1.155141,-2.766576\H,0.449122,1.79  
9243,-2.692152\C,-0.874037,3.492372,-2.433689\H,-1.808193,3.73946,-1.916337\H,-1.00444,3.708273,-  
3.49955\H,-0.0843,4.153276,-2.056236\C,-1.388581,0.942382,-4.16315\H,-2.152503,0.207894,-4.43065  
5\H,-0.397299,0.541436,-4.424824\H,-1.565374,1.861727,-4.740246\C,0.436264,0.6409 03,2.122856\C,  
1.049308,-0.553933,2.558216\H,2.066009,-0.606568,2.930168\C,-0.003991,-1.341413,3.287876\C,-0.98  
8523,0.600047,2.507149\H,0.93006,1.588928,1.962791\O,-1.856811,1.445837,2.347008\N,-1.199327,-0.  
645458,3.13405\O,0.1235,-2.393408,3.893103\C,-2.485429,-1.119288,3.611846\H,-2.820891,-1.978247,  
3.021095\H,-3.198911,-0.299649,3.508902\H,-2.405121,-1.419655,4.660448\\Version=AM64L-G03RevE  
.01\State=1-A\HF=-1170.7385351\RMSD=4.922e-09\RMSF=1.218e-06\Thermal=0.\Dipole=0.785015,0.3  
515636,-1.4940939

Zero-point correction=	0.410215 (Hartree/Particle)
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Thermal correction to Energy=	0.442880
Thermal correction to Enthalpy=	0.443998
Thermal correction to Gibbs Free Energy=	0.341666
Sum of electronic and zero-point Energies=	-1170.328320
Sum of electronic and thermal Energies=	-1170.295655
Sum of electronic and thermal Enthalpies=	-1170.294537
Sum of electronic and thermal Free Energies=	-1170.396869

### B3LYP/6-31+G\* ( $\epsilon=2.2706$ )

HF = -1170.713350

### BMK/6-31+G\*

H,5.6145356896,-0.0592414096,-0.3293134918\C,4.5304464921,0.0405737017,-0.3248863333\H,4.1920709512,-1.8445059874,0.6619738174\C,3.739343447,-0.9567472622,0.2204756537\C,2.5448805472,1.3402236523,-0.8714996896\C,2.3250717995,-0.8434836524,0.2012110864\C,3.9240623244,1.1993469848,-0.8712600299\C,1.7043190977,0.3121678235,-0.3542642787\C,1.4695224375,-1.7988161014,0.8549425718\H,4.5467276175,1.9870904755,-1.2923211075\C,-0.4036266464,1.7310080105,-0.6743282127\H,2.1088438883,2.2459754174,-1.2846732829\C,0.1203640791,-1.948216278,0.3950621389\H,1.9334096065,-2.6495860062,1.357171271\C,-0.622211113,-3.1408935875,0.6188439565\C,-0.5161749754,-0.7985995036,-0.1658372762\H,-2.4103559785,-0.025768977,-0.9111303356\C,0.2557215434,0.4213714658,-0.2641387427\C,-1.9561033135,-3.2063474821,0.2641792523\H,-0.1220088787,-3.9950875305,1.0731337876\H,-2.5177499676,-4.1270035047,0.4148902338\C,-2.5996312941,-2.0648748385,-0.2853563609\H,-3.6533814701,-2.1178640784,-0.5548500778\C,-1.9066448457,-0.8836064499,-0.4795058448\H,-1.41470874,1.7934144686,-0.2540827291\C,-0.4902468462,1.98912168,-2.2012386156\H,0.1622122261,2.5584544124,-0.2267660528\O,-1.5056226481,1.1607036307,-2.7229230316\H,0.4656910058,1.711353911,-2.6790177468\C,-0.7863373298,3.4768783606,-2.4723776134\H,-1.709218547,3.7738517138,-1.9562486173\H,-0.909272324,3.6694852762,-3.5455679851\H,0.036736415,4.1080180757,-2.1103614689\C,-1.4398347946,0.9416082349,-4.1078497737\H,-2.2417757576,0.2395331146,-4.3579640269\H,-0.4708075001,0.4981627236,-4.3924098544\H,-1.590148085,1.8697763032,-4.6824379525\C,0.4304099789,0.657084477,2.097029541\C,1.0623523861,-0.500239219,2.5698489817\H,2.0923668713,-0.5705189896,2.9025173151\C,0.0081971299,-1.3382697248,3.2448475562\C,-1.0212132262,0.5540487622,2.4285847354\H,0.8882359434,1.6241488774,1.9256439023\O,-1.9071771093,1.3566520125,2.220385266\N,-1.2030070316,-0.6886298138,3.0440648259\O,0.1435173323,-2.3884268464,3.8345904559\C,-2.4841079794,-1.2307444805,3.4384558096\H,-2.7242293336,-2.1128722943,2.8305821803\H,-3.2359246421,-0.4524104789,3.2767732851\H,-2.4565174324,-1.5192990692,4.4954059088\\Version=EM64L-G09RevA.02\State=1-A\HF=-1170.0000717\RMSD=4.808e-09\RMSF=2.162e-06\Dipole=0.7728704,0.3779515,-1.4287072

Zero-point correction=	0.416072 (Hartree/Particle)
Thermal correction to Energy=	0.447791
Thermal correction to Enthalpy=	0.448909
Thermal correction to Gibbs Free Energy=	0.349946
Sum of electronic and zero-point Energies=	-1169.583999
Sum of electronic and thermal Energies=	-1169.552280
Sum of electronic and thermal Enthalpies=	-1169.551163
Sum of electronic and thermal Free Energies=	-1169.650125



## **TS4N-B**

### **B3LYP/6-31+G\***

H,4.877862,-0.253561,0.257825\C,3.798496,-0.182268,0.15272\H,3.420005,-2.113257,1.021139\C,2.988887,-1.226388,0.563975\C,1.843491,1.087701,-0.525905\C,1.588134,-1.153128,0.398523\C,3.216514,0.98504,-0.385014\C,0.990936,0.007459,-0.174003\C,0.693946,-2.157087,0.916477\H,3.850211,1.815773,-0.684908\C,-1.131615,1.340938,-0.689424\H,1.42535,2.008572,-0.914876\C,-0.549917,-2.365782,0.21497\H,1.148444,-3.020985,1.398759\C,-1.222268,-3.605833,0.223897\C,-1.15677,-1.223581,-0.379621\H,-2.916371,-0.529011,-1.439807\C,-0.453458,0.044746,-0.286708\C,-2.467761,-3.731714,-0.368553\H,-0.745223,-4.463426,0.69363\H,-2.973709,-4.693679,-0.378137\C,-3.0781,-2.606189,-0.958597\H,-4.05445,-2.705044,-1.426198\C,-2.444465,-1.374088,-0.955112\H,-2.197406,1.296931,-0.440246\C,-1.025334,1.762726,-2.173834\H,-0.717045,2.147497,-0.075351\O,-1.874451,0.900997,-2.936928\H,0.00618,1.623479,-2.529561\C,-1.429733,3.231185,-2.346951\H,-2.441017,3.396761,-1.957371\H,-1.416813,3.525577,-3.401893\H,-0.740644,3.891855,-1.807654\C,-1.550578,0.80252,-4.313183\H,-2.22764,0.059439,-4.742369\H,-0.512137,0.46509,-4.453223\H,-1.690771,1.75565,-4.843783\C,-0.74518,0.013863,2.1264\C,-0.102387,-1.168373,2.555318\H,-0.632526,-2.041957,2.916743\C,1.133797,-0.743983,3.299763\C,0.090277,1.164844,2.516423\H,-1.804441,0.139987,1.953077\O,-0.110221,2.36017,2.345787\N,1.230206,0.637105,3.156788\O,1.928762,-1.444246,3.905591\C,2.339916,1.431705,3.650417\H,3.238813,1.252531,3.050636\H,2.549895,1.167908,4.690702\H,2.053309,2.482533,3.57865\\Version=AM64L-G03RevE.01\nState=1-A\HF=-1170.7395728\RMSD=5.493e-09\RMSF=2.852e-06\Thermal=0.\Dipole=-0.0988671,-0.1043528,-1.4211737

Zero-point correction=	0.410129 (Hartree/Particle)
Thermal correction to Energy=	0.442782
Thermal correction to Enthalpy=	0.443900
Thermal correction to Gibbs Free Energy=	0.341620
Sum of electronic and zero-point Energies=	-1170.329444
Sum of electronic and thermal Energies=	-1170.296790
Sum of electronic and thermal Enthalpies=	-1170.295673
Sum of electronic and thermal Free Energies=	-1170.397953

### **B3LYP/6-31+G\* ( $\epsilon=2.2706$ )**

HF = -1170.714543

### **BMK/6-31+G\***

H,4.8468314366,-0.158970385,0.4277688527\C,3.7685954042,-0.1143502863,0.2830774559\H,3.4107043072,-2.0882551506,1.0687017267\C,2.9753372454,-1.1936025655,0.6257357643\C,1.8014326491,1.1404620712,-0.4198943262\C,1.5711574924,-1.1507136574,0.4076062845\C,3.1703690934,1.0655723695,-0.2332848699\C,0.9623610872,0.0182059363,-0.1422359598\C,0.6966818017,-2.1922796776,0.8666515141\H,3.7938554826,1.9246740944,-0.4762758979\C,-1.1625893633,1.3424986462,-0.6689784177\H,1.3697255238,2.0680381683,-0.7842561808\C,-0.5638776453,-2.3793948428,0.1969050298\H,1.1494438133,-3.0516701942,1.3645581461\C,-1.2450602319,-3.6242641016,0.2134866425\C,-1.1797312046,-1.2285899336,-0.3757692419\H,-2.9625391698,-0.5233947934,-1.409590702\C,-0.4799266941,0.0417810842,-0.271112696\C,-2.5021655022,-3.7402334878,-0.3547383216\H,-0.7576122526,-4.4871722984,0.6671823743\H,-3.0152301074,-4.7004416115,-0.361022928\C,-3.1207610699,-2.602497

7221,-0.9319183269\H,-4.1056737418,-2.696548143,-1.386402481\C,-2.4834529545,-1.371921333,-0.9335120509\H,-2.2364003119,1.2893270907,-0.4463665618\C,-1.015953313,1.7465562488,-2.1579255931\H,-0.7579442681,2.1491514154,-0.0434601923\O,-1.802183765,0.8601018489,-2.9254005964\H,0.0367563821,1.6333310001,-2.4693939572\C,-1.455679453,3.208509869,-2.3604829188\H,-2.4920423035,3.3388970413,-2.0202089311\H,-1.3969727733,3.4989954277,-3.4170349569\H,-0.8116335612,3.8876957257,-1.786043183\C,-1.4722713891,0.8019998392,-4.2886420401\H,-2.0821164114,0.007707806,-4.7312451577\H,-0.4059235483,0.5550329903,-4.4251586159\H,-1.6896186448,1.7487526487,-4.8091748457\C,-0.7639087882,0.0209267877,2.1204593175\C,-0.1512978319,-1.1562959431,2.5721706538\H,-0.6677813926,-2.0512967543,2.9029130478\C,1.1330112165,-0.7540623307,3.2511134479\C,0.1359896236,1.1621872541,2.4511970047\H,-1.8199483614,0.1818426399,1.9392933231\O,-0.0246245926,2.3470514234,2.236218491\N,1.2670227049,0.6155368167,3.0664275905\O,1.9338850155,-1.4576553335,3.8277324167\C,2.433910642,1.3716311363,3.4627325076\H,3.304347456,1.0590052288,2.8712836959\H,2.6448407168,1.2061283136,4.5254873401\H,2.2196615525,2.4290116228,3.2798273233\\Version=EM64L-G09RevA.02\State=1-A\HF=-1170.0011501\RMSD=3.595e-09\RMSF=5.293e-06\Dipole=-0.1588798,-0.069196,-1.3481475

Zero-point correction=	0.415411 (Hartree/Particle)
Thermal correction to Energy=	0.447263
Thermal correction to Enthalpy=	0.448381
Thermal correction to Gibbs Free Energy=	0.349088
Sum of electronic and zero-point Energies=	-1169.585739
Sum of electronic and thermal Energies=	-1169.553887
Sum of electronic and thermal Enthalpies=	-1169.552769
Sum of electronic and thermal Free Energies=	-1169.652062

## **TS5'-endo**

### **B3LYP/6-31+G\***

C,2.3505096846,-1.5155768947,0.8694591001\C,3.8164972778,-1.4373501678,0.5426986853\H,4.3280887414,-0.6853773012,1.1522997151\H,3.9866287446,-1.1829554535,-0.5076092164\H,4.2977407423,-2.4054055913,0.7464768145\C,1.3950481494,-1.9025389254,-0.0683700871\H,2.1182372966,-1.6606653233,1.9212680662\C,0.0185223538,-1.9016996471,0.1948849143\H,1.715727236,-2.0373002309,-1.1009510102\C,-0.5120916983,-1.4985233972,1.4208063132\H,-0.659074235,-2.029705087,-0.6487419308\H,0.0711645146,-1.6617465423,2.3239299661\C,-2.0009038705,-1.4490281288,1.678002326\H,-2.4845793636,-0.8549127567,0.889393831\O,-2.1791899446,-0.788399334,2.9363781754\C,-2.6121923745,-2.860456585,1.7139575663\H,-2.5023350761,-3.3565453639,0.7432385849\H,-3.6815993887,-2.8117244516,1.9481934693\H,-2.1185695662,-3.4726337645,2.4769409642\C,-3.4366240215,-0.1442738134,3.0888833514\H,-4.2712870076,-0.8602207789,3.0718167984\H,-3.5874620819,0.6095172137,2.3037113862\H,-3.4178170018,0.3462191037,4.06563627\C,0.2226726223,0.5843895123,1.5168756462\C,1.606372531,0.6149058678,1.3071283362\H,2.3598070199,0.7078514474,2.0787602857\C,1.8636368059,1.1862533008,-0.035476684\C,-0.4348211833,1.1299054762,0.2968753883\H,-0.2807245428,0.6729262186,2.4709194776\O,-1.6221972218,1.3478704552,0.1157301213\N,0.5905028307,1.3612044723,-0.6459205878\O,2.9279388487,1.4817718453,-0.5483058022\C,0.3966161267,1.8523131106,-1.9718261041\C,0.0443361317,2.8068938728,-4.5794138341\C,1.1523281938,1.3167127184,-3.0223978992\C,-0.5345362052,2.8675879008,-2.2241551292\C,-0.7102350792,3.3344509574,-3.5285231081\C,0.9779879884,1.7996955215,-4.3198530919\H,1.8807672956,0.5395628871,-2.8203129152\H,-1.1219600512,3.2762314017,-1.4108421411\H,-1.438044517,4.1189345607,-3.7191075915\H,1.573

435181,1.3844208255,-5.128818163\H,-0.0923218856,3.1784208686,-5.5916402571\\Version=AM64L-G03RevD.01\State=1-A\HF=-978.9500478\RMSD=6.303e-09\RMSF=2.796e-06\Thermal=0.\Dipole=-0.2885517,-1.0827894,0.4068806

Zero-point correction=	0.354542 (Hartree/Particle)
Thermal correction to Energy=	0.375818
Thermal correction to Enthalpy=	0.376762
Thermal correction to Gibbs Free Energy=	0.303535
Sum of electronic and zero-point Energies=	-978.595506
Sum of electronic and thermal Energies=	-978.574230
Sum of electronic and thermal Enthalpies=	-978.573285
Sum of electronic and thermal Free Energies=	-978.646513

B3LYP/6-31+G\* ( $\epsilon=2.2706$ )

HF = -978.940663

BMK/6-31+G\*

C,2.3475303026,-1.503261547,0.8062778296\C,3.8198317615,-1.39855231,0.4813533468\H,4.3188303614,-0.6530899687,1.113181994\H,3.9803970825,-1.1091511781,-0.5634004196\H,4.3107450563,-2.3683055705,0.6579811931\C,1.3894814627,-1.7872424184,-0.1610560664\H,2.1071571868,-1.7125584183,1.8476920838\C,0.0036177866,-1.7906421098,0.1123012459\H,1.7038412456,-1.8232168775,-1.2058802584\C,-0.5095663014,-1.5009530001,1.3717971716\H,-0.6834033898,-1.8169556246,-0.7362839929\H,0.0842522123,-1.716780948,2.2598880637\C,-2.0018587245,-1.4275842216,1.6325305604\H,-2.4770456763,-0.8472232737,0.824843895\O,-2.1815507369,-0.7539547685,2.862012383\C,-2.6161608668,-2.8445274558,1.6926581824\H,-2.5152901563,-3.3500488176,0.7236708652\H,-3.6834617355,-2.7883976824,1.9442706695\H,-2.1067923789,-3.442648369,2.4595080025\C,-3.4172578978,-0.0896378517,2.9773569552\H,-4.2650575527,-0.7927833856,2.9327309352\H,-3.52633026,0.6652157468,2.1825749871\H,-3.4229261107,0.4037584176,3.9548849102\C,0.2639922911,0.5951611555,1.6191782151\C,1.6382816938,0.6131556277,1.3907980776\H,2.4208622862,0.6491119711,2.1409524653\C,1.8779594406,1.1842571868,0.0342605707\C,-0.4079749808,1.1513169671,0.4026281919\H,-0.2513274974,0.6150870271,2.573248466\O,-1.587662856,1.3799469559,0.2402773715\N,0.6025124758,1.3637292268,-0.5507677743\O,2.9297827285,1.4639264756,-0.4933311796\C,0.3921810744,1.811462943,-1.8832026787\C,0.0032369398,2.6739553548,-4.5222308676\C,1.1541630185,1.253703725,-2.9219465957\C,-0.5626970594,2.8019352711,-2.1597148477\C,-0.7555776517,3.2235650975,-3.4809565079\C,0.9599675399,1.6903988076,-4.2363695425\H,1.9007351738,0.497412393,-2.6949255951\H,-1.1518236822,3.2229286668,-1.3508775922\H,-1.4990131327,3.9904189634,-3.6917069549\H,1.5567790087,1.257785475,-5.0376022511\H,-0.147358482,3.0102823415,-5.5466075078\\Version=AM64L-G09RevA.02\State=1-A\HF=-978.3292015\RMSD=4.104e-09\RMSF=3.935e-06\Dipole=-0.2953155,-1.0519491,0.3766472

Zero-point correction=	0.360400 (Hartree/Particle)
Thermal correction to Energy=	0.388286
Thermal correction to Enthalpy=	0.389404
Thermal correction to Gibbs Free Energy=	0.297985
Sum of electronic and zero-point Energies=	-977.968802
Sum of electronic and thermal Energies=	-977.940915
Sum of electronic and thermal Enthalpies=	-977.939797

Sum of electronic and thermal Free Energies= -978.031217

### **TS5'-exo**

B3LYP/6-31+G\*

C,2.0990306692,-1.9589831136,-0.1067193051\C,2.4178299272,-3.3396493292,0.3989925699\H,2.4026317967,-4.0563488894,-0.4347580431\H,1.673636088,-3.6776025124,1.1275585418\H,3.4111284232,-3.3812398489,0.8603186613\C,3.0966522591,-1.0645694272,-0.4975393242\H,1.1167005351,-1.8523707107,-0.5618353807\C,2.8420509268,0.2508255588,-0.903123357\H,4.1335566359,-1.347408349,-0.3149253788\C,1.5604631254,0.7964686059,-0.9505871288\H,3.6973840331,0.9127054885,-1.0171329608\H,0.7292995498,0.1323981611,-1.1744124712\C,1.2577147684,2.2323641762,-1.3359898914\H,0.4608690909,2.5943188888,-0.6701262699\O,0.7221555759,2.1610141633,-2.6694785506\C,2.4452241166,3.1955809359,-1.2652543099\H,2.8767631995,3.2179228418,-0.2570138519\H,2.1229680849,4.2141282953,-1.5044403839\H,3.2268987421,2.9132248812,-1.9785144192\C,-0.1562779131,3.2241521591,-3.0093132617\H,0.3623056936,4.1934157685,-3.0467746208\H,-0.9927458549,3.2931591189,-2.2982098321\H,-0.5462799063,2.997645615,-4.0050766678\C,1.0055107839,0.5425295777,1.2280081174\C,1.2708406922,-0.7762787655,1.6269661675\H,2.0983792793,-1.0864708814,2.2504336004\C,-0.032231963,-1.4837791332,1.7593014662\C,-0.4697161037,0.6925385171,1.0969512213\H,1.5946287685,1.4070810493,1.5022156348\O,-1.1058508594,1.7048843291,0.8598504747\N,-1.0322462009,-0.5882758733,1.3094581625\O,-0.2366502083,-2.6129595759,2.1698348979\C,-2.424168951,-0.8895275263,1.2036266887\C,-5.151254494,-1.4650292751,0.9794971437\C,-3.0784427939,-1.5746302031,2.2340617538\C,-3.1308801456,-0.490979413,0.0627972739\C,-4.493322647,-0.774063875,-0.0419284545\C,-4.4388830283,-1.8655184549,2.1128555211\H,-2.5253183538,-1.8863524827,3.112330554\H,-2.619769458,0.04531944,-0.7296138354\H,-5.0384925409,-0.4572114911,-0.9271682731\H,-4.9419229216,-2.4032237113,2.9122815989\H,-6.2111684216,-1.6892047292,0.8925959221\\Version=AM64 L-G03RevE.01\State=1-A\HF=-978.9444477\RMSD=3.128e-10\RMSF=3.081e-06\Thermal=0.\Dipole=0.9049593,0.3089659,-0.2480857

Zero-point correction=	0.354678 (Hartree/Particle)
Thermal correction to Energy=	0.375958
Thermal correction to Enthalpy=	0.376902
Thermal correction to Gibbs Free Energy=	0.303142
Sum of electronic and zero-point Energies=	-978.589770
Sum of electronic and thermal Energies=	-978.568490
Sum of electronic and thermal Enthalpies=	-978.567546
Sum of electronic and thermal Free Energies=	-978.641305

B3LYP/6-31+G\* ( $\epsilon=2.2706$ )

HF = -978.935902

BMK/6-31+G\*

C,2.1019986617,-1.9679092583,-0.047194945\C,2.4159577848,-3.3439747489,0.4949634675\H,2.3839580995,-4.0823462945,-0.3208653812\H,1.6722176709,-3.6485019366,1.2424984763\H,3.4163462316,-3.3755334659,0.9458624235\C,3.1006062602,-1.0838128591,-0.4470841055\H,1.1072048308,-1.852

4014289,-0.4789464763\C,2.8423203074,0.2350232951,-0.8754848933\H,4.1389425184,-1.362819021  
,-0.2563420741\C,1.5618162833,0.7744823846,-0.9227117297\H,3.6980024534,0.8970402338,-1.0047  
043416\H,0.7168109923,0.107484878,-1.0942006397\C,1.2439163688,2.2127658243,-1.3128689427\  
H,0.6316456873,2.6548420503,-0.5084882106\O,0.4390466759,2.1171526889,-2.4745915563\C,2.478  
7994837,3.0997873166,-1.5475524612\H,3.0942938876,3.1632893417,-0.6397606245\H,2.167893543  
2,4.1191156792,-1.8064618197\H,3.0891539462,2.7032507653,-2.369053483\C,-0.367187798,3.24321  
81977,-2.7193410456\H,0.2321923413,4.1267476594,-2.992735943\H,-0.984863693,3.484367653,-1.8  
386489434\H,-1.0195751545,2.9893633573,-3.5613584128\C,1.0461984772,0.5620677845,1.2894958  
311\C,1.2956823412,-0.7507693658,1.6975122192\H,2.1200158584,-1.0897788797,2.3138136063\C,-  
0.0217331606,-1.4599747702,1.7804702408\C,-0.4335488282,0.7106016555,1.1113958152\H,1.64253  
18581,1.4346487641,1.5289603786\O,-1.0576954943,1.717223554,0.8652931443\N,-0.9972754325,-0.  
5688561425,1.2930325599\O,-0.2387691083,-2.5821249391,2.1786366691\C,-2.3797063116,-0.86736  
48576,1.1398992388\C,-5.1028083868,-1.4374246687,0.8176348559\C,-3.0592535441,-1.5975900332,  
2.1262722106\C,-3.0552304712,-0.421731655,-0.0062888635\C,-4.4168659597,-0.7035758191,-0.1595  
077007\C,-4.4188538161,-1.8847457937,1.9554289444\H,-2.5229664294,-1.9475817084,3.003377339  
6\H,-2.5197956853,0.1446588951,-0.7638527918\H,-4.938043698,-0.3529252767,-1.0485762755\H,-4.  
9431623513,-2.4560728207,2.7194821702\H,-6.1612142406,-1.6593152349,0.6925970697\\Version=A  
M64L-G09RevA.02\State=1-A\HF=-978.3215809\RMSD=5.732e-09\RMSF=3.796e-06\Dipole=1.0018648,  
0.3692525,-0.2343269

Zero-point correction=	0.360519 (Hartree/Particle)
Thermal correction to Energy=	0.387556
Thermal correction to Enthalpy=	0.388673
Thermal correction to Gibbs Free Energy=	0.298857
Sum of electronic and zero-point Energies=	-977.961062
Sum of electronic and thermal Energies=	-977.934025
Sum of electronic and thermal Enthalpies=	-977.932907
Sum of electronic and thermal Free Energies=	-978.022724

## **TS5-endo**

B3LYP/6-31+G\*

C,0.7330205763,-1.7222357895,2.42639854\C,1.9757258982,-1.9457334601,3.2508147524\H,2.65696  
22487,-1.0920643279,3.1921195516\H,2.5257063606,-2.8344819908,2.9235915906\H,1.702038801,-  
2.1004438152,4.3043691868\C,0.1092556363,-0.4706286453,2.3697771976\H,0.1007293065,-2.60005  
13596,2.3090838427\C,-1.0223884426,-0.2106436951,1.5866587162\H,0.6360245569,0.3816542275,2.  
798062671\C,-1.6467495737,-1.1812221835,0.8095455799\H,-1.3278880084,0.8214242908,1.4414882  
497\H,-1.605484959,-2.2187941098,1.1288459253\C,-2.815769227,-0.8679064011,-0.1004883982\H,-  
2.6143338033,-1.2998554266,-1.0931342875\O,-2.9357337328,0.5449425928,-0.2340461988\C,-4.115  
0900838,-1.4816530335,0.4529999191\H,-4.0311122059,-2.5726835549,0.5304803505\H,-4.95868026  
29,-1.2584011012,-0.2093337843\H,-4.3354895106,-1.0750725264,1.4458985604\C,-3.5035538742,0.9  
738575277,-1.4648754561\H,-4.5306034908,0.6010758922,-1.5936458857\H,-2.884137926,0.6521732  
446,-2.3119262489\H,-3.531505067,2.0659214065,-1.4281950661\C,1.2774215998,-2.0077458993,0.3  
462336641\C,0.1596959171,-1.8808484087,-0.4893999068\H,-0.4284331745,-2.6989555316,-0.885083  
5698\C,0.2967176121,-0.6350453477,-1.272189425\C,2.1485173797,-0.8152701693,0.1178767774\H,  
1.7459818354,-2.9495132968,0.6058922469\O,3.2547166711,-0.5952076608,0.5787216612\N,1.44132  
52447,0.0339935383,-0.7602133484\O,-0.3872048111,-0.2391591396,-2.2002829688\C,1.8782960023,



1.3210623112,-1.1955507937\C,2.7024367707,3.8545198985,-2.0463816098\C,0.9511153976,2.36771  
86953,-1.2738809062\C,3.2168368509,1.5378299163,-1.5436832882\C,3.6231838526,2.8071383035,-1  
.9613553539\C,1.3658071106,3.6283408014,-1.7049298773\H,-0.0851732569,2.189160172,-1.008188  
663\H,3.9315681114,0.7264841115,-1.4745691463\H,4.6646447236,2.9728163768,-2.22467391\H,0.6  
414079908,4.4362564869,-1.768570688\H,3.0231949558,4.8392470803,-2.3762602027\\Version=IA32  
L-G03RevD.01\State=1-A\HF=-978.9478683\RMSD=4.570e-09\RMSF=3.535e-06\Thermal=0.\Dipole=-  
0.9219732,-0.8162031,0.5969153

Zero-point correction=	0.354688 (Hartree/Particle)
Thermal correction to Energy=	0.375929
Thermal correction to Enthalpy=	0.376873
Thermal correction to Gibbs Free Energy=	0.303777
Sum of electronic and zero-point Energies=	-978.593181
Sum of electronic and thermal Energies=	-978.571939
Sum of electronic and thermal Enthalpies=	-978.570995
Sum of electronic and thermal Free Energies=	-978.644092

B3LYP/6-31+G\* ( $\epsilon=2.2706$ )

HF = -978.937205

BMK/6-31+G\*

C,0.7876986817,-1.7321499246,2.4237591781\C,2.0447476428,-2.0044999725,3.2236614323\H,2.7849  
929603,-1.2092170167,3.0769882433\H,2.5072198889,-2.9566627374,2.9342329257\H,1.7990178927,  
-2.0682131516,4.2947414798\C,0.2856231969,-0.4410200693,2.2707369041\H,0.0927655836,-2.5677  
301869,2.3394823406\C,-0.8430643683,-0.1390522853,1.476682735\H,0.9054752965,0.3920482192,2.  
6077347577\C,-1.5690897149,-1.1068968077,0.7993628206\H,-1.042491633,0.9047463596,1.2415159  
553\H,-1.5988996925,-2.1262478398,1.1809454344\C,-2.7085590942,-0.7521830702,-0.1405732644\  
H,-2.594981582,-1.339287638,-1.0685974824\O,-2.6342083599,0.6173640352,-0.4513377147\C,-4.067  
1380253,-1.1039117804,0.5104611042\H,-4.1219603571,-2.1756363959,0.7449653383\H,-4.89347200  
44,-0.8645764498,-0.1713568292\H,-4.1943807078,-0.5290150185,1.4364673754\C,-3.2268316166,0.9  
689674802,-1.6788122969\H,-4.3078584991,0.7531275368,-1.6860357049\H,-2.7351770529,0.441768  
1778,-2.5098625112\H,-3.0857831654,2.0480558745,-1.8006925281\C,1.3001812821,-2.1605095701,0  
.3215337107\C,0.1718238029,-2.0609640455,-0.4884250558\H,-0.4718148771,-2.8714740536,-0.8134  
095456\C,0.2834196858,-0.8213014483,-1.2983479885\C,2.1458863243,-0.9430123866,0.0702627802  
\H,1.7676217248,-3.0796894263,0.6594216295\O,3.2409752528,-0.6935389608,0.5217614291\N,1.40  
84605024,-0.1234895087,-0.7989085296\O,-0.4066067734,-0.4601673922,-2.2246167217\C,1.7393344  
742,1.21078359,-1.1578825517\C,2.3446233951,3.8631159722,-1.8262152784\C,0.7097280384,2.1638  
390875,-1.2369033425\C,3.0684405719,1.5766902136,-1.4159750477\C,3.3638534526,2.9064695931,-  
1.742831126\C,1.0178558158,3.4847926599,-1.5764103374\H,-0.3176074507,1.8607663716,-1.04255  
75926\H,3.8576829339,0.8347596815,-1.348211705\H,4.3971439713,3.1901301781,-1.9357254763\H,  
0.218025795,4.2209469184,-1.6383825961\H,2.5803288081,4.8940751876,-2.0846423475\\Version=E  
M64L-G09RevA.02\State=1-A\HF=-978.32763\RMSD=5.280e-09\RMSF=8.188e-06\Dipole=-0.9884355,-  
0.7994915,0.7015784

Zero-point correction=	0.362384 (Hartree/Particle)
Thermal correction to Energy=	0.382187

Thermal correction to Enthalpy=	0.383131
Thermal correction to Gibbs Free Energy=	0.315678
Sum of electronic and zero-point Energies=	-977.965246
Sum of electronic and thermal Energies=	-977.945443
Sum of electronic and thermal Enthalpies=	-977.944499
Sum of electronic and thermal Free Energies=	-978.011952

## **TS5-exo**

### B3LYP/6-31+G\*

C,1.3533295755,0.6549979333,2.3891853898\C,2.656795995,0.3838731935,3.0873028222\H,3.153126  
3406,1.3129676767,3.3894911525\H,3.3371436504,-0.1887954664,2.4473465292\H,2.4838967524,-0.  
2166002485,3.9923931365\C,0.6288057425,1.8287290983,2.5835529383\H,0.8131605085,-0.2300636  
998,2.060563532\C,-0.538725649,2.147478616,1.8784364718\H,1.0880635017,2.6150424428,3.18295  
64746\C,-1.094343403,1.3136896203,0.9078663136\H,-0.9185377695,3.1642076274,1.9457800855\H,  
-0.9927272476,0.2368321973,1.0249344784\C,-2.3136557297,1.7183194475,0.1116935808\H,-2.2844  
605188,1.1959920315,-0.8555744172\O,-2.2420946028,3.1281424779,-0.1172385009\C,-3.603571570  
9,1.3201089667,0.8524308802\H,-3.6176798996,0.2407829828,1.0439729748\H,-4.4900918235,1.558  
9630258,0.2545158906\H,-3.6728234286,1.8459976247,1.8109832911\C,-3.072697321,3.5996499573,  
-1.1667340393\H,-4.1407329173,3.50935002,-0.9226595758\H,-2.8731688653,3.0596981281,-2.10446  
56742\H,-2.8324976656,4.6573966484,-1.3022803901\C,0.6160238872,1.2533954158,-0.5236534382\  
C,1.8103876367,0.9672248361,0.1518432402\H,2.578730088,1.6828187753,0.4093654649\C,2.199922  
71,-0.4283305131,-0.1654914603\C,0.2281057687,0.0350177297,-1.290344862\H,0.3223099939,2.224  
4434,-0.8993302915\O,-0.7045403628,-0.0956072192,-2.0662286349\N,1.1500484933,-0.9794575575,  
-0.9482598719\O,3.2127259546,-1.0243251743,0.1574547425\C,1.108410598,-2.3274770203,-1.41598  
82808\C,1.0376780978,-4.976210072,-2.316502824\C,1.3859023743,-3.3760647119,-0.52997976\C,0.7  
981279884,-2.6021385072,-2.7537529184\C,0.7572362973,-3.9264031201,-3.1947760062\C,1.356061  
775,-4.6950305208,-0.9849972038\H,1.6381467508,-3.1591061145,0.5021329134\H,0.5791190265,-1.  
7893348274,-3.435787684\H,0.5100722364,-4.1340742906,-4.232644283\H,1.5796805784,-5.5033946  
753,-0.293727299\H,1.010336453,-6.0047061345,-2.6667848875\\Version=IA32L-G03RevD.01\State=1  
-A\HF=-978.9484106\RMSD=7.033e-09\RMSF=2.673e-06\Thermal=0.\Dipole=-0.7035784,0.5483137,0.  
6284814

Zero-point correction=	0.354407 (Hartree/Particle)
Thermal correction to Energy=	0.375789
Thermal correction to Enthalpy=	0.376733
Thermal correction to Gibbs Free Energy=	0.302778
Sum of electronic and zero-point Energies=	-978.594003
Sum of electronic and thermal Energies=	-978.572622
Sum of electronic and thermal Enthalpies=	-978.571678
Sum of electronic and thermal Free Energies=	-978.645633

### B3LYP/6-31+G\* ( $\epsilon=2.2706$ )

HF = -978.938628



## BMK/6-31+G\*

C,1.3447063329,0.6104500649,2.3648583589\C,2.6523336868,0.3275595751,3.0674229836\H,3.1065155864,1.2516206442,3.4475465236\H,3.360195227,-0.1696748874,2.3907633472\H,2.4840628178,-0.3494301038,3.9190225292\C,0.618359856,1.7752273928,2.5820863426\H,0.8225332642,-0.2648275359,1.9769299799\C,-0.5513359554,2.1124275606,1.8671252848\H,1.0715070941,2.5497219155,3.2043826411\C,-1.0964808304,1.2981487873,0.8810783463\H,-0.9268382388,3.131743199,1.9496670899\H,-0.9701002797,0.2169191004,0.9511869739\C,-2.2977534365,1.7260291093,0.0594342101\H,-2.2406274316,1.2272512532,-0.9227009356\O,-2.2292415477,3.1240547359,-0.1227760421\C,-3.6052969958,1.2938508138,0.7635033664\H,-3.5967377244,0.2122063377,0.9511919312\H,-4.4800535123,1.5169296165,0.1390528329\H,-3.7056820516,1.8193717959,1.7222276102\C,-3.0898437759,3.6262015505,-1.1134561736\H,-4.1482122861,3.5511290813,-0.8177052787\H,-2.9461186062,3.0935763961,-2.068377675\H,-2.8361922657,4.682778521,-1.2494242108\C,0.6610792835,1.2990368806,-0.5487479196\C,1.8414356105,1.0101928834,0.1360937762\H,2.6075504869,1.7136912681,0.438724373\C,2.2180385844,-0.4028693042,-0.1681071449\C,0.2646257207,0.0652706746,-1.303518158\H,0.3328299035,2.2700530324,-0.9024846483\O,-0.6581597465,-0.0649296421,-2.0773577237\N,1.1685437992,-0.9511390386,-0.9405255714\O,3.2172914607,-0.9985139624,0.1648723065\C,1.114003253,-2.3003164698,-1.3875983317\C,1.0092982621,-4.9685718577,-2.2469035772\C,1.4610428532,-3.3352984057,-0.5041350986\C,0.7178133438,-2.5964721358,-2.7019451407\C,0.6615327097,-3.9311918858,-3.1215103809\C,1.4127602959,-4.6637729425,-0.9399083053\H,1.7843050391,-3.0976999877,0.5054089694\H,0.4430235245,-1.7925123182,-3.3773930146\H,0.3459846402,-4.1553756069,-4.1390073173\H,1.688156124,-5.4608687219,-0.2514046978\H,0.9701469243,-6.0039783836,-2.5805934313\\Version=EM64L-G09RevA.02\State=1-A\HF=-978.3258534\RMSD=2.278e-09\RMSF=4.743e-06\Dipole=-0.7145262,0.5810962,0.5871114

Zero-point correction=	0.359084 (Hartree/Particle)
Thermal correction to Energy=	0.379966
Thermal correction to Enthalpy=	0.380910
Thermal correction to Gibbs Free Energy=	0.308247
Sum of electronic and zero-point Energies=	-977.966769
Sum of electronic and thermal Energies=	-977.945887
Sum of electronic and thermal Enthalpies=	-977.944943
Sum of electronic and thermal Free Energies=	-978.017607

## TS6'-endo

### B3LYP/6-31+G\*

C,-1.6968845187,0.1786045299,1.0416017019\H,-1.2743575179,0.9429762487,1.6939184481\C,-2.2793547482,0.595130012,-0.1528143955\H,-2.9589984986,-0.0717959018,-0.6777642863\C,-1.4195227615,-1.1595477592,1.3476795783\H,-0.8012238313,-1.3650958648,2.2211930514\C,-1.6862032342,-2.214015159,0.4677247487\H,-2.5393003364,-2.1015791349,-0.1978853167\C,-1.3303385083,-3.6386311936,0.8078459353\H,-1.277506381,-4.2679758609,-0.0866132247\H,-2.1004921662,-4.0684911621,1.4641823964\H,-0.365394363,-3.7046791887,1.3190199256\C,-2.4862233531,2.0712589409,-0.4585317318\H,-1.8007792632,2.6560340342,0.1736905145\O,-2.2520914342,2.3826336434,-1.8299422237\H,-1.2819698841,2.366559622,-1.9644816696\C,-3.9269481707,2.4853838414,-0.1449359461\H,-4.1734157595,2.2976742478,0.9059238777\H,-4.6293648163,1.9275221347,-0.775412148\H,-4.0526924227,3.

5527801844,-0.3550243737\C,-0.7710429486,-0.328059926,-1.6505059473\H,-1.4343366139,-0.04287  
70927,-2.4553182544\C,-0.4690026404,-1.6362440749,-1.2519995113\H,-0.7921741595,-2.528772912  
8,-1.773663245\N,1.2918582648,-0.2558185999,-0.5925777705\C,2.5243509702,0.203700836,-0.0341  
259871\C,4.9387830485,1.0821800638,1.0702534952\C,3.3311083606,1.0997836245,-0.7456682236\  
C,2.9245390599,-0.2562203258,1.2262069665\C,4.1329347513,0.1802778391,1.7707733565\C,4.5319  
424009,1.5401435562,-0.1853891638\H,3.0157347888,1.456668776,-1.7187991014\H,2.3015454579,-  
0.9596861752,1.76711697\H,4.4417158557,-0.1849226742,2.7467242396\H,5.1519882924,2.2404838  
58,-0.7387382301\H,5.8770294258,1.4237939739,1.4993415305\C,0.892464756,-1.6187448795,-0.642  
9262428\O,1.5661702962,-2.5569072461,-0.2636674952\C,0.3663848716,0.5427177151,-1.290669456  
4\O,0.511067731,1.7357574498,-1.5397427911\\Version=IA32L-G03RevD.01\State=1-A\HF=-939.6499  
846\RMSD=4.993e-09\RMSF=5.736e-06\Thermal=0.\Dipole=-0.6058654,-0.6540256,0.8120557

Zero-point correction=	0.327106 (Hartree/Particle)
Thermal correction to Energy=	0.346487
Thermal correction to Enthalpy=	0.347431
Thermal correction to Gibbs Free Energy=	0.278959
Sum of electronic and zero-point Energies=	-939.322879
Sum of electronic and thermal Energies=	-939.303498
Sum of electronic and thermal Enthalpies=	-939.302554
Sum of electronic and thermal Free Energies=	-939.371026

B3LYP/6-31+G\* ( $\epsilon=2.2706$ )

HF = -939.632600

BMK/6-31+G\*

C,-1.5908329933,0.2347060713,1.0474398645\H,-1.092453399,1.0120616261,1.6307059737\C,-2.2665  
22386,0.6183308872,-0.1054339137\H,-2.9819666118,-0.0615644438,-0.5686914988\C,-1.3075163705  
,-1.1093182741,1.3724078939\H,-0.6072234507,-1.3006306063,2.1880968068\C,-1.6783096712,-2.178  
2777273,0.5585206775\H,-2.5637310691,-2.0625943345,-0.0659925515\C,-1.2795615939,-3.60276316  
6,0.8768326861\H,-2.0140573311,-4.052831251,1.5622253622\H,-0.2889458631,-3.6423299875,1.344  
5200371\H,-1.2465337931,-4.2217335803,-0.0283780115\C,-2.4792302946,2.0937553496,-0.44330230  
22\H,-1.7428218101,2.6873001871,0.1224210255\O,-2.3484334487,2.3553182229,-1.8230798386\H,-  
1.3966408758,2.3858660448,-2.0209926935\C,-3.8985814686,2.5210076863,-0.0333670396\H,-4.0637  
193109,2.3623876003,1.0396574875\H,-4.6403048015,1.9397576882,-0.5978305964\H,-4.0402672898  
,3.5828848712,-0.2692878623\C,-0.8582978768,-0.3111814062,-1.6715945238\H,-1.5492851761,0.014  
8622351,-2.4405328018\C,-0.5597717272,-1.6223435412,-1.3069239176\H,-0.9360850945,-2.5228384  
556,-1.7807072958\N,1.1961551466,-0.2666040254,-0.5901206158\C,2.4033541727,0.1733677313,0.0  
216176821\C,4.7771400244,1.0202775132,1.2469234723\C,3.1974200657,1.1503770058,-0.59785151  
12\C,2.7945603462,-0.3845568874,1.2489617963\C,3.9829463214,0.0379566739,1.8538696183\C,4.37  
84421642,1.5737153379,0.0236609715\H,2.8832640608,1.5810260032,-1.5430734319\H,2.18205013,-  
1.1541969628,1.7105477347\H,4.2856478843,-0.4026726655,2.8021809425\H,4.988797539,2.336401  
2241,-0.4568456247\H,5.7001076833,1.3482442713,1.721757165\C,0.8007527457,-1.6233767604,-0.6  
85436227\O,1.4642560108,-2.5666864572,-0.3261869724\C,0.2917077996,0.5506263769,-1.27967465  
57\O,0.4398126426,1.739153465,-1.4998261812\\Version=EM64L-G09RevA.02\State=1-A\HF=-939.05  
99351\RMSD=6.422e-09\RMSF=3.543e-06\Dipole=-0.5962108,-0.5498298,0.7648791

Zero-point correction=	0.331707 (Hartree/Particle)
Thermal correction to Energy=	0.350481
Thermal correction to Enthalpy=	0.351425
Thermal correction to Gibbs Free Energy=	0.285151
Sum of electronic and zero-point Energies=	-938.728228
Sum of electronic and thermal Energies=	-938.709454
Sum of electronic and thermal Enthalpies=	-938.708510
Sum of electronic and thermal Free Energies=	-938.774784

## **TS6'-exo**

### B3LYP/6-31+G\*

C,1.3337072655,0.6787525997,0.7466609897\H,1.8772422633,1.5156688553,1.1638584341\C,1.42709  
81152,-0.6511421945,1.1859176793\H,2.0548041774,-0.9968416332,1.9961477103\N,0.9366970771,-  
0.6914143068,-1.0972329478\C,0.600635209,-1.1359937098,-2.4139698561\C,-0.0654815349,-1.9961  
755201,-4.9879086816\C,-0.4775841902,-0.5498386691,-3.0875652053\C,1.3484393644,-2.149704091  
9,-3.0237754231\C,1.005878359,-2.5801054199,-4.3072957124\C,-0.8018934054,-0.9781434558,-4.37  
54844642\H,-1.0470437922,0.2427770788,-2.6142319689\H,2.1785867039,-2.6032033167,-2.4950497  
366\H,1.5845313286,-3.3718373176,-4.7757291038\H,-1.6347967346,-0.5151175883,-4.8978388801\  
H,-0.3243668444,-2.3307512003,-5.9889913029\C,1.2533928757,-1.5345861174,-0.0017856261\O,1.35  
76553704,-2.7458017551,-0.0605868502\C,1.0735081196,0.6545942126,-0.7145011224\O,0.99503847  
69,1.6063371879,-1.4813591054\C,-0.485286735,1.1894962618,2.8537737159\H,-0.2594932513,1.928  
6165227,3.6227387059\C,-0.622610513,1.6334173018,1.5403649229\H,-1.1489570521,1.0091229486,  
0.8215713695\C,-0.4076831001,-0.1582812893,3.2212694933\H,-0.145198659,-0.3859215293,4.25451  
74456\C,-0.4214658183,-1.2155469593,2.3081660248\H,-0.968688062,-1.0761074611,1.3780307647\  
C,-0.2768876797,-2.647069018,2.7504841627\H,0.2301863234,-3.2505444651,1.9907795993\H,-1.269  
9862653,-3.0915828631,2.908597822\H,0.2793600702,-2.7234022792,3.6916820551\C,-0.6287860228  
,3.1184661392,1.1953883615\H,0.3195936696,3.5664210991,1.5402687405\O,-0.7987553872,3.34786  
49837,-0.1943471339\H,-0.0678529739,2.9319449373,-0.6944504551\C,-1.7856067124,3.8486852045,  
1.8901497476\H,-1.7042326009,3.7876902749,2.9800988639\H,-2.744399931,3.4167849721,1.583184  
7484\H,-1.7712975032,4.9024715813,1.5924522193\\Version=IA32L-G03RevD.01\State=1-A\HF=-939.  
6450705\RMSD=7.902e-09\RMSF=4.838e-06\Thermal=0.\Dipole=0.0243945,-0.389914,1.3462309

Zero-point correction=	0.326716 (Hartree/Particle)
Thermal correction to Energy=	0.346154
Thermal correction to Enthalpy=	0.347098
Thermal correction to Gibbs Free Energy=	0.278249
Sum of electronic and zero-point Energies=	-939.318355
Sum of electronic and thermal Energies=	-939.298917
Sum of electronic and thermal Enthalpies=	-939.297972
Sum of electronic and thermal Free Energies=	-939.366822

### B3LYP/6-31+G\* ( $\epsilon=2.2706$ )

HF = -939.628440

## BMK/6-31+G\*

C,-1.1305936827,0.2719776692,-1.3559103849\H,-1.8496130896,-0.059435  
1001,-2.0961035945\C,-0.7798271765,1.5929569353,-1.0711238456\H,-1.1836896214,2.4841101498,-  
1.5367566325\N,1.053614944,0.2473445568,-0.5272797424\C,2.3198266428,-0.2041629751,-0.05726  
0243\C,4.8008725186,-1.1056  
765763,0.8761046328\C,2.3844922451,-1.3363527828,0.769564384\C,3.48978  
44363,0.478330181,-0.4218795059\C,4.7261215768,0.0263590101,0.05463227  
45\C,3.6272708981,-1.7862660232,1.2275203301\H,1.4732096838,-1.8648293  
129,1.037662464\H,3.4286281825,1.3569347754,-1.056708316\H,5.632176266  
9,0.561404525,-0.2242522564\H,3.6746668519,-2.668930457,1.862697575\H,  
5.7660061166,-1.4553654029,1.2382901324\C,0.644333508,1.5969639168,-0.  
6080370904\O,1.3393151438,2.5507082281,-0.346565357\C,0.063820084,-0.5  
809935902,-1.0711834711\O,0.1901418348,-1.7731367859,-1.2691797054\C,-  
3.4104515772,0.5561879706,0.2924907906\H,-4.4100607689,0.4298272977,-0  
.1292401152\C,-2.5541479068,-0.5380978494,0.2902407496\H,-1.6782895902  
,-0.5386166753,0.9411495571\C,-3.0035447965,1.8697337794,0.6058285567\  
H,-3.7126011879,2.6793930253,0.4209862103\C,-1.6931816528,2.214248597,  
0.9238361578\H,-1.0498079291,1.4528265205,1.3664803847\C,-1.2784170701  
,3.6452051111,1.1806401731\H,-0.2599662154,3.8325212732,0.8167815383\H  
,-1.2825332112,3.8459297324,2.2630101845\H,-1.9679288758,4.3507284457,  
0.6992415356\C,-3.0326074236,-1.9337277282,-0.125721953\H,-3.367755698  
6,-1.8945561937,-1.1788013699\O,-2.0313598731,-2.904585554,0.034364383  
7\H,-1.286943364,-2.7181511048,-0.5628809355\C,-4.2166818997,-2.394378  
7531,0.7451910131\H,-5.076369744,-1.721430222,0.6440734532\H,-3.909579  
9141,-2.4265405349,1.7981971511\H,-4.5123984849,-3.4041086686,0.435097  
1766\\Version=EM64L-G09RevA.02\State=1-A\HF=-939.0525805\RMSD=3.880e-0  
9\RMSF=4.631e-06\Dipole=-0.911251,1.0089478,0.0027081

Zero-point correction=	0.331631 (Hartree/Particle)
Thermal correction to Energy=	0.350458
Thermal correction to Enthalpy=	0.351402
Thermal correction to Gibbs Free Energy=	0.284406
Sum of electronic and zero-point Energies=	-938.720949
Sum of electronic and thermal Energies=	-938.702122
Sum of electronic and thermal Enthalpies=	-938.701178
Sum of electronic and thermal Free Energies=	-938.768174

## TS6-endo

## B3LYP/6-31+G\*

C,-1.7384778322,0.4099572357,-0.5317469457\H,-2.5602487891,0.4085796067,-1.2371157227\C,-1.86  
58413009,0.5548597233,0.8558704289\H,-2.7999874753,0.627847873,1.3979619079\N,0.1984442308  
,1.434468034,0.2405143338\C,1.490466006,2.0414377317,0.3079065287\C,4.0182277021,3.22603809  
47,0.464275402\C,1.8590111523,3.0219062907,-0.6206946822\C,2.381242167,1.655676459,1.316447  
8089\C,3.63972289,2.2535018524,1.3940193045\C,3.1255370009,3.6044408503,-0.5416204786\H,1.1

678346902,3.314388534,-1.4022188799\H,2.0852726407,0.9041122732,2.0397655002\H,4.325600756  
9,1.9541166232,2.1821135136\H,3.4102099301,4.3603479041,-1.2687180916\H,5.0011661188,3.6857  
664204,0.5243275147\C,-0.6783648294,1.2853592796,1.3563835124\O,-0.4548748249,1.7109761864,  
2.4733294855\C,-0.4427599975,1.0214428234,-0.9344805293\O,0.0090751423,1.1498914495,-2.0671  
268945\C,-0.2420398326,-1.9686332147,-0.2328424239\H,0.7254098818,-2.0926606859,-0.714748211  
3\C,-1.3440479674,-1.7212095795,-1.0530849897\H,-2.3395660273,-1.902650178,-0.6522115379\C,-0.  
2877882068,-1.8312452087,1.1607500157\H,0.6557574164,-1.8571057927,1.7055536148\C,-1.435912  
6914,-1.4510021514,1.8563446009\H,-2.3986521176,-1.7141312183,1.4255999536\C,-1.4412797597,-  
1.2365988782,3.3453300835\H,-1.6598973402,-2.1850283636,3.8578289448\H,-2.2086537762,-0.5175  
005451,3.6496263776\H,-0.4778573208,-0.865533158,3.7070387854\C,-1.2722063206,-1.8448190708,  
-2.5693143816\H,-2.0388908774,-1.1822966002,-3.0043021968\O,0.0036542586,-1.5123608612,-3.09  
26092905\H,0.1403012236,-0.5526265253,-2.9649140319\C,-1.5830777499,-3.2808451589,-3.0074871  
461\H,-2.5641294435,-3.6048681561,-2.6411686811\H,-0.8204890097,-3.9663205999,-2.6224597813\  
H,-1.5808897182,-3.336679299,-4.1011227207\Version=IA32L-G03RevD.01\State=1-A\HF=-939.64952  
87\RMSD=9.624e-09\RMSF=2.794e-06\Thermal=0.\Dipole=-0.9418481,-0.6688942,0.601812

Zero-point correction=	0.326851 (Hartree/Particle)
Thermal correction to Energy=	0.346313
Thermal correction to Enthalpy=	0.347258
Thermal correction to Gibbs Free Energy=	0.278452
Sum of electronic and zero-point Energies=	-939.322678
Sum of electronic and thermal Energies=	-939.303215
Sum of electronic and thermal Enthalpies=	-939.302271
Sum of electronic and thermal Free Energies=	-939.371077

### B3LYP/6-31+G\* ( $\epsilon=2.2706$ )

HF = -939.632297

### BMK/6-31+G\*

C,-1.8612822634,0.4898969135,-0.4878869531\H,-2.6896505892,0.4343447758,-1.1860574029\C,-1.94  
67073995,0.6104637528,0.8984254805\H,-2.8549652085,0.6539709845,1.4898626647\N,0.115585416  
,1.4721954516,0.2384505569\C,1.4279603186,2.0209432471,0.2815841874\C,4.016595894,3.0856369  
563,0.3941846238\C,1.830866936,2.9727517641,-0.6668512754\C,2.3116312889,1.6050876586,1.289  
418827\C,3.6015596408,2.1428468506,1.3444925696\C,3.1287883578,3.4949202642,-0.6088077389\  
H,1.1431924842,3.2908959561,-1.4440687071\H,1.9779713958,0.8829036207,2.0300641407\H,4.2811  
638918,1.8216627922,2.1318541187\H,3.441224309,4.2289220707,-1.349582189\H,5.0222358422,3.4  
999638305,0.437797284\C,-0.7192342727,1.3149720272,1.3733475347\O,-0.4523790384,1.70035910  
81,2.4867302119\C,-0.5652313813,1.0928672725,-0.9219259659\O,-0.1517740362,1.2315322721,-2.0  
581084282\C,-0.219368136,-1.8210062683,-0.2325081182\H,0.7498256926,-1.8697930085,-0.7295500  
731\C,-1.3419994743,-1.6575227573,-1.0376192627\H,-2.3292491408,-1.8704114885,-0.626611348\C,  
-0.2630140901,-1.6856441424,1.1720269493\H,0.6861814863,-1.6339531852,1.7095935009\C,-1.4301  
023466,-1.384458495,1.8703893111\H,-2.3814425113,-1.6898804794,1.4361728122\C,-1.4364018918,  
-1.1477822216,3.3642275153\H,-1.5276667445,-2.1087063824,3.8939918132\H,-2.2819430787,-0.518  
1511368,3.6674957606\H,-0.5164298149,-0.6502557055,3.692746504\C,-1.262930547,-1.7432634139,  
-2.5620412111\H,-1.9973176271,-1.0370920077,-2.9878091774\O,0.0195373405,-1.4592942977,-3.05  
54610492\H,0.1766693494,-0.5048552265,-2.9646048208\C,-1.6298517248,-3.1644125328,-3.0265906  
065\H,-2.6317940542,-3.4483904321,-2.678848317\H,-0.8991966499,-3.8823238589,-2.6326001171\H



,-1.6081396525,-3.2047176891,-4.1224522351\\Version=EM64L-G09RevA.02\\State=1-A\\HF=-939.0591  
598\\RMSD=5.240e-09\\RMSF=9.093e-06\\Dipole=-0.9388833,-0.6297674,0.5297361

Zero-point correction=	0.331875 (Hartree/Particle)
Thermal correction to Energy=	0.350728
Thermal correction to Enthalpy=	0.351673
Thermal correction to Gibbs Free Energy=	0.284815
Sum of electronic and zero-point Energies=	-938.727284
Sum of electronic and thermal Energies=	-938.708431
Sum of electronic and thermal Enthalpies=	-938.707487
Sum of electronic and thermal Free Energies=	-938.774345

## **TS6-exo**

### B3LYP/6-31+G\*

C,-1.0607679669,3.6531502996,-2.6994278818\C,-1.3843140374,2.7413926159,-1.5080014585\H,-1.90  
77054436,3.3436798503,-0.7444757005\C,-0.1138272551,2.1685818503,-0.8910245468\O,-2.2455172  
48,1.7330066268,-2.0093251233\H,3.8648821324,1.4852577527,1.9604862705\H,4.3517086471,0.547  
9706791,0.5349866849\H,3.3558910607,-0.2110007179,1.7812263808\H,-2.4933445777,1.114199604  
1,-1.2930524423\C,0.8642375819,2.9945971398,-0.3426902986\H,0.1678779035,1.1914706507,-1.277  
6101296\H,0.6462311615,4.0597157196,-0.2610829809\C,2.0168013875,2.5277758777,0.2988759218  
\C,2.2993611209,1.1743716671,0.5011795287\H,2.634065329,3.2576370358,0.8229077511\C,3.53045  
65059,0.7266367008,1.2437115449\H,1.9185785861,0.4650457096,-0.2310988178\H,-0.4542499668,4  
.5125958193,-2.3962425965\H,-1.9981501758,4.0163679599,-3.1337769134\H,-0.5190539953,3.09217  
15079,-3.4687470632\O,-2.3903404656,-0.2265707213,0.0112219131\C,-1.3121825613,-0.1457769638  
,0.5880690264\C,-0.6458765463,1.0753613019,1.1023826736\N,-0.4792654393,-1.2389821147,0.8846  
957343\C,0.5325035189,0.6803318528,1.7545116739\H,-1.2530044827,1.9313728999,1.3635478134\  
H,0.9650621898,1.1775640629,2.6123103423\C,0.6044336967,-0.8081741894,1.6929237883\O,1.4124  
543262,-1.5465679572,2.2236335278\C,-0.7239898542,-2.5957239546,0.506577273\C,-1.1864350047,  
-5.2520766394,-0.2309189539\C,-2.0066001282,-3.1410120668,0.6360991385\C,0.3279157057,-3.376  
1577529,0.0126899689\C,0.0936870429,-4.703609469,-0.348318015\C,-2.2325762653,-4.4662218987,  
0.2589175903\H,-2.8188084093,-2.5309964275,1.013297784\H,1.3221274597,-2.9520846696,-0.07567  
06254\H,0.9148282419,-5.3070848016,-0.7259189632\H,-3.2314220889,-4.8837616562,0.3537420262  
\H,-1.3666716857,-6.284453184,-0.5186118462\\Version=AM64L-G03RevD.01\\State=1-A\\HF=-939.644  
64522\\RMSD=4.527e-09\\RMSF=4.920e-06\\Thermal=0.\\Dipole=0.9955296,0.871196,0.4292129

Zero-point correction=	0.326624 (Hartree/Particle)
Thermal correction to Energy=	0.346094
Thermal correction to Enthalpy=	0.347038
Thermal correction to Gibbs Free Energy=	0.278087
Sum of electronic and zero-point Energies=	-939.318021
Sum of electronic and thermal Energies=	-939.298552
Sum of electronic and thermal Enthalpies=	-939.297607
Sum of electronic and thermal Free Energies=	-939.366558



B3LYP/6-31+G\* ( $\epsilon=2.2706$ )

HF= -939.638653

BMK/6-31+G\*

C,4.2077885159,-2.3713849452,1.0343144159\C,3.0279535316,-2.0060567893,0.1135420597\H,3.3690  
466435,-2.0766102758,-0.9363869378\C,2.5514653324,-0.5724369813,0.3761324049\O,2.0277435298  
,-2.954705607,0.3711749068\H,2.0518122969,4.3461133103,0.2077545121\H,1.304586568,4.0408981  
276,1.7941186224\H,0.3288840532,3.8824478983,0.3239995103\H,1.2639196629,-2.8074775777,-0.2  
125820732\C,3.4169541717,0.5086419478,0.2582053221\H,1.6750733577,-0.5005755324,1.02204839  
52\H,4.4175222415,0.322413681,-0.1384931322\C,3.0259255758,1.8549284704,0.4102989139\C,1.71  
7727146,2.2564256813,0.6655194476\H,3.7506566728,2.626081798,0.1409357506\C,1.3297805424,3.  
7158141892,0.7427518285\H,1.0545284187,1.5648417917,1.186663237\H,5.0679194154,-1.71197665  
,0.8688422261\H,4.5056018155,-3.4078715661,0.8338987571\H,3.8941343292,-2.2942626895,2.0830  
659775\O,-0.2170931618,-1.9343459236,-1.0020504764\C,-0.0775907765,-0.7270575921,-0.96926032  
32\C,1.1340035571,0.0605590077,-1.3559764474\N,-1.0571889292,0.1811455663,-0.5532442995\C,0.  
8079058917,1.4136311512,-1.2433674946\H,1.8504033679,-0.3777468145,-2.0409496411\H,1.231849  
9436,2.2303455316,-1.8155325256\C,-0.6206650446,1.5029930267,-0.8011865209\O,-1.3033325739,2  
.4915225281,-0.674144653\C,-2.3464882293,-0.1629581235,-0.0564730233\C,-4.8846084392,-0.81742  
59734,0.9301067794\C,-3.0800767774,-1.1982124157,-0.6552141515\C,-2.8778826044,0.5477645289,  
1.030355969\C,-4.1483872393,0.221064399,1.5158158695\C,-4.34497928,-1.5245317366,-0.1520019  
814\H,-2.6589607075,-1.748041705,-1.4914074614\H,-2.3064866428,1.3568344891,1.4769251218\H,-  
4.5591232915,0.7794227183,2.3551092503\H,-4.9097554443,-2.332579463,-0.6134676698\H,-5.87098  
08494,-1.0731199208,1.3130022565\\Version=EM64L-G09RevA.02\State=1-A\HF=-939.0521029\RMS  
D=4.643e-09\RMSF=1.740e-06\Dipole=0.8875635,0.9957066,-0.1166602

Zero-point correction=	0.332380 (Hartree/Particle)
Thermal correction to Energy=	0.351159
Thermal correction to Enthalpy=	0.352103
Thermal correction to Gibbs Free Energy=	0.285611
Sum of electronic and zero-point Energies=	-938.719723
Sum of electronic and thermal Energies=	-938.700944
Sum of electronic and thermal Enthalpies=	-938.700000
Sum of electronic and thermal Free Energies=	-938.766492

**TS70-A**

B3LYP/6-31+G\*

C,0.5857296961,-3.5854812574,-0.1314759083\C,-0.102821856,-2.3930594746,-0.0068506059\C,0.586  
8950577,-1.1526118058,-0.049376669\C,2.0020545753,-1.1670618377,-0.1899816233\C,2.682125853  
6,-2.3904688919,-0.33294522\C,1.9843101093,-3.5879274809,-0.3041806412\C,-0.0897888155,0.1110  
851182,0.1501187625\C,2.6876803378,0.1172667761,-0.253764313\C,2.09631927,1.1961024208,0.53  
44345202\C,0.6749411468,1.2536688732,0.6139606942\C,0.0807333266,2.4609792205,1.0653431718  
\H,-0.9930543527,2.5844193715,1.0063104151\C,0.8582109537,3.5047880209,1.535131485\C,2.2635  
227875,3.4003875376,1.5393845549\C,2.8700455157,2.2708930966,1.0102316807\H,0.0459138982,-4  
.5270623445,-0.0790404395\H,-1.1684997092,-2.4025550741,0.1855622241\H,3.7607586292,-2.38459

61651,-0.4639833986\H,2.5180316396,-4.5291450154,-0.4033685837\H,3.7752564523,0.0516641441,-  
0.2126019766\H,0.3816582576,4.4163537317,1.8855543514\H,2.8694291435,4.217042179,1.9226063  
418\H,3.9543231805,2.20948969,0.94822514\C,-2.2952230156,-0.266813466,-1.0395922434\C,-2.2839  
428719,0.2994997568,1.3430231145\C,-3.6679347728,-0.5602331479,-0.4204235383\H,-1.848269154  
6,-1.1425674383,-1.51778201\C,-3.7209069158,0.3532893347,0.8116751118\H,-2.0105590964,1.1820  
09114,1.9314607938\H,-4.4604091158,-0.3651076131,-1.1456192159\H,-3.7224380113,-1.611080788  
5,-0.1139853586\H,-3.9674209291,1.3812410579,0.5214216996\H,-4.4401605688,0.0272034648,1.568  
3873678\N,-1.4847207138,0.155005953,0.1369015959\O,-2.049020639,-0.8519564268,2.1684486878\  
O,-2.3903130116,0.7756381206,-1.9799366331\H,-1.795294574,0.5636634964,-2.7334761625\C,1.051  
8987497,1.0106331369,-2.3036387331\C,2.4223919625,0.7658992364,-1.9809418446\H,0.468107972  
1,1.8920939302,-2.085970478\H,3.1394811753,1.5834798893,-1.9379903262\C,0.6037576711,0.00413  
07152,-3.209729288\O,-0.4768615045,-0.2063236735,-3.742080625\C,2.8223813715,-0.374504039,-2.  
8906069836\O,3.9170132203,-0.8406902727,-3.0781697035\O,1.6903151626,-0.8684700916,-3.49510  
91596\C,-2.3945570196,-0.668567542,3.5330395089\H,-2.1110755305,-1.5865815625,4.0530564981\  
H,-3.4735613544,-0.5018273725,3.6691453509\H,-1.8454535833,0.1787653956,3.972198612\\Version  
=AM64L-G03RevE.01\State=1-A\HF=-1319.9654134\RMSD=4.192e-09\RMSF=5.018e-06\ZeroPoint=0.3  
990841\Thermal=0.4224457\Dipole=-0.4075554,0.7379536,2.996532

Zero-point correction=	0.399084 (Hartree/Particle)
Thermal correction to Energy=	0.422446
Thermal correction to Enthalpy=	0.423390
Thermal correction to Gibbs Free Energy=	0.347163
Sum of electronic and zero-point Energies=	-1319.566329
Sum of electronic and thermal Energies=	-1319.542968
Sum of electronic and thermal Enthalpies=	-1319.542024
Sum of electronic and thermal Free Energies=	-1319.618251

B3LYP/6-31+G\* ( $\epsilon=2.2706$ )

HF = -1319.9800898

## **TS70-B**

B3LYP/6-31+G\*

C,0.6720395698,-3.6263742881,0.0845916077\C,-0.0512381451,-2.4462443557,0.1248577625\C,0.607  
2639591,-1.1928954742,0.0740156715\C,2.0267621753,-1.1746026119,0.008823517\C,2.7439968846,-  
2.3820945896,-0.0521326583\C,2.0769400896,-3.5985943514,-0.0115626697\C,-0.1096521192,0.0692  
472376,0.139340417\C,2.6711432614,0.1275824722,-0.104743803\C,2.0172754592,1.226462341,0.59  
65068584\C,0.5917700149,1.246840832,0.6001627128\C,-0.0625567199,2.4451215789,0.9890467836  
\H,-1.1355397209,2.5314866482,0.8757074537\C,0.6623250918,3.5177027701,1.4752992778\C,2.067  
7740006,3.4532557012,1.5558404418\C,2.7361031724,2.3335575243,1.0863882498\H,0.152748089,-4  
.5790188302,0.1453950664\H,-1.1261460304,-2.4753362375,0.2481836682\H,3.8296883199,-2.35237  
73166,-0.1142917347\H,2.6386871294,-4.5285642769,-0.0372861988\H,3.7591965318,0.1216225542,-  
0.03671129\H,0.1448752495,4.4246421453,1.7757665929\H,2.6293311796,4.2984446234,1.94407275  
11\H,3.822268926,2.3082252518,1.0714075234\C,-2.2633813845,-0.4071015848,-1.1207004028\C,-2.3  
575252503,0.1777306414,1.2437414753\C,-3.5393898662,-0.9878258705,-0.5105431099\H,-1.654907

6323,-1.1393943543,-1.6645354673\C,-3.773694945,-0.0700867855,0.699341311\H,-2.267162132,1.14  
3235559,1.7560175703\H,-4.3578752292,-0.9718571462,-1.2334075977\H,-3.3736020476,-2.0210526  
818,-0.1860200876\H,-4.2180943442,0.8769191243,0.3758358293\H,-4.416014483,-0.5102532587,1.4  
675014218\N,-1.5112715742,0.0825298309,0.0568930307\O,-1.939972747,-0.8371048734,2.16525725  
51\O,-2.6594360261,0.6433042327,-1.9740314802\H,-1.8906841991,1.1692208233,-2.2884232052\C,1  
.0278470223,0.4746618848,-2.3090865578\C,2.4043068184,0.4902870484,-1.9338343526\H,0.448216  
05,-0.3777713709,-2.6296965826\H,3.1035227874,-0.2452410313,-2.3252729991\C,0.589086137,1.82  
2526758,-2.5208911616\O,-0.4975920853,2.2935147715,-2.806399002\C,2.824896529,1.9291981511,-  
2.1135410853\O,3.9284268116,2.4070645259,-2.0614496162\O,1.6955626389,2.6892908548,-2.33098  
52534\C,-2.3267157686,-0.5944301374,3.509497365\H,-1.8913415282,-1.3971988951,4.1090781925\  
H,-3.4197430695,-0.6091316576,3.6344032675\H,-1.9405168507,0.3728760934,3.8655732417\\Versio  
n=AM64L-G09RevA.02\State=1-A\HF=-1319.9636368\RMSD=7.004e-09\RMSF=9.817e-06\ZeroPoint=0.  
3987307\Thermal=0.4220844\Dipole=-0.2135374,-1.9895052,2.1450888

Zero-point correction=	0.398731 (Hartree/Particle)
Thermal correction to Energy=	0.422084
Thermal correction to Enthalpy=	0.423029
Thermal correction to Gibbs Free Energy=	0.346784
Sum of electronic and zero-point Energies=	-1319.564906
Sum of electronic and thermal Energies=	-1319.541552
Sum of electronic and thermal Enthalpies=	-1319.540608
Sum of electronic and thermal Free Energies=	-1319.616852

B3LYP/6-31+G\* ( $\epsilon=2.2706$ )  
HF = -1319.9784182

## PRODUCTS

### 1N-A

B3LYP/6-31+G\*

N,-2.48643446,0.3742500372,-1.5357774196\C,-2.176564311,-0.9818183324,-1.5338203283\C,-0.6779  
272113,-1.1306047652,-1.3138162258\C,-0.1349826335,0.3151730355,-1.2048834649\C,-1.375489815  
1,1.1973408404,-1.3493047156\O,-2.992926037,-1.8720364557,-1.6875789524\O,-1.4271137614,2.415  
2974072,-1.335791303\C,-3.8427923597,0.872885136,-1.7153184014\C,-0.3365984811,-1.9332154682  
, -0.0085849808\C,1.1727637822,-1.9158455496,0.0662625533\C,1.7214185645,-0.6200770904,0.1110  
668156\C,0.6660474634,0.5080082847,0.1598672659\C,-0.3658607208,0.1637836695,1.254126101\C,  
-0.8836960914,-1.1422090691,1.1562858583\C,1.9883478736,-3.0443536024,0.0065566211\C,3.37837  
19896,-2.8923359784,-0.0248535171\C,3.9310362442,-1.6107180269,-0.0347470228\C,3.1093634907,  
-0.4776944463,0.0184035932\C,-1.8630096877,-1.5962728547,2.0386021906\C,-2.3497593979,-0.742  
7465197,3.0336789768\C,-1.8725205725,0.5663520193,3.1145450472\C,-0.8935162799,1.0232002223  
,2.2234274522\C,1.2257527038,1.9501049631,0.2746748035\C,2.0721252097,2.2484748203,1.526150  
1011\O,1.9823956915,2.214535543,-0.9144798541\C,1.9930595571,3.5781606832,-1.3149302506\H,5.  
0091187051,-1.4839738039,-0.0944878415\H,3.5589105656,0.5042536622,-0.0487691697\H,4.021883  
7298,-3.7675932934,-0.0627588251\H,1.5411826236,-4.0358055728,-0.0253263917\H,-2.2530075131,

-2.6066880087,1.9395013099\H,-0.5682768868,2.0548891295,2.2953120133\H,-2.2638632626,1.2434  
140003,3.869589655\H,-3.1081524626,-1.0931817105,3.7289517569\H,0.3571357787,2.6203191376,0  
.2746459461\H,2.287001342,3.322084529,1.5745624199\H,3.0246648152,1.7169802196,1.514232022  
4\H,1.5548476684,1.9746538712,2.4486723448\H,2.509349438,4.217215984,-0.5836672947\H,0.9705  
043002,3.9499582722,-1.4669876977\H,2.5394381494,3.6194477619,-2.2611008635\H,-4.4597735412  
,0.6075886653,-0.851378207\H,-4.2820804353,0.4262098264,-2.6109597173\H,-3.7890969823,1.9577  
403296,-1.815579618\H,0.5495624186,0.5683930664,-2.0183279787\H,-0.2582514173,-1.6675555556,  
-2.1706554555\H,-0.7515877835,-2.9429890129,-0.0612293515\\Version=AM64L-G03RevE.01\State=1  
-A\HF=-1131.4790627

Zero-point correction=	0.386083 (Hartree/Particle)
Thermal correction to Energy=	0.408095
Thermal correction to Enthalpy=	0.409039
Thermal correction to Gibbs Free Energy=	0.334916
Sum of electronic and zero-point Energies=	-1131.092980
Sum of electronic and thermal Energies=	-1131.070968
Sum of electronic and thermal Enthalpies=	-1131.070023
Sum of electronic and thermal Free Energies=	-1131.144146

## **1N-B**

### **B3LYP/6-31+G\***

N,-2.7446754267,0.0811241535,-1.3415519401\C,-1.5936346586,-0.6520499705,-1.6218562343\C,-0.3  
729052523,0.2246603665,-1.3263147377\C,-0.9739351949,1.5612655079,-0.8298745548\C,-2.482979  
0233,1.3672852815,-0.8789285325\O,-1.5991384635,-1.7911071511,-2.0551751775\O,-3.3413369126,  
2.1764780047,-0.5797836935\C,-4.0948296671,-0.4417970683,-1.498989124\C,-0.4494216363,1.8670  
370763,0.6082472413\C,1.0576315919,1.9341487617,0.4756566704\C,1.6483290952,0.7376003464,0.  
0246487292\C,0.628348733,-0.3908184985,-0.2514039833\C,-0.2065083466,-0.5364275003,1.034717  
9372\C,-0.7846232386,0.6698058704,1.4750176923\C,1.832832766,3.0554102726,0.7643381078\C,3.2  
227097474,2.9928046086,0.6157355012\C,3.8182742049,1.8057653521,0.1864211596\C,3.038595068  
9,0.6792602794,-0.1065108925\C,-1.6002525418,0.7009697866,2.604873936\C,-1.8381477622,-0.4787  
71694,3.3186680485\C,-1.2651735005,-1.6777817828,2.8895675749\C,-0.4538576247,-1.7102340706,  
1.7484887959\C,1.2240557538,-1.7287037936,-0.7614631662\C,1.7991555453,-1.6801697359,-2.1866  
329242\O,2.2081767613,-2.1440435753,0.1962380808\C,2.4671294478,-3.5360714,0.2178184324\H,4.  
8991646359,1.7456053893,0.0862748022\H,3.5237611382,-0.2425479438,-0.4012540605\H,3.834424  
7603,3.861701569,0.8448308776\H,1.3563780463,3.9696531989,1.1124858246\H,-2.0477374486,1.63  
90666983,2.9255321147\H,-0.0138406451,-2.6504047881,1.4371410772\H,-1.4452802929,-2.5953645  
124,3.4440689118\H,-2.4670761316,-0.4598747624,4.2050285274\H,0.411516118,-2.467029657,-0.76  
47274412\H,2.387951838,-2.5829311145,-2.3796104936\H,2.4472446876,-0.814219396,-2.350176237  
6\H,0.9913569903,-1.664551732,-2.9239839464\H,2.9340897184,-3.8910375988,-0.712311816\H,1.54  
45439492,-4.1143396718,0.3868756954\H,3.1570065099,-3.712311425,1.0472303133\H,-4.566334248  
6,-0.5663227923,-0.5194612853\H,-4.0230138767,-1.4064629275,-2.0029556364\H,-4.6913675351,0.2  
569423661,-2.0909360873\H,-0.7160946281,2.4001718581,-1.4847387395\H,0.1722112391,0.3620119  
863,-2.2639817699\H,-0.8857242902,2.7946058284,0.9877164227\\Version=AM64L-G03RevD.01\Stat  
e=1-A\HF=-1131.4795527

Zero-point correction=	0.386188 (Hartree/Particle)
------------------------	-----------------------------

Thermal correction to Energy=	0.407936
Thermal correction to Enthalpy=	0.408880
Thermal correction to Gibbs Free Energy=	0.336269
Sum of electronic and zero-point Energies=	-1131.093365
Sum of electronic and thermal Energies=	-1131.071616
Sum of electronic and thermal Enthalpies=	-1131.070672
Sum of electronic and thermal Free Energies=	-1131.143283

## **10-A**

B3LYP/6-31+G\*

H,0.1072654867,3.1465312949,3.5575791594\C,0.5453605169,2.3869659076,2.9151273533\H,-1.1929  
910018,2.2700189526,1.6564293836\C,-0.2024761521,1.8773481561,1.8458057486\C,2.4122842179,0  
.978037167,2.3066835412\C,0.3425495709,0.8932569632,1.017859303\C,1.8445807958,1.936030451  
9,3.1538484286\C,1.6639314154,0.466184363,1.2488471752\C,-0.3256461992,0.2253109509,-0.20181  
98012\H,2.4186253033,2.334860526,3.9861718815\H,3.4320626309,0.6347277011,2.4677731813\C,-  
0.1317263852,-1.2964910144,-0.0659799767\C,-1.7931577675,0.6292094703,-0.4763155962\C,-1.107  
2663264,-2.2875212009,-0.2078181969\C,1.2044621158,-1.6806786309,0.1581766687\H,2.593918065  
6,-3.3043156781,0.4259769061\C,2.1741024878,-0.5205148346,0.2214640263\C,-0.7559798882,-3.638  
3732966,-0.0939881405\H,-2.1418579092,-2.0315231794,-0.4104864042\H,-1.5236684281,-4.4003135  
553,-0.2003136888\C,0.5679344143,-4.0090475908,0.1466407525\H,0.8347072732,-5.0591050422,0.2  
311227185\C,1.5554138356,-3.0253281829,0.2636110069\H,-2.104305658,0.0735855798,-1.36942115  
57\O,-1.7961226841,2.020416242,-0.8126973812\C,-2.7838131109,0.3242982843,0.676218586\H,-3.7  
135738198,-0.111101747,0.2938587943\H,-3.0447165307,1.2462188774,1.2035446174\H,-2.36803782  
77,-0.3699639585,1.4114789624\C,-2.9308074226,2.4276893149,-1.5647536077\H,-3.861875836,2.32  
03335693,-0.9891071287\H,-3.0113814269,1.8500110827,-2.496562867\H,-2.7843773811,3.48394140  
44,-1.8045388187\C,0.6115656318,0.6463600474,-1.4196535279\C,2.0750839721,0.2431094052,-1.14  
63422587\C,2.4656648391,-0.6294894224,-2.3258865532\C,0.2812659302,-0.0482354052,-2.7352077  
031\O,-0.736526061,-0.031148124,-3.3714039524\O,1.3885101977,-0.7565294788,-3.1925295673\O,3.  
5170498658,-1.1610919557,-2.5506840577\H,0.4827100697,1.7209792111,-1.5710401506\H,2.753007  
8388,1.1020385475,-1.1196573802\H,3.2022513412,-0.8406911729,0.4079897198\\Version=AM64L-  
G03RevD.01\State=1-A\HF=-1112.0193476

Zero-point correction=	0.345293 (Hartree/Particle)
Thermal correction to Energy=	0.365183
Thermal correction to Enthalpy=	0.366127
Thermal correction to Gibbs Free Energy=	0.297923
Sum of electronic and zero-point Energies=	-1111.674055
Sum of electronic and thermal Energies=	-1111.654165
Sum of electronic and thermal Enthalpies=	-1111.653220
Sum of electronic and thermal Free Energies=	-1111.721425

## **10-B**

B3LYP/6-31+G\*



H,1.2348741958,4.5599077208,0.2478498187\C,1.3972884296,3.4988559378,0.4196341866\H,-0.5915  
393482,2.9651689223,-0.2033235926\C,0.3526160368,2.5973794099,0.1776982206\C,2.8499399916,1  
.6773768042,1.0603480578\C,0.5482788056,1.2294472764,0.3856628613\C,2.6409754747,3.0466726  
492,0.8632578846\C,1.8117056361,0.7806966165,0.8170157001\C,-0.4748533093,0.0904882597,0.17  
5221887\H,3.4478565068,3.7518964834,1.0448862326\H,3.8190267514,1.3100606831,1.3916546432  
\C,0.1983120423,-0.924408037,-0.7680682794\C,-1.8894986046,0.5275617928,-0.2870429848\C,-0.32  
65761695,-1.4490850449,-1.9501910455\C,1.4633225889,-1.357248026,-0.3266994806\H,3.16110587  
98,-2.6320650982,-0.69120313\C,1.912643382,-0.7225238582,0.9743590812\C,0.4066941008,-2.39020  
52053,-2.6829357061\H,-1.2936812165,-1.127267159,-2.318474578\H,-0.0069067902,-2.7891351591,-  
3.6055363291\C,1.6603158357,-2.8155716042,-2.2390889653\H,2.2234911468,-3.5475291506,-2.8118  
882452\C,2.19027284,-2.299863285,-1.0516976459\H,-2.4468763004,-0.3849590437,-0.5382799069\  
O,-1.718131151,1.2946374136,-1.4850928788\C,-2.7121715497,1.2876328053,0.7668544123\H,-3.587  
0326729,1.7438179387,0.292664818\H,-2.1411486044,2.0829027511,1.2548319251\H,-3.0909306647,  
0.6018353031,1.5305728564\C,-2.8493180912,1.331400257,-2.3378337869\H,-3.6947669463,1.87231  
31706,-1.8892534332\H,-3.1853444541,0.3165442092,-2.6037774171\H,-2.5379052657,1.8551913761,  
-3.2451300978\C,0.8499006513,-1.0886743256,2.0606569917\C,-0.5482029925,-0.6432107792,1.5873  
602437\C,-1.3572192121,-1.9377239663,1.5735936871\C,0.7286131827,-2.5858507975,2.2822098721  
\O,1.5611791023,-3.3592718136,2.6632879836\O,-0.5632810335,-3.0016025678,1.9786778661\O,-2.5  
133244914,-2.1042661613,1.2964971294\H,1.1393394295,-0.6285634377,3.0109774758\H,-1.0184719  
599,0.0330417299,2.3059177738\H,2.9074288176,-1.0538049906,1.2828258945\\Version=AM64L-G03  
RevE.01\State=1-A\HF=-1112.0190237

Zero-point correction=	0.345364 (Hartree/Particle)
Thermal correction to Energy=	0.365105
Thermal correction to Enthalpy=	0.366049
Thermal correction to Gibbs Free Energy=	0.298472
Sum of electronic and zero-point Energies=	-1111.673660
Sum of electronic and thermal Energies=	-1111.653918
Sum of electronic and thermal Enthalpies=	-1111.652974
Sum of electronic and thermal Free Energies=	-1111.720551

## 2N-A

### B3LYP/6-31+G\*

C,0.9065443233,1.3143176697,2.0627076041\C,0.319058641,0.4236971913,1.1570129739\C,0.616708  
1144,-0.9471278266,1.2691990432\C,1.4660029023,-1.4225371416,2.2670090607\C,2.0300792344,-0.  
5262399519,3.1801931152\C,1.751660475,0.8373811178,3.0725843666\C,-0.6181858577,0.77457254  
11,-0.0166147508\C,-1.8487892025,-0.1520133979,0.0707324361\C,-1.5198684886,-1.5160563264,0.2  
114627697\C,-0.0304541484,-1.7970210571,0.2019417844\C,-3.1913950087,0.2040176373,-0.076797  
4556\C,-4.1900437622,-0.7767028144,-0.0096341942\C,-3.8574938883,-2.1188843107,0.178385426\C,  
-2.5120674293,-2.4922032918,0.2724441387\C,-0.8618348143,2.3095291466,-0.1219305713\O,-1.394  
2388093,2.6838167316,-1.3972448191\C,-1.7632164219,2.9224248595,0.9591544952\C,0.4738683667  
,-1.2588283339,-1.1791303024\C,0.0930767329,0.2308950604,-1.3373139743\C,1.397857908,0.92636  
16718,-1.6933957119\N,2.4296599603,-0.0005713952,-1.6357792786\C,1.9902242682,-1.2925893722,  
-1.3332617835\O,2.7248706101,-2.2568702359,-1.2429533094\O,1.534257611,2.1008025624,-2.00818  
65652\C,3.8284318781,0.3178878386,-1.8907948098\H,3.8787126571,1.3527527451,-2.2318392453\



H,4.2251739854,-0.3555581091,-2.6548586975\H,4.4144499099,0.1955063463,-0.9751648464\H,-4.6372728166,-2.8741849479,0.2328602826\H,-2.2377922407,-3.5393985294,0.3830523739\H,-5.2316834998,-0.4840247747,-0.1144868196\H,-3.4741164038,1.2304544665,-0.2700984717\H,0.7190711262,2.3810340083,2.0064682211\H,1.6910370038,-2.4849284943,2.3257202829\H,2.6873382403,-0.890483897,3.9654638366\H,2.1920332751,1.5401473543,3.7752894054\H,0.1289660373,2.7659443527,-0.0321713985\H,-1.6407160218,2.4324328501,1.9292940277\H,-2.815813096,2.8592217894,0.6784217796\H,-1.5232343055,3.9853175983,1.0717547524\H,-0.6352512018,2.8068210998,-1.9944196681\H,0.0425608374,-1.8753270351,-1.975639089\H,-0.6078296999,0.3941704263,-2.1598608478\H,0.203653019,-2.8589558222,0.3114244339\Version=AM64L-G03RevE.01\State=1-A\HF=-1092.1764668

Zero-point correction=	0.358195 (Hartree/Particle)
Thermal correction to Energy=	0.378534
Thermal correction to Enthalpy=	0.379478
Thermal correction to Gibbs Free Energy=	0.308850
Sum of electronic and zero-point Energies=	-1091.818271
Sum of electronic and thermal Energies=	-1091.797933
Sum of electronic and thermal Enthalpies=	-1091.796989
Sum of electronic and thermal Free Energies=	-1091.867616

## **2N-B**

### **B3LYP/6-31+G\***

C,3.229879594,0.2021106334,-0.456442451\C,1.9158855753,-0.0996848994,-0.0794088411\C,1.6566446396,-1.3678933918,0.4718452361\C,2.6819475658,-2.2807001764,0.711271536\C,3.9983709351,-1.9457898381,0.3789665803\C,4.2634149026,-0.713703657,-0.2197851118\C,0.6511681142,0.7757872564,-0.2993425316\C,-0.2057357554,0.7379573714,0.9779812291\C,-0.4345585274,-0.5579038647,1.478017844\C,0.1853382813,-1.6574742409,0.6481651403\C,-0.8183595113,1.8247095887,1.612667991\C,-1.5935331518,1.6174409312,2.7600309485\C,-1.7864414649,0.3311040108,3.2687716698\C,-1.2158838456,-0.7648394492,2.6146586587\C,1.0297875893,2.2006354711,-0.8248200196\O,-0.0825190782,3.0407114205,-1.1019423512\C,1.9011205636,3.0303391594,0.1328237778\C,-0.3954802728,-1.5383459947,-0.8017071422\C,-0.1591640228,-0.1089196676,-1.3661282019\C,-1.5638739592,0.3579079709,-1.760383054\N,-2.4830100348,-0.6194990219,-1.4213446072\C,-1.8995450533,-1.7531512508,-0.855498168\O,-2.5222321394,-2.7332534719,-0.496772758\O,-1.8653627038,1.3925234602,-2.3417160248\C,-3.9178829238,-0.5035208632,-1.6524727193\H,-4.2501127419,-1.2939771783,-2.3312885576\H,-4.1080721971,0.4758199485,-2.0923112935\H,-4.4517967283,-0.6058033201,-0.7041705265\H,-2.390832918,0.1788143397,4.159355818\H,-1.3848710384,-1.7754434789,2.9797275471\H,-2.0560717803,2.4704374894,3.2502757862\H,-0.7227037258,2.8218408076,1.2027072155\H,3.4769438009,1.1401144891,-0.9396434726\H,2.4521768174,-3.2526467226,1.1428457336\H,4.8054224422,-2.6484795074,0.5691611927\H,5.2792041111,-0.4553185187,-0.5077761837\H,1.5943024852,2.0348977615,-1.7578286948\H,2.7354011485,2.4740770963,0.5614122228\H,1.2987817811,3.4159175634,0.9577042592\H,2.2962894194,3.8918255117,-0.4159576114\H,-0.6802622439,2.6152441615,-1.7490241483\H,0.4336037323,-0.1313177832,-2.2880740981\H,0.0740464374,-2.3046218599,-1.4279098024\H,-0.0094241182,-2.6529282861,1.0553579837\Version=AM64L-G03RevE.01\State=1-A\HF=-1092.1753458

Zero-point correction=	0.358773 (Hartree/Particle)
Thermal correction to Energy=	0.378630
Thermal correction to Enthalpy=	0.379575

Thermal correction to Gibbs Free Energy=	0.311598
Sum of electronic and zero-point Energies=	-1091.816573
Sum of electronic and thermal Energies=	-1091.796715
Sum of electronic and thermal Enthalpies=	-1091.795771
Sum of electronic and thermal Free Energies=	-1091.863747

## **20-A**

### **B3LYP/6-31+G\***

C,-1.0940312634,0.5058231381,-1.3025887371\C,0.1869719265,0.5961267541,-2.1539511965\C,0.2889647128,2.0644925931,-2.5337655533\C,-1.6732187533,1.9070915341,-1.356665782\O,-2.7227975946,2.2982445103,-0.9143364138\O,-0.823662765,2.7540715964,-2.04440921\O,1.1387710604,2.6259519518,-3.1631206889\H,3.3716928146,3.1626832719,1.6816277293\C,2.529588377,2.5328702189,1.4076596301\H,3.4685350773,1.7745364648,-0.3878553671\C,2.5887092761,1.7498036098,0.2508107295\C,0.2895623704,1.7060713076,1.8521500244\C,1.504979071,0.942385524,-0.0896815224\C,1.3807584762,2.5117426876,2.2001090207\C,0.3466840234,0.9018680189,0.7086381065\C,1.4188319844,0.0828802254,-1.3290119628\H,1.3252078806,3.1268406128,3.0943622945\C,-2.0370585491,0.0079209797,1.0586477697\H,-0.5896747342,1.7216620919,2.48692316\C,1.0437456338,-1.3238748229,-0.9096327215\C,1.7261139785,-2.4762378706,-1.2936274433\C,-0.1320652074,-1.3972729653,-0.135907607\H,-1.5912803183,-2.7500298355,0.7068968278\C,-0.7623832848,-0.0223003283,0.1660330078\C,1.2296942517,-3.7301831684,-0.9204462654\H,2.6348232105,-2.3980269869,-1.8868694723\H,1.7601811269,-4.6336718044,-1.2094612518\C,0.0394763939,-3.8142154364,-0.1968356549\H,-0.3672967754,-4.7862899862,0.0697638445\C,-0.6481064089,-2.6547578156,0.1851827821\H,-2.2526963332,1.0668415775,1.230674618\C,-1.907280427,-0.6799135533,2.4261751903\O,-3.1682396059,-0.5644374413,0.388260853\H,-0.8986763864,-0.5982511879,2.8409859152\H,-2.1597789562,-1.739320222,2.3558759089\H,-2.6120345334,-0.2264146635,3.1314289431\H,-3.6285139073,0.1508977524,-0.0810984278\H,0.1131868934,0.015531658,-3.07983892\H,-1.8349148112,-0.1772845183,-1.7257557688\H,2.3292320758,0.1201445275,-1.9323463881\\Version=AM64L-G03RevD.01\State=1-A\HF=-1072.7150722

Zero-point correction=	0.317211 (Hartree/Particle)
Thermal correction to Energy=	0.335575
Thermal correction to Enthalpy=	0.336519
Thermal correction to Gibbs Free Energy=	0.271685
Sum of electronic and zero-point Energies=	-1072.397861
Sum of electronic and thermal Energies=	-1072.379497
Sum of electronic and thermal Enthalpies=	-1072.378553
Sum of electronic and thermal Free Energies=	-1072.443387

## **20-B**

### **B3LYP/6-31+G\***

C,0.576297994,0.7005104463,1.5473402323\C,1.9176329482,0.8326728307,0.783605418\C,2.2140278631,2.3196075844,0.7599050975\C,0.2761550849,2.1388654051,1.9658425122\O,-0.6024609838,2.5495527462,2.6819961911\O,1.223837898,3.0027707409,1.4673875566\O,3.130384084,2.9012248183,0.

2558152915\H,2.4426881478,-4.4586233134,-0.6209028285\C,1.8361167739,-3.5987503187,-0.34940  
64937\H,3.1351340699,-2.1637743467,-1.3161346527\C,2.2193280634,-2.3145211115,-0.748587412\  
C,-0.1110239057,-2.6622871936,0.7615725857\C,1.4272686612,-1.2210295245,-0.404406194\C,0.6831  
641079,-3.7644126641,0.4187987851\C,0.2325421052,-1.3786244304,0.3215617024\C,1.7934569866,  
0.2220825412,-0.6557034111\H,0.3920502489,-4.7552354151,0.7576279989\C,-1.8674888163,-0.3105  
011317,1.3668367104\H,-0.9884274239,-2.8335310584,1.3740571518\C,0.6345937272,0.9105926282,  
-1.3383601044\C,0.7345033686,1.6543126016,-2.5137472734\C,-0.5903986367,0.787697625,-0.65552  
49782\H,-2.6431161262,1.4559335745,-0.6004442871\C,-0.509945144,-0.049638952,0.6334103347\C,  
-0.3991946358,2.2951560445,-3.0214552374\H,1.6924201933,1.7414731778,-3.0213587541\H,-0.3314  
831931,2.8737089951,-3.9389712229\C,-1.6104442647,2.2085455313,-2.3319833336\H,-2.487605589  
8,2.7284170488,-2.7084685288\C,-1.7093272724,1.4696761484,-1.1472679922\H,-1.6124312157,-0.87  
34738137,2.2799974604\C,-2.8879035301,-1.1261538968,0.5558871925\O,-2.5741338275,0.86788791  
74,1.7331315278\H,-2.4581316542,-1.9985613899,0.0630783939\H,-3.3485801244,-0.5020330056,-0.2  
121876859\H,-3.6835732105,-1.4578583251,1.231153877\H,-2.0357216374,1.4244776275,2.32617062  
67\H,0.6845488673,0.1229639034,2.4724231136\H,2.7423108014,0.3367793521,1.3064934582\H,2.7  
339291973,0.3381006025,-1.2001828286\Version=AM64L-G03RevD.01\State=1-A\HF=-1072.7129209

Zero-point correction=	0.317659 (Hartree/Particle)
Thermal correction to Energy=	0.335662
Thermal correction to Enthalpy=	0.336606
Thermal correction to Gibbs Free Energy=	0.272756
Sum of electronic and zero-point Energies=	-1072.395262
Sum of electronic and thermal Energies=	-1072.377259
Sum of electronic and thermal Enthalpies=	-1072.376315
Sum of electronic and thermal Free Energies=	-1072.440165

### **3N-A**

#### **B3LYP/6-31+G\***

C,-0.6205701767,-0.9050700121,-1.9519773852\C,-0.0821074682,0.4066545704,-1.3281755275\C,1.33  
57103139,0.5374859694,-1.8915022837\C,0.5129633264,-1.4350010129,-2.8183939663\O,0.51282666  
84,-2.4474643401,-3.4947325297\N,1.5844027325,-0.5544434367,-2.7244784695\O,2.1332503875,1.4  
367191084,-1.6947130257\C,2.8412483614,-0.7642822288,-3.429641937\H,3.3315232981,-1.6696123  
375,-3.0598259001\H,3.4741981602,0.1054926874,-3.2491332327\H,2.64952657,-0.8808576717,-4.49  
97058084\H,2.481620871,-4.287722331,1.262508981\C,1.9731738953,-3.3433829407,1.0860081564\  
H,0.4531527924,-4.2088059843,-0.1882085216\C,0.830526151,-3.3027565338,0.2804664838\C,1.8123  
845509,-0.9440592677,1.4271352412\C,0.178887633,-2.0888072006,0.0676575385\C,2.4624051551,-2  
.1643570071,1.6509556483\C,0.6527109744,-0.896117973,0.6470637079\C,-1.0310908377,-1.9019664  
165,-0.8202204639\H,3.3565046034,-2.1869918708,2.2688969358\C,0.4077037441,1.6612794439,0.92  
83517874\H,2.2264236579,-0.0445787761,1.8692213803\C,-2.0900261168,-1.1749873545,-0.0237357  
543\C,-3.4050954779,-1.6096335034,0.1273730796\C,-1.6472828879,0.0356329194,0.5466074843\H,-  
2.2785296397,1.7468241829,1.7088862592\C,-0.1609779122,0.3642836997,0.2666386606\C,-4.31231  
46656,-0.8360026116,0.8591113787\H,-3.7202757771,-2.5484381327,-0.3235095847\H,-5.338138930  
1,-1.1720647542,0.9863136871\C,-3.8908333282,0.3695445643,1.4200792391\H,-4.5887748705,0.980  
2693954,1.987249761\C,-2.568673123,0.8055944536,1.2621302939\H,1.4789297487,1.6390432094,0.  
700618285\C,0.262322047,1.6637644102,2.4753200675\C,-0.0918295675,2.9929222522,0.316372229  
\H,0.1449273441,0.6575788121,2.886773733\H,-0.6000300049,2.2508458455,2.8081145791\H,1.1460

563342,2.1106178487,2.9442021081\C,0.6193709539,4.2229634953,0.8999404368\H,-1.175931978,3.1026755684,0.4491936356\H,0.0961523668,2.9907345772,-0.7616896787\H,0.4160204411,4.3554671485,1.9685954004\H,0.2914299902,5.1348844195,0.3870430427\H,1.706048781,4.1420741096,0.7701499363\H,-1.4886341129,-0.7296014567,-2.5961545787\H,-0.658340369,1.2681078948,-1.6750627176\H,-1.38894461,-2.8424554318,-1.2471177924\\Version=AM64L-G03RevE.01\State=1-A\HF=-1095.5806044

Zero-point correction=	0.410798 (Hartree/Particle)
Thermal correction to Energy=	0.432639
Thermal correction to Enthalpy=	0.433583
Thermal correction to Gibbs Free Energy=	0.361088
Sum of electronic and zero-point Energies=	-1095.169806
Sum of electronic and thermal Energies=	-1095.147965
Sum of electronic and thermal Enthalpies=	-1095.147021
Sum of electronic and thermal Free Energies=	-1095.219517

### **3N-B**

#### **B3LYP/6-31+G\***

C,-0.9414540817,0.3465175602,-1.1924625387\C,-1.4448647629,-1.0917735072,-1.4700503204\C,-2.9018729245,-1.1026686572,-1.0300695286\C,-2.1589164083,1.0629292909,-0.6007397776\O,-2.2396378238,2.2266537371,-0.250394416\N,-3.2226646252,0.161132041,-0.5483392418\O,-3.6807186271,-2.0370947767,-1.082536329\C,-4.5428364719,0.499686447,-0.0352390785\H,-4.5775283894,1.5799895768,0.1113986904\H,-4.7205419552,-0.011269038,0.9160826511\H,-5.3048388204,0.1842504302,-0.7522811784\H,-1.5153983715,-2.6144600555,3.9273904998\C,-1.13277558,-2.0015164536,3.1153999358\H,-1.485834646,-3.5008377092,1.5955540045\C,-1.1089468377,-2.5033285153,1.8099325054\C,-0.1818529659,0.0882068571,2.3241064666\C,-0.6085038711,-1.7138640924,0.7759088217\C,-0.674614628,-0.7071204348,3.3665163089\C,-0.1266436331,-0.4131650036,1.0205324843\C,-0.5709045535,-2.1196261543,-0.6804670452\H,-0.7013599311,-0.3063073788,4.3766822265\C,0.8506149132,1.7859000875,0.0519699165\H,0.1499989282,1.0952205918,2.548040734\C,0.836706244,-1.9083470143,-1.1878417847\C,1.5958748871,-2.878948561,-1.8377821488\C,1.3323044725,-0.6054341558,-0.9782141072\H,3.0326380206,0.6868740075,-1.3311417202\C,0.3459029599,0.3379880872,-0.2452719424\C,2.8793688729,-2.5644837395,-2.2963481068\H,1.1875756766,-3.8768535012,-1.9841391978\H,3.4799907175,-3.3184887616,-2.7984995064\C,3.3790237231,-1.2761088452,-2.1065962004\H,4.3733162133,-1.0192322723,-2.4632132987\C,2.6107700942,-0.3012604427,-1.4562243696\H,0.0577098936,2.2404283291,0.655940193\C,0.9708168432,2.681221802,-1.2001353133\C,2.1532846015,1.848918073,0.9025073278\H,-0.0127795636,2.9547155728,-1.5924831758\H,1.5459594499,2.2118156375,-2.0057721836\H,1.4776149476,3.6173186293,-0.9380971299\C,2.1835686408,3.0578148017,1.8492163635\H,3.0279417378,1.9133006662,0.245096439\H,2.28467573,0.9293534966,1.4839026108\H,2.0706755075,4.0016777988,1.3018124018\H,3.1330079531,3.1044447916,2.3959517384\H,1.3752464104,3.0132794,2.5902317156\H,-0.6755198819,0.8576965675,-2.1215789122\H,-1.4078739174,-1.3456006714,-2.5346742384\H,-0.9347041672,-3.1375445388,-0.8425812448\\Version=AM64L-G03RevE.01\State=1-A\HF=-1095.5815598

Zero-point correction=	0.410710 (Hartree/Particle)
Thermal correction to Energy=	0.432566
Thermal correction to Enthalpy=	0.433511

Thermal correction to Gibbs Free Energy=	0.360880
Sum of electronic and zero-point Energies=	-1095.170849
Sum of electronic and thermal Energies=	-1095.148993
Sum of electronic and thermal Enthalpies=	-1095.148049
Sum of electronic and thermal Free Energies=	-1095.220680

## **4N-A**

### B3LYP/6-31+G\*

H,5.5059018442,-0.2420113941,-0.6382255196\C,4.4426152688,-0.0657362588,-0.4977068283\H,4.146124286,-1.8209781581,0.7327468815\C,3.6789902417,-0.9561178605,0.2661563716\C,2.4617783134,1.2813536774,-0.8925627635\C,2.3151029538,-0.7282012976,0.4337120339\C,3.8339541549,1.0534057076,-1.0664095739\C,1.6843868667,0.3831313722,-0.1581137552\C,1.3903678997,-1.5636192287,1.2889191282\H,4.4231999334,1.7570674398,-1.648994375\C,-0.5028204905,1.7453545655,-0.4730581664\H,2.0218508739,2.1671020269,-1.334673095\C,0.1951406204,-1.9566300919,0.4493349424\C,-0.2860557224,-3.2568806071,0.307938503\C,-0.4629324169,-0.8698297235,-0.1604582087\H,-2.1628440691,-0.2773558709,-1.3439800707\C,0.1742314081,0.4978219114,0.1451265975\C,-1.4397894829,-3.4885821122,-0.4491346062\H,0.2291601701,-4.081678887,0.7951444855\H,-1.8173245887,-4.5011384138,-0.567556619\C,-2.1094469853,-2.4140274205,-1.0371095887\H,-3.0151861665,-2.5883889924,-1.612899121\C,-1.631456328,-1.1048827093,-0.8887886182\H,-1.5331404539,1.810117743,-0.1126815451\C,-0.5430669819,1.9070156259,-2.013077156\H,0.0083393411,2.6186627145,-0.0486071664\O,-1.8583989035,1.5337796647,-2.4601127773\H,0.1820221422,1.2337860227,-2.4939389976\C,-0.2646973502,3.358668786,-2.4281276138\H,-0.97937154,4.0275667448,-1.9345313115\H,-0.3623846685,3.4926243575,-3.5106376278\H,0.7469745435,3.6739304438,-2.1479785856\C,-1.9384647589,1.1609692835,-3.8249679284\H,-2.9758044048,0.8693611234,-4.0100564794\H,-1.2789247478,0.3064445736,-4.0430805076\H,-1.6820492702,1.9895778341,-4.5006203966\C,0.1350278703,0.6101281848,1.7386484461\C,0.8725834486,-0.5828183209,2.395812483\C,-0.152804344,-1.2321110937,3.3154430154\C,-1.2707798545,0.5665808088,2.3447438368\O,-2.1875816955,1.3429781579,2.1488280739\N,-1.3415400244,-0.5183930062,3.2199136278\O,0.010343046,-2.2047179645,4.0294696328\C,-2.5390388456,-0.8752218155,3.9679193771\H,-2.9307319158,-1.8336125204,3.6140883115\H,-3.2779437859,-0.0886624175,3.8093818897\H,-2.2963484435,-0.9641937551,5.0300185765\H,1.7234096568,-0.2603709553,3.0050147165\H,0.5836278828,1.5704997598,2.0151705148\H,1.887795473,-2.424767654,1.7425575571\\Version=AM64L-G03RevD.01\State=1-A\HF=-1170.7934038

Zero-point correction=	0.414847 (Hartree/Particle)
Thermal correction to Energy=	0.437898
Thermal correction to Enthalpy=	0.438842
Thermal correction to Gibbs Free Energy=	0.362813
Sum of electronic and zero-point Energies=	-1170.378556
Sum of electronic and thermal Energies=	-1170.355506
Sum of electronic and thermal Enthalpies=	-1170.354562
Sum of electronic and thermal Free Energies=	-1170.430590

## **4N-B**

### B3LYP/6-31+G\*



H,4.9086764048,-0.6075900303,-0.351809998\C,3.838456437,-0.4330499032,-0.2771879242\H,3.4643  
223259,-2.2115287469,0.8974401136\C,3.0282599301,-1.3388672784,0.4164728494\C,1.8899775402,  
0.9306188748,-0.7640051872\C,1.6554050216,-1.1139165633,0.5006431529\C,3.268685281,0.700547  
1308,-0.8590069258\C,1.067808719,0.0164389177,-0.1017041195\C,0.6782383202,-1.986514223,1.25  
73121546\H,3.8951796822,1.4157523091,-1.386028931\C,-1.1234604044,1.3855784336,-0.482416444  
\H,1.4770206526,1.8299937685,-1.2045091542\C,-0.455822653,-2.3434809178,0.324050036\C,-0.9227  
224849,-3.6341270795,0.0877032383\C,-1.0763137221,-1.2253339255,-0.2659980358\H,-2.697281926  
8,-0.5760511987,-1.5306473794\C,-0.450325329,0.1307290135,0.1253577087\C,-2.0307690872,-3.826  
5941683,-0.7460838511\H,-0.4295769262,-4.4846713633,0.5540399697\H,-2.3977089971,-4.8313836  
19,-0.93983639\C,-2.6650832415,-2.7226904936,-1.3169330852\H,-3.5332528379,-2.8657021759,-1.95  
58033023\C,-2.196359425,-1.4229981673,-1.0762259506\H,-2.1803165132,1.389258276,0.188502249  
4\C,-1.0850675222,1.6069593842,-2.0162212683\H,-0.6833062686,2.2565305754,0.0091086206\O,-2.  
3862428092,1.2817119552,-2.5405368005\H,-0.352165723,0.9343214465,-2.4867454762\C,-0.753582  
7695,3.0652689699,-2.3615782028\H,-1.48864165,3.731656695,-1.8955058036\H,-0.7706657193,3.23  
77914496,-3.4430300266\H,0.2395860066,3.3507967854,-1.9978564534\C,-2.4131815032,0.98586579  
33,-3.9264740934\H,-3.4451062455,0.7191048538,-4.1703726478\H,-1.754890601,0.1355767748,-4.16  
42441655\H,-2.1190097223,1.8465746218,-4.5436708427\C,-0.6118958044,0.1645824477,1.71626522  
04\C,0.0169376727,-1.0945742771,2.3627548756\C,1.0310254484,-0.5696061313,3.3687446696\C,0.0  
943873926,1.3349699962,2.4094692289\O,-0.0993458831,2.5260017116,2.2433246414\N,1.01178814  
58,0.8197203876,3.3255267115\O,1.7482198873,-1.2249115599,4.1025809387\C,1.8688475933,1.648  
6185665,4.1617790908\H,2.9064270561,1.5854884238,3.819214348\H,1.8170206493,1.2979208375,5.  
1953461158\H,1.5159873922,2.6780553023,4.0868200963\H,-1.6818571264,0.2472482104,1.9360263  
416\H,-0.7207451202,-1.6974480978,2.9021898231\H,1.1564404573,-2.8606419925,1.7067647629\\V  
ersion=AM64L-G03RevD.01\State=1-A\HF=-1170.7937453

Zero-point correction=	0.414776 (Hartree/Particle)
Thermal correction to Energy=	0.437876
Thermal correction to Enthalpy=	0.438820
Thermal correction to Gibbs Free Energy=	0.362562
Sum of electronic and zero-point Energies=	-1170.378969
Sum of electronic and thermal Energies=	-1170.355869
Sum of electronic and thermal Enthalpies=	-1170.354925
Sum of electronic and thermal Free Energies=	-1170.431183

## 5'-endo/unlike

### B3LYP/6-31+G\*

C,-0.7769342292,-0.8226979187,-2.1418168368\C,-0.7085056261,-0.4832805054,-3.6402917127\H,-1.0  
225203037,-1.345448056,-4.2410965311\H,0.3069090401,-0.2066856015,-3.938833411\H,-1.3771400  
014,0.3539536986,-3.8771194651\C,-2.175338025,-1.2075117255,-1.724156226\H,-0.1236619561,-1.6  
955203314,-1.9723550263\C,-2.6897973875,-0.9900157666,-0.5111740981\H,-2.7811703537,-1.70965  
3667,-2.4784528048\C,-1.9584053415,-0.3525577043,0.6438554432\H,-3.7093145843,-1.3142384206,-  
0.3014961702\H,-1.7467464329,-1.139901393,1.3829451245\C,-2.8665760707,0.664503591,1.377151  
3026\H,-3.8618103418,0.1992672909,1.4830786619\O,-2.9899975409,1.8047208393,0.5228058066\C,  
-2.355853321,1.0397350271,2.7719136478\H,-2.2635768738,0.1447149796,3.3972386582\H,-3.04486  
39821,1.7280306344,3.2728802723\H,-1.3728324371,1.5209048248,2.7252629502\C,-4.0987873639,2.



6464602245,0.7855889447\H,-4.0149266742,3.1594154247,1.7544858823\H,-5.0422756731,2.078651  
2515,0.7636875989\H,-4.116943572,3.3971393245,-0.0088141836\C,-0.6027620326,0.2662098718,0.2  
299703685\C,-0.2499554846,0.3559092918,-1.2705723364\H,-0.6028239171,1.2938944996,-1.708958  
3351\C,1.2740051084,0.3331553366,-1.2668763133\C,0.6188962044,-0.406219435,0.8477040433\H,-  
0.570738899,1.2945223886,0.6138028825\O,0.6881948093,-0.9610671591,1.9259244642\N,1.695752  
4804,-0.2215110409,-0.0394013111\O,2.0194663638,0.6742068174,-2.1630386066\C,3.0568360436,-0  
.5493840324,0.2685603803\C,5.7082262717,-1.1851639903,0.8699888362\C,4.0652143046,0.3938786  
898,0.0437196185\C,3.3670917528,-1.8088730873,0.7923471736\C,4.6940157332,-2.1195415677,1.09  
60519368\C,5.3898481788,0.0687972732,0.3415362131\H,3.8162835375,1.3638533746,-0.371357152  
3\H,2.5780112267,-2.5303105203,0.9712877751\H,4.9326182511,-3.0964274648,1.5081299235\H,6.1  
725840019,0.8007157549,0.1608032305\H,6.7403051171,-1.4326310212,1.1040893809\Version=AM  
64L-G03RevE.01\State=1-A\HF=-979.0249414

Zero-point correction=	0.359840 (Hartree/Particle)
Thermal correction to Energy=	0.380339
Thermal correction to Enthalpy=	0.381283
Thermal correction to Gibbs Free Energy=	0.308516
Sum of electronic and zero-point Energies=	-978.665102
Sum of electronic and thermal Energies=	-978.644603
Sum of electronic and thermal Enthalpies=	-978.643659
Sum of electronic and thermal Free Energies=	-978.716425

## **5'-exo/unlike**

### **B3LYP/6-31+G\***

C,0.8167447553,0.2909741171,-2.6818801376\C,0.0651587411,0.36922083,-4.0162580233\H,-0.05809  
90173,1.4066511437,-4.3453099666\H,-0.9329543817,-0.0729381162,-3.9528909337\H,0.6327378642,  
-0.1668446307,-4.7866895438\C,1.006911509,-1.1214895685,-2.1758507828\H,1.8196616608,0.71641  
42855,-2.850764937\C,1.6189768986,-1.312480471,-0.9991092085\H,0.6420713179,-1.9549891492,-2.  
7739884366\C,2.0631954508,-0.0941799524,-0.2215884902\H,1.7680775605,-2.3091486434,-0.58981  
15494\H,2.8321069123,0.4344527172,-0.810143341\C,2.7172979718,-0.3995799887,1.1376164292\H,  
1.9990592238,-0.9295267841,1.776302234\O,3.0202071083,0.8679537459,1.7328609632\C,3.9956894  
352,-1.2314894552,0.9830267509\H,3.7859226687,-2.2230071035,0.5663932501\H,4.4791809941,-1.3  
805707197,1.9545811387\H,4.7068204696,-0.720766684,0.3227019742\C,3.0557882822,0.860583274  
8,3.1517287268\H,3.8495496968,0.2057928475,3.5413115977\H,2.0884194551,0.5442767527,3.56583  
68689\H,3.2669682238,1.8868837573,3.4642988583\C,0.8620890737,0.9007589641,-0.1495571714\C,  
0.2194642568,1.1818452055,-1.5342397945\H,0.343168243,2.2297846675,-1.8313653759\C,-1.27635  
26608,0.9634414688,-1.3206349915\C,-0.2888079292,0.3923375948,0.7180750626\H,1.2219451907,1.  
8232586585,0.3180093378\O,-0.2257569935,0.0051086257,1.8692864735\N,-1.4798866804,0.473044  
6518,-0.0199924771\O,-2.167216871,1.1843879496,-2.1165540406\C,-2.7683061597,0.1314445875,0.  
506837415\C,-5.2786352203,-0.5383234925,1.5267245974\C,-3.1885402207,0.671726616,1.72609851  
55\C,-3.5964761045,-0.7414074313,-0.2051652603\C,-4.852870086,-1.0701221651,0.3064026838\C,-4.  
4431575356,0.3303128437,2.2342368657\H,-2.5359703763,1.3417008639,2.27500263\H,-3.26397656  
96,-1.1496491776,-1.1532923664\H,-5.4975970431,-1.7447103388,-0.2505784052\H,-4.7665470244,0.  
7470474335,3.1843636069\H,-6.2560620898,-0.7991797308,1.9239692533\Version=AM64L-G03RevE  
.01\State=1-A\HF=-979.0220181

Zero-point correction=	0.359798 (Hartree/Particle)
Thermal correction to Energy=	0.380073
Thermal correction to Enthalpy=	0.381017
Thermal correction to Gibbs Free Energy=	0.309957
Sum of electronic and zero-point Energies=	-978.662220
Sum of electronic and thermal Energies=	-978.641945
Sum of electronic and thermal Enthalpies=	-978.641001
Sum of electronic and thermal Free Energies=	-978.712061

## **5-endo/like**

### **B3LYP/6-31+G\***

C,-0.7378332438,2.3229165219,0.0482387312\C,-0.8646919679,3.5980120394,-0.8034400779\H,-1.7509607088,3.546576221,-1.4483851493\H,0.0151563382,3.7356687402,-1.4394491511\H,-0.9670516187,4.4806400813,-0.1606755991\C,-1.9379676676,2.1291725272,0.9432827983\H,0.1373525079,2.4582381317,0.7062621652\C,-2.4640562377,0.946209397,1.2757131999\H,-2.3700974885,3.039510735,1.3593017341\C,-1.958334013,-0.3903205293,0.8019737713\H,-3.3219368296,0.9185284082,1.9483118163\H,-1.5930155865,-0.9332097767,1.6852689607\C,-3.1263962013,-1.2489293755,0.2239712601\H,-3.8793013622,-1.3479276498,1.0253102654\O,-2.6892535995,-2.5527790836,-0.1533760294\C,-3.794281867,-0.6474432948,-1.0090476756\H,-4.176855532,0.3557186847,-0.7966581123\H,-4.6263124245,-1.2835377333,-1.3270563531\H,-3.0893491691,-0.5793058437,-1.8458151904\C,-2.3931761171,-3.4387717147,0.9193603853\H,-3.2320485857,-3.4872455585,1.6310039067\H,-1.4778221859,-3.1538232651,1.4533693426\H,-2.2495562304,-4.4259626912,0.4723207113\C,-0.7734664652,-0.2828220025,-0.1761505544\C,-0.4803613288,1.0742066595,-0.8506935431\H,-1.0330397981,1.1964186333,-1.7870467637\C,1.0123707562,0.9931691173,-1.1503557186\C,0.5765702274,-0.68336645,0.4125846981\H,-0.9328620133,-1.0278127065,-0.969988953\O,0.7880642223,-1.4965997326,1.2894275784\N,1.5697124211,0.0208868637,-0.2940051278\O,1.6448023733,1.6711191552,-1.9347426598\C,2.9749472783,-0.2228720137,-0.1590867541\C,5.7127719261,-0.7019462736,0.1091304023\C,3.4577846461,-1.535040241,-0.1961429713\C,3.8549653262,0.8508187388,0.0101139185\C,5.2232304161,0.6065906789,0.1394177173\C,4.8265049434,-1.7697623045,-0.0566168093\H,2.7684630993,-2.3631356837,-0.3200395599\H,3.4747588591,1.8662968053,0.0275395482\H,5.9056032092,1.4428565283,0.2656729372\H,5.1986419812,-2.7904901173,-0.080328908\H,6.7783277108,-0.8884506267,0.2135258128\\Version=AM64L-G03RevD.01\State=1-A\HF=-979.0258527

Zero-point correction=	0.360267 (Hartree/Particle)
Thermal correction to Energy=	0.380537
Thermal correction to Enthalpy=	0.381481
Thermal correction to Gibbs Free Energy=	0.310485
Sum of electronic and zero-point Energies=	-978.665585
Sum of electronic and thermal Energies=	-978.645316
Sum of electronic and thermal Enthalpies=	-978.644372
Sum of electronic and thermal Free Energies=	-978.715367

## 5-exo/like

B3LYP/6-31+G\*

C,-1.163044202,2.5245780283,-0.066162152\C,-0.6343831168,3.9269219187,-0.391877397\H,0.30388  
35553,3.8928074062,-0.9525125015\H,-0.4507363724,4.5077060956,0.5185066664\H,-1.377113869,4.  
4641066352,-0.9940927791\C,-1.422473784,1.6763889342,-1.2918020553\H,-2.1285661279,2.655933  
1286,0.4499618395\C,-1.8393375109,0.4135985622,-1.1332982484\H,-1.2816994084,2.1147860826,-2  
.2784262732\C,-1.9958020968,-0.1263124095,0.269693225\H,-2.0705568123,-0.2304722163,-1.97767  
13374\H,-2.8149520855,0.4241472605,0.7624329301\C,-2.4273873815,-1.6058025118,0.3041018454\  
H,-1.7188509703,-2.2101252818,-0.2786750561\O,-3.7017120011,-1.6183915193,-0.3582920718\C,-2.  
5401222362,-2.1801202663,1.7183791748\H,-1.5525006118,-2.2979178999,2.1745762902\H,-3.00443  
61081,-3.1716865821,1.6965858823\H,-3.1588610058,-1.533345141,2.3532131423\C,-4.0792775923,-  
2.8701628744,-0.9023956283\H,-3.3288495187,-3.2369694711,-1.6202809179\H,-5.0269263566,-2.71  
16444166,-1.4240259438\H,-4.2282962889,-3.6361351398,-0.1271943773\C,-0.2946804941,1.7181019  
164,0.9624822614\C,-0.7098288248,0.2256679062,1.0782361502\H,-0.8669318148,-0.0419853713,2.1  
298039881\C,0.520146144,-0.5573885886,0.6137992671\C,1.1889544824,1.6792946901,0.602122167  
\H,-0.3676494876,2.2301501618,1.9292195021\O,1.9482781094,2.6248190825,0.5375722663\N,1.564  
687314,0.3445023913,0.3725434099\O,0.6139544817,-1.7641060178,0.497973169\C,2.8835896021,-0.  
0566640446,-0.0225860069\C,5.4460470755,-0.8442142713,-0.7950581853\C,3.0477642088,-0.88378  
78138,-1.1377259439\C,3.9923837586,0.380136043,0.7084486991\C,5.2729202897,-0.0132867673,0.3  
151256526\C,4.331485549,-1.2791528556,-1.5175318308\H,2.1795568584,-1.2200508351,-1.6938240  
795\H,3.854493469,1.0291374872,1.5661230076\H,6.1350907605,0.330629205,0.8801951612\H,4.45  
8394581,-1.9259002907,-2.381566225\H,6.4443458392,-1.1507903497,-1.0960966872\\Version=AM6  
4L-G03RevE.01\State=1-A\HF=-979.0210754

Zero-point correction=	0.359740 (Hartree/Particle)
Thermal correction to Energy=	0.380038
Thermal correction to Enthalpy=	0.380982
Thermal correction to Gibbs Free Energy=	0.309796
Sum of electronic and zero-point Energies=	-978.661336
Sum of electronic and thermal Energies=	-978.641037
Sum of electronic and thermal Enthalpies=	-978.640093
Sum of electronic and thermal Free Energies=	-978.711280

## 6'-endo/unlike

B3LYP/6-31+G\*

C,2.0164227784,0.3359649681,1.2119768259\H,2.0946659987,-0.1206596844,2.1971324332\C,2.2042  
015186,-0.522373892,-0.0185064837\H,3.1220301173,-0.1940517874,-0.5333435133\C,1.752997875,1  
.6412072821,1.0663750923\H,1.6085525673,2.2971029508,1.9234151923\C,1.6287973902,2.2092650  
777,-0.3291847716\H,2.6113081696,2.1123176266,-0.8206402295\C,1.2524660981,3.6957244544,-0.3  
627333593\H,1.168327314,4.0599688526,-1.3931527048\H,2.0320718361,4.2820897363,0.138553657  
1\H,0.2979996702,3.8875465211,0.1335479263\C,2.4036106505,-2.0227219684,0.3202835363\H,1.63  
28916431,-2.3201114052,1.0474330628\O,2.2978057192,-2.8474161875,-0.8380717631\H,1.34313714

63,-2.9537815554,-1.0135629916\C,3.7826657445,-2.2745565677,0.9253228366\H,3.9562826213,-1.6557665684,1.8129272454\H,4.5628332184,-2.0488042845,0.1882666978\H,3.8775918561,-3.3269900797,1.2104579362\C,1.0616426503,-0.2275822803,-1.056133609\H,1.394015239,-0.6240498237,-2.0208409087\C,0.6892578923,1.2760056279,-1.156848049\H,0.7124349237,1.6097364718,-2.2026648418\N,-1.2403265055,0.0270176634,-0.5042826318\C,-2.5949533834,-0.2850144804,-0.1474530673\C,-5.2296867093,-0.8763958301,0.5492732868\C,-3.3209627829,-1.2074854987,-0.9065212222\C,-3.1767829243,0.3441251052,0.9569271125\C,-4.497329348,0.0481750641,1.2989243945\C,-4.6379635724,-1.5035945724,-0.5504941091\H,-2.8576029222,-1.6955899966,-1.7568199899\H,-2.605078705,1.0627030162,1.5339200736\H,-4.9516627907,0.5412302733,2.1540563494\H,-5.2009167822,-2.224626949,-1.1369802225\H,-6.2565011237,-1.1068196899,0.8206144762\C,-0.7767684551,1.3415850365,-0.7256074953\O,-1.4714903056,2.3298412939,-0.6196408212\C,-0.2508201477,-0.9278316675,-0.7225556062\O,-0.4341641802,-2.1353822528,-0.6703697439\\Version=AM64L-G03RevD.01\State=1-A\HF=-939.7218864

Zero-point correction=	0.332333 (Hartree/Particle)
Thermal correction to Energy=	0.350720
Thermal correction to Enthalpy=	0.351664
Thermal correction to Gibbs Free Energy=	0.285447
Sum of electronic and zero-point Energies=	-939.389554
Sum of electronic and thermal Energies=	-939.371166
Sum of electronic and thermal Enthalpies=	-939.370222
Sum of electronic and thermal Free Energies=	-939.436439

## **6'-exo/unlike**

### **B3LYP/6-31+G\***

C,-0.9251280318,-0.1680307693,-0.7524724376\H,-1.0756043119,-0.4788767849,-1.7946292035\C,-0.5925410603,1.3424659723,-0.7217546636\H,-0.8887186066,1.8321450303,-1.6558313274\N,1.3954732789,0.09158119,-0.3145326226\C,2.7704142535,-0.2207345291,-0.0449808553\C,5.4419627173,-0.824208563,0.4815541603\C,3.1058564725,-0.9222360842,1.1169382403\C,3.7611454727,0.1817983142,-0.9455111549\C,5.0972699087,-0.1190103374,-0.6746716892\C,4.4439974372,-1.2260076031,1.3735005691\H,2.3283564165,-1.2361916063,1.8046207604\H,3.4905896576,0.7329091381,-1.8392538539\H,5.8680022057,0.1980235489,-1.3719415565\H,4.7042046428,-1.7764148896,2.273567841\H,6.4829598242,-1.059571824,0.6864092723\C,0.9292812244,1.388478615,-0.6238991577\O,1.646533452,2.3578682367,-0.7571009978\C,0.3648479996,-0.8494556282,-0.3120658885\O,0.4974499374,-2.0252197905,-0.0106906016\C,-3.1197163861,0.4648626083,0.3426439676\H,-4.1769051993,0.2182137358,0.4193653988\C,-2.1553581865,-0.6646893483,0.0632168601\H,-1.7816893085,-1.0341991824,1.0324322385\C,-2.7159037387,1.7255261397,0.5290036348\H,-3.4419833654,2.5057464909,0.7538663199\C,-1.2613246587,2.1308125746,0.4453012268\H,-0.7640142593,1.8300078093,1.3831475302\C,-1.1010407667,3.6500350107,0.289269591\H,-0.049207647,3.9408292916,0.2301637318\H,-1.5571712717,4.1667556501,1.1422805951\H,-1.6024112523,3.9996827895,-0.6224602556\C,-2.8658533482,-1.8656120956,-0.6273854072\H,-3.4911619752,-1.4671593392,-1.4383161405\O,-1.951448127,-2.7422742269,-1.2810294255\H,-1.1615368919,-2.8675696544,-0.7188772374\C,-3.7484022098,-2.6466998659,0.3513197313\H,-4.5167800157,-2.015487215,0.814245079\H,-3.1366613808,-3.0826970022,1.1515665894\H,-4.2487829016,-3.4643958067,-0.1770088616\\Version=AM64L-G03RevD.01\State=1-A\HF=-939.7230939

Zero-point correction=	0.332050 (Hartree/Particle)
Thermal correction to Energy=	0.350616
Thermal correction to Enthalpy=	0.351560
Thermal correction to Gibbs Free Energy=	0.284690
Sum of electronic and zero-point Energies=	-939.391044
Sum of electronic and thermal Energies=	-939.372478
Sum of electronic and thermal Enthalpies=	-939.371534
Sum of electronic and thermal Free Energies=	-939.438404

## **6-endo/like**

B3LYP/6-31+G\*

C,-1.0364453888,-0.2811519818,-1.0260475576\H,-1.2557576315,-0.7679619719,-1.9864782924\C,-0.5985934455,1.1926315332,-1.251446797\H,-0.7510483821,1.5039799067,-2.2912755481\N,1.2841383191,-0.0807959517,-0.529712234\C,2.6246761252,-0.4237712536,-0.1467877202\C,5.2253135372,-1.0861711201,0.6056787205\C,3.6748037829,-0.2305712322,-1.0481696707\C,2.8639849417,-0.9442549809,1.1280757483\C,4.1674496245,-1.2786058309,1.4987247558\C,4.9762929252,-0.5603130254,-0.6649166713\H,3.4770462251,0.1831102701,-2.0310650792\H,2.0387261712,-1.0924663231,1.8163323245\H,4.3541108555,-1.6878872387,2.4878378656\H,5.7947748431,-0.4059606841,-1.3627702391\H,6.23933275,-1.3446357386,0.8989840554\C,0.9087763771,1.1880878027,-1.0156519435\O,1.6868252736,2.0957722614,-1.2196719115\C,0.2167148362,-0.9728512895,-0.4870448038\O,0.3144027097,-2.1327956797,-0.1166230402\C,-2.0422493391,0.37254284,1.1539390111\H,-2.2022492824,-0.1079684077,2.115278557\C,-2.2969901175,-0.4095058985,-0.1130774158\H,-3.0846137066,0.1064627873,-0.6881959194\C,-1.5753632934,1.6235367152,1.041477385\H,-1.348775594,2.2321242799,1.9155386178\C,-1.3698231151,2.2137640912,-0.3366257617\H,-2.3622723722,2.2901002732,-0.8104467882\C,-0.7745263444,3.627076648,-0.3135082731\H,-1.4568361828,4.2991565427,0.2207040073\H,-0.6323717321,4.0206551628,-1.3255844677\H,0.1969163255,3.6553212711,0.1880241335\C,-2.8370226519,-1.8481765246,0.1118321154\H,-2.7686286128,-2.3842978896,-0.8502370496\O,-2.1291376782,-2.5690783119,1.1115273598\H,-1.214524705,-2.6949990087,0.7920794722\C,-4.3015353453,-1.8246738643,0.5477706571\H,-4.9343846883,-1.3517316167,-0.2123130795\H,-4.4190915774,-1.2759072278,1.4893953227\H,-4.6530444366,-2.8487893337,0.7074501547\\Version=AM64L-G03RevD.01\State=1-A\HF=-939.7208751

Zero-point correction=	0.332360 (Hartree/Particle)
Thermal correction to Energy=	0.350719
Thermal correction to Enthalpy=	0.351664
Thermal correction to Gibbs Free Energy=	0.285316
Sum of electronic and zero-point Energies=	-939.388515
Sum of electronic and thermal Energies=	-939.370156
Sum of electronic and thermal Enthalpies=	-939.369212
Sum of electronic and thermal Free Energies=	-939.435559

## 6-exo/like

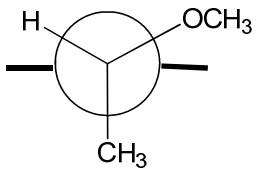
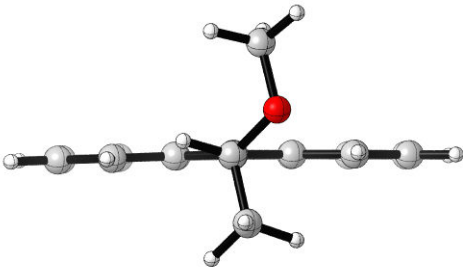
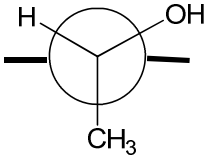
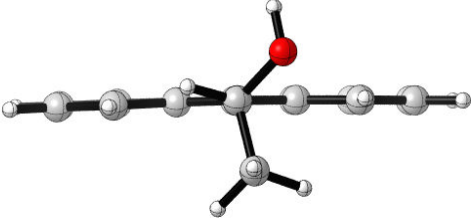
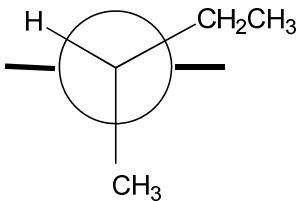
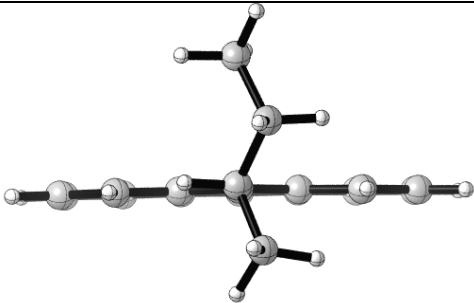
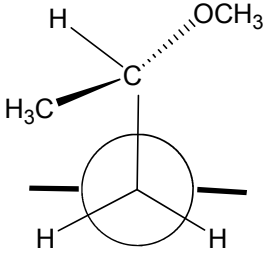
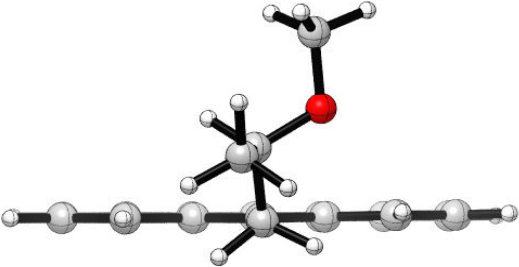
B3LYP/6-31+G\*

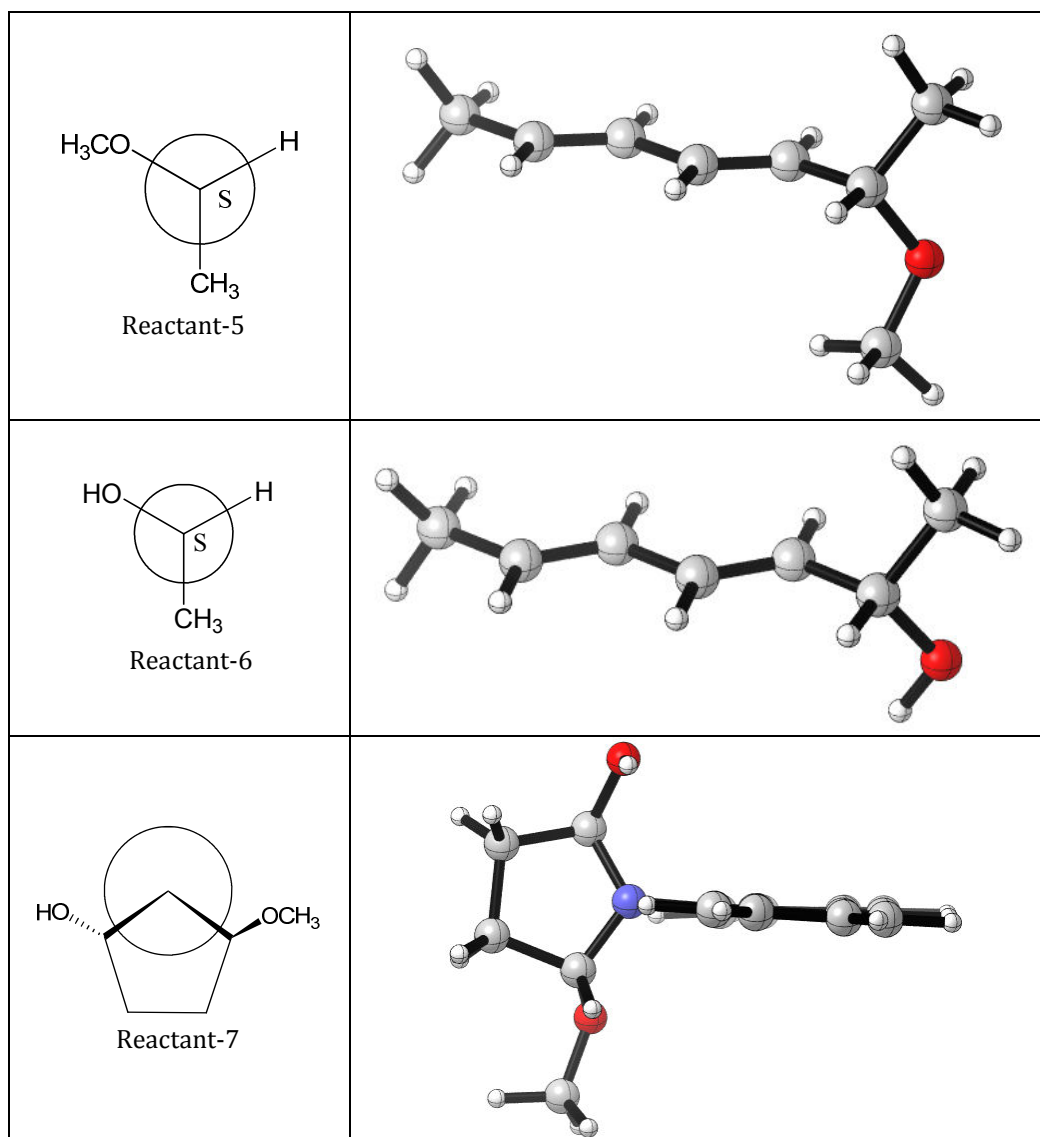
C,-1.0120236973,-0.0610027389,0.5778283344\H,-1.4086638118,-0.18540811,1.5908544321\C,-0.5905  
523262,1.4177351167,0.3621460788\H,-0.6938028922,1.9603468578,1.3115490645\N,1.3378692733,  
0.0265954091,0.1992162525\C,2.7011577582,-0.3895452619,0.0268968597\C,5.3487461935,-1.19390  
76911,-0.3126876258\C,2.9987010024,-1.4374605933,-0.848851215\C,3.717132983,0.2600815471,0.7  
33210974\C,5.0417433836,-0.1436880368,0.5567163523\C,4.3253449993,-1.8396006772,-1.01196948  
77\H,2.2012669142,-1.9383062606,-1.3873856116\H,3.4754153686,1.0782851629,1.4030759283\H,5.  
8328073462,0.3641892175,1.1016541161\H,4.5566898076,-2.6575903251,-1.6886980397\H,6.380816  
9099,-1.5074568914,-0.445034589\C,0.9041589178,1.3615641876,0.0609936702\O,1.6300145739,2.28  
59720651,-0.2393058256\C,0.2962014159,-0.8423010399,0.5232891292\O,0.4424858948,-2.03634367  
42,0.7340426971\C,-3.1543513357,0.4842914936,-0.5795367652\H,-4.1972896972,0.172790741,-0.61  
63930671\C,-2.0968357825,-0.5873308227,-0.4158770611\H,-1.6138721888,-0.7434291671,-1.394017  
9855\C,-2.8267007126,1.7730578206,-0.7148488057\H,-3.5957031165,2.5303228868,-0.8618292554\  
C,-1.3840585071,2.2239803868,-0.7083436235\H,-0.9512723153,1.9839912595,-1.6935407068\C,-1.25  
03575274,3.7393749375,-0.4967202032\H,-1.7848921363,4.2822030645,-1.285524236\H,-0.20238898  
1,4.0492885806,-0.5139000543\H,-1.6847094103,4.0358856336,0.4673848007\C,-2.7420563823,-1.95  
90039638,-0.0572817194\H,-3.6027039828,-2.0563743069,-0.7306947678\O,-1.911918858,-3.0609632  
134,-0.399663409\H,-1.0854882307,-2.9957810086,0.1174453342\C,-3.2509751856,-2.0682927749,1.3  
853934098\H,-3.8932464679,-1.2203346467,1.6562917921\H,-2.4218984496,-2.1162303283,2.101301  
2918\H,-3.8317907471,-2.9896048357,1.4948135363\\Version=AM64L-G03RevD.01\State=1-A\HF=-93  
9.7219965

Zero-point correction=	0.332354 (Hartree/Particle)
Thermal correction to Energy=	0.350855
Thermal correction to Enthalpy=	0.351800
Thermal correction to Gibbs Free Energy=	0.284485
Sum of electronic and zero-point Energies=	-939.389643
Sum of electronic and thermal Energies=	-939.371141
Sum of electronic and thermal Enthalpies=	-939.370197
Sum of electronic and thermal Free Energies=	-939.437511

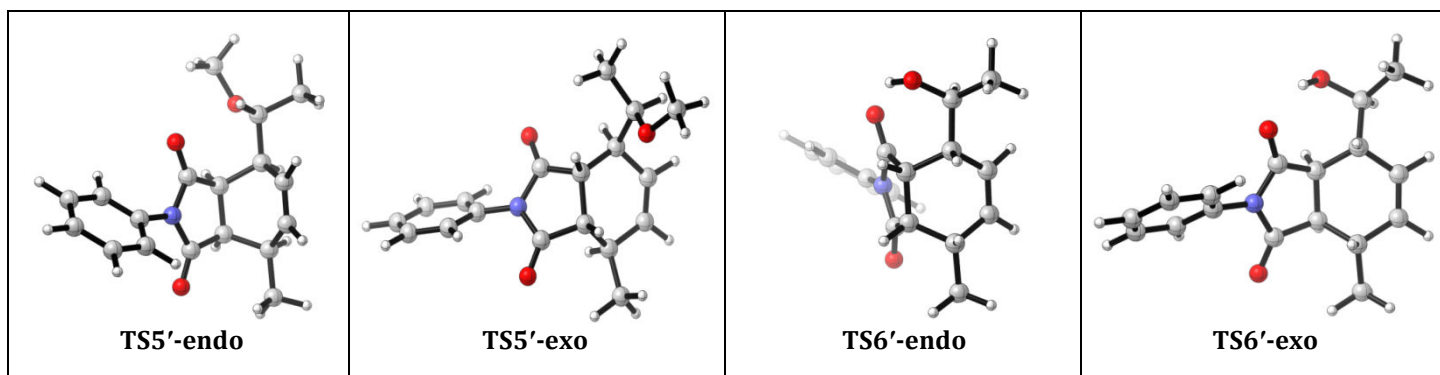


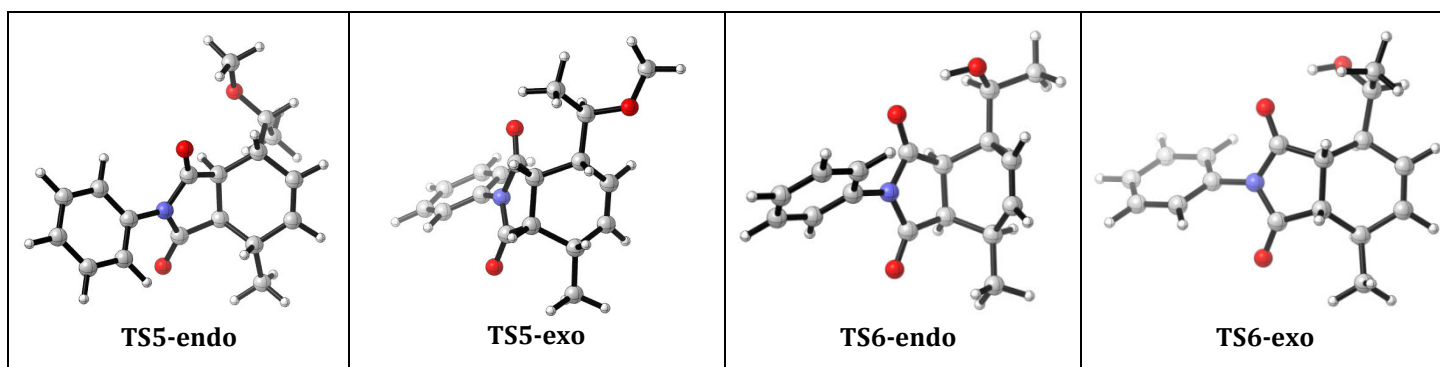
## CONFORMATIONS of the REACTANTS, TRANSITION STATES and PRODUCTS

Conformation	3D structure
 <p>Reactant-1 (Y=CH<sub>3</sub>)</p>	
 <p>Reactant-2 (Y=H)</p>	
 <p>Reactant-3</p>	
 <p>Reactant-4</p>	

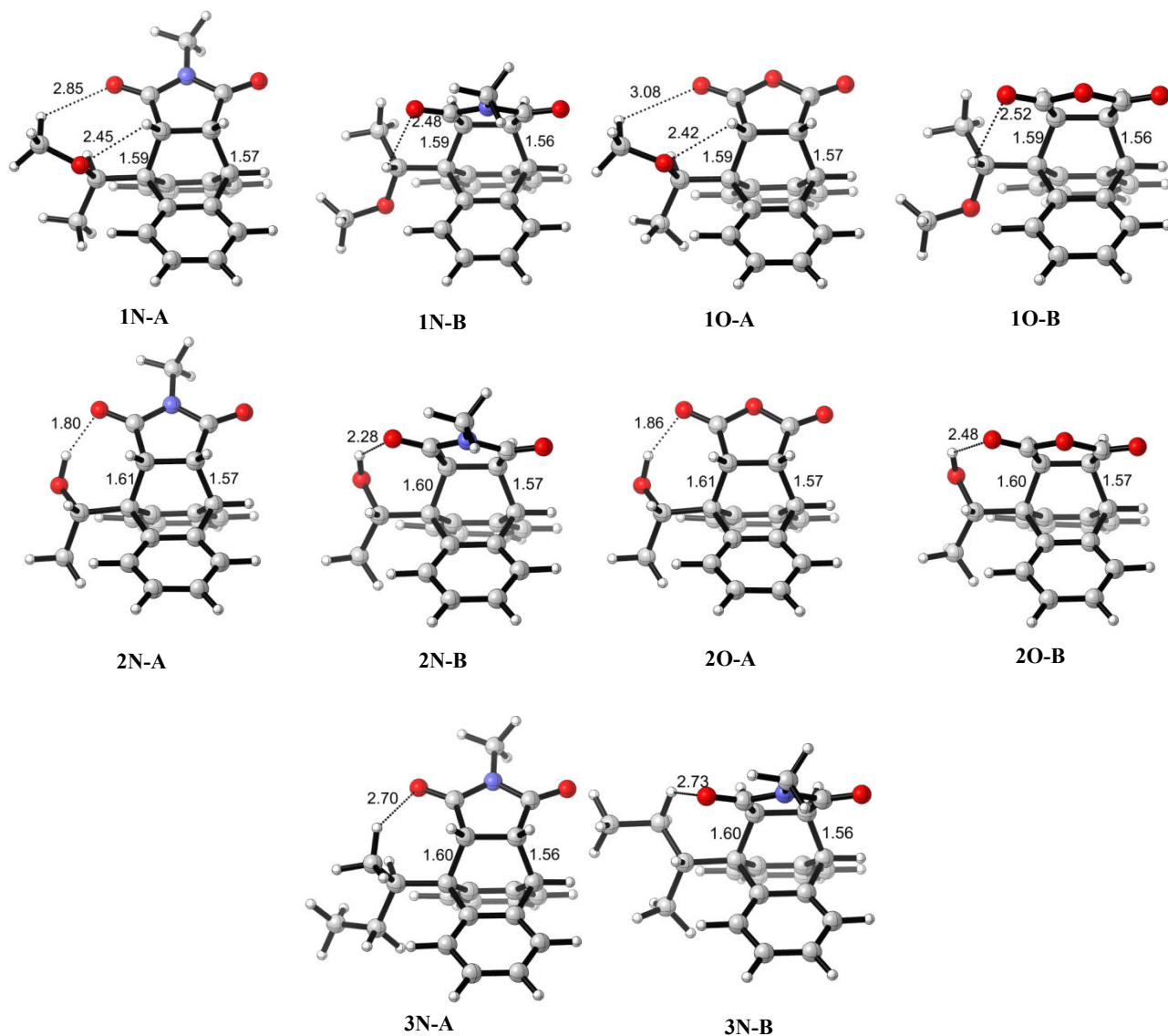


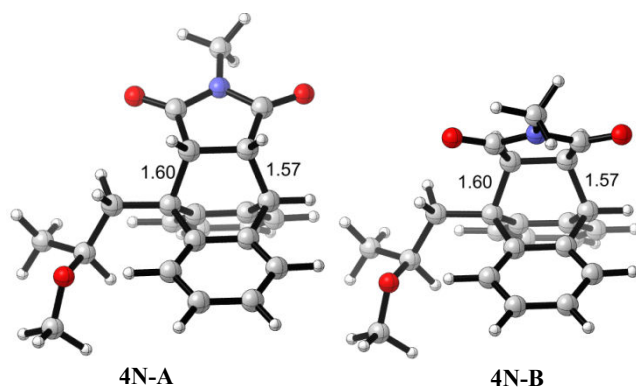
**Figure S1.** Best conformations of the all the reactants.



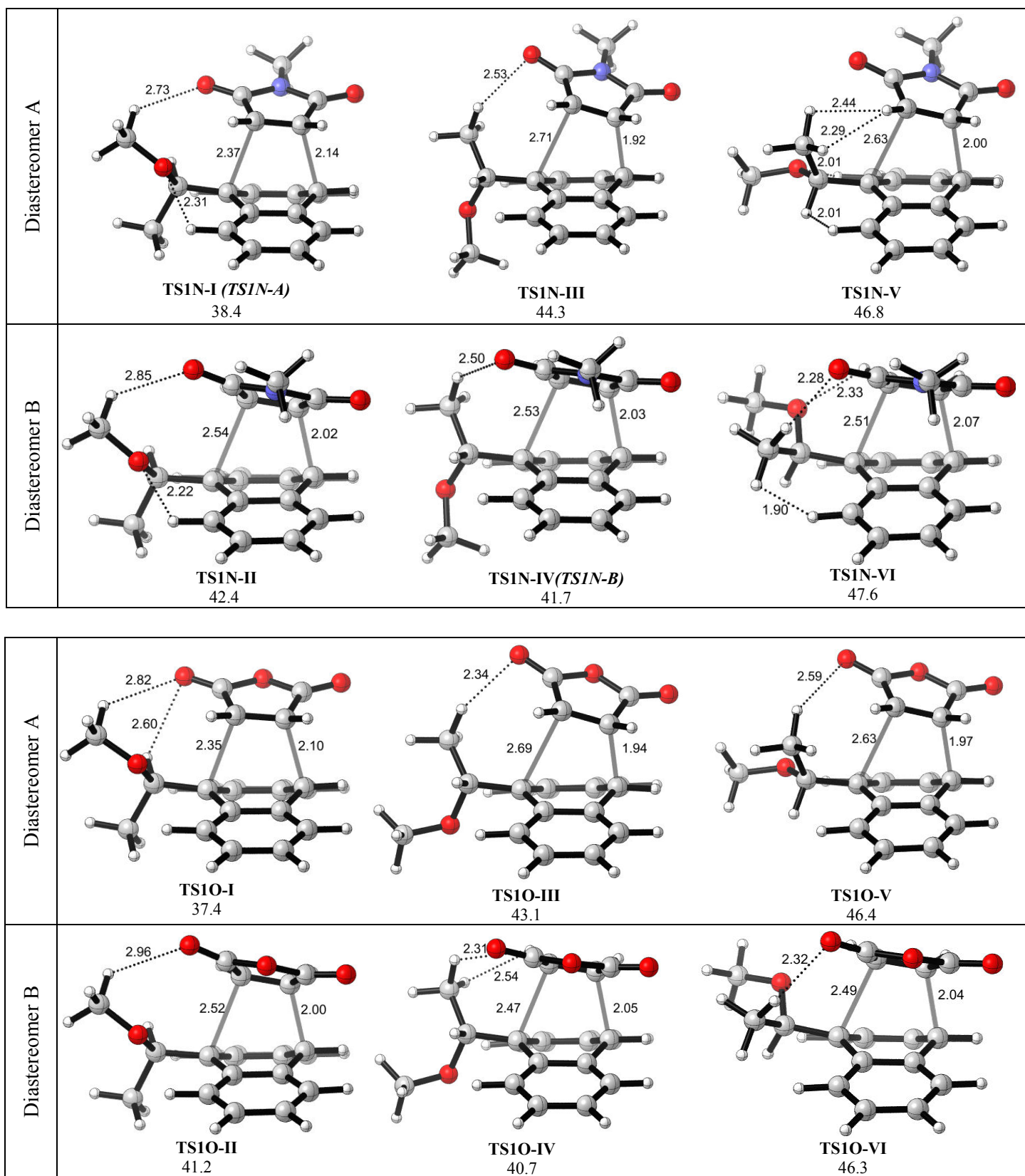


**Figure S2.** Product conformations of all the species in Part II.

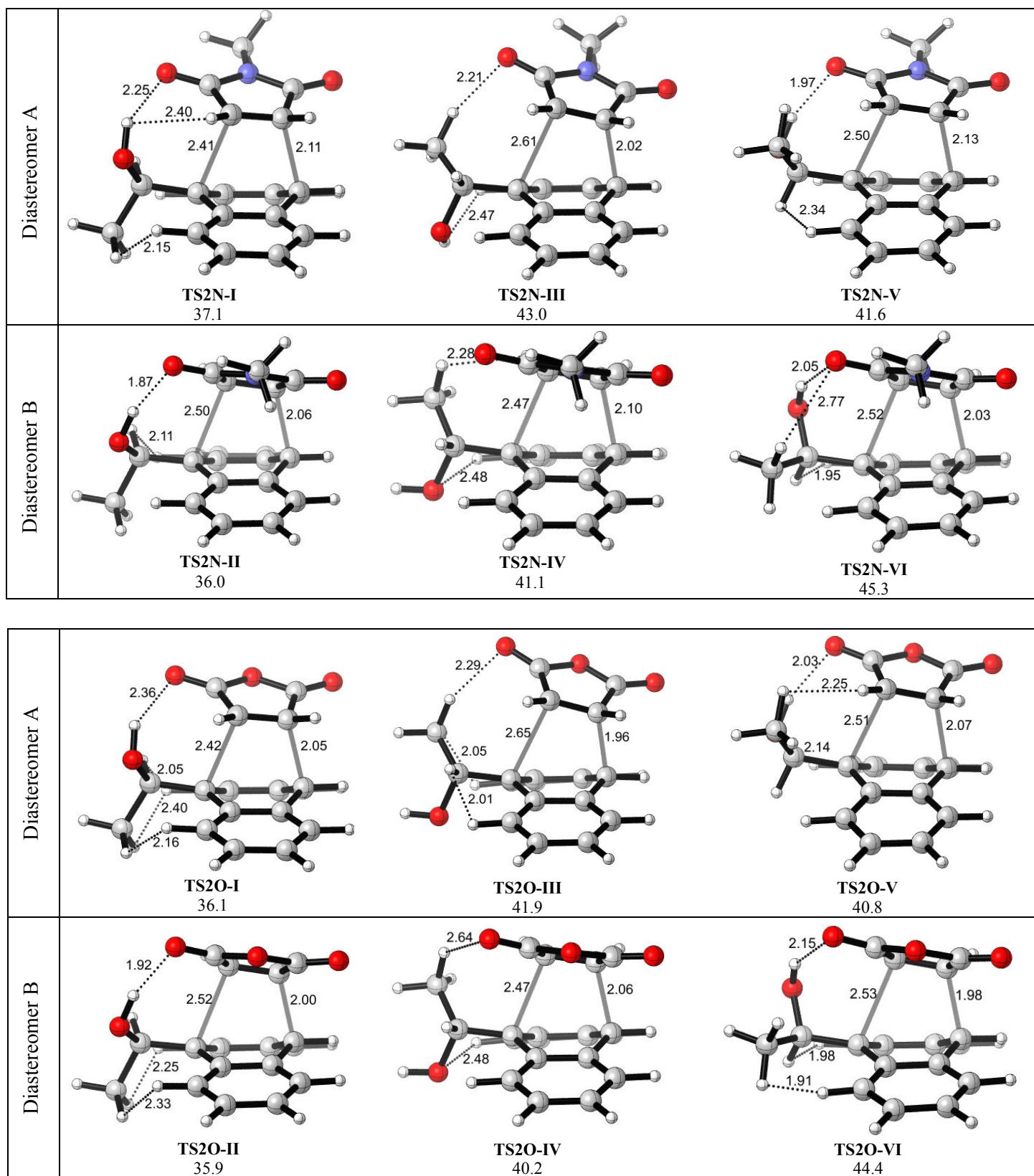




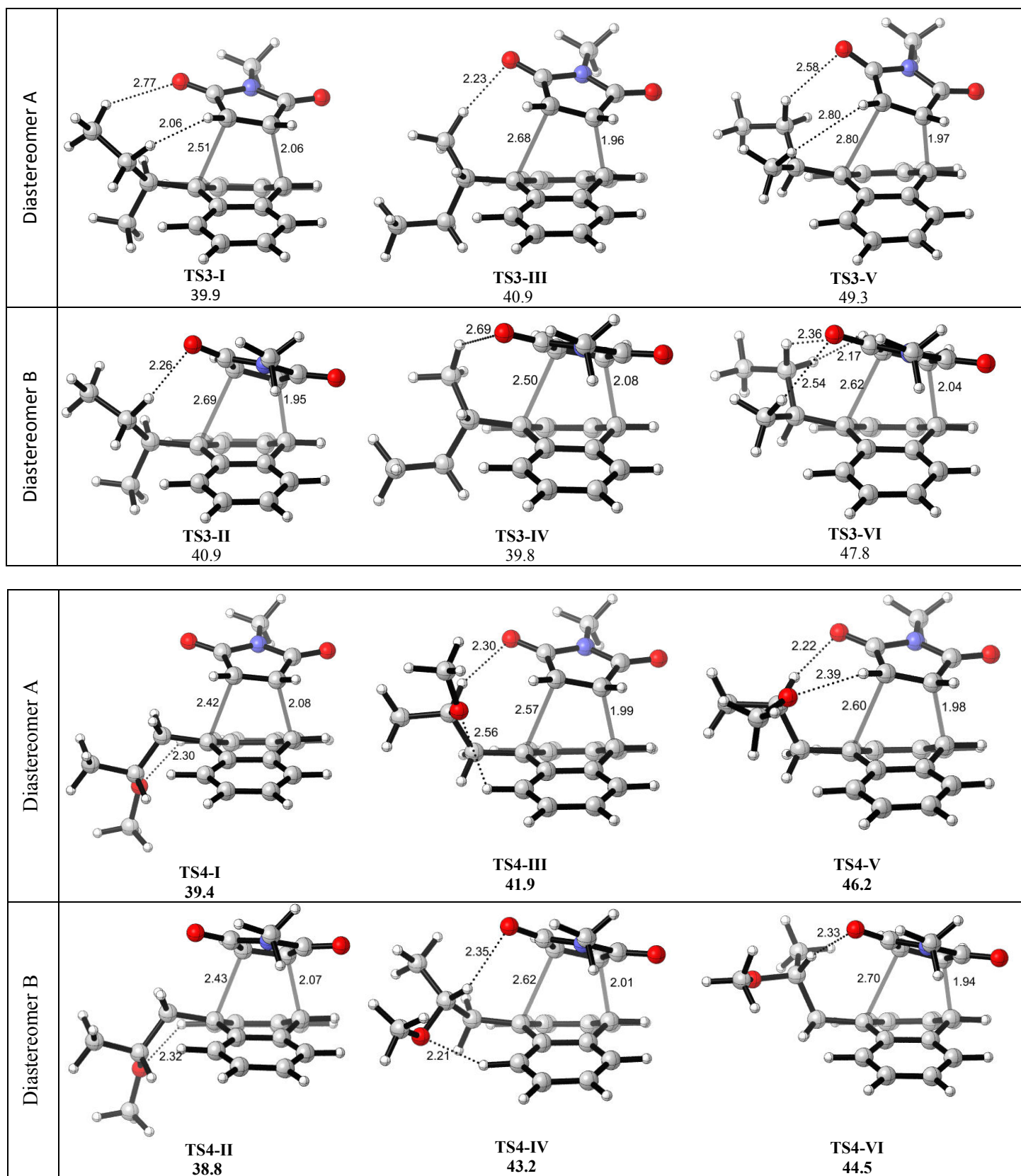
**Figure S3.** Product conformations of all the species in Part I.

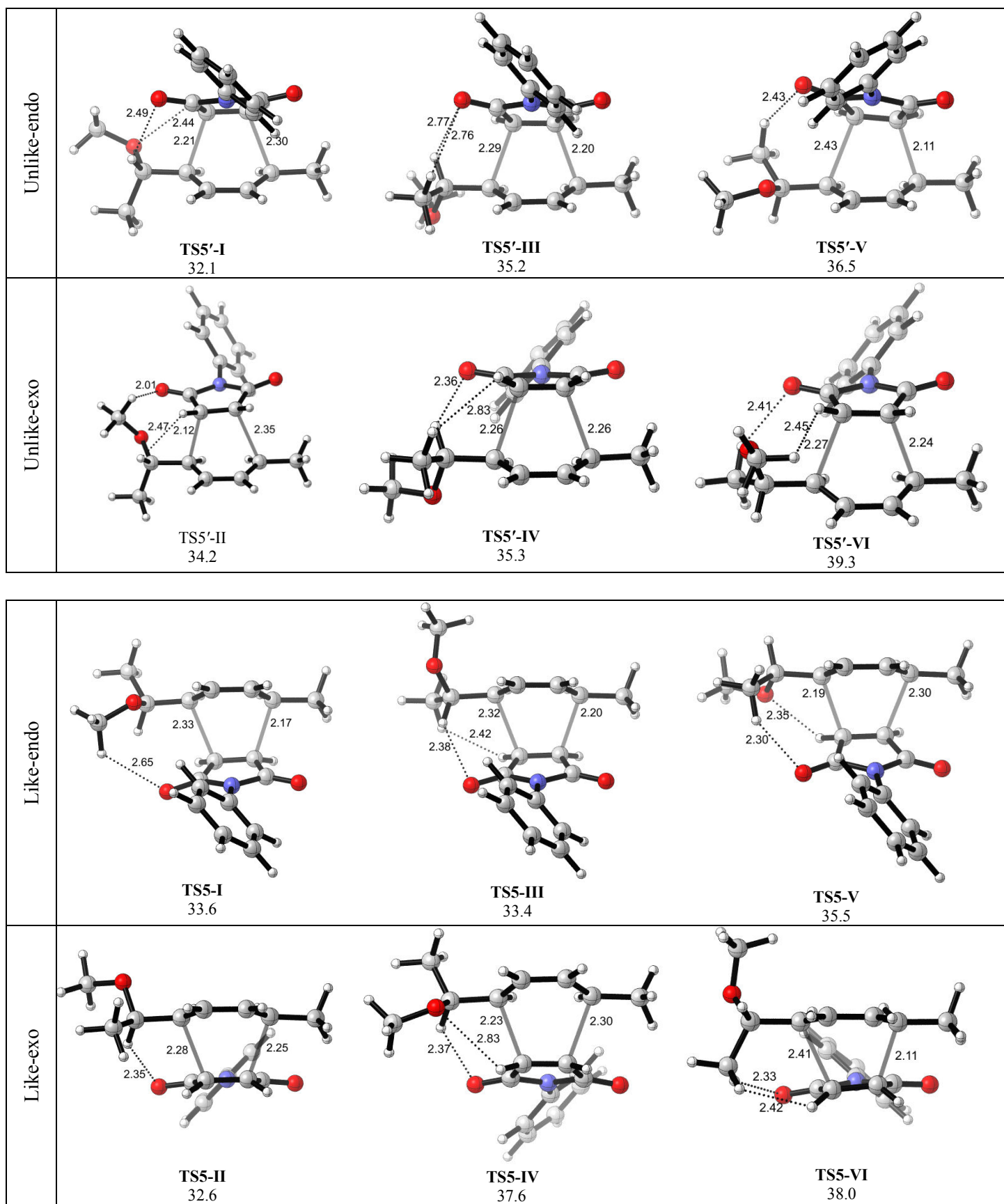


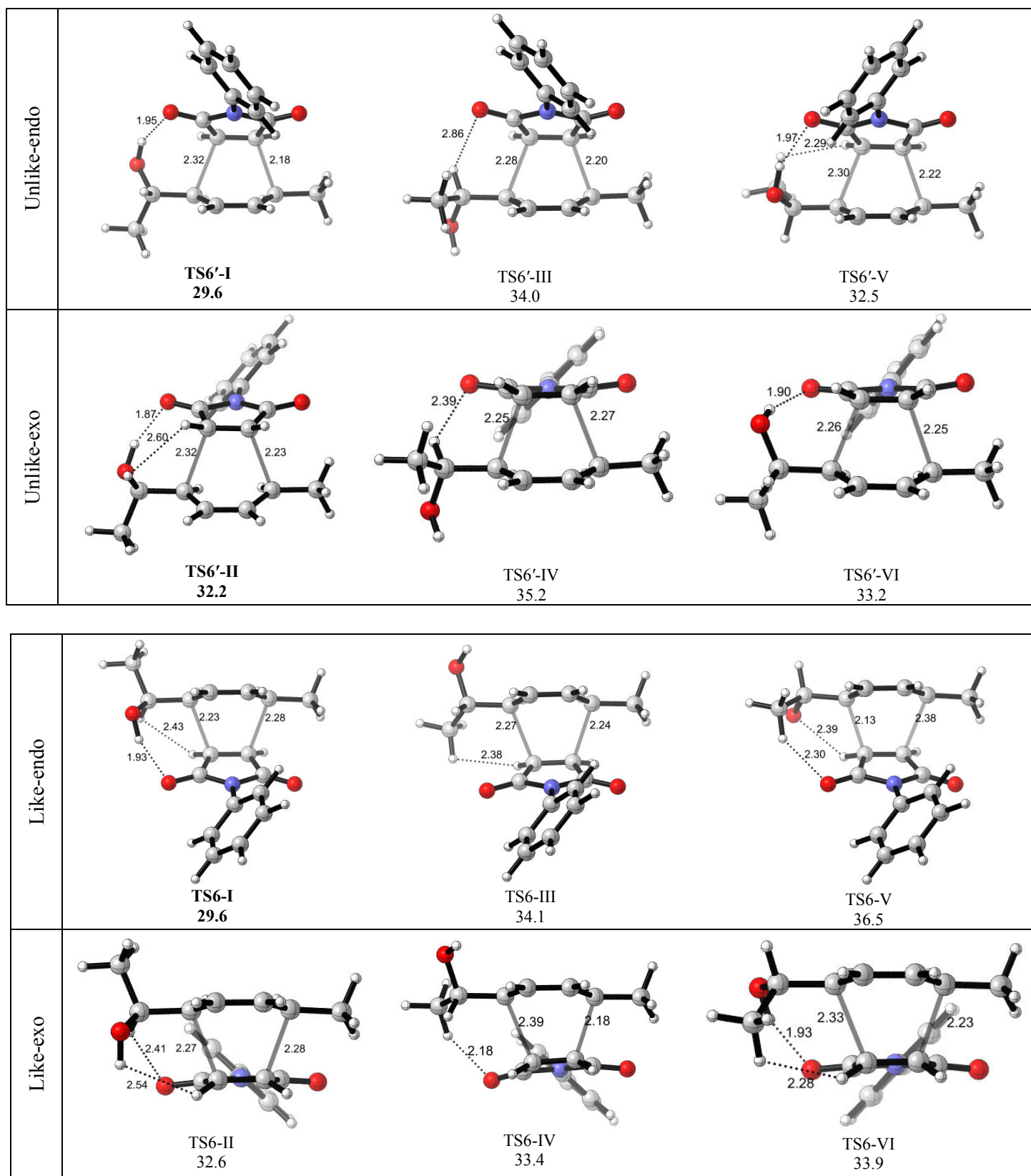




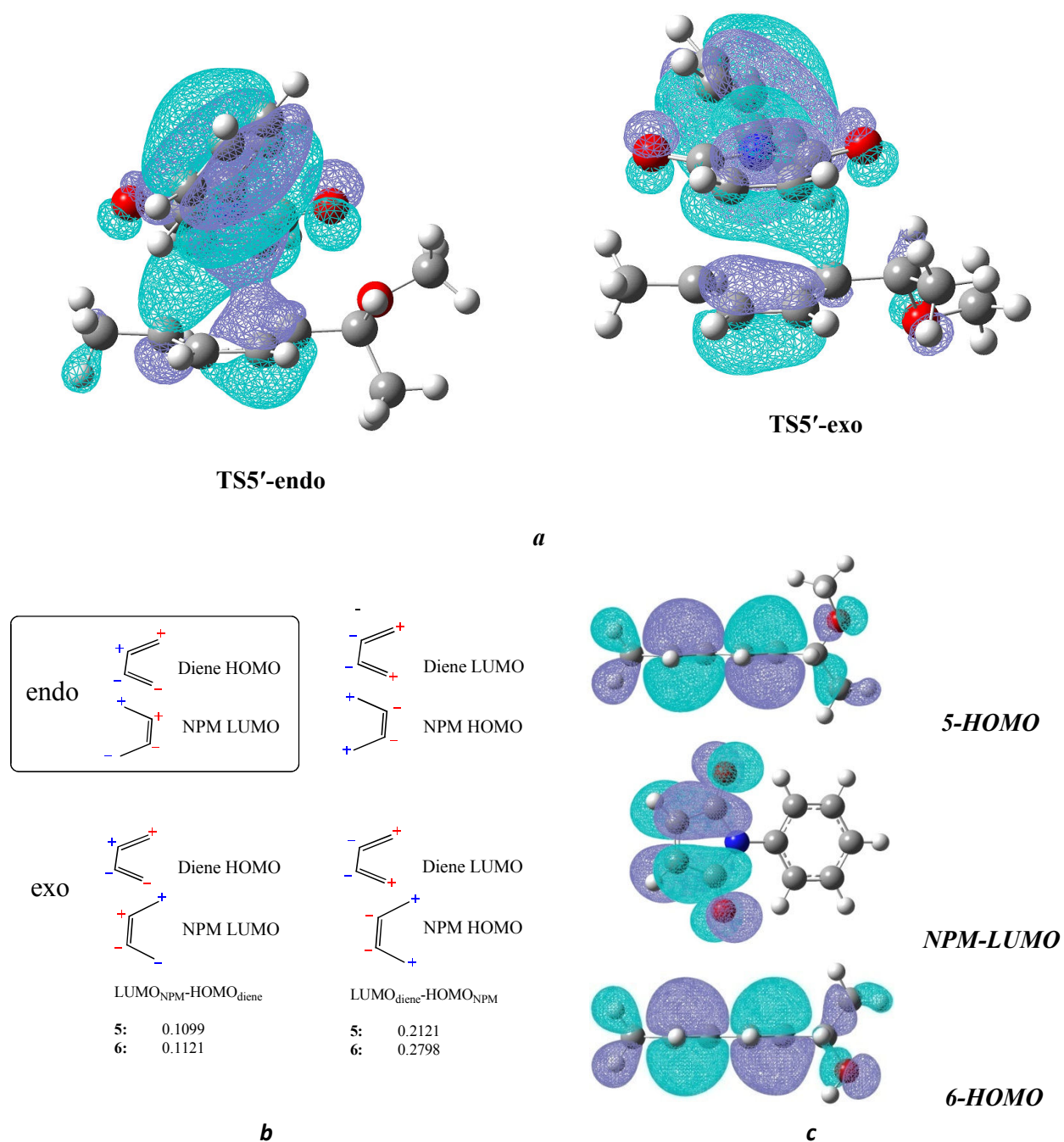








**Figure S4.** Transition state structures of 1-5 with NMM, MA, NPM



**Figure S5. (a)** Highest occupied molecular orbitals for *endo* and *exo* transition states of **5-NPM**.

**(b)** Frontier orbital interactions in Diels-Alder reactions of **5** and **6** with **NPM**: primary interactions are in red, secondary interactions are in blue. **(c)** HOMO of dienes and LUMO of dienophile (**NPM**).



### TABLES for PART I and II

**Table S1.** Gibbs Free Energies of Activation ( $\Delta G^\ddagger$ ), Diastereomeric ratios and Dipole moments,  $\mu$  (Debye) for the transition states of reactions **1-4** (B3LYP/6-31+G(d)).

	$\Delta G^\ddagger$ (gas phase)	$\Delta G^\ddagger$ (benzene)	Diastereomeric Ratio*	$\mu$
<b>TS1N-A</b>	38.4	45.5	0.97 (0.98) - 0.98 - <b>0.94</b> [0.99]	2.6
<b>TS1N-B</b>	41.7	48.2	0.03 (0.02) - 0.02 - <b>0.06</b> [0.01]	2.7
<b>TS1O-A</b>	37.4	43.3	0.97 (0.98) - 0.99 - <b>0.93</b> [0.99]	5.4
<b>TS1O-B</b>	40.7	45.9	0.03 (0.02) - 0.01 - <b>0.07</b> [0.01]	5.6
<b>TS2N-A</b>	37.1	44.0	0.26 (0.26) - 0.56 - <b>0.27</b> [0.37]	2.3
<b>TS2N-B</b>	36.0	43.0	0.74 (0.74) - 0.44 - <b>0.73</b> [0.63]	3.2
<b>TS2O-A</b>	36.1	42.7	0.45 (0.47) - 0.78 - <b>0.38</b> [0.32]	4.9
<b>TS2O-B</b>	35.9	42.2	0.55 (0.53) - 0.22 - <b>0.62</b> [0.68]	6.6
<b>TS3N-A</b>	39.9	46.6	0.46 (0.47) - 0.49 - <b>0.41</b> [0.40]	3.1
<b>TS3N-B</b>	39.7	46.3	0.54 (0.53) - 0.51 - <b>0.59</b> [0.60]	3.3
<b>TS4N-A</b>	39.4	45.9	0.34 (0.23) - 0.32 - <b>0.31</b> [0.40]	4.4
<b>TS4N-B</b>	38.8	45.1	0.66 (0.77) - 0.68 - <b>0.69</b> [0.60]	3.6

\*Values in benzene are given in bold, BMK/6-31+G(d) values are given in parentheses, M06-2X/6-31+G(d)//B3LYP/6-31+G(d) values are given in italic, experimental values in benzene at 80°C are given

in brackets. For compound **20** in toluene at 30°C the nature of the diastereomers in has not been identified.<sup>5a</sup>

**Table S2.** Gibbs Free Energies of Activation ( $\Delta G^\ddagger$ ), Diastereomeric ratios and Dipole moments,  $\mu$  (Debye) for the transition states of reactions **5** and **6** (B3LYP/6-31+G(d)).

		$\Delta G^\ddagger$ Gas phase	$\Delta G^\ddagger$ benzene	Diastereomeric Ratio*	$\mu$
<i>unlike</i>	<b>TS5'-endo</b>	32.1	38.2	0.55 (0.50) <i>0.77 - <b>0.62</b></i>	3.0
	<b>TS5'-exo</b>	35.3	40.9	0.02 (0.00) <i>0.00 - <b>0.04</b></i>	2.5
				[0.83]	
<i>like</i>	<b>TS5-endo</b>	33.6	40.5	0.12 (0.01) <i>0.18 - <b>0.06</b></i>	3.5
	<b>TS5-exo</b>	32.6	39.0	0.31 (0.48) <i>0.05 - <b>0.28</b></i>	2.8
				[0.17]	
<i>unlike</i>	<b>TS6'-endo</b>	29.6	36.0	0.46 (0.56) <i>0.51 - <b>0.42</b></i>	3.1
	<b>TS6'-exo</b>	32.2	35.8	0.03 (0.01) <i>0.00 - <b>0.05</b></i>	3.6
				[0.70]	
<i>like</i>	<b>TS6-endo</b>	29.6	38.2	0.48 (0.43) <i>0.49 - <b>0.47</b></i>	3.3
	<b>TS6-exo</b>	32.6	37.7	0.03 (0.00) <i>0.00 - <b>0.07</b></i>	2.9
				[0.30]	

Experiments are conducted in benzene.

Values in benzene are given in bold, BMK/6-31+G(d) values are given in parentheses, M06-2X/6-31+G(d)//B3LYP/6-31+G(d) values are given in italic, experimental values are given in brackets.