

Supporting Information

**Computational insight into the mechanism and origins of
highly selectivities in acylation of polyamines with 5-
benzoyl-5-phenyl-1,5-dihydro-4*H*-pyrazol-4-one**

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Table of Contents

Coordinates of all stationary points.....	S2
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Coordinates of all stationary points:

BCPP-gas

Sum of electronic and thermal Free Energies= -1070.264506

0 1

C	5.79173200	0.30677300	0.03038000
C	5.25502700	0.68584600	-1.36665700
C	3.72742500	0.82096900	-1.19863500
H	6.64070700	-0.38221100	-0.01681800
H	6.13458000	1.18894300	0.58834700
H	5.46495600	-0.13226600	-2.06196600
H	5.71833900	1.58839600	-1.77036600
H	3.42195900	1.86140600	-1.02609400
H	3.16817800	0.47479900	-2.07005400
C	4.58399100	-0.29092200	0.70306700
H	4.62073300	-0.84389900	1.63568500
C	3.45486300	-0.00651700	0.04287000
C	-0.25673700	-0.62297200	0.65832500
C	0.86787800	-0.19234400	-0.31083000
O	0.73511500	0.18610300	-1.45252900
C	2.10774700	-0.36788100	0.47598200
N	0.53275400	-1.25419000	1.71041000
H	0.17750100	-1.13087900	2.65297300
N	1.83923000	-0.90521100	1.62719300
C	-1.28961900	-1.58257900	0.08776400
C	-2.46699000	-1.79980900	0.80759200
C	-1.07063900	-2.28665600	-1.09679400
C	-3.41543000	-2.70774500	0.35001000
H	-2.64293700	-1.25596400	1.73269100
C	-2.02329000	-3.19376300	-1.55330300
H	-0.16730200	-2.11874900	-1.67255300
C	-3.19564600	-3.40624000	-0.83407000
H	-4.32662500	-2.86603000	0.91728300
H	-1.84561400	-3.73556300	-2.47649100
H	-3.93596900	-4.11239100	-1.19532600
C	-0.94585000	0.64625500	1.26154100
O	-0.83027400	0.84532600	2.45243500
C	-1.75470100	1.55367600	0.39854200
C	-2.00052900	1.32271900	-0.95899200
C	-2.28891000	2.69109800	1.01871600
C	-2.77121100	2.22743200	-1.68246300
H	-1.58658200	0.45476800	-1.45592100
C	-3.05611200	3.58888300	0.29161800
H	-2.08562100	2.84865700	2.07225600

C	-3.29867400	3.35594500	-1.06196600
H	-2.95914800	2.04684900	-2.73528600
H	-3.46586900	4.46892900	0.77592400
H	-3.89984700	4.05657900	-1.63294400

BCPP-DCM

Sum of electronic and thermal Free Energies= -1070.292108

O 1

C	5.80911100	0.34528600	0.00476900
C	5.27176000	0.68851300	-1.40078700
C	3.74247700	0.81488500	-1.23922800
H	6.65932200	-0.34315700	-0.02443400
H	6.14785900	1.24124700	0.54279200
H	5.49032200	-0.14249300	-2.07807500
H	5.72688300	1.58746400	-1.82177800
H	3.42661300	1.85715500	-1.10005900
H	3.19249300	0.43381600	-2.10242500
C	4.60467700	-0.23995900	0.69291100
H	4.65098500	-0.76799000	1.64045700
C	3.47235600	0.02161000	0.02580800
C	-0.23748900	-0.59909500	0.66656200
C	0.88119900	-0.18891800	-0.31870300
O	0.73895500	0.17141600	-1.46537600
C	2.12591600	-0.33469400	0.46862800
N	0.55919000	-1.20452000	1.72598500
H	0.20330000	-1.10914900	2.67247200
N	1.86055800	-0.84721900	1.63259900
C	-1.27360600	-1.57285800	0.13183200
C	-2.47711600	-1.73000100	0.82503100
C	-1.02184800	-2.35718100	-0.99558600
C	-3.42154800	-2.65593800	0.39194100
H	-2.68044200	-1.12848300	1.70820000
C	-1.97037200	-3.28125000	-1.42788900
H	-0.09283100	-2.24585900	-1.54478200
C	-3.17100500	-3.43154100	-0.73815300
H	-4.35368300	-2.76828200	0.93626200
H	-1.76699200	-3.88405300	-2.30725900
H	-3.90870000	-4.15050200	-1.07994600
C	-0.86817400	0.72439000	1.22340000
O	-0.59787200	1.05225700	2.35900400
C	-1.77612300	1.54583500	0.37102500
C	-2.06775800	1.24931400	-0.96573600
C	-2.34972700	2.67517900	0.97199300
C	-2.92128400	2.07850200	-1.68748900

H	-1.62407600	0.38924500	-1.45142400
C	-3.20492700	3.49519100	0.24907600
H	-2.11338900	2.89359800	2.00790100
C	-3.49199800	3.19631700	-1.08330800
H	-3.14206000	1.84683800	-2.72414400
H	-3.64829700	4.36595500	0.72088100
H	-4.16133000	3.83592100	-1.65033600

2-gas

Sum of electronic and thermal Free Energies= -726.113875

0 1

C	-5.07418600	0.33550400	0.17231600
C	-4.71627700	-1.14539600	-0.07856200
C	-3.20145000	-1.25174200	0.19103000
H	-5.84921500	0.70040500	-0.50934500
H	-5.45398900	0.49466900	1.19113800
H	-4.90787900	-1.38371600	-1.12910300
H	-5.30605500	-1.83572000	0.52864000
H	-2.98349100	-1.58774300	1.21289200
H	-2.69796200	-1.95581200	-0.47721500
C	-3.75102700	1.03467200	-0.00681000
H	-3.64006600	2.11072800	-0.08577600
C	-2.72636400	0.17518700	0.00322900
C	0.92672400	0.47777100	-0.12461400
C	-0.18743500	-0.32295900	0.05134400
O	-0.23103200	-1.65525500	0.33679000
C	-1.31154200	0.52697300	-0.09896400
N	0.42264500	1.72548900	-0.34526100
H	0.94550800	2.54741000	-0.60312200
N	-0.90759600	1.77274700	-0.35877800
C	2.35232700	0.15971100	-0.05518200
C	3.28017200	1.08341800	0.44286800
C	2.80605900	-1.09596600	-0.48263200
C	4.63084300	0.76165700	0.50145100
H	2.93502100	2.04671800	0.80788700
C	4.15671700	-1.41895000	-0.40611700
H	2.09680800	-1.80112100	-0.90727800
C	5.07317500	-0.49159400	0.08264600
H	5.33960000	1.48651800	0.88854800
H	4.49577000	-2.39302100	-0.74355800
H	6.12708500	-0.74298800	0.13664000
H	0.59535000	-1.90165300	0.77158700

2-DCM

Sum of electronic and thermal Free Energies= -726.140659

0 1

C	-5.08014100	0.35187700	0.15722500
C	-4.73057300	-1.12943900	-0.09898400
C	-3.21970200	-1.24722000	0.18678700
H	-5.84750200	0.72733600	-0.52738300
H	-5.46376100	0.50924200	1.17492100
H	-4.91266400	-1.36064800	-1.15319100
H	-5.33029800	-1.81859700	0.49987800
H	-3.01832400	-1.58386600	1.21200000
H	-2.71547200	-1.95496300	-0.47707600
C	-3.75117200	1.04285100	-0.01026500
H	-3.64061200	2.12032400	-0.08394100
C	-2.72951700	0.17690800	0.00563900
C	0.92877100	0.46549200	-0.10827100
C	-0.19062100	-0.33608500	0.06113000
O	-0.24692400	-1.66961300	0.32931100
C	-1.30973300	0.51842900	-0.08716900
N	0.43183300	1.71237100	-0.32836500
H	0.96645500	2.54298700	-0.54705900
N	-0.89780800	1.76683000	-0.33789300
C	2.35861200	0.15144700	-0.04716500
C	3.28665900	1.09547900	0.41349500
C	2.81225900	-1.11226700	-0.45037600
C	4.64061500	0.78167800	0.46159500
H	2.94421300	2.07045300	0.74947600
C	4.16685600	-1.42488000	-0.38691200
H	2.10501900	-1.83956700	-0.83890200
C	5.08465500	-0.47968200	0.06653200
H	5.35016200	1.52115000	0.81911200
H	4.50595200	-2.40597600	-0.70409400
H	6.14114500	-0.72382100	0.11163700
H	0.55109300	-1.92909300	0.81437400

3-gas

Sum of electronic and thermal Free Energies= -726.116470

0 1

C	-5.06510200	0.32149100	0.21498100
C	-4.71321600	-1.14214900	-0.12651400
C	-3.19865500	-1.26874700	0.13046600
H	-5.84442000	0.72891000	-0.43664200

H	-5.43260400	0.42163100	1.24542900
H	-4.91048600	-1.31700300	-1.18822800
H	-5.30206600	-1.86444600	0.44248600
H	-2.97580300	-1.65105100	1.13413900
H	-2.69638100	-1.93696400	-0.57381900
C	-3.74074100	1.02633500	0.06431700
H	-3.65212700	2.10909900	0.06156700
C	-2.71673000	0.16362000	0.01465300
C	0.93464900	0.53089600	-0.13870800
C	-0.18140300	-0.32257300	0.04656300
O	-0.19551000	-1.65690800	0.32266000
C	-1.30260800	0.47802400	-0.08445600
N	0.52788800	1.77981300	-0.36479400
H	-1.33080500	2.55314300	-0.54329600
N	-0.80122500	1.72344400	-0.33001900
C	2.35938200	0.17692800	-0.06570900
C	3.29902500	1.11914000	0.36875100
C	2.79628900	-1.10353100	-0.42701600
C	4.64437700	0.78338700	0.44569000
H	2.95358300	2.11094400	0.64118400
C	4.14502300	-1.43885100	-0.33835500
H	2.08368200	-1.82383400	-0.81993600
C	5.07154900	-0.49865500	0.10062100
H	5.36467900	1.52215300	0.78258500
H	4.47197400	-2.43283700	-0.62655500
H	6.12264900	-0.75953800	0.16818300
H	0.63451500	-1.87962300	0.76362100

3-DCM

Sum of electronic and thermal Free Energies= -726.141844

O 1

C	-5.06433700	0.35280200	0.22126800
C	-4.74023700	-1.11012600	-0.14861400
C	-3.22761700	-1.26967600	0.10407100
H	-5.83587600	0.78911400	-0.42086600
H	-5.42741600	0.44111500	1.25446900
H	-4.94210300	-1.26190800	-1.21339700
H	-5.34000400	-1.83213900	0.40956300
H	-3.01572300	-1.67669600	1.10060600
H	-2.74127100	-1.93378200	-0.61576900
C	-3.72906100	1.03790900	0.08293400
H	-3.61547000	2.11846900	0.09369400
C	-2.72096500	0.15693400	0.01425600
C	0.93676300	0.50709000	-0.12656800

C	-0.18229700	-0.34508500	0.04614500
O	-0.21033200	-1.68431900	0.29384900
C	-1.30191900	0.46331000	-0.08141800
N	0.52795200	1.75974400	-0.34392200
H	-1.33662500	2.54412800	-0.51033600
N	-0.80222400	1.70743100	-0.31745100
C	2.36682000	0.16624900	-0.05717800
C	3.30397000	1.13368900	0.32939200
C	2.81345200	-1.12292000	-0.37548000
C	4.65581000	0.81684100	0.39585600
H	2.95900900	2.13221700	0.57935600
C	4.16800300	-1.43872500	-0.29837200
H	2.10416600	-1.87349500	-0.71196700
C	5.09261300	-0.47212700	0.08866500
H	5.37143800	1.57594100	0.69637000
H	4.49965100	-2.44112800	-0.55074300
H	6.14789500	-0.71919000	0.14787700
H	0.54889600	-1.91531300	0.85021400

A-TS-gas

Sum of electronic and thermal Free Energies= -1299.850029

Imaginary frequency= -252.03

0 1

C	5.85800800	-0.92989200	1.27995200
C	5.81875000	-0.77973700	-0.25602200
C	4.35465400	-0.43528600	-0.59571900
H	6.55899500	-1.70395800	1.60831700
H	6.16880300	0.00292000	1.77097200
H	6.07250700	-1.74096100	-0.71321900
H	6.52892200	-0.03911900	-0.63072800
H	4.19378900	0.64805200	-0.67935900
H	4.01499100	-0.86999500	-1.53836200
C	4.42424800	-1.24500000	1.62084800
H	4.09726000	-1.60328200	2.59103900
C	3.59804300	-0.96882800	0.60495100
C	-0.11196300	-1.04048700	0.08331800
C	1.23627100	-0.86114500	-0.48797100
O	1.48705500	-0.43983500	-1.63658200
C	2.14393900	-1.08185200	0.62373600
N	0.16495200	-1.49058900	1.40800400
H	-0.46126000	-1.26506000	2.17231400
N	1.45839400	-1.34288700	1.71320500
C	-1.17430600	-1.74410800	-0.68100800
C	-2.17355500	-2.45538400	-0.00444900

C	-1.25060300	-1.65226700	-2.07912800
C	-3.23607500	-3.02462900	-0.69638900
H	-2.12252900	-2.55527300	1.07504600
C	-2.31959100	-2.22043000	-2.76692400
H	-0.44908100	-1.16587200	-2.62566900
C	-3.32437100	-2.89768400	-2.08033900
H	-4.00145200	-3.56544600	-0.14881900
H	-2.35858500	-2.14230500	-3.84909300
H	-4.15780200	-3.33572400	-2.61940000
C	-0.55243500	0.80632900	0.40290100
O	0.31739100	1.33656800	1.10764100
C	-1.98375400	0.74613200	0.92200800
C	-3.12713100	0.46639700	0.16667700
C	-2.11985300	0.97778900	2.29427600
C	-4.37937600	0.42992200	0.77373200
H	-3.07012800	0.23041700	-0.89377000
C	-3.37047100	0.92876500	2.90153600
H	-1.22210300	1.21872300	2.85486800
C	-4.50512900	0.65816400	2.14101500
H	-5.25587100	0.20852400	0.17355900
H	-3.45975900	1.11280000	3.96735600
H	-5.48295800	0.62450800	2.61031500
C	-0.28107700	2.74410500	-1.30596300
N	1.47896300	4.36941100	-1.64003100
H	2.28541400	4.79418200	-1.19681300
H	1.71352000	4.25164100	-2.62106000
N	-0.53011600	1.27536900	-1.10747700
H	0.24858900	0.73821100	-1.56668400
H	-1.39876700	1.00032600	-1.56650900
C	1.18975100	3.07721600	-1.02445900
H	1.82367500	2.24962100	-1.38037900
H	1.33219800	3.14243600	0.05422800
H	-0.45484100	2.91095500	-2.37741200
C	-1.24375400	3.59493800	-0.49641100
H	-2.28754800	3.38645100	-0.74914100
H	-1.09424300	3.41518800	0.57076800
H	-1.02396200	4.64088500	-0.71776200

A-TS-DCM

Sum of electronic and thermal Free Energies= -1299.891882

Imaginary frequency= -225.13

0 1

C	5.86740900	-0.89404400	1.31949200
C	5.84667800	-0.74143800	-0.21597500

C	4.38704800	-0.39410000	-0.57105100
H	6.56495800	-1.66739500	1.65670700
H	6.16861100	0.03910100	1.81595200
H	6.10464400	-1.70220200	-0.67246900
H	6.56018500	0.00112900	-0.58026600
H	4.22957500	0.68999500	-0.65039300
H	4.06092700	-0.82629100	-1.51977200
C	4.43019200	-1.21274800	1.64245400
H	4.09874100	-1.57574200	2.61049500
C	3.61305500	-0.93325800	0.61735300
C	-0.10554500	-0.99221900	0.06828300
C	1.25420600	-0.82489100	-0.50145000
O	1.51950500	-0.44495700	-1.65481400
C	2.15702800	-1.04065800	0.61897900
N	0.17401100	-1.44289200	1.39494100
H	-0.46915300	-1.28403200	2.16319600
N	1.46077300	-1.30229900	1.70354000
C	-1.13987700	-1.74987600	-0.69392400
C	-2.10638700	-2.49917800	-0.00887700
C	-1.20809200	-1.68948300	-2.09327000
C	-3.12330900	-3.15064300	-0.69904900
H	-2.06756800	-2.56953200	1.07396600
C	-2.23033100	-2.34107100	-2.77992500
H	-0.44509700	-1.15209700	-2.64652100
C	-3.19707900	-3.06750100	-2.08816300
H	-3.86247500	-3.72261600	-0.14659900
H	-2.26378400	-2.28485100	-3.86374300
H	-3.99357300	-3.57169900	-2.62589600
C	-0.56917600	0.80984700	0.37990400
O	0.30601000	1.36326000	1.07512200
C	-1.99146200	0.73232200	0.93096500
C	-3.14427000	0.44771100	0.19065400
C	-2.10914700	0.94794400	2.30759900
C	-4.38771200	0.39501100	0.81725300
H	-3.10067900	0.23997100	-0.87597200
C	-3.35001900	0.88344200	2.93503500
H	-1.20805700	1.18336300	2.86446400
C	-4.49471900	0.60949900	2.18947800
H	-5.27289600	0.17640300	0.22828600
H	-3.42319200	1.05589000	4.00435000
H	-5.46509200	0.56389900	2.67368200
C	-0.38378900	2.78611600	-1.30998300
N	1.33399200	4.44929800	-1.70625300
H	2.21465600	4.82435200	-1.36600200

H	1.45173500	4.32196200	-2.70874900
N	-0.59270000	1.30645000	-1.11867900
H	0.17247800	0.81163900	-1.61755700
H	-1.46530200	1.03569500	-1.57711400
C	1.08420000	3.15599800	-1.07465500
H	1.72452200	2.34280800	-1.45219200
H	1.26451000	3.23494300	-0.00227100
H	-0.59893100	2.94801500	-2.37311900
C	-1.34706900	3.60025500	-0.46585200
H	-2.38990400	3.36333500	-0.69513800
H	-1.16405400	3.42507100	0.59707800
H	-1.17343700	4.65633600	-0.68336400

B-TS-gas (a-TS-gas)

Sum of electronic and thermal Free Energies= -1299.855405

Imaginary frequency=-224.13

0 1

C	5.79094300	-0.89555600	1.17605400
C	5.73600400	-0.97446500	-0.36515000
C	4.26028100	-0.72724300	-0.73877600
H	6.50849000	-1.60175900	1.60653000
H	6.09187600	0.10362300	1.52152200
H	6.01743900	-1.98431100	-0.67881100
H	6.42139800	-0.27691900	-0.85217200
H	4.06269200	0.31969300	-1.00455600
H	3.92577500	-1.31869900	-1.59391500
C	4.36622600	-1.17997700	1.57706700
H	4.05434100	-1.38704200	2.59513700
C	3.52576000	-1.08237700	0.53977200
C	-0.17205600	-1.17215700	0.06955900
C	1.15763200	-1.03562300	-0.53320200
O	1.41597200	-0.67957300	-1.70043500
C	2.07402700	-1.21693300	0.58520600
N	0.10381000	-1.58422400	1.39747600
H	-0.51889100	-1.35608800	2.16277000
N	1.40432200	-1.44208100	1.69186500
C	-1.32432700	-1.74150100	-0.65117900
C	-2.38876200	-2.32794900	0.04816900
C	-1.42079500	-1.63727600	-2.04992700
C	-3.52532800	-2.76453500	-0.62095200
H	-2.32870400	-2.43404300	1.12718000
C	-2.56659300	-2.07051400	-2.71279300
H	-0.56957900	-1.25449900	-2.60638700
C	-3.62896600	-2.62489300	-2.00356700

H	-4.33841800	-3.21066700	-0.05682000
H	-2.62007700	-1.98650300	-3.79399600
H	-4.52079000	-2.95938600	-2.52300100
C	-0.48424300	0.82504700	0.41261300
O	0.43184400	1.26483200	1.11590700
C	-1.89901500	0.81480200	0.93719000
C	-3.05484000	0.69150600	0.16028300
C	-2.01953100	0.91534000	2.32750800
C	-4.30750000	0.66935600	0.76691600
H	-3.00665900	0.57670500	-0.92001900
C	-3.27130300	0.87823000	2.93146100
H	-1.11016500	1.04084200	2.90696400
C	-4.41939000	0.75762000	2.15123100
H	-5.19546600	0.56719000	0.15188300
H	-3.35178000	0.95485800	4.01093200
H	-5.39770800	0.73309900	2.61997800
C	0.54980900	4.89566100	-1.31641000
C	0.53303100	3.50988600	-0.68415300
H	1.29235300	5.53060600	-0.82621200
H	0.80570800	4.82017100	-2.37827700
H	-0.42352400	5.38604800	-1.22658800
C	-0.61846200	2.70333400	-1.30287400
H	0.34485900	3.59979200	0.39195000
H	-1.58961000	2.99119200	-0.89111800
H	-0.62229700	2.84693600	-2.38807500
N	1.77722200	2.79576400	-0.96138300
H	2.55447600	3.44367200	-1.03181700
H	1.96697900	2.16239300	-0.18537900
N	-0.42875000	1.24390500	-1.07551600
H	0.51179300	0.96787700	-1.43540900
H	-1.09889100	0.69090800	-1.61744100

B-TS-DCM (a-TS-DCM)

Sum of electronic and thermal Free Energies= -1299.898385

Imaginary frequency=-248.90

0 1

C	5.81742100	-0.85194700	1.24107600
C	5.78574100	-0.96173700	-0.29816500
C	4.32139800	-0.69036600	-0.69822800
H	6.51733400	-1.55856300	1.69883300
H	6.12409800	0.15073300	1.57105600
H	6.05029500	-1.98376500	-0.58740700
H	6.49112200	-0.28655500	-0.78796200
H	4.15356600	0.35874200	-0.97588600

H	3. 99175600	-1. 28881500	-1. 55094300
C	4. 38263500	-1. 10929500	1. 62449000
H	4. 05870900	-1. 29488700	2. 64403700
C	3. 55750500	-1. 01505800	0. 57221800
C	-0. 15506500	-1. 06706900	0. 06707800
C	1. 19274600	-0. 94296500	-0. 52826400
O	1. 46173200	-0. 61240300	-1. 69539200
C	2. 10275500	-1. 13083400	0. 59468900
N	0. 12590400	-1. 48935600	1. 39717500
H	-0. 51223700	-1. 32482800	2. 16750700
N	1. 41764600	-1. 35775600	1. 69419300
C	-1. 25460400	-1. 75259900	-0. 65822900
C	-2. 26639200	-2. 41512000	0. 05202400
C	-1. 33756000	-1. 70810600	-2. 05852200
C	-3. 33614100	-3. 00125700	-0. 61569900
H	-2. 22020500	-2. 46938300	1. 13590500
C	-2. 41446000	-2. 29335700	-2. 72172600
H	-0. 54021500	-1. 23491100	-2. 62332800
C	-3. 42115800	-2. 93665400	-2. 00586900
H	-4. 10878300	-3. 50804000	-0. 04560300
H	-2. 45881100	-2. 25133400	-3. 80583700
H	-4. 25955600	-3. 39025100	-2. 52457700
C	-0. 53581900	0. 81900700	0. 37897700
O	0. 37483800	1. 32179300	1. 06719400
C	-1. 94688900	0. 79190700	0. 93770500
C	-3. 11499400	0. 64378800	0. 18198900
C	-2. 04622400	0. 90431000	2. 32835100
C	-4. 35753000	0. 61240600	0. 81144700
H	-3. 08447500	0. 53794300	-0. 89957700
C	-3. 28712500	0. 85799000	2. 95648400
H	-1. 13245300	1. 04048700	2. 89788900
C	-4. 44718400	0. 71390300	2. 19785200
H	-5. 25628100	0. 49979400	0. 21344100
H	-3. 34853800	0. 94390500	4. 03684500
H	-5. 41727900	0. 68301700	2. 68373800
C	0. 36057900	4. 95202600	-1. 39267200
C	0. 40058200	3. 57341500	-0. 74868300
H	1. 11661200	5. 60419400	-0. 94640000
H	0. 56059600	4. 87354700	-2. 46660100
H	-0. 61726700	5. 42274300	-1. 25512700
C	-0. 76385000	2. 74211000	-1. 30011800
H	0. 26695200	3. 67413000	0. 33405900
H	-1. 71409200	3. 00833000	-0. 83198900
H	-0. 84050200	2. 88439200	-2. 38198700

N	1. 65410700	2. 88660500	-1. 07701000
H	2. 41388300	3. 56186100	-1. 10552200
H	1. 86259600	2. 24263700	-0. 31370100
N	-0. 53774200	1. 27897800	-1. 10212300
H	0. 39155000	1. 04518100	-1. 49808700
H	-1. 21853400	0. 74829000	-1. 65205700

C-TS-gas

Sum of electronic and thermal Free Energies= -1299. 853781

Imaginary frequency= -259. 34

O 1

C	5. 74814500	-1. 15413700	1. 26722900
C	5. 72276700	-0. 90718000	-0. 25631800
C	4. 26749100	-0. 51521400	-0. 58272800
H	6. 43442500	-1. 95824100	1. 55150600
H	6. 06847500	-0. 25855500	1. 81754200
H	5. 96313900	-1. 84218800	-0. 77159500
H	6. 44748700	-0. 15638900	-0. 57871900
H	4. 13123900	0. 57507100	-0. 59840400
H	3. 92813500	-0. 88392700	-1. 55310900
C	4. 30726800	-1. 46679600	1. 57834200
H	3. 96731900	-1. 88035300	2. 52180700
C	3. 49300400	-1. 11264900	0. 57697500
C	-0. 21264700	-1. 06760500	0. 04204800
C	1. 14037800	-0. 91219900	-0. 52134100
O	1. 41584400	-0. 44973700	-1. 64955700
C	2. 03635400	-1. 19790700	0. 58536600
N	0. 04375000	-1. 57345400	1. 34864000
H	-0. 58157400	-1. 37265000	2. 12002300
N	1. 33947200	-1. 47875000	1. 66361000
C	-1. 31592900	-1. 67323700	-0. 74263000
C	-2. 36560900	-2. 33560000	-0. 09265200
C	-1. 37643300	-1. 53406000	-2. 13845200
C	-3. 45771600	-2. 81256000	-0. 80772700
H	-2. 33003500	-2. 47104800	0. 98374500
C	-2. 47621100	-2. 00866300	-2. 84886600
H	-0. 53712600	-1. 08595300	-2. 66216700
C	-3. 52744100	-2. 63895700	-2. 18803800
H	-4. 26101400	-3. 31810200	-0. 28123000
H	-2. 50217400	-1. 89600600	-3. 92835100
H	-4. 38392300	-3. 00517000	-2. 74415100
C	-0. 56515000	0. 81110500	0. 43567200
O	0. 35317000	1. 27883100	1. 12419800
C	-1. 97691800	0. 80227400	0. 99361600

C	-3.15129500	0.63203900	0.25378200
C	-2.06406600	0.95947300	2.38066900
C	-4.38793400	0.62180500	0.89349100
H	-3.13340300	0.46903500	-0.82141900
C	-3.29938700	0.93591200	3.01878300
H	-1.14082500	1.11879800	2.92874300
C	-4.46547900	0.76951400	2.27517800
H	-5.29051200	0.48553700	0.30690600
H	-3.35252500	1.05861300	4.09569900
H	-5.43133100	0.75564100	2.76957800
C	0.82884000	4.82487000	-1.36085000
C	0.73586300	3.43934900	-0.72934400
H	1.68923200	5.35577300	-0.95190400
H	0.96424200	4.74298500	-2.44551600
H	-0.07419900	5.41480800	-1.17472100
C	-0.56957400	2.77219400	-1.22373600
H	0.66486300	3.53492600	0.35550000
H	-1.44565500	3.16545400	-0.69927700
H	-0.69577200	2.95502100	-2.29759600
N	1.94590100	2.68356100	-0.98953800
H	1.98319800	1.86864000	-0.38209400
H	2.03061300	2.38046300	-1.95654000
N	-0.56297700	1.29339900	-1.05381900
H	0.30533000	0.88439600	-1.47721500
H	-1.34268500	0.86674800	-1.55721200

C-TS-DCM

Sum of electronic and thermal Free Energies= -1299.896035

Imaginary frequency= -252.62

0 1

C	5.75611900	-1.08953800	1.31064700
C	5.74480700	-0.87402800	-0.21737000
C	4.28888800	-0.50562300	-0.56714700
H	6.44722600	-1.88032100	1.61957600
H	6.05994900	-0.17929300	1.84637600
H	6.00152500	-1.81641700	-0.71140000
H	6.46350700	-0.12035100	-0.54673400
H	4.13688900	0.58203100	-0.60851500
H	3.96599800	-0.90143400	-1.53267500
C	4.31521800	-1.41158700	1.61309700
H	3.97559900	-1.80875500	2.56482600
C	3.50531600	-1.08534500	0.59614900
C	-0.20574800	-1.03368000	0.03703600
C	1.15717200	-0.89783500	-0.52675900

O	1. 44429400	-0. 48216500	-1. 66481700
C	2. 04803600	-1. 17191600	0. 58900500
N	0. 05232200	-1. 52589900	1. 35026300
H	-0. 59177700	-1. 38961700	2. 12134200
N	1. 34086800	-1. 44134700	1. 66608100
C	-1. 28874500	-1. 69550100	-0. 74046100
C	-2. 30961300	-2. 39024500	-0. 07664800
C	-1. 34624400	-1. 59399600	-2. 13849100
C	-3. 36582300	-2. 95093000	-0. 78713700
H	-2. 28172500	-2. 49090500	1. 00424700
C	-2. 40849700	-2. 15420700	-2. 84485200
H	-0. 54234200	-1. 09675000	-2. 67230600
C	-3. 42642500	-2. 82837900	-2. 17429300
H	-4. 14638600	-3. 48328800	-0. 25239300
H	-2. 43291900	-2. 06808300	-3. 92690200
H	-4. 25378100	-3. 26189500	-2. 72679800
C	-0. 57245700	0. 80929400	0. 39713200
O	0. 36058400	1. 30442400	1. 06285000
C	-1. 97013000	0. 80001200	0. 99899200
C	-3. 16353000	0. 62694100	0. 28926900
C	-2. 02395300	0. 95907600	2. 38777200
C	-4. 38460900	0. 62004900	0. 96072000
H	-3. 17272500	0. 47319200	-0. 78668200
C	-3. 24309800	0. 93966900	3. 05810600
H	-1. 09107600	1. 10952000	2. 92123700
C	-4. 42826900	0. 77229000	2. 34445900
H	-5. 30256200	0. 48674300	0. 39708700
H	-3. 26788500	1. 06357500	4. 13623600
H	-5. 38179000	0. 76146400	2. 86295000
C	0. 64790500	4. 88367800	-1. 40778700
C	0. 62053700	3. 49303200	-0. 78390500
H	1. 48987100	5. 45474600	-1. 01071400
H	0. 76361600	4. 81359100	-2. 49548300
H	-0. 27583800	5. 43229200	-1. 19878500
C	-0. 66310400	2. 78227400	-1. 25602100
H	0. 57393800	3. 58220400	0. 30270500
H	-1. 54362300	3. 15109200	-0. 72383800
H	-0. 80831700	2. 94684000	-2. 32889000
N	1. 85598300	2. 78031200	-1. 08792900
H	1. 89979700	1. 93519800	-0. 52124200
H	1. 89484400	2. 50665800	-2. 06889200
N	-0. 61547000	1. 29964200	-1. 08384800
H	0. 24137800	0. 93030900	-1. 53998200
H	-1. 39886800	0. 87959400	-1. 58966600

D-TS1-gas

Sum of electronic and thermal Free Energies= -1299.823518

Imaginary frequency= -1425.97

0 1

C	-4.76320600	-2.26411600	0.69918700
C	-4.19703900	-2.54262700	-0.70934400
C	-2.68204900	-2.30099900	-0.57698500
H	-5.78288200	-1.86658600	0.67430100
H	-4.79230400	-3.17486800	1.31334200
H	-4.61456300	-1.80543900	-1.40477800
H	-4.44319800	-3.53896500	-1.08213400
H	-2.15095100	-3.21321100	-0.27283900
H	-2.19938500	-1.94702600	-1.49012800
C	-3.75744100	-1.29100700	1.26456400
H	-3.91595700	-0.69093000	2.15581000
C	-2.61604000	-1.29826600	0.56043600
C	0.73939200	0.38725200	0.80812500
C	-0.47579500	0.10962600	-0.14902100
O	-0.32449900	-0.39085900	-1.39050200
C	-1.43343500	-0.49380400	0.86960800
N	-0.03017600	0.73875500	2.00682900
H	0.50483400	0.55734200	2.85300900
N	-1.14851100	-0.09882700	2.05777600
C	1.66094400	1.49891300	0.34044800
C	2.21717100	1.46018300	-0.94469400
C	1.95901300	2.57606000	1.17995000
C	3.06176300	2.47929100	-1.37204700
H	1.96594500	0.64007900	-1.60849300
C	2.81014000	3.59081900	0.74826500
H	1.51090000	2.62585600	2.16626700
C	3.36626300	3.54338400	-0.52612700
H	3.48356200	2.43990100	-2.37106700
H	3.03585600	4.41955200	1.41156300
H	4.03036600	4.33350700	-0.86107300
C	1.64722300	-0.84836200	1.19142700
O	1.72521100	-1.11012100	2.37404900
C	2.54811900	-1.57165000	0.23609500
C	2.21580300	-1.89382300	-1.08235600
C	3.77735400	-1.98917800	0.76384000
C	3.11616500	-2.61810000	-1.86059200
H	1.25333600	-1.58936800	-1.48203400
C	4.67734700	-2.69213800	-0.02463000

H	4.00879000	-1.75155700	1.79642000
C	4.34618000	-3.00919100	-1.34130500
H	2.84985200	-2.87792000	-2.88008700
H	5.63350000	-2.99832500	0.38702300
H	5.04577900	-3.56461200	-1.95827000
C	-2.58400500	3.39373700	-0.51023600
C	-2.43236300	1.88247500	-0.39948300
H	-2.02367500	3.90968800	0.27475600
H	-2.23227300	3.74545800	-1.48542000
H	-3.63554600	3.67422100	-0.40659800
C	-3.29936800	1.13284600	-1.42797700
H	-2.71832300	1.56385500	0.61085900
H	-3.19299400	1.63436700	-2.39869000
H	-2.90136800	0.12326500	-1.56132400
N	-1.01240700	1.51606000	-0.61096200
H	-0.70779100	0.87689100	-1.60294500
H	-0.38411600	2.26923600	-0.32541100
N	-4.70941300	1.02810500	-1.10124400
H	-4.80950000	0.53227000	-0.21826800
H	-5.13285500	1.94456800	-0.99184700

D-TS1-DCM

Sum of electronic and thermal Free Energies= -1299.860198

Imaginary frequency=-1507.40

0 1

C	-4.88631700	-2.12789800	0.68112800
C	-4.31903800	-2.45553000	-0.71591500
C	-2.79683800	-2.26793600	-0.57828700
H	-5.88377300	-1.67925100	0.63950900
H	-4.96657600	-3.02656800	1.30841100
H	-4.70227600	-1.71790800	-1.43039100
H	-4.59919200	-3.44954600	-1.07125800
H	-2.29972800	-3.19842900	-0.27185300
H	-2.30447000	-1.93207700	-1.49305400
C	-3.84372400	-1.19480700	1.24454900
H	-3.99668300	-0.56921700	2.11955200
C	-2.69710400	-1.25871200	0.55161400
C	0.71532200	0.31641100	0.80757300
C	-0.51601100	0.10451800	-0.14757600
O	-0.37179400	-0.42342800	-1.38706100
C	-1.48571100	-0.49834900	0.86603600
N	-0.02867400	0.64529800	2.02986400
H	0.50510200	0.43366600	2.86971700
N	-1.17226800	-0.15820800	2.06312100

C	1. 69346400	1. 40858600	0. 40907900
C	2. 09297800	1. 57436100	-0. 92281600
C	2. 23308300	2. 24774800	1. 38872600
C	3. 01054200	2. 56392700	-1. 26435500
H	1. 67091000	0. 93592600	-1. 69204700
C	3. 15644000	3. 23235400	1. 04460500
H	1. 92883700	2. 13960800	2. 42506000
C	3. 54840300	3. 39282700	-0. 28193800
H	3. 30470300	2. 68500500	-2. 30213200
H	3. 56675400	3. 87550900	1. 81664400
H	4. 26688700	4. 16101800	-0. 54971200
C	1. 53424100	-0. 99880200	1. 10067700
O	1. 44524000	-1. 47581100	2. 21420000
C	2. 53874500	-1. 57420900	0. 14728900
C	2. 35955500	-1. 65395100	-1. 23657500
C	3. 70468000	-2. 09307500	0. 72674400
C	3. 34328900	-2. 24461300	-2. 02680700
H	1. 43624900	-1. 28628400	-1. 67284000
C	4. 69113300	-2. 66186700	-0. 06924000
H	3. 82814700	-2. 03706800	1. 80338000
C	4. 51043900	-2. 73952100	-1. 45008900
H	3. 19403000	-2. 31891200	-3. 09945700
H	5. 59730300	-3. 04876600	0. 38582800
H	5. 27734300	-3. 18881800	-2. 07363900
C	-2. 53098200	3. 42168100	-0. 50928300
C	-2. 43029100	1. 90725800	-0. 40510500
H	-1. 95582800	3. 91196000	0. 28147800
H	-2. 16148400	3. 76547500	-1. 48094900
H	-3. 57435200	3. 73352400	-0. 40904900
C	-3. 31254600	1. 19561100	-1. 44461800
H	-2. 73519900	1. 59414700	0. 60121200
H	-3. 16453400	1. 69054400	-2. 41283000
H	-2. 96642500	0. 16514700	-1. 56680300
N	-1. 01804800	1. 49774100	-0. 61492200
H	-0. 73629600	0. 82833900	-1. 61593900
H	-0. 37694400	2. 24827300	-0. 34977000
N	-4. 73423900	1. 16907000	-1. 13579700
H	-4. 86293600	0. 70782100	-0. 23620400
H	-5. 08705100	2. 11739400	-1. 02833200

D-INT1-gas

Sum of electronic and thermal Free Energies= -1299.865042

0 1

C	-5. 15209300	-1. 36409800	0. 84034600
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C	-4. 54987400	-2. 09704500	-0. 37684500
C	-3. 02979100	-2. 07949200	-0. 13220700
H	-6. 06859700	-0. 81779500	0. 59456900
H	-5. 40726700	-2. 06198300	1. 64959100
H	-4. 76757600	-1. 51873400	-1. 28180700
H	-4. 95075800	-3. 10364600	-0. 51271100
H	-2. 69841400	-2. 95461600	0. 44347300
H	-2. 43882200	-2. 06366800	-1. 04971300
C	-4. 01860300	-0. 46632900	1. 27260300
H	-4. 12258000	0. 35414700	1. 97625600
C	-2. 85246000	-0. 84130600	0. 73104300
C	0. 73974800	0. 31047200	0. 96797900
C	-0. 49484300	0. 18690400	-0. 00141900
O	-0. 33321500	-0. 80827700	-0. 98416100
C	-1. 55227700	-0. 22348700	1. 02763100
N	0. 04911500	0. 69203400	2. 20438600
H	0. 53481400	0. 35450100	3. 03157300
N	-1. 21253400	0. 09589100	2. 21905200
C	1. 78827600	1. 32167300	0. 54613200
C	2. 30568400	1. 30977000	-0. 75536000
C	2. 26475300	2. 27101300	1. 45187200
C	3. 28628000	2. 21701000	-1. 13524300
H	1. 94632800	0. 57423200	-1. 46771100
C	3. 25531900	3. 17572600	1. 07257000
H	1. 84503400	2. 31223200	2. 45080700
C	3. 76974000	3. 14962000	-0. 21898600
H	3. 67582700	2. 19330200	-2. 14763700
H	3. 61836300	3. 90465700	1. 78975800
H	4. 53914900	3. 85538900	-0. 51465400
C	1. 36670100	-1. 11323300	1. 16468700
O	1. 06284600	-1. 74987000	2. 14595000
C	2. 34528200	-1. 68779400	0. 17599900
C	1. 94446000	-2. 74533000	-0. 64227500
C	3. 67433800	-1. 25977700	0. 15898900
C	2. 86291800	-3. 35084500	-1. 49314000
H	0. 91034100	-3. 07092500	-0. 61761900
C	4. 59214600	-1. 87673000	-0. 68645000
H	3. 99104800	-0. 44426800	0. 80249800
C	4. 18667700	-2. 91717800	-1. 51736400
H	2. 54550000	-4. 16666800	-2. 13441200
H	5. 62404200	-1. 54143800	-0. 69483600
H	4. 90214100	-3. 39296300	-2. 18036400
C	-2. 12421300	3. 36511300	-1. 24767300
C	-2. 14367100	1. 90071800	-0. 82720400

H	-1.70525600	3.99995400	-0.46095500
H	-1.52045000	3.48846600	-2.15194500
H	-3.13764800	3.72090000	-1.45171800
C	-2.84580200	1.02667800	-1.87885400
H	-2.71414600	1.81605400	0.11152900
H	-2.45496000	1.28975900	-2.87025300
H	-2.58477700	-0.02142900	-1.71267800
N	-0.75291000	1.46602000	-0.64396000
H	-0.13441500	-0.33039400	-1.80142000
H	-0.22947300	2.19681900	-0.17071700
N	-4.29848100	1.12415700	-1.89797400
H	-4.65010600	0.90027600	-0.96871700
H	-4.59291000	2.07399100	-2.10601600

D-INT1-DCM

Sum of electronic and thermal Free Energies= -1299.901974

0 1

C	-5.16499400	-1.32389500	0.87065400
C	-4.57038300	-2.08318600	-0.33364300
C	-3.04851500	-2.07220100	-0.09824800
H	-6.06959600	-0.76317700	0.61480700
H	-5.43440900	-2.00655200	1.68837100
H	-4.78841300	-1.52139400	-1.24884900
H	-4.97751900	-3.08991300	-0.44977300
H	-2.71851300	-2.95000800	0.47437800
H	-2.46583400	-2.05869100	-1.02128300
C	-4.02131900	-0.43706300	1.29545700
H	-4.12474400	0.39910200	1.98137200
C	-2.85870800	-0.83028300	0.75802900
C	0.74253300	0.31335000	0.96541600
C	-0.50382400	0.20141300	0.00585300
O	-0.36256800	-0.79259800	-0.97648200
C	-1.55264200	-0.21773600	1.04385200
N	0.06307900	0.69121500	2.20948000
H	0.56550800	0.38064000	3.03775800
N	-1.19634700	0.08926600	2.23469700
C	1.80322600	1.31729800	0.55510100
C	2.26415200	1.37406000	-0.76609300
C	2.36405700	2.17518400	1.50393800
C	3.26591700	2.26746200	-1.12791000
H	1.84594300	0.70870500	-1.51470900
C	3.37530100	3.06493200	1.14251100
H	2.00662200	2.15581100	2.52822700
C	3.82860800	3.11316300	-0.17237600

H	3.60942400	2.29997000	-2.15689700
H	3.80346400	3.72280500	1.89216600
H	4.61396600	3.80733700	-0.45426000
C	1.34980100	-1.11924800	1.13545300
O	1.01552900	-1.78722300	2.08896900
C	2.33083900	-1.68627000	0.14619400
C	1.93476300	-2.77204200	-0.63974800
C	3.65329200	-1.23733900	0.09812900
C	2.84854800	-3.38270400	-1.49279500
H	0.90746000	-3.11803800	-0.59040100
C	4.56802700	-1.86262200	-0.74655400
H	3.97069600	-0.40762800	0.72244300
C	4.16577900	-2.92855600	-1.54767400
H	2.53366600	-4.21738900	-2.11098100
H	5.59516800	-1.51348700	-0.77708100
H	4.87853200	-3.40827200	-2.21118900
C	-2.13423900	3.37002000	-1.26613100
C	-2.15665800	1.90786700	-0.83924100
H	-1.72505500	4.00625000	-0.47493100
H	-1.51715200	3.49182000	-2.16234600
H	-3.14480900	3.72437700	-1.48698900
C	-2.82443400	1.02505700	-1.90398300
H	-2.75267700	1.82442800	0.08322000
H	-2.39008800	1.26836300	-2.88217000
H	-2.58794800	-0.02420600	-1.71071400
N	-0.76471300	1.48827500	-0.61471900
H	-0.10895600	-0.33490600	-1.79340100
H	-0.28133800	2.21882500	-0.09812300
N	-4.27707400	1.14948400	-1.98010000
H	-4.66348100	0.94249000	-1.05946400
H	-4.53298200	2.11365400	-2.18172400

D-TS2-gas

Sum of electronic and thermal Free Energies= -1299.685982

Imaginary frequency= -351.17

O 1

C	4.62314100	-3.11847700	0.64824900
C	4.23182800	-2.34838000	1.92834700
C	2.82584800	-1.78233600	1.64578500
H	5.69322400	-3.05585400	0.42962400
H	4.38110100	-4.18733800	0.72465200
H	4.92694600	-1.51597700	2.06906700
H	4.26756200	-2.96683200	2.82705900
H	2.03865700	-2.44322000	2.03383200

H	2. 65880300	-0. 80031400	2. 10039600
C	3. 77016200	-2. 46842700	-0. 40978500
H	3. 91353700	-2. 60802900	-1. 47604000
C	2. 78963000	-1. 73172800	0. 12891300
C	0. 08143500	0. 56690300	-1. 09343400
C	0. 50082200	-0. 46050800	-0. 04637300
O	-0. 17682700	-1. 45290800	0. 55972100
C	1. 78213400	-0. 95650500	-0. 58276800
N	0. 69101900	-0. 06176000	-2. 26203900
H	0. 84000600	0. 46490800	-3. 11453300
N	1. 76827800	-0. 77745200	-1. 88224500
C	0. 87456400	1. 93237600	-0. 90544000
C	2. 25379600	1. 99340700	-1. 16661100
C	0. 24024400	3. 13521700	-0. 56167400
C	2. 96885500	3. 17927700	-1. 04522900
H	2. 81247900	1. 12014700	-1. 47734500
C	0. 96192300	4. 32299600	-0. 44492500
H	-0. 83665200	3. 14325900	-0. 44420100
C	2. 32929700	4. 35676300	-0. 67332200
H	4. 03485200	3. 17387200	-1. 24903100
H	0. 42859800	5. 23110800	-0. 18218700
H	2. 88697200	5. 28282800	-0. 57838600
C	-1. 49382000	0. 75303400	-0. 73667900
O	-2. 10254600	1. 82463100	-1. 03066300
C	-2. 34773100	-0. 50075700	-1. 02805100
C	-1. 91490900	-1. 68528400	-1. 62616400
C	-3. 71416400	-0. 35451200	-0. 76683600
C	-2. 81100300	-2. 71840600	-1. 89660600
H	-0. 87490700	-1. 81323800	-1. 90726100
C	-4. 60716900	-1. 39092600	-1. 01189700
H	-4. 05659200	0. 60533600	-0. 39585900
C	-4. 15674100	-2. 58425300	-1. 57271300
H	-2. 45298900	-3. 62806200	-2. 36931100
H	-5. 66068100	-1. 26053200	-0. 78406900
H	-4. 85194000	-3. 39256500	-1. 77648500
C	-2. 24659200	-0. 89694600	2. 29441700
C	-1. 92814100	0. 55181000	1. 93232100
H	-2. 51505700	-1. 48643900	1. 41863500
H	-1. 39208900	-1. 37101100	2. 78709800
H	-3. 09588200	-0. 90676700	2. 98351900
C	-1. 43717000	1. 33327800	3. 16559700
H	-2. 85758200	1. 03307600	1. 57373000
H	-0. 47668400	0. 90622800	3. 48132100
N	-0. 95531200	0. 73922400	0. 85024400

H	-0.58970700	1.68332400	0.94972400
N	-2.32727600	1.36353700	4.31483800
H	-3.24308600	1.70640600	4.03717800
H	-2.46248000	0.42688700	4.68192300
H	-1.23744300	2.37066400	2.86711400
H	0.26163000	-2.29619500	0.36105300

D-TS2-DCM

Sum of electronic and thermal Free Energies= -1299.729147

Imaginary frequency= -301.01

O 1

C	4.75642900	-2.98622800	0.52758200
C	4.18607300	-2.46225800	1.86329800
C	2.74640200	-2.01353700	1.54045000
H	5.82458500	-2.77950500	0.41303200
H	4.63235600	-4.07334000	0.42892300
H	4.76622200	-1.59129700	2.18134500
H	4.22738000	-3.20341700	2.66366600
H	2.02077100	-2.80961800	1.75821400
H	2.43333000	-1.13227200	2.11062700
C	3.91353600	-2.28008500	-0.50065800
H	4.15582300	-2.24080800	-1.55817400
C	2.81402600	-1.74580700	0.04842000
C	0.07950700	0.57564900	-1.05961200
C	0.48271100	-0.53005200	-0.08547800
O	-0.22913500	-1.53976000	0.40003400
C	1.77770800	-0.98957400	-0.63881900
N	0.61932000	-0.04597200	-2.26984900
H	0.78999200	0.52796000	-3.09120100
N	1.72131100	-0.77582600	-1.92469500
C	0.93868000	1.89288900	-0.83029300
C	2.26995300	1.95806000	-1.27731800
C	0.41543500	3.06531000	-0.25952300
C	3.04705900	3.10130600	-1.11727900
H	2.74563500	1.12061100	-1.77174300
C	1.19424100	4.21158900	-0.10281200
H	-0.63383900	3.10819000	-0.00230800
C	2.51863700	4.23939300	-0.51748800
H	4.07226700	3.09284300	-1.47366600
H	0.74031500	5.09281100	0.34027300
H	3.12313400	5.13208900	-0.39165500
C	-1.46370700	0.82264900	-0.64610100
O	-2.00389300	1.96078500	-0.89441700
C	-2.41762200	-0.34057000	-1.02171600

C	-2.08771600	-1.51269800	-1.70702500
C	-3.76949200	-0.10866600	-0.73567700
C	-3.06997400	-2.44322100	-2.05077900
H	-1.06241000	-1.71432800	-1.99401100
C	-4.74826900	-1.04461000	-1.05098600
H	-4.03650600	0.83820000	-0.27944600
C	-4.40088200	-2.22380500	-1.70993400
H	-2.78754100	-3.34238100	-2.59053900
H	-5.78606000	-0.84620300	-0.79919900
H	-5.16173400	-2.95341700	-1.97012900
C	-2.26116100	-1.04524000	2.22982300
C	-1.93135000	0.42324900	1.97275000
H	-2.54754700	-1.56751900	1.31701800
H	-1.40713900	-1.56655500	2.67383100
H	-3.10024800	-1.09936300	2.92949500
C	-1.40330900	1.09871500	3.25180600
H	-2.86116700	0.94208600	1.68005800
H	-0.44078800	0.63829400	3.50956000
N	-0.96079300	0.67530300	0.89733000
H	-0.55799200	1.58831700	1.08881500
N	-2.27379900	1.03929400	4.41852000
H	-3.19440500	1.39745600	4.17165600
H	-2.41327800	0.07085800	4.69495100
H	-1.20274100	2.15463700	3.02939400
H	0.26205300	-2.37686400	0.30136100

I-TS-gas

Sum of electronic and thermal Free Energies= -726.044351

Imaginary frequency=-1654.82

0 1

C	-5.06492500	0.32305000	0.16435600
C	-4.70368300	-1.17552500	0.07460800
C	-3.18472200	-1.24957300	0.33397000
H	-5.84643800	0.61042000	-0.54584400
H	-5.43428000	0.59425300	1.16295900
H	-4.90854500	-1.53014900	-0.93971400
H	-5.28213500	-1.79491700	0.76323100
H	-2.95306200	-1.47709100	1.38258100
H	-2.68837100	-2.01625800	-0.26588200
C	-3.74744500	1.00254900	-0.10335200
H	-3.64396200	2.06252600	-0.30994000
C	-2.71856900	0.15219800	-0.00580000
C	0.93202900	0.52932100	-0.17471900
C	-0.17910700	-0.30926900	-0.04940900

O	-0.20156400	-1.64909000	0.15564400
C	-1.31005100	0.50982700	-0.14098800
N	0.51817800	1.79153400	-0.41497100
H	-0.18893800	2.37797700	0.40802100
N	-0.91592700	1.77553100	-0.40282900
C	2.35484900	0.17621300	-0.07180100
C	3.27135400	1.08324000	0.47226000
C	2.81116600	-1.07179700	-0.51438700
C	4.61268900	0.74129900	0.58431600
H	2.91747900	2.05509900	0.80082900
C	4.15548600	-1.41339300	-0.39282300
H	2.12187600	-1.75599100	-1.00283500
C	5.05764400	-0.51065300	0.16075000
H	5.31532000	1.45198400	1.00722200
H	4.49868900	-2.38050700	-0.74557900
H	6.10555000	-0.77591400	0.25373400
H	0.66328400	-1.92308700	0.48877000

I-TS-DCM

Sum of electronic and thermal Free Energies= -726.068468

Imaginary frequency= -1667.26

O 1

C	-5.06847200	0.34394200	0.15980500
C	-4.72061300	-1.15667100	0.06273600
C	-3.20295900	-1.24515900	0.32443000
H	-5.84682800	0.64351000	-0.54890500
H	-5.43308800	0.61478700	1.16025900
H	-4.92694200	-1.50464400	-0.95382000
H	-5.30431200	-1.77377300	0.74902800
H	-2.97588100	-1.47679400	1.37324400
H	-2.71460400	-2.01444700	-0.27876900
C	-3.74553300	1.01383000	-0.10414300
H	-3.63962100	2.07615500	-0.30166800
C	-2.72231200	0.15396000	-0.00990100
C	0.93432000	0.50707200	-0.16479000
C	-0.18334700	-0.32573600	-0.04071600
O	-0.22522700	-1.66193000	0.16273600
C	-1.30913000	0.50090700	-0.14109500
N	0.52613100	1.77060500	-0.40814500
H	-0.18150700	2.35722000	0.42493500
N	-0.90687400	1.76484100	-0.40187000
C	2.36044500	0.16233100	-0.06130300
C	3.27174100	1.08905100	0.46087900
C	2.82457900	-1.08733900	-0.49184500

C	4. 61970300	0. 76497400	0. 56056200
H	2. 91318400	2. 06016800	0. 78882400
C	4. 17524100	-1. 40967200	-0. 38317100
H	2. 13925600	-1. 79474300	-0. 95103600
C	5. 07434400	-0. 48701500	0. 14517800
H	5. 31816400	1. 48932200	0. 96747300
H	4. 52462500	-2. 37904900	-0. 72409000
H	6. 12688900	-0. 73855800	0. 22788100
H	0. 61963700	-1. 95869000	0. 53509600

II-TS-gas

Sum of electronic and thermal Free Energies= -1452. 201760

Imaginary frequency= -514. 62

0 1

C	-4. 97224500	2. 62237800	0. 47190100
C	-4. 56399200	3. 88945900	-0. 31055000
C	-3. 13282100	3. 61674200	-0. 81868200
H	-5. 59850400	2. 84372000	1. 34074900
H	-5. 53672300	1. 91821400	-0. 15414700
H	-4. 54230100	4. 74017600	0. 37643100
H	-5. 25854900	4. 13242600	-1. 11663500
H	-3. 12663600	3. 22539400	-1. 84404700
H	-2. 49946700	4. 50657600	-0. 81323300
C	-3. 64554300	2. 01548700	0. 84536300
H	-3. 53804800	1. 22095100	1. 57823100
C	-2. 64249100	2. 54544600	0. 13405300
C	1. 00237400	1. 92358300	0. 10108400
C	-0. 07094500	2. 78605700	-0. 17470600
O	-0. 01976600	4. 04464200	-0. 68250400
C	-1. 25062100	2. 11900100	0. 18764700
N	0. 45983900	0. 79919000	0. 58831300
H	-1. 25239200	-0. 01828900	0. 96032400
N	-0. 86184800	0. 91814900	0. 64577500
C	2. 43869400	2. 12688900	-0. 11261700
C	3. 27732700	1. 05646200	-0. 44330900
C	2. 97022800	3. 41817300	0. 00462200
C	4. 63086000	1. 28572700	-0. 66250100
H	2. 87659600	0. 04989200	-0. 53776700
C	4. 32443600	3. 63752900	-0. 22196200
H	2. 32807500	4. 23904700	0. 31132000
C	5. 15513900	2. 57245000	-0. 55989500
H	5. 27157000	0. 44810600	-0. 91557000
H	4. 73141000	4. 63833500	-0. 12308900
H	6. 21176500	2. 74365700	-0. 73731400

H	0.75854400	4.11801500	-1.25093600
C	-5.11937900	-2.80276700	-0.58911500
C	-4.85811100	-1.90622700	0.63980800
C	-3.35442600	-1.57691000	0.58085900
H	-5.87697700	-3.56830800	-0.39172300
H	-5.48404000	-2.21630200	-1.44479500
H	-5.06010600	-2.47897800	1.54980900
H	-5.49107300	-1.01439100	0.66391200
H	-3.17844100	-0.62281400	0.05818500
H	-2.88835800	-1.50254400	1.56841400
C	-3.75465200	-3.37370900	-0.88190500
H	-3.57864100	-4.19353500	-1.56953300
C	-2.78062500	-2.70862100	-0.24849600
C	0.87903600	-2.85371100	-0.15267000
C	-0.29116200	-2.30433900	0.38436200
O	-0.37003800	-1.39250100	1.33565100
C	-1.34220300	-2.92890500	-0.36820400
N	-0.84872800	-3.78994700	-1.26314700
C	2.26724700	-2.54786600	0.14919100
C	3.28865800	-2.71803500	-0.80067900
C	2.60880400	-2.03667800	1.41541500
C	4.60720400	-2.40250400	-0.49034400
H	3.04265600	-3.07907600	-1.79567100
C	3.92658200	-1.70665100	1.71080600
H	1.82132000	-1.91899300	2.15306800
C	4.93391300	-1.89183200	0.76523500
H	5.38276700	-2.54838200	-1.23677000
H	4.17152500	-1.31320900	2.69255400
H	5.96247600	-1.64004800	1.00317000
H	0.69437500	-0.18789500	0.93156500
N	0.47126100	-3.71456000	-1.13731000
H	1.04421700	-4.36848500	-1.64537200

II-TS-DCM

Sum of electronic and thermal Free Energies= -1452.248255

Imaginary frequency= -114.17

0 1

C	-5.00942000	2.66736600	0.43358800
C	-4.60566100	3.95059000	-0.32420600
C	-3.16883700	3.70002400	-0.82862400
H	-5.63230400	2.86979300	1.30957700
H	-5.57375200	1.97374000	-0.20440500
H	-4.59571100	4.78975700	0.37722300
H	-5.29619100	4.19983800	-1.13201000

H	-3. 15023200	3. 33747600	-1. 86424200
H	-2. 54402400	4. 59523000	-0. 79149100
C	-3. 68287300	2. 05373700	0. 79324100
H	-3. 57505000	1. 24312700	1. 50926400
C	-2. 67881000	2. 60648200	0. 09915600
C	0. 96440000	1. 97627900	0. 06400000
C	-0. 10337500	2. 85153900	-0. 19251000
O	-0. 05379300	4. 12194400	-0. 65476100
C	-1. 28647100	2. 17938000	0. 14766200
N	0. 41635200	0. 83914500	0. 51624300
H	-1. 37919200	0. 10697300	0. 89848800
N	-0. 90471600	0. 96374800	0. 57329200
C	2. 40591000	2. 17461000	-0. 12137000
C	3. 23198800	1. 11913700	-0. 52573000
C	2. 95279600	3. 44529200	0. 09988700
C	4. 59249700	1. 34135700	-0. 71139400
H	2. 81111300	0. 13287200	-0. 70769400
C	4. 31441600	3. 65777900	-0. 08992900
H	2. 31834300	4. 25621100	0. 44606100
C	5. 13450600	2. 60800100	-0. 49810200
H	5. 22759200	0. 52100700	-1. 02927900
H	4. 73473000	4. 64218900	0. 08760700
H	6. 19608400	2. 77562400	-0. 64867300
H	0. 73218700	4. 23477900	-1. 21275600
C	-5. 09013300	-2. 97644400	-0. 52556500
C	-4. 83656800	-2. 05574000	0. 68644600
C	-3. 34467700	-1. 68189200	0. 59802600
H	-5. 82322700	-3. 76053700	-0. 30874300
H	-5. 48052100	-2. 41246600	-1. 38503300
H	-5. 00691600	-2. 62206700	1. 60750000
H	-5. 49476300	-1. 18314000	0. 70721100
H	-3. 20301000	-0. 73209700	0. 05856000
H	-2. 86496600	-1. 57209400	1. 57456500
C	-3. 71401600	-3. 51556200	-0. 82812200
H	-3. 53403000	-4. 34628400	-1. 50364400
C	-2. 74714900	-2. 81169200	-0. 22018600
C	0. 91932200	-2. 87199100	-0. 15249200
C	-0. 26206400	-2. 33556800	0. 39479900
O	-0. 36121500	-1. 43281700	1. 33601300
C	-1. 30313500	-2. 99299200	-0. 35128100
N	-0. 79234300	-3. 84979100	-1. 24794200
C	2. 30786600	-2. 55156900	0. 14473400
C	3. 33370600	-2. 76219600	-0. 79341300
C	2. 64296400	-1. 99043100	1. 39113500

C	4. 65081000	-2. 43329700	-0. 48920600
H	3. 09455800	-3. 17178500	-1. 77143500
C	3. 96135000	-1. 65448300	1. 68303600
H	1. 85262600	-1. 83231500	2. 11776300
C	4. 97249400	-1. 87590800	0. 74896500
H	5. 42966100	-2. 60497900	-1. 22661300
H	4. 20166400	-1. 22268300	2. 65017500
H	6. 00004900	-1. 61323000	0. 98014600
H	0. 72741900	-0. 09812700	0. 86023700
N	0. 52608300	-3. 75088900	-1. 12448100
H	1. 11928100	-4. 36617400	-1. 66343400

III-TS-gas

Sum of electronic and thermal Free Energies= -1452. 205071

Imaginary frequency= -509. 12

O 1

C	-4. 92224400	-2. 70802100	-0. 47616400
C	-4. 48916200	-3. 96695400	0. 30621000
C	-3. 06380000	-3. 66632600	0. 81482500
H	-5. 54283600	-2. 94206000	-1. 34575900
H	-5. 50236200	-2. 01639800	0. 14966900
H	-4. 45052100	-4. 81680200	-0. 38103400
H	-5. 17915000	-4. 22392800	1. 11188000
H	-3. 06492100	-3. 27613600	1. 84064700
H	-2. 41282900	-4. 54332600	0. 80872400
C	-3. 60737700	-2. 07471000	-0. 84834500
H	-3. 51471500	-1. 27964400	-1. 58275300
C	-2. 59422400	-2. 58503000	-0. 13693600
C	1. 03812800	-1. 89335300	-0. 10178300
C	-0. 01941700	-2. 77463600	0. 17838400
O	0. 05469000	-4. 02668400	0. 69799000
C	-1. 21036300	-2. 13358400	-0. 19091200
N	0. 47580800	-0. 78312200	-0. 59856200
H	-1. 25514700	-0. 00915800	-0. 98210900
N	-0. 84321600	-0. 92851500	-0. 65687600
C	2. 47693200	-2. 07378100	0. 11708700
C	3. 29721300	-0. 99310300	0. 45937000
C	3. 02787900	-3. 35672400	-0. 00531500
C	4. 65255100	-1. 20466400	0. 68629400
H	2. 88254700	0. 00747000	0. 55656300
C	4. 38355100	-3. 55799400	0. 22858000
H	2. 40010200	-4. 18485100	-0. 32257400
C	5. 19606300	-2. 48286500	0. 57913100
H	5. 27864900	-0. 35875700	0. 94809400

H	4. 80588000	-4. 55200000	0. 12547100
H	6. 25394900	-2. 63971100	0. 76234600
H	0. 84967000	-4. 08802700	1. 24458200
C	-5. 16218700	2. 77888100	0. 58427800
C	-4. 89787400	1. 88547600	-0. 64575400
C	-3. 39689400	1. 54953500	-0. 57950800
H	-5. 91947300	3. 54438100	0. 38658600
H	-5. 52702400	2. 18989500	1. 43803800
H	-5. 09337000	2. 46180000	-1. 55466800
H	-5. 53357400	0. 99625000	-0. 67404900
H	-3. 22233400	0. 59756000	-0. 05411200
H	-2. 92221000	1. 47691200	-1. 56284500
C	-3. 79767400	3. 35264000	0. 87596200
H	-3. 65101200	4. 18919900	1. 55288900
C	-2. 81901700	2. 68069400	0. 24883300
C	0. 84004900	2. 85609700	0. 19987800
C	-0. 33890900	2. 28632100	-0. 38506200
O	-0. 38626500	1. 39278400	-1. 35548600
C	-1. 38715200	2. 86481000	0. 34304800
N	0. 53903100	3. 69845100	1. 19030700
H	-1. 24362900	4. 26959100	1. 94165000
N	-0. 78577500	3. 69549200	1. 25342800
C	2. 23160100	2. 55566500	-0. 14999900
C	3. 25962700	2. 75704200	0. 78382000
C	2. 55984700	2. 04432800	-1. 41570700
C	4. 57694500	2. 45434100	0. 45992700
H	3. 00202200	3. 15812800	1. 75874200
C	3. 88064900	1. 73158200	-1. 72882300
H	1. 76730500	1. 91207900	-2. 14534700
C	4. 89391300	1. 93425000	-0. 79620100
H	5. 36257400	2. 62356200	1. 19102700
H	4. 11915600	1. 33696400	-2. 71176800
H	5. 92283900	1. 69243100	-1. 04447600
H	0. 69015300	0. 21012400	-0. 94425100

III-TS-DCM

Sum of electronic and thermal Free Energies= -1452. 249932

Imaginary frequency=-108. 16

O 1

C	-4. 92336100	2. 78953900	0. 40333700
C	-4. 48420400	4. 05879800	-0. 35849600
C	-3. 05012800	3. 77188400	-0. 85145700
H	-5. 54631100	3. 01146200	1. 27456700
H	-5. 50068600	2. 10629600	-0. 23428000

H	-4. 45953200	4. 90143000	0. 33840000
H	-5. 16315900	4. 31967600	-1. 17242400
H	-3. 03250300	3. 40419800	-1. 88529600
H	-2. 40447700	4. 65216900	-0. 81373900
C	-3. 61415100	2. 14620400	0. 77451100
H	-3. 53008500	1. 33777100	1. 49612200
C	-2. 59260200	2. 67155800	0. 08478500
C	1. 03486000	1. 95276900	0. 07595000
C	-0. 00969200	2. 85453700	-0. 18640400
O	0. 07389300	4. 12402600	-0. 64629600
C	-1. 21114300	2. 21160500	0. 14447900
N	0. 45593200	0. 82928100	0. 52393500
H	-1. 35906100	0. 14416200	0. 89840100
N	-0. 86211800	0. 98665500	0. 57123000
C	2. 48173200	2. 11926600	-0. 10061400
C	3. 28957200	1. 04642900	-0. 49613300
C	3. 05243900	3. 37975900	0. 11948500
C	4. 65491400	1. 24223600	-0. 67615000
H	2. 85211400	0. 06697800	-0. 67535800
C	4. 41884700	3. 56546400	-0. 06380900
H	2. 43223300	4. 20409700	0. 45973600
C	5. 22044500	2. 49879300	-0. 46467800
H	5. 27556100	0. 40875800	-0. 98823300
H	4. 85725200	4. 54208000	0. 11305000
H	6. 28581400	2. 64512100	-0. 61070100
H	0. 86566500	4. 21782800	-1. 19970800
C	-5. 17928700	-2. 85255600	-0. 49916800
C	-4. 90406400	-1. 99362300	0. 75280500
C	-3. 40664900	-1. 64321800	0. 67572300
H	-5. 92701600	-3. 63107000	-0. 31504900
H	-5. 56109200	-2. 24167700	-1. 32998100
H	-5. 08340100	-2. 59728500	1. 64787000
H	-5. 54417600	-1. 10972500	0. 81449200
H	-3. 24623100	-0. 67326500	0. 18065900
H	-2. 91794500	-1. 58769900	1. 65230400
C	-3. 81515000	-3. 40591100	-0. 83139600
H	-3. 66667500	-4. 21296200	-1. 54390000
C	-2. 83230500	-2. 74429200	-0. 19621300
C	0. 83225100	-2. 89926100	-0. 21888400
C	-0. 33772300	-2. 31884100	0. 38523600
O	-0. 37494600	-1. 42394700	1. 33876300
C	-1. 39949700	-2. 92011900	-0. 31907500
N	0. 51000700	-3. 76130000	-1. 19004100
H	-1. 28969000	-4. 35825600	-1. 89470000

N	-0.81699900	-3.76257200	-1.23032100
C	2.23187700	-2.60482900	0.10668100
C	3.25166400	-2.82510100	-0.83335800
C	2.57828000	-2.08454600	1.36463800
C	4.57668900	-2.53963800	-0.52166700
H	2.98962200	-3.22195800	-1.80952300
C	3.90661500	-1.79447100	1.66905100
H	1.79178700	-1.91958200	2.09371100
C	4.91120700	-2.02052900	0.73074100
H	5.35317900	-2.71785300	-1.26020400
H	4.15758700	-1.39489800	2.64730000
H	5.94553600	-1.79230200	0.96932000
H	0.73772800	-0.12001600	0.86429400

IV-TS-gas

Sum of electronic and thermal Free Energies= -1452.220652

Imaginary frequency= -1384.37

O 1

C	-2.70116200	4.86239700	0.19289600
C	-1.59305000	5.93612300	0.25021100
C	-0.29836500	5.21418100	-0.17610100
H	-3.44803000	4.98668900	0.98307300
H	-3.24579200	4.89078000	-0.76120300
H	-1.48502900	6.27967100	1.28310900
H	-1.81451000	6.80975300	-0.36640600
H	-0.08094900	5.34766600	-1.24391900
H	0.58382600	5.56150800	0.36663000
C	-1.92584800	3.57545100	0.31273500
H	-2.39481400	2.61632400	0.51431500
C	-0.61638600	3.75896800	0.10170400
C	2.28567200	1.49942000	0.00991500
C	1.79869000	2.81268000	0.01025100
O	2.51316800	3.97519200	-0.03576000
C	0.40164900	2.71580100	0.06992500
N	1.22302100	0.67996600	0.05524000
H	0.87911100	-0.52829700	0.08871500
N	0.09905800	1.40494200	0.10007200
C	3.66241700	1.00217900	-0.06775700
C	3.93581800	-0.22899100	-0.67746500
C	4.71871000	1.74725600	0.46992800
C	5.23821500	-0.70871400	-0.73637800
H	3.12040900	-0.79963600	-1.11355400
C	6.02370500	1.26907900	0.39433800
H	4.50765000	2.68219200	0.98146100

C	6. 28708900	0. 04130500	-0. 20609000
H	5. 43702300	-1. 66654700	-1. 20657200
H	6. 83457300	1. 85174600	0. 81943200
H	7. 30437700	-0. 33208300	-0. 25893100
H	3. 32174300	3. 81376900	-0. 53836800
C	2. 69701600	-4. 86976800	0. 19544500
C	1. 58593900	-5. 94061000	0. 24859600
C	0. 29462500	-5. 21440300	-0. 18022500
H	3. 44183500	-4. 99804500	0. 98706200
H	3. 24374000	-4. 89893500	-0. 75756000
H	1. 47425100	-6. 28480100	1. 28093700
H	1. 80671800	-6. 81439300	-0. 36818200
H	0. 08022400	-5. 34520100	-1. 24904400
H	-0. 59036000	-5. 56050500	0. 35872000
C	1. 92422800	-3. 58119200	0. 31611700
H	2. 39442700	-2. 62361500	0. 52166500
C	0. 61469600	-3. 76020500	0. 10119100
C	-2. 28296200	-1. 49863700	0. 00771500
C	-1. 79864800	-2. 81260700	0. 00998700
O	-2. 51528500	-3. 97487500	-0. 03398600
C	-0. 40185500	-2. 71545800	0. 06815300
N	-1. 22013600	-0. 67822900	0. 05016400
H	-0. 85482900	0. 56211700	0. 08972400
N	-0. 09613200	-1. 40463500	0. 09546900
C	-3. 65966800	-1. 00113700	-0. 06875700
C	-3. 93458800	0. 22810300	-0. 68206000
C	-4. 71621100	-1. 74300100	0. 47329500
C	-5. 23664500	0. 70893500	-0. 73980000
H	-3. 11937500	0. 79540600	-1. 12274400
C	-6. 02109900	-1. 26418200	0. 39883200
H	-4. 50491000	-2. 67652400	0. 98734900
C	-6. 28524800	-0. 03816100	-0. 20480100
H	-5. 43581200	1. 66512500	-1. 21337400
H	-6. 83145800	-1. 84507300	0. 82745300
H	-7. 30239800	0. 33577000	-0. 25681200
H	-3. 32578100	-3. 81060500	-0. 53241900

IV-TS-DCM

Sum of electronic and thermal Free Energies= -1452. 254514

Imaginary frequency= -38. 57

0 1

C	-2. 05912900	-5. 13808300	-0. 19882900
C	-0. 84498600	-6. 08399900	-0. 31711700
C	0. 37792100	-5. 24350800	0. 10627700

H	-2. 80718800	-5. 30830300	-0. 97873100
H	-2. 57537800	-5. 25096000	0. 76432900
H	-0. 72685200	-6. 38183900	-1. 36305500
H	-0. 95643100	-6. 99333700	0. 27674600
H	0. 63807100	-5. 39094400	1. 16232100
H	1. 27286000	-5. 47511500	-0. 47584800
C	-1. 43289700	-3. 77168600	-0. 28274000
H	-2. 01052600	-2. 86277300	-0. 43259500
C	-0. 10549000	-3. 82345400	-0. 10804000
C	2. 52789300	-1. 23862300	0. 01779300
C	2. 18750300	-2. 59898900	-0. 00656400
O	3. 01773100	-3. 67139800	0. 00027900
C	0. 78621400	-2. 67155800	-0. 05993600
N	1. 37197500	-0. 55965700	-0. 00693800
H	1. 06881200	0. 46937300	-0. 02487400
N	0. 34216300	-1. 40368000	-0. 06216300
C	3. 83246200	-0. 57277000	0. 08385500
C	3. 95458500	0. 67378900	0. 71092400
C	4. 95822100	-1. 17636200	-0. 48859300
C	5. 18894100	1. 31169600	0. 75313600
H	3. 08602200	1. 13531100	1. 17341700
C	6. 19265000	-0. 53569200	-0. 43355000
H	4. 86147200	-2. 12876700	-1. 00148700
C	6. 31007800	0. 70728000	0. 18454600
H	5. 27728100	2. 27842100	1. 23824600
H	7. 06116000	-1. 00505400	-0. 88396000
H	7. 27321900	1. 20583900	0. 22298200
H	3. 80217000	-3. 46715000	0. 53332100
C	1. 94227600	5. 30376000	-0. 16858800
C	0. 68592600	6. 18351000	-0. 34030100
C	-0. 49779200	5. 29026400	0. 08128000
H	2. 70101300	5. 50358300	-0. 93249000
H	2. 42580700	5. 47316100	0. 80415800
H	0. 57601900	6. 44336300	-1. 39779500
H	0. 73741200	7. 11665700	0. 22546400
H	-0. 77869400	5. 44462800	1. 13193500
H	-1. 39866000	5. 47056300	-0. 51053200
C	1. 38150600	3. 90596100	-0. 24330900
H	2. 00280100	3. 02231900	-0. 36030400
C	0. 04803700	3. 88584100	-0. 09944400
C	-2. 47971300	1. 23079400	0. 03027400
C	-2. 20182900	2. 60332100	-0. 00590200
O	-3. 08097900	3. 65347900	-0. 00253900
C	-0. 80384700	2. 70054500	-0. 04948900

N	-1.30517700	0.56577500	0.01929000
H	-0.61426600	-0.87180800	-0.04868700
N	-0.29698400	1.44667000	-0.03816600
C	-3.76755600	0.53046900	0.09332200
C	-3.85888000	-0.72862900	0.70592100
C	-4.92528100	1.09293500	-0.46271300
C	-5.06952900	-1.41125800	0.74652700
H	-2.97034900	-1.16063600	1.15805100
C	-6.13978000	0.41325400	-0.40659400
H	-4.86658600	2.05268700	-0.96846800
C	-6.21721900	-0.84121900	0.19432300
H	-5.12063300	-2.38686400	1.22106000
H	-7.02556900	0.86168600	-0.84616100
H	-7.16344000	-1.37151100	0.23261300
H	-3.86910200	3.39152400	0.49545200

Al-Et-TS-gas

Sum of electronic and thermal Free Energies= -1339.123420

Imaginary frequency= -221.10

0 1

C	5.85700600	-0.95007600	1.09982300
C	5.79523500	-0.90521100	-0.44253000
C	4.30699700	-0.69895000	-0.79066800
H	6.60905000	-1.65531100	1.46858300
H	6.11451300	0.03027200	1.52517900
H	6.12211500	-1.87138100	-0.83878700
H	6.44358000	-0.13829600	-0.87264900
H	4.05821200	0.35520800	-0.97160300
H	3.99481800	-1.23549200	-1.68934200
C	4.44951700	-1.33138500	1.48079000
H	4.15422600	-1.63355400	2.47985200
C	3.59833200	-1.18920400	0.45745900
C	-0.09526900	-1.39401900	-0.00309200
C	1.22318200	-1.15974900	-0.60022200
O	1.45945800	-0.70665800	-1.73791000
C	2.15418600	-1.39073600	0.49704200
N	0.20648600	-1.90173600	1.28529200
H	-0.41860100	-1.76085200	2.06943600
N	1.50252100	-1.73071400	1.58497400
C	-1.23374900	-1.94136900	-0.76135100
C	-2.27071200	-2.62160400	-0.10719700
C	-1.34635300	-1.72347200	-2.14568400
C	-3.39731400	-3.04064700	-0.80375800
H	-2.19719200	-2.81534700	0.95872600

C	-2.48219800	-2.14020700	-2.83567800
H	-0.51386700	-1.26544000	-2.67274400
C	-3.51807100	-2.78955900	-2.16914100
H	-4.18926400	-3.56111700	-0.27428100
H	-2.54840300	-1.96790200	-3.90567200
H	-4.40222300	-3.11107500	-2.70948700
C	-0.47682200	0.55682600	0.50879900
O	0.42133800	0.96467000	1.25308900
C	-1.89153700	0.45273600	1.02386900
C	-3.04171600	0.36204000	0.23425100
C	-2.01743700	0.42523600	2.41701900
C	-4.29376000	0.24474900	0.83093000
H	-2.98850300	0.34647000	-0.85173400
C	-3.26815700	0.29358000	3.00986200
H	-1.11372600	0.52922300	3.00942500
C	-4.41056100	0.20530500	2.21711000
H	-5.17696300	0.16912200	0.20529500
H	-3.35261700	0.27121800	4.09153500
H	-5.38814400	0.10693500	2.67761600
C	0.47999700	4.78926200	-0.87906800
C	0.47031300	3.35262800	-0.35954400
H	1.28637800	5.32595300	-0.36589400
H	0.74082400	4.76909100	-1.94522600
C	-0.67241800	2.57192500	-1.03113000
H	0.28198500	3.36425900	0.72169500
H	-1.64497500	2.78570700	-0.58075500
H	-0.70208800	2.81301300	-2.09937600
N	1.72349600	2.67696500	-0.68720500
H	2.48900700	3.34113700	-0.73036000
H	1.93166700	2.00199400	0.04785000
N	-0.43360100	1.10544900	-0.93720500
H	0.51584700	0.89744100	-1.31755100
H	-1.08517200	0.58037500	-1.52726300
C	-0.83896900	5.52923800	-0.66662800
H	-1.64827500	5.09845000	-1.26380800
H	-1.14197900	5.49295900	0.38444900
H	-0.74725000	6.57907300	-0.95312400

AI-Et-TS-DCM

Sum of electronic and thermal Free Energies= -1339.166544

Imaginary frequency= -237.90

0 1

C	5.92195000	-0.92659400	1.12450200
C	5.86258500	-0.77912400	-0.41070900

C	4. 37816600	-0. 52379100	-0. 74121100
H	6. 66560600	-1. 66216000	1. 44796600
H	6. 18549200	0. 02143000	1. 61418900
H	6. 17192100	-1. 72278900	-0. 87096600
H	6. 52240300	0. 00503700	-0. 78892100
H	4. 15053200	0. 54682800	-0. 83541700
H	4. 06128400	-0. 98718200	-1. 67812300
C	4. 51039400	-1. 31924800	1. 47795200
H	4. 21774200	-1. 68868100	2. 45604600
C	3. 65900600	-1. 09509500	0. 46697800
C	-0. 05491300	-1. 28231400	-0. 00299700
C	1. 27685700	-1. 04312900	-0. 60007200
O	1. 51497700	-0. 60771800	-1. 73828500
C	2. 21106800	-1. 27941400	0. 49482800
N	0. 26523000	-1. 81138100	1. 28032400
H	-0. 36708500	-1. 72584400	2. 06870300
N	1. 55406800	-1. 63523500	1. 57624500
C	-1. 13554700	-1. 94540100	-0. 77603200
C	-2. 09987400	-2. 72398600	-0. 11981200
C	-1. 25519600	-1. 75898900	-2. 16148900
C	-3. 15861800	-3. 28647100	-0. 82410100
H	-2. 02597500	-2. 88714300	0. 95141900
C	-2. 32080000	-2. 32160800	-2. 86160700
H	-0. 49340300	-1. 19436700	-2. 69048400
C	-3. 28042700	-3. 08189300	-2. 19794400
H	-3. 89455000	-3. 88409300	-0. 29490000
H	-2. 39328700	-2. 16841200	-3. 93410400
H	-4. 11041600	-3. 51736200	-2. 74496300
C	-0. 52868900	0. 53856400	0. 48887000
O	0. 34598400	1. 01093900	1. 24322400
C	-1. 94361800	0. 38496500	1. 01766800
C	-3. 09695800	0. 28675800	0. 23205400
C	-2. 06110100	0. 31216400	2. 40950700
C	-4. 34237700	0. 11783600	0. 83304500
H	-3. 05103100	0. 32592800	-0. 85342300
C	-3. 30403400	0. 12658900	3. 00746600
H	-1. 16064200	0. 41751400	3. 00643900
C	-4. 44921900	0. 03074500	2. 21920700
H	-5. 22949700	0. 04602900	0. 21184100
H	-3. 37911600	0. 06784200	4. 08877100
H	-5. 42087200	-0. 10798900	2. 68264600
C	0. 25342200	4. 86386000	-0. 89602400
C	0. 30229900	3. 43564800	-0. 35535300
H	1. 05976400	5. 43210700	-0. 41776100

H	0.47786300	4.83293500	-1.97016500
C	-0.83287600	2.61269200	-0.98310500
H	0.14578900	3.46096500	0.73029300
H	-1.79023500	2.78011500	-0.48543600
H	-0.92902000	2.86137800	-2.04485200
N	1.57760100	2.80312800	-0.70579400
H	2.32084500	3.49646000	-0.67644200
H	1.78814300	2.11298800	0.01546300
N	-0.53463200	1.15037200	-0.93648900
H	0.41136400	1.01398600	-1.33662500
H	-1.17570800	0.64544000	-1.55451300
C	-1.08004000	5.56584600	-0.65292100
H	-1.89584400	5.09315900	-1.20849700
H	-1.34339100	5.54942300	0.40987100
H	-1.03097500	6.61084000	-0.96976000

Al-H-TS-gas

Sum of electronic and thermal Free Energies= -1260.582087

Imaginary frequency= -224.66

0 1

C	-5.83002800	-0.21574000	-1.22809000
C	-5.76794000	-0.77368400	0.21050300
C	-4.28606400	-0.67881600	0.62658900
H	-6.56247700	-0.74091500	-1.84984600
H	-6.11501500	0.84582200	-1.24063000
H	-6.06573700	-1.82651000	0.19555400
H	-6.43800500	-0.25321000	0.89870800
H	-4.06772300	0.22888600	1.20469300
H	-3.95747900	-1.51350100	1.24969400
C	-4.41281100	-0.38208600	-1.71337900
H	-4.11034800	-0.26515300	-2.74851100
C	-3.56504500	-0.62673100	-0.70675000
C	0.13285400	-0.92024400	-0.32736400
C	-1.19154300	-0.96334800	0.30089400
O	-1.43798500	-0.99736300	1.52306800
C	-2.11615000	-0.76212200	-0.80737400
N	-0.15668800	-0.88148600	-1.71444300
H	0.46659900	-0.43077100	-2.37309600
N	-1.45568700	-0.63173800	-1.93463100
C	1.27753800	-1.70909100	0.16152500
C	2.32682700	-2.05938600	-0.70002400
C	1.38268300	-2.05901500	1.51913200
C	3.45762700	-2.70650700	-0.21779400
H	2.25945500	-1.81406700	-1.75568800

C	2.52277800	-2.70117200	1.99642400
H	0.54139800	-1.86023000	2.17753600
C	3.57048400	-3.01809200	1.13576400
H	4.25901800	-2.96303700	-0.90361300
H	2.58304300	-2.96826600	3.04713600
H	4.45782300	-3.51668600	1.51136300
C	0.48203400	1.07542700	-0.01692400
O	-0.42659800	1.73345000	-0.53569600
C	1.89529400	1.20800500	-0.52888000
C	3.05063400	0.82798200	0.16062100
C	2.01405400	1.73784000	-1.81834700
C	4.30109700	0.97601200	-0.43276700
H	3.00274400	0.38089000	1.15076700
C	3.26329100	1.87060100	-2.41400400
H	1.10584300	2.05453500	-2.32169400
C	4.41097400	1.49177500	-1.72061700
H	5.18864900	0.67126300	0.11183100
H	3.34231500	2.28035700	-3.41573800
H	5.38735300	1.59865000	-2.18176900
C	0.65256700	2.30700900	2.20686900
H	1.62991300	2.69223700	1.90586000
H	0.65472000	2.09494600	3.27899100
N	-1.75052600	2.54374900	1.91243000
H	-2.50826200	3.14122000	2.21890500
H	-1.96600600	2.21232700	0.97325400
N	0.43651300	0.99824100	1.52732600
H	-0.51040100	0.64156200	1.78529200
H	1.09451200	0.28837600	1.86147300
C	-0.48760800	3.27140000	1.86113200
H	-0.29386400	3.72881100	0.88623500
H	-0.47797800	4.06231700	2.61670500

AI-H-TS-DCM

Sum of electronic and thermal Free Energies= -1260.623892

Imaginary frequency=-244.57

O 1

C	-5.85264000	-0.30164200	-1.29060800
C	-5.80507500	-0.73200400	0.19124400
C	-4.33312200	-0.56704200	0.62129600
H	-6.56013800	-0.89586600	-1.87809600
H	-6.15921500	0.74809300	-1.39972300
H	-6.08022100	-1.78875500	0.26362400
H	-6.49636800	-0.16705800	0.82069700
H	-4.14890500	0.39337800	1.12136000

H	-4. 00047100	-1. 34126800	1. 31643400
C	-4. 42363800	-0. 47505400	-1. 73668600
H	-4. 11254300	-0. 44138000	-2. 77635800
C	-3. 58604800	-0. 60997300	-0. 69883500
C	0. 12944700	-0. 82228000	-0. 25487600
C	-1. 21454300	-0. 85925500	0. 36081800
O	-1. 47596600	-0. 87064100	1. 57502100
C	-2. 13166400	-0. 71617400	-0. 76339900
N	-0. 16155000	-0. 85105100	-1. 64866400
H	0. 47340100	-0. 46798000	-2. 34038800
N	-1. 45401000	-0. 62766000	-1. 88676300
C	1. 22470700	-1. 69347200	0. 24098100
C	2. 21808700	-2. 14973200	-0. 63728400
C	1. 32537000	-2. 02805800	1. 59999400
C	3. 28815200	-2. 90442400	-0. 16912000
H	2. 15627800	-1. 90867100	-1. 69465200
C	2. 40174600	-2. 78203600	2. 06381400
H	0. 54179100	-1. 71760700	2. 28423100
C	3. 39082900	-3. 21818600	1. 18558500
H	4. 04703500	-3. 24583900	-0. 86651500
H	2. 46030200	-3. 03440400	3. 11830400
H	4. 22901100	-3. 80308700	1. 55055400
C	0. 53997200	1. 06554100	-0. 02926900
O	-0. 35805100	1. 75458700	-0. 55397400
C	1. 95400200	1. 16945100	-0. 57187400
C	3. 11483100	0. 81174200	0. 12174300
C	2. 06416300	1. 64002100	-1. 88438100
C	4. 36132500	0. 92890700	-0. 48926900
H	3. 07442300	0. 42489600	1. 13682400
C	3. 30859200	1. 74014600	-2. 49935700
H	1. 15649000	1. 93465600	-2. 40168300
C	4. 46174600	1. 38726400	-1. 80078200
H	5. 25425700	0. 65234200	0. 06226800
H	3. 37843100	2. 10330100	-3. 51992000
H	5. 43440900	1. 47024400	-2. 27530000
C	0. 76344100	2. 45119500	2. 11695700
H	1. 71329000	2. 83781600	1. 74262200
H	0. 83879600	2. 28540100	3. 19378400
N	-1. 66420700	2. 64223700	1. 91111000
H	-2. 42164100	3. 27544200	2. 14766200
H	-1. 87291000	2. 25820200	0. 98986900
N	0. 54113000	1. 09789500	1. 52185200
H	-0. 38971100	0. 76711600	1. 83721800
H	1. 22251100	0. 43720600	1. 90570400

C	-0.40744000	3.38291200	1.79939500
H	-0.26272900	3.83032700	0.81175200
H	-0.38639200	4.18491300	2.54208400

Al-alkenyl-TS-gas

Sum of electronic and thermal Free Energies= -1337.911984

Imaginary frequency=-211.49

O 1

C	5.81352200	-1.10201600	1.05482200
C	5.74808700	-1.00872200	-0.48527000
C	4.26474900	-0.75315900	-0.82143800
H	6.54655300	-1.83911800	1.39876700
H	6.10048900	-0.14288000	1.50877600
H	6.04819500	-1.97057000	-0.91196600
H	6.41517300	-0.24646100	-0.89455200
H	4.04290100	0.31189800	-0.97091300
H	3.93550200	-1.25494200	-1.73396900
C	4.39714300	-1.45526200	1.42999000
H	4.09682200	-1.77847000	2.42093200
C	3.54689000	-1.26024700	0.41459900
C	-0.15149500	-1.34708500	-0.03655200
C	1.17029600	-1.13096600	-0.63251800
O	1.41614500	-0.65166400	-1.75707700
C	2.09792100	-1.42357200	0.45338800
N	0.13958000	-1.90714400	1.23174700
H	-0.47882800	-1.77595800	2.02280100
N	1.44110500	-1.78232300	1.53202000
C	-1.31210700	-1.82608500	-0.80599200
C	-2.36916300	-2.49308600	-0.17041200
C	-1.42440500	-1.55298700	-2.18062900
C	-3.51367100	-2.84565200	-0.87441000
H	-2.29694800	-2.72883700	0.88714400
C	-2.57819700	-1.90330800	-2.87787200
H	-0.57846600	-1.10625900	-2.69595600
C	-3.63283000	-2.53989000	-2.22883400
H	-4.32091000	-3.35692100	-0.35924400
H	-2.64402800	-1.68917400	-3.94032000
H	-4.53080100	-2.80974100	-2.77466100
C	-0.46989500	0.60197100	0.55370400
O	0.43974500	0.94482400	1.31642600
C	-1.88899200	0.52294200	1.05775100
C	-3.03601600	0.50945100	0.25852300
C	-2.02514700	0.43370000	2.44731200
C	-4.29535200	0.40679000	0.84212400

H	-2.97486000	0.54348800	-0.82654600
C	-3.28376200	0.31703900	3.02643000
H	-1.12284000	0.47863400	3.04924200
C	-4.42296400	0.30557200	2.22421300
H	-5.17622500	0.39097500	0.20887100
H	-3.37657300	0.24651000	4.10532800
H	-5.40645800	0.21903200	2.67436300
C	0.54715700	3.37507000	-0.18401600
C	-0.60312700	2.67561600	-0.92228300
H	0.36260400	3.26957300	0.89190800
H	-1.58080200	2.91026300	-0.49350100
H	-0.58342400	2.95210900	-1.98049000
N	1.79295300	2.69532300	-0.54680200
H	2.54259200	3.34734700	-0.74241700
H	2.06865800	2.06840500	0.20549300
N	-0.39989200	1.20297000	-0.86958800
H	0.55538900	0.99909900	-1.23672500
H	-1.04778500	0.70935900	-1.49024600
C	0.60188200	4.84683400	-0.49440000
H	1.43941800	5.36443500	-0.02710600
C	-0.25573000	5.54335200	-1.23332400
H	-1.11736100	5.09235700	-1.71626700
H	-0.13008800	6.61099400	-1.37460200

Al-alkenyl-TS-DCM

Sum of electronic and thermal Free Energies= -1337.955168

Imaginary frequency= -241.96

O 1

C	5.90695100	-0.98281700	1.08207700
C	5.84479200	-0.79768900	-0.44879500
C	4.36302700	-0.51366300	-0.76691900
H	6.64388300	-1.73345800	1.38560100
H	6.18150500	-0.04943500	1.59349500
H	6.13880900	-1.73454900	-0.93246800
H	6.51434000	-0.01415100	-0.81086800
H	4.14986000	0.56213800	-0.83022500
H	4.03695400	-0.94634000	-1.71537900
C	4.49208500	-1.36914700	1.42974200
H	4.19829200	-1.76077000	2.39880500
C	3.64036300	-1.10860200	0.42774200
C	-0.07563800	-1.23596800	-0.03471700
C	1.25566100	-0.98659000	-0.62660300
O	1.49410400	-0.50578500	-1.74675100
C	2.19059300	-1.27802400	0.45386700

N	0. 24157000	-1. 81380600	1. 22710700
H	-0. 38841100	-1. 75952800	2. 02010100
N	1. 53323300	-1. 66683000	1. 52410100
C	-1. 16779500	-1. 85346900	-0. 82762500
C	-2. 14020500	-2. 64509400	-0. 19931500
C	-1. 28761600	-1. 61435300	-2. 20539100
C	-3. 20649200	-3. 16843500	-0. 92234100
H	-2. 06624200	-2. 84959900	0. 86479800
C	-2. 36090700	-2. 13751900	-2. 92394400
H	-0. 51895300	-1. 04111000	-2. 71470900
C	-3. 32820500	-2. 91101000	-2. 28730100
H	-3. 94829700	-3. 77731300	-0. 41462400
H	-2. 43295400	-1. 94334000	-3. 98981700
H	-4. 16408300	-3. 31585200	-2. 84871700
C	-0. 52078600	0. 58108900	0. 52710300
O	0. 37350400	1. 01692700	1. 27939700
C	-1. 92758900	0. 42160300	1. 07073500
C	-3. 09139700	0. 36183800	0. 29675500
C	-2. 02703300	0. 30095400	2. 46045200
C	-4. 33055000	0. 18387000	0. 90802300
H	-3. 05752000	0. 43781700	-0. 78729600
C	-3. 26389300	0. 10608600	3. 06782100
H	-1. 11764700	0. 37515500	3. 04851800
C	-4. 42004900	0. 04952400	2. 29170100
H	-5. 22646900	0. 14243800	0. 29676900
H	-3. 32577100	0. 00944200	4. 14723200
H	-5. 38698100	-0. 09590800	2. 76291500
C	0. 25954900	3. 48339700	-0. 20910400
C	-0. 85862500	2. 68991000	-0. 89214700
H	0. 13099900	3. 38133700	0. 87565700
H	-1. 82762700	2. 84010800	-0. 41161500
H	-0. 92480700	2. 96813600	-1. 94707000
N	1. 55027100	2. 91651100	-0. 62735800
H	2. 26050100	3. 64192900	-0. 66814900
H	1. 83950800	2. 24535100	0. 08299300
N	-0. 54274800	1. 23209800	-0. 87959000
H	0. 40480600	1. 11790800	-1. 28395800
H	-1. 17980200	0. 73342600	-1. 50735200
C	0. 18060000	4. 95137800	-0. 53780600
H	1. 01177600	5. 53695900	-0. 14424700
C	-0. 78697700	5. 56868700	-1. 20993800
H	-1. 64801400	5. 04638600	-1. 61770400
H	-0. 75397400	6. 64215400	-1. 36810500

Al-Ph-TS-gas

Sum of electronic and thermal Free Energies= -1491.472939

Imaginary frequency= -236.85

0 1

C	-0.88544500	6.00744800	-1.11731800
C	-0.58242700	5.92858000	0.39476600
C	-0.54108700	4.42361800	0.72930100
H	-1.52293800	6.86009900	-1.37309700
H	0.03327200	6.11598600	-1.71089400
H	-1.40587400	6.39249600	0.94618600
H	0.33509200	6.45200300	0.67332300
H	0.48018900	4.02017000	0.72596400
H	-0.95043300	4.18823000	1.71425100
C	-1.53456300	4.67672000	-1.39872500
H	-2.04871900	4.43804300	-2.32355900
C	-1.34392200	3.80639500	-0.39979400
C	-2.03751300	0.18574900	0.16657500
C	-1.49558400	1.44704700	0.68198200
O	-0.80822200	1.59686600	1.71342000
C	-1.76647900	2.41047300	-0.37558800
N	-2.69971900	0.57139200	-1.02612400
H	-2.79913900	-0.06399600	-1.80817400
N	-2.38443800	1.82585900	-1.37625800
C	-2.63504900	-0.84545100	1.03451000
C	-3.57493200	-1.75244900	0.52505600
C	-2.21869000	-0.99355700	2.36899800
C	-4.05830900	-2.79230600	1.30960900
H	-3.92344900	-1.64696000	-0.49789700
C	-2.70204200	-2.04291000	3.14699500
H	-1.54855600	-0.25153300	2.79444900
C	-3.61402100	-2.95394500	2.62036800
H	-4.78217500	-3.48462200	0.89121800
H	-2.37262600	-2.13756300	4.17722300
H	-3.98692900	-3.77118500	3.22870800
C	-0.29084800	-0.50740300	-0.63459900
O	0.15180500	0.32801700	-1.43167700
C	-0.70853200	-1.87110500	-1.12811100
C	-0.88059600	-3.00829200	-0.33322900
C	-0.95708100	-1.95565600	-2.50245500
C	-1.29380500	-4.20755600	-0.90671400
H	-0.73104200	-2.98084500	0.74358600
C	-1.38340800	-3.15118600	-3.06978500

H	-0.78786000	-1.06757300	-3.10335700
C	-1.55028800	-4.28162500	-2.27246800
H	-1.42787500	-5.08079100	-0.27694300
H	-1.57481500	-3.20386800	-4.13663900
H	-1.87824100	-5.21711900	-2.71371400
C	2.72793500	-0.07243600	-0.23287400
C	1.87818500	-1.05584700	0.59235500
H	2.51196800	-0.24300500	-1.29437900
H	1.87717200	-2.05610400	0.15108200
H	2.27423600	-1.10504400	1.61041500
N	2.38325900	1.28253800	0.19466200
H	3.14840300	1.91347100	-0.02385800
H	1.57661000	1.58383800	-0.35342000
N	0.46682400	-0.59221600	0.71109900
H	0.44769800	0.36514900	1.13225400
H	-0.05652400	-1.17949400	1.36669700
C	4.18412500	-0.39388100	0.03042900
C	4.89613700	-1.21014000	-0.84804400
C	4.81882400	0.08952500	1.17837200
C	6.22383700	-1.53985300	-0.58795800
H	4.40765500	-1.58217600	-1.74509600
C	6.14711600	-0.23443600	1.43570700
H	4.26290300	0.72754100	1.86013900
C	6.85196900	-1.05116900	0.55401000
H	6.76897800	-2.17215100	-1.28131800
H	6.63358600	0.15139200	2.32591300
H	7.88826300	-1.30258100	0.75512400

AI-Ph-TS-DCM

Sum of electronic and thermal Free Energies= -1491.521430

Imaginary frequency= -258.29

0 1

C	-0.96267200	6.01175300	-1.17123900
C	-0.59861600	5.94462700	0.32737100
C	-0.51266400	4.44195500	0.66341300
H	-1.62882800	6.84872200	-1.40477000
H	-0.07092300	6.13696000	-1.80132600
H	-1.40834700	6.39359500	0.91088300
H	0.31981800	6.48561900	0.56641000
H	0.51683900	4.06211000	0.61812300
H	-0.88101100	4.20528700	1.66438700
C	-1.59333100	4.66657300	-1.42423500
H	-2.13768600	4.42110200	-2.33103500
C	-1.34522700	3.80079700	-0.43129600

C	-1. 94854100	0. 15075500	0. 15787800
C	-1. 42469800	1. 43543200	0. 66508600
O	-0. 74610800	1. 60548000	1. 69344100
C	-1. 73056000	2. 39355900	-0. 38836800
N	-2. 64121800	0. 53698700	-1. 02385100
H	-2. 80685300	-0. 10146700	-1. 79408800
N	-2. 35864800	1. 79016200	-1. 37456500
C	-2. 60477400	-0. 82616700	1. 06325600
C	-3. 60707200	-1. 67882200	0. 57812000
C	-2. 20257500	-0. 95952200	2. 40157200
C	-4. 17752400	-2. 64530500	1. 39958500
H	-3. 94176000	-1. 58989000	-0. 45131200
C	-2. 77474200	-1. 93242300	3. 21850800
H	-1. 45764700	-0. 28012100	2. 80422600
C	-3. 75872900	-2. 78409500	2. 72202100
H	-4. 95060400	-3. 29566300	1. 00188600
H	-2. 45207900	-2. 01680300	4. 25181000
H	-4. 20072800	-3. 54251200	3. 36014000
C	-0. 30339300	-0. 55982400	-0. 62273600
O	0. 17485100	0. 27080200	-1. 42073200
C	-0. 73729200	-1. 91553800	-1. 14705000
C	-0. 92587700	-3. 06322100	-0. 36992800
C	-0. 98344000	-1. 97737900	-2. 52266000
C	-1. 34954600	-4. 25017300	-0. 96381000
H	-0. 76532400	-3. 05634200	0. 70504000
C	-1. 42072400	-3. 15979800	-3. 11157600
H	-0. 81326100	-1. 08383400	-3. 11462500
C	-1. 60263400	-4. 30099500	-2. 33253500
H	-1. 48959400	-5. 13400700	-0. 34963300
H	-1. 61075500	-3. 19222500	-4. 17980100
H	-1. 93892500	-5. 22638400	-2. 78931600
C	2. 75989400	-0. 08438700	-0. 21232100
C	1. 91564800	-1. 14334400	0. 51891500
H	2. 57402100	-0. 18349800	-1. 28711300
H	1. 91507200	-2. 09733700	-0. 01341400
H	2. 30472200	-1. 29147200	1. 52937600
N	2. 37683600	1. 23710900	0. 29354300
H	3. 12082500	1. 90072700	0. 09089100
H	1. 56610000	1. 53849200	-0. 24891200
N	0. 49898700	-0. 70276600	0. 69504900
H	0. 50146900	0. 22599600	1. 16045000
H	0. 03001400	-1. 33848500	1. 34551200
C	4. 22045200	-0. 38680300	0. 05569200
C	4. 96080300	-1. 13724300	-0. 85927800

C	4. 83449900	0. 04662300	1. 23536300
C	6. 29474000	-1. 45003000	-0. 60399500
H	4. 48842900	-1. 47299100	-1. 77915400
C	6. 16880600	-0. 25975100	1. 48857800
H	4. 26155800	0. 63057900	1. 95041700
C	6. 90201300	-1. 00992700	0. 56992700
H	6. 86059900	-2. 03112000	-1. 32564000
H	6. 63735100	0. 08803200	2. 40417400
H	7. 94250700	-1. 24771700	0. 76796600

BCPP-OMe-gas

Sum of electronic and thermal Free Energies= -1184.713307

O 1

C	-5. 88866900	-2. 27558900	0. 77580700
C	-6. 14407400	-1. 33572300	-0. 42241900
C	-4. 74762900	-0. 88643300	-0. 90011700
H	-6. 65190800	-2. 18325600	1. 55476800
H	-5. 87799900	-3. 33120200	0. 47115800
H	-6. 69979800	-0. 45991500	-0. 07467300
H	-6. 73161800	-1. 80569600	-1. 21370200
H	-4. 37604800	-1. 50069300	-1. 73042800
H	-4. 72474000	0. 14805600	-1. 24830900
C	-4. 51779000	-1. 86075600	1. 24173600
H	-4. 07748700	-2. 17066200	2. 18364000
C	-3. 88810600	-1. 11129300	0. 32868800
C	-0. 41546300	0. 44759300	0. 01417700
C	-1. 85862400	0. 31333100	-0. 52180100
O	-2. 30180900	0. 85846800	-1. 49799100
C	-2. 52099700	-0. 60978800	0. 43828000
N	-0. 54000700	-0. 22776500	1. 30542800
H	0. 24557600	-0. 77495600	1. 63707800
N	-1. 70928400	-0. 93255600	1. 39306100
C	-0. 02533600	1. 91112500	0. 08974200
C	0. 01825500	2. 59462200	1. 30468700
C	0. 24059600	2. 58878800	-1. 10185000
C	0. 34759000	3. 94714900	1. 32711900
H	-0. 20740800	2. 06037900	2. 22204400
C	0. 56784300	3. 94039900	-1. 07232000
H	0. 17374800	2. 05754500	-2. 04684700
C	0. 62633100	4. 62123500	0. 14125800
H	0. 38298800	4. 47511300	2. 27467100
H	0. 77530100	4. 46256500	-2. 00054000
H	0. 88454100	5. 67496200	0. 16214200
C	0. 53284300	-0. 34704400	-0. 92327900

O	0.13407300	-0.75281100	-1.99219900
C	1.92312600	-0.61639900	-0.45447900
C	2.50494000	-0.00616000	0.66868400
C	2.67957000	-1.53049600	-1.19075300
C	3.80028500	-0.31330600	1.04122200
H	1.95585000	0.73456800	1.24219500
C	3.98037700	-1.85007700	-0.82629900
H	2.22272000	-1.98995600	-2.06097200
C	4.54559100	-1.23889900	0.29854300
H	4.26941400	0.15380200	1.89955600
H	4.54029300	-2.56648300	-1.41430800
O	5.79847200	-1.47347700	0.74456800
C	6.59668100	-2.39024000	0.02223000
H	7.55422200	-2.42866200	0.53925400
H	6.14576500	-3.38892400	0.01473300
H	6.75167200	-2.05401300	-1.00904600

BCPP-OMe-DCM

Sum of electronic and thermal Free Energies= -1184.744759

O 1

C	5.96209800	-2.19139900	-0.76582800
C	6.20215700	-1.22352000	0.41227400
C	4.79770800	-0.80867000	0.89723600
H	6.71318700	-2.09083900	-1.55564800
H	5.98385100	-3.24142500	-0.44274100
H	6.72705200	-0.33710500	0.04355100
H	6.81018800	-1.66278800	1.20588300
H	4.45414000	-1.42103200	1.74119400
H	4.75198500	0.23165700	1.22683600
C	4.57543800	-1.82542800	-1.22490900
H	4.14165100	-2.16926100	-2.15899100
C	3.93127100	-1.07721100	-0.31877500
C	0.41254800	0.38347000	-0.00729600
C	1.84506700	0.25385700	0.55382100
O	2.25573800	0.77117600	1.56308700
C	2.54934300	-0.61336200	-0.42144900
N	0.56787000	-0.27597300	-1.30082900
H	-0.20190400	-0.80644800	-1.69426500
N	1.75242900	-0.93108300	-1.39468600
C	0.02797700	1.85123400	-0.07891700
C	0.06802300	2.55694300	-1.28202700
C	-0.31053400	2.51104300	1.10517300
C	-0.24655400	3.91389000	-1.30046900
H	0.33877500	2.03993500	-2.19713400

C	-0.62228700	3.86755500	1.08063400
H	-0.32432500	1.96563500	2.04470800
C	-0.59313300	4.57131000	-0.12192200
H	-0.21793400	4.45763200	-2.23952300
H	-0.88775900	4.37426300	2.00303500
H	-0.83946300	5.62819000	-0.14011500
C	-0.55544200	-0.42420800	0.90260000
O	-0.15597000	-0.86677600	1.95988200
C	-1.94897900	-0.64573100	0.43489600
C	-2.49659000	-0.04364600	-0.71090300
C	-2.75128400	-1.50853800	1.18887600
C	-3.80053000	-0.30631800	-1.08636100
H	-1.91618900	0.65106800	-1.31016000
C	-4.06173800	-1.78177700	0.82424800
H	-2.32766300	-1.97076800	2.07444900
C	-4.59207100	-1.17866200	-0.32385500
H	-4.23612500	0.15554300	-1.96566200
H	-4.65707700	-2.45636900	1.42701600
O	-5.84622600	-1.37410800	-0.77206900
C	-6.69360700	-2.24136800	-0.02989200
H	-7.64401100	-2.25782000	-0.56209500
H	-6.28232400	-3.25520800	0.01191100
H	-6.84975900	-1.86458700	0.98621800

BCPP-OMe-TS-gas

Sum of electronic and thermal Free Energies= -1414.306476

Imaginary frequency= -237.41

O 1

C	-5.98620400	-0.31877800	-2.08419900
C	-6.20549300	-0.59287600	-0.58039500
C	-4.80562200	-0.51495600	0.06190900
H	-6.65785500	-0.90566100	-2.71934200
H	-6.16337400	0.73665400	-2.33515400
H	-6.59634000	-1.60760800	-0.45816900
H	-6.92293600	0.09217000	-0.12264900
H	-4.59621100	0.47116600	0.49725800
H	-4.66050600	-1.23361100	0.87143200
C	-4.53239000	-0.66563300	-2.27936600
H	-4.06030400	-0.76931200	-3.25045800
C	-3.88143600	-0.76605700	-1.11404700
C	-0.33568900	-1.21957100	-0.05194600
C	-1.74053100	-1.05694700	0.33391600
O	-2.18051300	-0.84226600	1.48088500
C	-2.45433600	-1.01032600	-0.93651300

N	-0.39537800	-1.42500400	-1.45426900
H	0.36253500	-1.13217600	-2.05910500
N	-1.61384300	-1.13644900	-1.93670500
C	0.63283200	-1.98044700	0.75733900
C	1.76496200	-2.55707000	0.16428700
C	0.48836200	-2.07510200	2.15264900
C	2.73837900	-3.17445800	0.93979300
H	1.88735600	-2.51156300	-0.91364500
C	1.47166500	-2.68982000	2.92413500
H	-0.42210800	-1.69911600	2.61134500
C	2.60668300	-3.23121200	2.32588200
H	3.60976100	-3.60718600	0.45831800
H	1.33988500	-2.75721600	3.99980800
H	3.37230600	-3.70625800	2.93016100
C	0.16206100	0.76204600	-0.04163300
O	-0.58972700	1.36900300	-0.81351800
C	1.64265800	0.71569400	-0.31424600
C	2.64108400	0.36813500	0.60753200
C	2.02421800	1.03352700	-1.61768600
C	3.97267000	0.34659900	0.23178000
H	2.40010600	0.07777100	1.62758400
C	3.35850800	1.00012100	-2.01400100
H	1.24574300	1.32765200	-2.31490700
C	4.34083500	0.65717800	-1.08241100
H	4.75112500	0.07386300	0.93533700
H	3.61754700	1.25280400	-3.03482200
C	-0.90364300	4.64106000	2.06679700
C	-0.86078200	3.35530100	1.25107300
H	-1.50418300	5.39836000	1.55613600
H	-1.35085700	4.44799300	3.04733600
H	0.09902600	5.05143500	2.21590800
C	0.10680300	2.37580600	1.93146000
H	-0.47577800	3.56989300	0.24731900
H	1.15228400	2.62912200	1.73575300
H	-0.07514700	2.37416300	3.01093800
N	-2.17744100	2.72335100	1.20587600
H	-2.91126300	3.42331200	1.22870600
H	-2.25954000	2.21215400	0.32738500
N	-0.12991200	0.98190900	1.46521800
H	-1.13347200	0.74146900	1.62006900
H	0.40093700	0.30741100	2.02353700
O	5.66772900	0.59732600	-1.35168900
C	6.08189900	0.90037400	-2.66720800
H	5.81609700	1.92775800	-2.94203800

H	7.16563200	0.79220100	-2.67641900
H	5.64068300	0.20766600	-3.39328600

BCPP-OMe-TS-DCM

Sum of electronic and thermal Free Energies= -1414.348832

Imaginary frequency=-244.92

0 1

C	-6.00100200	-0.38598900	-2.12788100
C	-6.23212200	-0.60314000	-0.61740400
C	-4.84157300	-0.46506700	0.03449300
H	-6.65483100	-1.00859600	-2.74719100
H	-6.18982800	0.65613400	-2.42202400
H	-6.60054100	-1.62110400	-0.45681900
H	-6.96827500	0.08507200	-0.19589800
H	-4.65985300	0.54783900	0.41868300
H	-4.69470800	-1.14283900	0.87854100
C	-4.53980800	-0.71673300	-2.29379900
H	-4.06217800	-0.85441800	-3.25908100
C	-3.89702900	-0.75328600	-1.11786700
C	-0.33285600	-1.11029400	-0.01331500
C	-1.75690100	-0.97161200	0.36011500
O	-2.21020200	-0.77164800	1.49848100
C	-2.46625700	-0.96072000	-0.91475100
N	-0.39760100	-1.35927700	-1.41568800
H	0.36800700	-1.11445000	-2.03472900
N	-1.61231700	-1.09873500	-1.90386500
C	0.58909400	-1.95113300	0.79275900
C	1.67041700	-2.60012500	0.17983600
C	0.43946900	-2.06494200	2.18308200
C	2.58430800	-3.32636400	0.93558500
H	1.80121100	-2.53104700	-0.89622800
C	1.36021000	-2.79115400	2.93599500
H	-0.41486300	-1.60108300	2.66610100
C	2.43958800	-3.41922200	2.31921300
H	3.41613000	-3.81824400	0.44072900
H	1.22564300	-2.86984000	4.01061700
H	3.15704000	-3.98137300	2.90837000
C	0.19653000	0.74902200	-0.02476300
O	-0.54139700	1.38582400	-0.80588000
C	1.68411300	0.69395200	-0.30723800
C	2.68273300	0.36929300	0.62276300
C	2.06744400	0.96913800	-1.61974600
C	4.01515600	0.33144800	0.24639800
H	2.44127200	0.12877900	1.65485700

C	3.40170100	0.92070900	-2.01819800
H	1.29512900	1.23977400	-2.33303800
C	4.38443300	0.60199100	-1.07771900
H	4.79139000	0.08491300	0.96314800
H	3.66051200	1.14059200	-3.04700700
C	-0.85053300	4.72822900	2.00987100
C	-0.81733700	3.43200400	1.21220300
H	-1.47798000	5.47023600	1.50795400
H	-1.26003100	4.54651100	3.00922500
H	0.15336300	5.14934700	2.11733900
C	0.18462700	2.47738700	1.87300400
H	-0.46997100	3.64028600	0.19427100
H	1.21621900	2.72996400	1.61808500
H	0.06220500	2.50643400	2.95959400
N	-2.13709600	2.79215000	1.21161000
H	-2.85989900	3.50576800	1.16304700
H	-2.20951500	2.24225700	0.35505700
N	-0.06173800	1.05851800	1.47874200
H	-1.05768900	0.84870600	1.67089200
H	0.47807300	0.43489300	2.08523200
O	5.70919600	0.53355700	-1.34716900
C	6.12707500	0.83458500	-2.66885700
H	5.85419000	1.85811000	-2.94804600
H	7.21260500	0.73732300	-2.67166400
H	5.69879700	0.13173600	-3.39174900

BCPP-Cl-gas

Sum of electronic and thermal Free Energies= -1529.841477

0 1

C	-5.94997900	-2.12565000	0.80950600
C	-6.20054000	-1.13316600	-0.34660200
C	-4.80099300	-0.71812000	-0.84607000
H	-6.68774900	-2.03342000	1.61252800
H	-5.98806300	-3.16896600	0.46727200
H	-6.71371400	-0.25101600	0.04730700
H	-6.82541800	-1.55165900	-1.13807800
H	-4.47522400	-1.31326300	-1.70878900
H	-4.74880500	0.32748500	-1.15601300
C	-4.55232200	-1.78079500	1.25166700
H	-4.09958800	-2.14250100	2.16890800
C	-3.91893600	-1.02120600	0.34955000
C	-0.39600400	0.41415100	-0.00306300
C	-1.85414200	0.34278300	-0.51344800
O	-2.29286800	0.92237800	-1.47104100

C	-2.53158400	-0.57507900	0.44157400
N	-0.51924300	-0.28674800	1.27442500
H	0.25086800	-0.86902700	1.58147400
N	-1.71335500	-0.94923000	1.37134900
C	0.04743500	1.86099900	0.09777700
C	0.13078100	2.51450400	1.32722700
C	0.32342800	2.55484600	-1.08208200
C	0.51043600	3.85304600	1.37505800
H	-0.10367200	1.96837700	2.23534300
C	0.70157600	3.89238800	-1.02689600
H	0.22447700	2.04930000	-2.03839800
C	0.80026800	4.54266500	0.20071600
H	0.57636900	4.35817900	2.33330200
H	0.91711000	4.42738900	-1.94583300
H	1.09805900	5.58522400	0.24158000
C	0.50234500	-0.39258400	-0.97299600
O	0.07130900	-0.78086400	-2.03403700
C	1.90554000	-0.70763200	-0.54733300
C	2.52735800	-0.12503000	0.56216600
C	2.61015200	-1.63490300	-1.32231100
C	3.83229200	-0.46849500	0.89712700
H	2.01199600	0.62068400	1.15952700
C	3.91090600	-1.98686100	-0.99582300
H	2.11472600	-2.07058300	-2.18326100
C	4.51019000	-1.39820600	0.11576400
H	4.32487600	-0.01680400	1.75019900
H	4.46264200	-2.70716700	-1.58865000
Cl	6.14191400	-1.83167200	0.53251500

BCPP-Cl-DCM

Sum of electronic and thermal Free Energies= -1529.872630

0 1

C	6.02084800	-2.02581800	-0.82294600
C	6.23911000	-1.05650900	0.35807800
C	4.82614600	-0.69998000	0.86379700
H	6.75865800	-1.89417200	-1.62049600
H	6.08361000	-3.07612300	-0.50612400
H	6.72372900	-0.14796900	-0.01213300
H	6.87431400	-1.47632700	1.14080500
H	4.51635200	-1.33321800	1.70552200
H	4.74488000	0.33469800	1.20397400
C	4.61666000	-1.70771700	-1.26403600
H	4.18517400	-2.05994200	-2.19607200
C	3.95612400	-0.99082600	-0.34449200

C	0.39343600	0.35090400	0.00954500
C	1.84055600	0.27942500	0.54703800
O	2.24832800	0.82684900	1.54095100
C	2.55658500	-0.57919300	-0.42739400
N	0.54721400	-0.32895500	-1.27301000
H	-0.20987600	-0.89018600	-1.64775400
N	1.75305000	-0.94233500	-1.37876100
C	-0.04036600	1.80370700	-0.08292200
C	-0.03293100	2.48800400	-1.29903700
C	-0.38759400	2.47348100	1.09288200
C	-0.38849300	3.83425300	-1.33793400
H	0.24577700	1.96310500	-2.20725100
C	-0.74136000	3.81914900	1.04737500
H	-0.37467900	1.94609500	2.04277300
C	-0.74418300	4.50162900	-0.16762700
H	-0.38449600	4.36212800	-2.28636800
H	-1.01341000	4.33406700	1.96321400
H	-1.02213600	5.55020400	-0.20204200
C	-0.52620600	-0.47097500	0.94979000
O	-0.09586100	-0.89928600	1.99804000
C	-1.93687300	-0.73560400	0.52492900
C	-2.52444300	-0.15596800	-0.60502700
C	-2.68553800	-1.61365500	1.31728500
C	-3.84081600	-0.45048800	-0.94262400
H	-1.97720000	0.54427400	-1.22794700
C	-3.99907300	-1.91662900	0.99146800
H	-2.22257000	-2.05725200	2.19208400
C	-4.56040400	-1.32840600	-0.13951300
H	-4.30149600	-0.00037500	-1.81451300
H	-4.58119300	-2.59799200	1.60164000
Cl	-6.21259600	-1.70207100	-0.55827400

BCPP-Cl-TS-gas

Sum of electronic and thermal Free Energies= -1759.435888

Imaginary frequency=-221.47

0 1

C	-6.02527100	-0.51187800	-1.89130900
C	-6.19139500	-0.74230200	-0.37336800
C	-4.77286700	-0.62413700	0.22038800
H	-6.70623700	-1.12957800	-2.48588500
H	-6.22907500	0.53191100	-2.16913600
H	-6.56250200	-1.75814500	-0.20724900
H	-6.90409800	-0.05377500	0.08645300
H	-4.56488800	0.37683300	0.62125100

H	-4. 59042400	-1. 31692700	1. 04491000
C	-4. 57280000	-0. 84014400	-2. 12357600
H	-4. 13069900	-0. 96469300	-3. 10626700
C	-3. 88324100	-0. 89571500	-0. 97761800
C	-0. 29676500	-1. 23315700	-0. 02253500
C	-1. 69046300	-1. 08136400	0. 40486900
O	-2. 09542500	-0. 81800900	1. 55542000
C	-2. 44713400	-1. 11081800	-0. 83979100
N	-0. 39985400	-1. 51179100	-1. 40679200
H	0. 33413400	-1. 26294900	-2. 05796100
N	-1. 63894200	-1. 27468100	-1. 86173400
C	0. 72892500	-1. 90577700	0. 79245800
C	1. 85929600	-2. 47956200	0. 19321800
C	0. 63959700	-1. 91334400	2. 19571100
C	2. 88382500	-3. 00959500	0. 96790300
H	1. 93999700	-2. 50333100	-0. 88947200
C	1. 67392000	-2. 44006700	2. 96558300
H	-0. 26801800	-1. 54266400	2. 66436500
C	2. 80601300	-2. 97858100	2. 35891300
H	3. 75176100	-3. 44323300	0. 48110400
H	1. 58467100	-2. 44193600	4. 04768500
H	3. 61083400	-3. 38560300	2. 96185700
C	0. 12640600	0. 78182600	-0. 13648500
O	-0. 65277200	1. 31441500	-0. 93361900
C	1. 60341900	0. 75014300	-0. 44005400
C	2. 62342400	0. 50102600	0. 48270800
C	1. 94052600	0. 96838100	-1. 77995100
C	3. 95334700	0. 46997900	0. 07747900
H	2. 41196600	0. 29057600	1. 52802400
C	3. 26415500	0. 92609200	-2. 19947500
H	1. 13774700	1. 18888800	-2. 47642700
C	4. 26174700	0. 67795300	-1. 26170800
H	4. 74338900	0. 26874200	0. 79162000
H	3. 52691600	1. 09403000	-3. 23773800
C	-1. 09172100	4. 72316400	1. 76594600
C	-0. 99799900	3. 39798000	1. 02057400
H	-1. 74335400	5. 41789700	1. 22986800
H	-1. 50559500	4. 56209100	2. 76670100
H	-0. 10962500	5. 19343400	1. 86698700
C	0. 03667200	2. 50975600	1. 72920100
H	-0. 64800700	3. 57701200	-0. 00248000
H	1. 06287900	2. 80095100	1. 48874700
H	-0. 11599400	2. 56366100	2. 81174400
N	-2. 27884500	2. 69538400	1. 04159800

H	-3.05018800	3.35332100	1.06966400
H	-2.36430000	2.14627500	0.18695100
N	-0.14575600	1.08000100	1.35350400
H	-1.13679500	0.80956700	1.54560300
H	0.41952800	0.46129700	1.94208500
Cl	5.92621500	0.62550200	-1.77281900

BCPP-Cl-TS-DCM

Sum of electronic and thermal Free Energies= -1759.479169

Imaginary frequency=-254.02

O 1

C	-6.03565100	-0.56181200	-1.98123500
C	-6.22990800	-0.76083700	-0.46316800
C	-4.83036600	-0.57498600	0.15636900
H	-6.68767800	-1.20872700	-2.57706100
H	-6.25503700	0.47108700	-2.28667200
H	-6.56649900	-1.78594500	-0.27945400
H	-6.97577700	-0.08625900	-0.03670100
H	-4.66621000	0.44982300	0.51547100
H	-4.64870900	-1.23082300	1.01124100
C	-4.57077900	-0.86141200	-2.17293600
H	-4.11057000	-1.00426900	-3.14586800
C	-3.90337300	-0.86392000	-1.01014000
C	-0.31412700	-1.11499100	0.02687000
C	-1.72891700	-0.96351200	0.42418100
O	-2.15736800	-0.68812500	1.55823500
C	-2.46596700	-1.04163900	-0.83002000
N	-0.40630300	-1.44189200	-1.35313200
H	0.34970600	-1.28013500	-2.00894800
N	-1.63241200	-1.23449400	-1.82976300
C	0.64798500	-1.87338500	0.86258000
C	1.72449800	-2.54872000	0.26959400
C	0.53916500	-1.88220800	2.26187300
C	2.67349900	-3.19752000	1.05240800
H	1.82280800	-2.56554900	-0.81211700
C	1.49513100	-2.53073200	3.04099400
H	-0.31254700	-1.39969600	2.73158100
C	2.56974900	-3.18464900	2.44271700
H	3.50015700	-3.71240500	0.57254100
H	1.39204000	-2.52878700	4.12190900
H	3.31455400	-3.68644700	3.05202500
C	0.17131200	0.78282600	-0.10643000
O	-0.60130600	1.35596900	-0.89810300
C	1.64793400	0.71936700	-0.44591300

C	2. 67976900	0. 46696600	0. 46313500
C	1. 96379500	0. 90771200	-1. 79471100
C	4. 00268200	0. 40507600	0. 03557700
H	2. 48302200	0. 29829200	1. 51791500
C	3. 27873200	0. 83316900	-2. 24016600
H	1. 15788700	1. 12345800	-2. 48845200
C	4. 28500500	0. 58309100	-1. 31365600
H	4. 80115400	0. 21108300	0. 74298000
H	3. 51981500	0. 97597300	-3. 28776200
C	-0. 88698000	4. 83719000	1. 75107400
C	-0. 85562500	3. 50037600	1. 02308200
H	-1. 54071300	5. 54099300	1. 22839600
H	-1. 26612000	4. 70274200	2. 76964900
H	0. 11199400	5. 27910600	1. 80801000
C	0. 18123800	2. 59819200	1. 70237100
H	-0. 54372900	3. 65934600	-0. 01511100
H	1. 20175700	2. 85866300	1. 41318000
H	0. 08230600	2. 67339900	2. 78902800
N	-2. 16287900	2. 84100100	1. 10111700
H	-2. 89962900	3. 53989100	1. 04968700
H	-2. 26152000	2. 25054400	0. 27513700
N	-0. 04494100	1. 15617400	1. 37995700
H	-1. 03117200	0. 93205900	1. 61174500
H	0. 52551500	0. 57303100	1. 99925700
Cl	5. 94503100	0. 48937900	-1. 85686100

BCPP-CF3-gas

Sum of electronic and thermal Free Energies= -1407.197821

0 1

C	-6. 19861400	-2. 60062500	0. 82961700
C	-6. 57797900	-1. 59481000	-0. 27880500
C	-5. 24061900	-1. 02499600	-0. 79567100
H	-6. 91846600	-2. 61234900	1. 65380000
H	-6. 14396000	-3. 62891500	0. 44661200
H	-7. 16343100	-0. 78319000	0. 16299100
H	-7. 18136100	-2. 04278500	-1. 07078900
H	-4. 88317900	-1. 55196000	-1. 68962500
H	-5. 30004500	0. 03159000	-1. 06446300
C	-4. 82934300	-2. 13629100	1. 25077400
H	-4. 31749300	-2. 48595200	2. 14122200
C	-4. 29943600	-1. 28418000	0. 36474600
C	-0. 94396000	0. 50148300	-0. 02105800
C	-2. 40166600	0. 30220900	-0. 49968300
O	-2. 91914700	0. 86374100	-1. 42813100

C	-2.96071700	-0.70603300	0.44046600
N	-0.96542800	-0.24461200	1.23571700
H	-0.13444900	-0.75379100	1.51214400
N	-2.08594300	-1.02429600	1.33909300
C	-0.63905600	1.98136400	0.11296300
C	-0.57715900	2.60330200	1.35992800
C	-0.47118500	2.73284300	-1.05189200
C	-0.32637200	3.97034600	1.43940500
H	-0.72777300	2.01077600	2.25665500
C	-0.22173700	4.09860800	-0.96482600
H	-0.55433500	2.24864500	-2.02062600
C	-0.14421000	4.71899800	0.27959600
H	-0.27691000	4.45114300	2.41103100
H	-0.09045500	4.67883900	-1.87213600
H	0.05328400	5.78386300	0.34504000
C	0.00181900	-0.18205700	-1.03809200
O	-0.41017800	-0.56194200	-2.10876400
C	1.43955200	-0.39009800	-0.64872600
C	2.03181100	0.22041200	0.46119900
C	2.19824200	-1.23648000	-1.46427300
C	3.36935500	-0.02188700	0.75663800
H	1.46709000	0.90834100	1.08235000
C	3.53076400	-1.48083100	-1.16948100
H	1.71997900	-1.68790300	-2.32649500
C	4.10983300	-0.87280200	-0.05658600
H	3.84004400	0.45835200	1.60700000
H	4.12702100	-2.13230200	-1.79917400
C	5.54028500	-1.18461100	0.28999400
F	6.28358700	-1.36414100	-0.80987500
F	6.10203200	-0.20456100	1.00927600
F	5.63004500	-2.30992200	1.01377100

BCPP-CF3-DCM

Sum of electronic and thermal Free Energies= -1407.227715

0 1

C	6.29279000	-2.49139300	-0.81453000
C	6.64252300	-1.48087200	0.29849300
C	5.28920100	-0.94272500	0.80735800
H	7.01749500	-2.48458400	-1.63459600
H	6.25721200	-3.52185500	-0.43496600
H	7.21241600	-0.65478600	-0.13738300
H	7.24880700	-1.91853200	1.09428600
H	4.93807000	-1.48082600	1.69738900
H	5.32779500	0.11505200	1.07715800

C	4. 91654200	-2. 05714100	-1. 24418500
H	4. 42289100	-2. 42236600	-2. 13968700
C	4. 36019300	-1. 21804800	-0. 35996300
C	0. 94564300	0. 46052200	0. 01029500
C	2. 39483800	0. 28151500	0. 51848900
O	2. 87175500	0. 82298400	1. 48420900
C	3. 00758700	-0. 67121000	-0. 43856000
N	1. 01629300	-0. 25400900	-1. 26010400
H	0. 20466400	-0. 74325800	-1. 62130100
N	2. 15699100	-0. 98144300	-1. 36750400
C	0. 61450600	1. 93831100	-0. 09780400
C	0. 64496700	2. 60137100	-1. 32533400
C	0. 33227500	2. 64786900	1. 07193300
C	0. 37819500	3. 96727800	-1. 38128500
H	0. 87098000	2. 04445400	-2. 22908500
C	0. 06646700	4. 01294300	1. 00934100
H	0. 32493200	2. 13640200	2. 03056100
C	0. 08641600	4. 67468400	-0. 21681000
H	0. 39961700	4. 47849200	-2. 33856100
H	-0. 15654900	4. 55869300	1. 92054500
H	-0. 12450600	5. 73824900	-0. 26445200
C	-0. 00310500	-0. 27874400	0. 98949400
O	0. 42350200	-0. 71758800	2. 03418400
C	-1. 44396800	-0. 45618400	0. 60862700
C	-2. 02662400	0. 16110600	-0. 50292100
C	-2. 21833000	-1. 28072200	1. 43324600
C	-3. 37196600	-0. 04697700	-0. 78858500
H	-1. 45242800	0. 82099600	-1. 14532400
C	-3. 55942300	-1. 49102000	1. 15086000
H	-1. 75347500	-1. 74836700	2. 29403700
C	-4. 12830900	-0. 87045800	0. 03915400
H	-3. 82878400	0. 43661500	-1. 64492900
H	-4. 16299700	-2. 12682100	1. 78986600
C	-5. 56907300	-1. 13918200	-0. 29258000
F	-6. 31211500	-1. 30589900	0. 81141100
F	-6. 11759500	-0. 14164600	-0. 99987400
F	-5. 70687600	-2. 25780200	-1. 02440800

BCPP-CF3-TS-gas

Sum of electronic and thermal Free Energies= -1636.794622

Imaginary frequency=-214.61

0 1

C	-6. 29179800	-0. 38295800	-2. 19466100
C	-6. 56016300	-0. 68044100	-0. 70327800

C	-5.18262000	-0.61141500	-0.01321000
H	-6.93905400	-0.96285900	-2.86063700
H	-6.46486800	0.67526300	-2.43636200
H	-6.95361400	-1.69711200	-0.60967700
H	-7.29323200	-0.00315900	-0.25910200
H	-4.98884200	0.36623500	0.44785500
H	-5.06384800	-1.34492500	0.78739800
C	-4.83091600	-0.72108300	-2.34685900
H	-4.32615300	-0.80535300	-3.30330800
C	-4.21933900	-0.84060300	-1.16214200
C	-0.70406800	-1.25024100	0.00462000
C	-2.12176800	-1.10392000	0.34902600
O	-2.59765900	-0.88014800	1.48040500
C	-2.79771700	-1.08141400	-0.94129400
N	-0.72219200	-1.48402100	-1.39072400
H	0.05448000	-1.23026500	-1.98787400
N	-1.92775300	-1.21998300	-1.91517500
C	0.26971500	-1.94863700	0.86082100
C	1.43410400	-2.50752500	0.31525300
C	0.09497700	-1.99458100	2.25499600
C	2.40938900	-3.06123900	1.13544000
H	1.58127100	-2.50089500	-0.76074700
C	1.08000300	-2.54567700	3.07111400
H	-0.83939100	-1.63521300	2.67764800
C	2.24643100	-3.06958900	2.51946400
H	3.30547700	-3.48207600	0.69019800
H	0.92519600	-2.57795800	4.14529700
H	3.01265700	-3.49551800	3.15851300
C	-0.27390400	0.76918700	-0.02134500
O	-0.98132800	1.32485100	-0.86787800
C	1.22325900	0.72596700	-0.20690200
C	2.16210100	0.47366300	0.79720700
C	1.66382900	0.93365500	-1.51904900
C	3.51772700	0.41827700	0.49270000
H	1.86440600	0.28094600	1.82431800
C	3.01554900	0.86693700	-1.82808000
H	0.91953300	1.16655800	-2.27371600
C	3.93985000	0.60779200	-0.81826800
H	4.24406500	0.21835900	1.27251400
H	3.35861200	1.03199200	-2.84395000
C	-1.66193900	4.66123400	1.86930900
C	-1.49788000	3.35644400	1.10055000
H	-2.27431400	5.36555400	1.30055900
H	-2.15273700	4.47177000	2.82951200

H	-0.69494200	5.13472700	2.06063400
C	-0.51246000	2.45743200	1.86531400
H	-1.07133900	3.56395000	0.11276100
H	0.52717400	2.75703700	1.70703100
H	-0.74386700	2.48765700	2.93473100
N	-2.76963200	2.64350700	1.00193300
H	-3.54882300	3.29259900	1.00199600
H	-2.78865000	2.12677700	0.12343700
N	-0.66274800	1.03577000	1.44688800
H	-1.66664200	0.76694700	1.55545200
H	-0.14834500	0.40192100	2.06523500
C	5.39577300	0.47675100	-1.16359800
F	5.69375600	-0.76821300	-1.56707500
F	5.74350000	1.30338500	-2.15979500
F	6.18331600	0.74865200	-0.11348000

BCPP-CF3-TS-DCM

Sum of electronic and thermal Free Energies= -1636.835492

Imaginary frequency=-231.71

0 1

C	-6.31466900	-0.51520800	-2.27105100
C	-6.60274100	-0.72040800	-0.76863000
C	-5.24117700	-0.55760500	-0.06325600
H	-6.93440500	-1.15378100	-2.90891100
H	-6.50690600	0.52079100	-2.58384500
H	-6.96409500	-1.74150500	-0.61195400
H	-7.36393300	-0.03787400	-0.38399800
H	-5.08731100	0.45988700	0.32035500
H	-5.11927900	-1.22741000	0.79119800
C	-4.84337700	-0.82520700	-2.37562400
H	-4.32491600	-0.96197600	-3.31975000
C	-4.24789300	-0.84221900	-1.17473400
C	-0.72445300	-1.11498800	0.07020800
C	-2.16342800	-0.97432900	0.38563900
O	-2.66060100	-0.72451400	1.49612200
C	-2.82419500	-1.02837800	-0.91173600
N	-0.73788600	-1.42905100	-1.31706300
H	0.05378400	-1.25691800	-1.92624000
N	-1.93351000	-1.21024000	-1.86212100
C	0.18932400	-1.88647500	0.95048800
C	1.31456400	-2.52930400	0.41434700
C	-0.01510300	-1.93636600	2.33752200
C	2.21645900	-3.18915300	1.24192000
H	1.49156700	-2.51029500	-0.65736900

C	0.89430600	-2.59607800	3.16223700
H	-0.90350600	-1.47769400	2.76059800
C	2.01632300	-3.21911700	2.62148900
H	3.08217700	-3.67809200	0.80569400
H	0.71702200	-2.62708500	4.23300700
H	2.72438100	-3.72953300	3.26642300
C	-0.23383400	0.77021700	-0.00768100
O	-0.92505500	1.35091800	-0.86830000
C	1.27023600	0.69932500	-0.20762400
C	2.21372300	0.51459000	0.80593600
C	1.70237900	0.79983100	-1.53540200
C	3.56855300	0.41856800	0.49748300
H	1.92366800	0.43247200	1.84991500
C	3.04912900	0.68833400	-1.85055100
H	0.96072300	0.97547200	-2.30763900
C	3.97855400	0.49654300	-0.82815000
H	4.29582100	0.27485700	1.28861100
H	3.37991700	0.75975200	-2.88253300
C	-1.47938700	4.81634400	1.75788000
C	-1.37370800	3.48287800	1.03109700
H	-2.10255200	5.51261900	1.18978600
H	-1.93028000	4.67429600	2.74575500
H	-0.49355000	5.27202900	1.88839100
C	-0.38061400	2.59132000	1.78735600
H	-0.98420400	3.64954300	0.02108600
H	0.65599900	2.85838400	1.57034700
H	-0.55767000	2.66884700	2.86400200
N	-2.67304000	2.80344800	1.00165400
H	-3.41638200	3.49127800	0.91151700
H	-2.70191600	2.22749300	0.16024200
N	-0.57732700	1.14810000	1.45286400
H	-1.57993200	0.93054400	1.60341900
H	-0.06282700	0.56278500	2.11702000
C	5.42619400	0.36603300	-1.19752300
F	5.64204700	-0.70836900	-1.97706700
F	5.85993800	1.43044300	-1.89463800
F	6.22192500	0.24228200	-0.12661800

m-TS-gas

Sum of electronic and thermal Free Energies= -1283.804767

Imaginary frequency= -257.08

0 1

C	5.41193400	-0.97429000	1.33017500
C	5.29738000	-1.72119100	-0.01803500

C	3. 84468600	-1. 50700200	-0. 49199600
H	6. 03472700	-1. 51107100	2. 05331800
H	5. 86568700	0. 01935100	1. 20920900
H	5. 46633200	-2. 78892900	0. 14958900
H	6. 03375200	-1. 38403100	-0. 75142500
H	3. 76035200	-0. 68593600	-1. 21417200
H	3. 41768400	-2. 38589000	-0. 98297000
C	3. 97687100	-0. 85016500	1. 77364800
H	3. 67593500	-0. 52426100	2. 76360500
C	3. 11905700	-1. 14592900	0. 78901700
C	-0. 58344600	-0. 85740700	0. 35370600
C	0. 73880100	-1. 08683400	-0. 25577600
O	0. 99475900	-1. 10149800	-1. 47622600
C	1. 66217800	-1. 08825100	0. 86743900
N	-0. 31383300	-0. 98547100	1. 74795100
H	-0. 85563000	-0. 45584500	2. 42080000
N	1. 00220200	-0. 93516800	1. 99163300
C	-1. 79448900	-1. 53156700	-0. 18430400
C	-2. 88805600	-1. 78063200	0. 65416900
C	-1. 89903200	-1. 86457300	-1. 54113100
C	-4. 06463500	-2. 31799100	0. 14781400
H	-2. 82189600	-1. 54052300	1. 71083300
C	-3. 08160900	-2. 40160600	-2. 04413600
H	-1. 04294500	-1. 72202800	-2. 19138900
C	-4. 17247000	-2. 62063100	-1. 20773600
H	-4. 90211800	-2. 49658100	0. 81469500
H	-3. 14474500	-2. 65773300	-3. 09734200
H	-5. 09318800	-3. 03559300	-1. 60460200
C	-0. 69823000	1. 07085200	0. 23230400
O	0. 09641000	1. 58922700	1. 02076100
C	-2. 18447000	1. 36122300	0. 38144400
C	-3. 16399300	1. 11539600	-0. 58541800
C	-2. 56739300	1. 88724400	1. 61714400
C	-4. 50085800	1. 39160600	-0. 31824600
H	-2. 91413800	0. 64856900	-1. 53507600
C	-3. 90621000	2. 15411500	1. 88679700
H	-1. 78849400	2. 09900200	2. 34246000
C	-4. 87637900	1. 90750800	0. 91924400
H	-5. 25041100	1. 18332700	-1. 07464400
H	-4. 19039300	2. 56397900	2. 85071300
H	-5. 92089600	2. 11497000	1. 12773700
C	3. 23215500	2. 83419300	-1. 25232400
H	3. 23576800	3. 35046100	-2. 22090900
H	3. 01017200	3. 59169700	-0. 49128700

C	0.75963600	2.34551200	-1.46809600
H	0.52920500	3.11288200	-0.72650900
H	0.68000900	2.77039100	-2.47348600
N	-0.29575500	1.29320500	-1.33743100
H	0.06976300	0.40014600	-1.73511500
H	-1.13441900	1.56952000	-1.84535900
C	2.14414000	1.76530300	-1.22514500
H	2.35232500	0.99223700	-1.97481700
H	2.14757700	1.27991100	-0.24375300
C	4.60322600	2.21890300	-0.98099700
H	4.87513400	1.50897500	-1.76897200
H	5.38588200	2.97949300	-0.92744500
H	4.58856600	1.67099500	-0.03241300

m-TS-DCM

Sum of electronic and thermal Free Energies= -1283.844811

Imaginary frequency=-182.73

O 1

C	5.37573900	-1.28142700	1.47565400
C	5.32045100	-1.70112000	-0.00956800
C	3.89403900	-1.35657300	-0.48571000
H	5.96929200	-1.97107400	2.08471100
H	5.82591700	-0.28715100	1.60275400
H	5.47059000	-2.78250900	-0.08138900
H	6.09317600	-1.22016100	-0.61383800
H	3.84936000	-0.38771200	-0.99994800
H	3.48639400	-2.09311600	-1.18308500
C	3.92305000	-1.24795100	1.87382100
H	3.58624400	-1.15230500	2.90156800
C	3.10878500	-1.28405900	0.80997300
C	-0.57630500	-0.84353000	0.24847800
C	0.77472000	-1.06027600	-0.32889200
O	1.07772300	-1.01006700	-1.52990200
C	1.65159700	-1.18822400	0.82851800
N	-0.36095100	-1.12300700	1.63654200
H	-0.93551800	-0.67774600	2.34510400
N	0.94306600	-1.12839900	1.93134500
C	-1.75671500	-1.49928300	-0.38931200
C	-2.83453900	-1.91934000	0.40166900
C	-1.84574500	-1.65158200	-1.77921200
C	-3.97634600	-2.45923500	-0.18033400
H	-2.78454500	-1.81800600	1.48160500
C	-2.99251300	-2.19197000	-2.35821200
H	-1.00999700	-1.36699200	-2.40838400

C	-4.06529300	-2.59096800	-1.56515900
H	-4.80033600	-2.77553600	0.45192700
H	-3.04167800	-2.30474500	-3.43708700
H	-4.95799900	-3.00868700	-2.01973400
C	-0.69149300	1.01415200	0.29108700
O	0.13961400	1.48427700	1.09052400
C	-2.17082500	1.30493600	0.55049200
C	-3.20572700	1.19185800	-0.38439700
C	-2.48355500	1.67754400	1.86075700
C	-4.52248200	1.45240500	-0.01340400
H	-3.01549800	0.86755100	-1.40419900
C	-3.80161600	1.92660400	2.23465900
H	-1.67025000	1.78103100	2.57174800
C	-4.82566700	1.81598900	1.29698200
H	-5.31309400	1.35893100	-0.75137700
H	-4.02692600	2.21425500	3.25697000
H	-5.85404300	2.01177500	1.58402400
C	3.07086200	3.12219300	-1.26117800
H	2.97009600	3.67984200	-2.20082000
H	2.84694800	3.82698900	-0.45132100
C	0.63112500	2.49505000	-1.35691300
H	0.39599600	3.19902300	-0.55729700
H	0.47406600	2.97822400	-2.32463600
N	-0.36236000	1.38109200	-1.25585100
H	0.02287800	0.55892600	-1.74988600
H	-1.22100000	1.65462300	-1.73480600
C	2.05684700	1.98179400	-1.22733300
H	2.26455500	1.27253900	-2.03856400
H	2.14822800	1.43424900	-0.28286100
C	4.49992300	2.60826800	-1.11366600
H	4.75769800	1.92726500	-1.93184500
H	5.22462800	3.42729800	-1.11899900
H	4.61791700	2.06021000	-0.17236900

s-TS-gas

Sum of electronic and thermal Free Energies= -1339.108505

Imaginary frequency=-160.43

0 1

C	-5.60340100	-0.95521100	-0.98712200
C	-5.42995100	-1.62653000	0.39255400
C	-3.94036100	-1.45128900	0.74935100
H	-6.33229000	-1.47416400	-1.61801500
H	-5.95944400	0.08144200	-0.89250200
H	-5.64980000	-2.69407100	0.29611500

H	-6. 10193800	-1. 22029300	1. 15226900
H	-3. 75455400	-0. 56598200	1. 37118100
H	-3. 52188800	-2. 29924100	1. 29603300
C	-4. 20477600	-0. 98190400	-1. 55025000
H	-3. 96416100	-0. 76237900	-2. 58519100
C	-3. 29227400	-1. 25374700	-0. 60740100
C	0. 43186100	-1. 17337200	-0. 42373900
C	-0. 84461900	-1. 37151700	0. 27799200
O	-1. 03966600	-1. 45471400	1. 50325300
C	-1. 84324600	-1. 27171800	-0. 78484800
N	0. 06544500	-1. 22751800	-1. 79326700
H	0. 58372200	-0. 70019600	-2. 48502100
N	-1. 26072500	-1. 11089200	-1. 94966900
C	1. 68207700	-1. 85616700	-0. 02162200
C	2. 77243300	-1. 90862100	-0. 90001200
C	1. 81547300	-2. 44292800	1. 24546600
C	3. 97157400	-2. 49591600	-0. 51448600
H	2. 69052200	-1. 46879300	-1. 88975800
C	3. 02107200	-3. 02178900	1. 63039000
H	0. 95977700	-2. 44933000	1. 91331900
C	4. 10769000	-3. 04338600	0. 75872500
H	4. 80502100	-2. 51753400	-1. 20953400
H	3. 10633300	-3. 47091900	2. 61517700
H	5. 04630200	-3. 49465400	1. 06338500
C	0. 48692500	0. 92600900	-0. 30407200
O	-0. 27497500	1. 31687500	-1. 19517400
C	1. 96046500	1. 29512600	-0. 39366600
C	3. 00712900	0. 83193300	0. 41486700
C	2. 26421100	2. 18609100	-1. 43197900
C	4. 31084600	1. 26853900	0. 19741400
H	2. 83702200	0. 09706400	1. 19050700
C	3. 56762700	2. 61915200	-1. 64721400
H	1. 44966300	2. 52607600	-2. 06159800
C	4. 59708500	2. 16341000	-0. 82877600
H	5. 10730600	0. 88526400	0. 82691600
H	3. 77746800	3. 31306500	-2. 45490000
H	5. 61698100	2. 49535200	-0. 99467000
C	-2. 51930400	4. 12009100	1. 10780400
C	-1. 78603500	2. 97212500	0. 42434300
H	-3. 36757300	4. 45002800	0. 50248600
H	-2. 89363000	3. 79908500	2. 08583000
H	-1. 85800000	4. 97830200	1. 25774000
C	-0. 50603100	2. 65158000	1. 22937900
H	-1. 48544000	3. 27649200	-0. 58124900

H	0.34914300	3.25447700	0.90961300
H	-0.69207000	2.83753400	2.29275800
N	-2.61865000	1.76958000	0.38433100
H	-3.60635200	1.99555700	0.43364700
H	-2.45071900	1.26968000	-0.48749700
N	-0.12060300	1.21123300	1.13263900
H	-1.02618600	0.70674200	1.14926400
C	0.63787100	0.77703000	2.32830500
H	-0.03606100	0.82460000	3.18464100
H	0.95653400	-0.25282800	2.19215500
H	1.48713800	1.44356400	2.47560700

s-TS-DCM

Sum of electronic and thermal Free Energies= -1339.147101

Imaginary frequency= -127.80

O 1

C	-5.65236900	-0.97610300	-1.05176500
C	-5.50491000	-1.52449100	0.38315000
C	-4.02175200	-1.31762100	0.75069800
H	-6.36843600	-1.54839200	-1.65029200
H	-6.00383300	0.06555200	-1.05505500
H	-5.72388300	-2.59678100	0.37791200
H	-6.18788900	-1.05108000	1.09221200
H	-3.84997400	-0.38159200	1.29887800
H	-3.61912900	-2.12035700	1.37298100
C	-4.24448500	-1.04745300	-1.58489100
H	-3.99192400	-0.90752300	-2.63157200
C	-3.34694200	-1.23171200	-0.60591300
C	0.39647000	-1.04992000	-0.36212400
C	-0.90498900	-1.27810800	0.32450000
O	-1.11221000	-1.35528900	1.53909500
C	-1.89352800	-1.24081700	-0.75656700
N	0.03859100	-1.21416500	-1.74376200
H	0.54702700	-0.68754400	-2.44707400
N	-1.28895000	-1.12328500	-1.91163800
C	1.59795600	-1.84264100	0.05093400
C	2.65995900	-1.99960900	-0.85042200
C	1.69868400	-2.44194100	1.31251100
C	3.79897400	-2.71327700	-0.49407900
H	2.60365900	-1.54909500	-1.83730400
C	2.84402300	-3.15144400	1.66944700
H	0.87129300	-2.36099600	2.00925800
C	3.90108100	-3.28582400	0.77280600
H	4.61030300	-2.81798900	-1.20780500

H	2. 90222800	-3. 60962000	2. 65214000
H	4. 79180400	-3. 83893600	1. 05348000
C	0. 53491200	0. 86196600	-0. 31639700
O	-0. 23046700	1. 31247800	-1. 19940300
C	2. 02088000	1. 22511700	-0. 43726100
C	3. 06805200	0. 78783800	0. 38570500
C	2. 32830000	2. 07447900	-1. 50704700
C	4. 37559100	1. 20621600	0. 14931900
H	2. 89083100	0. 09685300	1. 19961000
C	3. 63576000	2. 48842300	-1. 74593300
H	1. 51450600	2. 40239100	-2. 14392100
C	4. 66600000	2. 05672000	-0. 91472400
H	5. 17121800	0. 85032200	0. 79652300
H	3. 84749300	3. 14888500	-2. 58123300
H	5. 68801100	2. 37435500	-1. 09674900
C	-2. 31333800	4. 24744700	1. 12409400
C	-1. 64005500	3. 07667000	0. 42049200
H	-3. 18090300	4. 59355400	0. 55507100
H	-2. 64926800	3. 94574400	2. 12214300
H	-1. 62124900	5. 08763100	1. 23351000
C	-0. 33140900	2. 73166400	1. 16636000
H	-1. 38085500	3. 36576800	-0. 60092500
H	0. 52764600	3. 27643900	0. 76656600
H	-0. 44216000	2. 98100900	2. 22628500
N	-2. 51958600	1. 89984200	0. 42558700
H	-3. 49439100	2. 18817000	0. 41838200
H	-2. 34927200	1. 37541800	-0. 43193500
N	-0. 01924400	1. 26923200	1. 13238000
H	-0. 95220700	0. 83054700	1. 19252300
C	0. 73048600	0. 86214100	2. 34364500
H	0. 06718900	0. 97791200	3. 20204800
H	1. 02572000	-0. 18041000	2. 25709700
H	1. 60208800	1. 50456200	2. 46253500

a-TS[‡] -gas

Sum of electronic and thermal Free Energies= -1299.854557

Imaginary frequency= -212.20

0 1

C	5. 82339200	-0. 21090800	1. 13462800
C	5. 78024800	-0. 87589100	-0. 25875700
C	4. 29456900	-0. 87342600	-0. 67308700
H	6. 57464800	-0. 66201000	1. 79106800
H	6. 07077000	0. 85813600	1. 06877200
H	6. 12245400	-1. 91117800	-0. 16795300

H	6. 42640400	-0. 38022400	-0. 98696500
H	4. 02968100	-0. 02635800	-1. 31898900
H	4. 00133300	-1. 76868100	-1. 22715000
C	4. 41385100	-0. 39101900	1. 63747500
H	4. 10730000	-0. 20079300	2. 66046500
C	3. 57608500	-0. 75158000	0. 65730700
C	-0. 12449400	-1. 02850300	0. 29112600
C	1. 20317700	-1. 05516000	-0. 34388600
O	1. 44582400	-1. 02032600	-1. 56236400
C	2. 13318700	-0. 93354000	0. 77143800
N	0. 17719500	-1. 13429000	1. 67736900
H	-0. 43210900	-0. 71340600	2. 36942900
N	1. 47891300	-0. 89657000	1. 90735100
C	-1. 25760400	-1. 80035900	-0. 26376500
C	-2. 27169800	-2. 28127600	0. 57377700
C	-1. 38349300	-1. 99249900	-1. 64904200
C	-3. 39512800	-2. 90485700	0. 04390100
H	-2. 18366900	-2. 15590700	1. 64859700
C	-2. 51310600	-2. 61489200	-2. 17354500
H	-0. 57121100	-1. 68275300	-2. 29921000
C	-3. 52992500	-3. 06271600	-1. 33346600
H	-4. 17211700	-3. 26375900	0. 71154800
H	-2. 59201600	-2. 76012000	-3. 24671600
H	-4. 41047200	-3. 54378100	-1. 74638200
C	-0. 47894700	0. 92642400	0. 20640900
O	0. 37646800	1. 53229400	0. 87115600
C	-1. 93068800	0. 99358600	0. 64638900
C	-3. 04452200	0. 64407900	-0. 12365200
C	-2. 12696500	1. 42578900	1. 96181400
C	-4. 32547200	0. 73224400	0. 41218900
H	-2. 94181900	0. 25862100	-1. 13508300
C	-3. 40793300	1. 50132100	2. 49998500
H	-1. 25208400	1. 72055500	2. 53266300
C	-4. 51192400	1. 15735600	1. 72478200
H	-5. 17756700	0. 44997900	-0. 19745700
H	-3. 54343700	1. 83909900	3. 52242300
H	-5. 51255000	1. 21832000	2. 14006100
C	-0. 20474300	2. 53314200	-1. 80594600
N	2. 17195200	2. 13195500	-1. 31152300
H	3. 07192700	2. 54573000	-1. 52209300
H	2. 22749600	1. 70691500	-0. 38647900
N	-0. 33038500	1. 10905200	-1. 33549600
H	0. 54763500	0. 62127400	-1. 62645100
H	-1. 09375600	0. 63428900	-1. 82204000

C	1. 11644200	3. 13469100	-1. 29381300
H	0. 94558900	3. 56250900	-0. 30082500
H	1. 36650000	3. 95214100	-1. 97832300
H	-0. 13691300	2. 43814900	-2. 89556800
C	-1. 40616600	3. 37642500	-1. 41824400
H	-2. 34589700	2. 95924700	-1. 78953200
H	-1. 47409600	3. 47092500	-0. 33164800
H	-1. 28295500	4. 37571000	-1. 84451600

a-TS' -DCM

Sum of electronic and thermal Free Energies= -1299.894911

Imaginary frequency= -151.65

0 1

C	5. 88489600	-0. 36044500	1. 22773300
C	5. 84078300	-0. 74966000	-0. 26559900
C	4. 36086200	-0. 62428700	-0. 68223400
H	6. 61322500	-0. 94977000	1. 79421100
H	6. 16053200	0. 69437200	1. 36624900
H	6. 15287400	-1. 79315000	-0. 37078000
H	6. 50679600	-0. 14232900	-0. 88267800
H	4. 13936000	0. 33922000	-1. 16038500
H	4. 05105500	-1. 39404700	-1. 39304200
C	4. 46494400	-0. 58744500	1. 67753100
H	4. 15939500	-0. 58421200	2. 71932500
C	3. 62532600	-0. 72342100	0. 64153600
C	-0. 10174600	-0. 91391100	0. 21172400
C	1. 24738700	-0. 92063100	-0. 41472600
O	1. 49881700	-0. 86094700	-1. 62385900
C	2. 17391100	-0. 86658900	0. 71331000
N	0. 20687000	-1. 10171500	1. 59739900
H	-0. 40979000	-0. 74092800	2. 31857100
N	1. 50401300	-0. 88451900	1. 84062900
C	-1. 16927100	-1. 78392100	-0. 36120100
C	-2. 10342500	-2. 40251300	0. 48039400
C	-1. 29956000	-1. 95272600	-1. 74672000
C	-3. 14748300	-3. 15456400	-0. 04835800
H	-2. 01623100	-2. 29149300	1. 55718100
C	-2. 34849200	-2. 70445400	-2. 27187100
H	-0. 56310400	-1. 51231600	-2. 41033500
C	-3. 28097700	-3. 30306900	-1. 42784900
H	-3. 86124800	-3. 62355700	0. 62197900
H	-2. 43085200	-2. 82588000	-3. 34777400
H	-4. 09862500	-3. 88600000	-1. 83970900
C	-0. 53645100	0. 91322900	0. 20599100

O	0.31159600	1.55829200	0.86784900
C	-1.98300600	0.92519700	0.69691600
C	-3.11035400	0.58462000	-0.05853500
C	-2.15301400	1.27868100	2.03888700
C	-4.37761200	0.60440900	0.51893000
H	-3.02814000	0.28506400	-1.09988200
C	-3.41861900	1.28422400	2.62024000
H	-1.27289300	1.56339400	2.60660000
C	-4.53620000	0.94871300	1.85994100
H	-5.24190600	0.34049700	-0.08242800
H	-3.53083800	1.55938600	3.66441600
H	-5.52513200	0.95579700	2.30730300
C	-0.41962900	2.66912500	-1.72523900
N	2.00420700	2.37632400	-1.36819100
H	2.87635000	2.88538400	-1.47528000
H	2.06197300	1.87090200	-0.48367100
N	-0.46327100	1.21188900	-1.33116200
H	0.41707500	0.79761400	-1.68850600
H	-1.22269100	0.75345800	-1.84149500
C	0.89118800	3.31542200	-1.25557300
H	0.75354700	3.69817600	-0.23887500
H	1.06628700	4.16851400	-1.91850100
H	-0.41038300	2.62644300	-2.81907600
C	-1.63553900	3.43641300	-1.24298300
H	-2.56980100	3.00079600	-1.60624600
H	-1.66384200	3.47758700	-0.15109900
H	-1.56655100	4.46008000	-1.62220400

b-TS-gas

Sum of electronic and thermal Free Energies= -1606.143792

Imaginary frequency= -241.05

0 1

C	1.53369000	5.78702300	0.20998600
C	2.55806300	4.79819400	0.80639200
C	1.92396000	3.40278700	0.63841700
H	1.50828000	6.74001100	0.74815200
H	1.76289200	6.02506300	-0.83818800
H	2.67461400	5.00817600	1.87394700
H	3.54540500	4.87637200	0.34545400
H	2.26567600	2.90402800	-0.27991100
H	2.14930900	2.72286500	1.46287900
C	0.23926700	5.02048500	0.29942200
H	-0.73867300	5.46432000	0.14737500
C	0.44451800	3.71717600	0.52378100

C	-1. 71202800	0. 66747500	0. 73970300
C	-0. 38481600	1. 27989100	0. 91325500
O	0. 67948900	0. 67120300	1. 14464100
C	-0. 58084800	2. 68121400	0. 58406800
N	-2. 55676200	1. 79572100	0. 52181200
H	-3. 38142700	1. 71443700	-0. 06214600
N	-1. 83884400	2. 89810800	0. 27569600
C	-2. 18520100	-0. 40331600	1. 64996200
C	-3. 54894900	-0. 52969600	1. 94345300
C	-1. 29890700	-1. 35990700	2. 16952800
C	-4. 01988500	-1. 59787900	2. 69805600
H	-4. 24738700	0. 21197800	1. 56938100
C	-1. 77658800	-2. 42948900	2. 92158600
H	-0. 23261900	-1. 24372400	2. 00556000
C	-3. 13900600	-2. 56307700	3. 17910000
H	-5. 08221300	-1. 67775500	2. 90604500
H	-1. 07523100	-3. 15785200	3. 31717000
H	-3. 50764700	-3. 40074300	3. 76185600
C	-1. 52408300	0. 02723400	-1. 08592300
O	-1. 22615200	0. 96213500	-1. 83847700
C	-2. 82390600	-0. 72829800	-1. 33909300
C	-3. 18588600	-1. 95815300	-0. 77978400
C	-3. 71630900	-0. 09000800	-2. 20590200
C	-4. 41324400	-2. 53724100	-1. 08994000
H	-2. 54905300	-2. 46781500	-0. 05997700
C	-4. 94707200	-0. 66465900	-2. 50572600
H	-3. 40234400	0. 85119700	-2. 64579100
C	-5. 29728500	-1. 89279600	-1. 95041700
H	-4. 68120100	-3. 48895700	-0. 64276000
H	-5. 62870800	-0. 15788100	-3. 18136300
H	-6. 25505600	-2. 34581300	-2. 18525400
C	3. 84608000	-0. 59595400	-1. 40663200
H	3. 87748200	0. 30277200	-0. 77426000
H	4. 85454100	-0. 74039600	-1. 80248500
N	2. 33060700	-1. 57669200	0. 30015500
H	2. 35180600	-2. 23020900	1. 08126100
H	2. 37627000	-0. 65332600	0. 73219500
C	2. 89319200	-0. 35194400	-2. 58264300
H	3. 33151100	0. 45183800	-3. 18282300
H	2. 88370400	-1. 23766500	-3. 23296000
C	1. 45858400	0. 04792300	-2. 21080400
H	1. 47085300	0. 62384000	-1. 27777100
H	1. 03704900	0. 71992000	-2. 95846200
N	-0. 34908700	-0. 99560100	-0. 83855600

H	-0.71665900	-1.89962400	-0.54324400
H	0.27193300	-0.66436500	-0.07243300
C	3.51950300	-1.79815900	-0.50998900
H	3.35476000	-2.67045000	-1.16279000
C	0.51224900	-1.15029800	-2.04821600
H	1.07526400	-2.07296100	-1.89977700
H	-0.15436600	-1.26208400	-2.90623700
C	4.71506900	-2.18075300	0.36605100
O	4.65313800	-2.36203200	1.55750100
O	5.83821600	-2.34587300	-0.34717600
C	6.97831700	-2.75381900	0.41184800
H	7.79500000	-2.84359100	-0.30167900
H	7.21155700	-2.00912500	1.17504900
H	6.78486900	-3.71044500	0.90108100

b-TS-DCM

Sum of electronic and thermal Free Energies= -1606.190896

Imaginary frequency= -203.70

0 1

C	1.51677800	5.80624000	-0.56144700
C	2.50820000	4.94678600	0.25149700
C	1.88773800	3.53561900	0.29473100
H	1.45396500	6.83599300	-0.19519200
H	1.80516000	5.86674100	-1.62028800
H	2.56725900	5.34019300	1.27109300
H	3.51815100	4.95336900	-0.16455200
H	2.28673700	2.88367500	-0.49531500
H	2.06128400	3.02003700	1.24174500
C	0.22194600	5.04823500	-0.41991600
H	-0.74442400	5.45184400	-0.70673300
C	0.41665900	3.80254600	0.03479800
C	-1.74150400	0.77959400	0.59049300
C	-0.44194600	1.45926500	0.81386900
O	0.57561500	0.96661500	1.31951800
C	-0.60397200	2.76985000	0.19033500
N	-2.55642800	1.83469300	0.07047800
H	-3.33231100	1.63736300	-0.55338300
N	-1.81691100	2.88608000	-0.29608400
C	-2.33230000	-0.06485100	1.66435900
C	-3.72376100	-0.13893000	1.82024200
C	-1.52294800	-0.85058800	2.49884500
C	-4.28954300	-0.98346200	2.76956800
H	-4.36918300	0.46674300	1.19102700
C	-2.09480800	-1.69712700	3.44643700

H	-0.44310900	-0.77717500	2.41592800
C	-3.47891600	-1.77376400	3.58304100
H	-5.36973200	-1.02558800	2.87113200
H	-1.45118200	-2.29484500	4.08492700
H	-3.92172700	-2.43626800	4.31986200
C	-1.36722800	-0.19307100	-0.99859600
O	-0.95431600	0.57661200	-1.88952300
C	-2.65805700	-0.96651600	-1.26073500
C	-3.06719700	-2.12441300	-0.58997300
C	-3.48821400	-0.43137300	-2.25093000
C	-4.28119500	-2.73029400	-0.90679100
H	-2.46522600	-2.56934200	0.19840700
C	-4.70784900	-1.02860400	-2.55717000
H	-3.14552200	0.45213700	-2.78017600
C	-5.10686000	-2.18267300	-1.88590200
H	-4.58247600	-3.62921300	-0.37828000
H	-5.34176000	-0.59841600	-3.32632800
H	-6.05435500	-2.65519500	-2.12501700
C	3.78499700	-1.40943300	-1.59474900
H	3.92765600	-0.31987000	-1.61527500
H	4.72698400	-1.85892500	-1.92284500
N	2.48470700	-1.03782000	0.47836600
H	2.41920400	-1.26967400	1.46819000
H	2.74461100	-0.05189900	0.46585000
C	2.69174400	-1.79753400	-2.59562400
H	3.05629600	-1.51006800	-3.58712500
H	2.58690100	-2.89049300	-2.61661500
C	1.32224300	-1.14211400	-2.36799200
H	1.45508400	-0.15351800	-1.91908400
H	0.82562500	-0.96552000	-3.32405200
N	-0.28215800	-1.15478200	-0.43480900
H	-0.68134500	-1.76886900	0.27880700
H	0.47349700	-0.62713700	0.04273400
C	3.54691400	-1.82225300	-0.13306600
H	3.26955200	-2.88442400	-0.10834100
C	0.39241300	-1.98058800	-1.47969000
H	0.95583900	-2.74015100	-0.93388300
H	-0.38964700	-2.48049500	-2.05586000
C	4.85551800	-1.69521600	0.64422300
O	5.05058100	-0.90440000	1.53782600
O	5.77545700	-2.56764900	0.21662500
C	7.04316900	-2.49999900	0.87883500
H	7.66471800	-3.26303200	0.41323400
H	7.49097300	-1.51282800	0.74662900

H 6.92720300 -2.70374700 1.94539900

b-TS' -gas

Sum of electronic and thermal Free Energies= -1606.143761

Imaginary frequency= -234.17

O 1

C	-5.28043400	-2.10087300	-2.09648800
C	-5.48013300	-1.83089900	-0.59046300
C	-4.11973700	-1.30485900	-0.09266000
H	-5.86234200	-2.95752700	-2.45097900
H	-5.58683600	-1.23896200	-2.70576100
H	-5.70075400	-2.77680300	-0.08630300
H	-6.30469100	-1.14480500	-0.38360100
H	-4.07988100	-0.20603500	-0.11913200
H	-3.88466800	-1.60233900	0.93189300
C	-3.79171200	-2.31063800	-2.20020100
H	-3.29725200	-2.72284600	-3.07308700
C	-3.14836700	-1.87278600	-1.11098200
C	0.43655900	-1.59427800	-0.08250800
C	-0.98037700	-1.49658800	0.29253700
O	-1.42541600	-1.05940900	1.37374500
C	-1.70213900	-1.86732800	-0.91354100
N	0.38737200	-2.21292100	-1.36343600
H	1.10386000	-2.02335400	-2.05481700
N	-0.85296100	-2.18809200	-1.86413400
C	1.45650800	-2.05146000	0.89116700
C	2.59189600	-2.74412300	0.45210800
C	1.35087200	-1.73634700	2.25424400
C	3.60651700	-3.08396500	1.33853600
H	2.68477500	-3.01102600	-0.59592500
C	2.37171000	-2.07712300	3.13741000
H	0.45272800	-1.25092600	2.62017600
C	3.50900800	-2.74100500	2.68484900
H	4.47970000	-3.61527300	0.97339300
H	2.27156900	-1.82832100	4.18959200
H	4.30389800	-3.00113500	3.37603400
C	0.77111800	0.25643300	-0.65708700
O	0.06327200	0.54209400	-1.62868400
C	2.28374000	0.26649000	-0.82845000
C	3.22900800	0.30042700	0.20039800
C	2.72440200	0.24691600	-2.15399800
C	4.58801500	0.32751700	-0.09567500
H	2.92968200	0.26300500	1.24527200
C	4.08520700	0.25891200	-2.44881300

H	1. 97313100	0. 25451700	-2. 93776600
C	5. 02138700	0. 30461600	-1. 41960900
H	5. 30913700	0. 34914700	0. 71494100
H	4. 41239300	0. 24437500	-3. 48361500
H	6. 08272100	0. 31892700	-1. 64532400
C	-3. 48472100	2. 47744300	1. 94208400
H	-3. 94949600	1. 48574200	1. 84256100
H	-4. 29333700	3. 16792600	2. 20694200
N	-1. 53840300	1. 34660600	3. 00767100
H	-1. 08413900	1. 20060500	3. 90513700
H	-2. 01225300	0. 47295700	2. 78081800
C	-2. 92053800	2. 89677200	0. 57936600
H	-3. 76465500	2. 98137400	-0. 11247900
H	-2. 48773300	3. 90423100	0. 64114800
C	-1. 89872100	1. 92740600	-0. 02919900
H	-2. 13320700	0. 90703700	0. 28715200
H	-1. 94304500	1. 94444400	-1. 11782700
C	-0. 46369700	2. 25184500	0. 39093500
H	-0. 47672300	2. 79265000	1. 34203400
N	0. 35249900	1. 02647300	0. 67469200
H	1. 19452200	1. 30251200	1. 18136700
H	-0. 23540700	0. 44344400	1. 30310400
C	-2. 51684300	2. 43559800	3. 12467800
H	-1. 97292600	3. 38876900	3. 18313300
H	-3. 11342900	2. 35998800	4. 04584500
C	0. 25599700	3. 12443900	-0. 62308700
O	-0. 28182600	3. 84961900	-1. 41472900
O	1. 58439800	3. 02880200	-0. 45478500
C	2. 38322500	3. 65558800	-1. 45986100
H	2. 30126200	4. 74174200	-1. 38618700
H	3. 40374200	3. 32322600	-1. 27239000
H	2. 05017900	3. 33063100	-2. 44741100

b-TS' -DCM

Sum of electronic and thermal Free Energies= -1606.186463

Imaginary frequency= -227.95

0 1

C	-5. 28980000	-2. 22977400	-2. 07407700
C	-5. 51006800	-1. 79821600	-0. 60901300
C	-4. 14918900	-1. 24612500	-0. 14059600
H	-5. 87222700	-3. 11645600	-2. 34417300
H	-5. 57911500	-1. 43663300	-2. 77775500
H	-5. 76093000	-2. 68043600	-0. 01189000
H	-6. 32258600	-1. 07722000	-0. 49417500

H	-4. 08797600	-0. 15580400	-0. 26655600
H	-3. 93603100	-1. 45265400	0. 91077600
C	-3. 80157300	-2. 46006600	-2. 13350300
H	-3. 30459300	-2. 96321000	-2. 95727100
C	-3. 16807700	-1. 91937800	-1. 08318700
C	0. 41339100	-1. 55177900	-0. 03326300
C	-1. 01471800	-1. 46421900	0. 33178500
O	-1. 47572400	-1. 02495300	1. 39839000
C	-1. 72359800	-1. 89029900	-0. 86826300
N	0. 37440800	-2. 23251000	-1. 28530700
H	1. 11170000	-2. 12029300	-1. 97347300
N	-0. 85889200	-2. 24522500	-1. 79340600
C	1. 41452300	-2. 00358400	0. 96928900
C	2. 51470300	-2. 77403300	0. 56881800
C	1. 31733800	-1. 62354100	2. 31611200
C	3. 49710200	-3. 14138100	1. 48229800
H	2. 60657900	-3. 08547300	-0. 46741400
C	2. 30535500	-1. 99223200	3. 22653400
H	0. 45545300	-1. 05972500	2. 65627400
C	3. 40238000	-2. 74579800	2. 81543700
H	4. 34116600	-3. 73741600	1. 14893600
H	2. 21137300	-1. 69128100	4. 26572600
H	4. 17117200	-3. 02909500	3. 52720100
C	0. 75457600	0. 23831500	-0. 65738200
O	0. 03109900	0. 50908500	-1. 63329700
C	2. 26588600	0. 22009000	-0. 86466900
C	3. 23189500	0. 32463600	0. 14099400
C	2. 68284200	0. 07789800	-2. 19085800
C	4. 58662000	0. 29484200	-0. 17913200
H	2. 95218600	0. 40849000	1. 18808800
C	4. 03837900	0. 03178500	-2. 50932200
H	1. 92334400	0. 02419200	-2. 96448500
C	4. 99511500	0. 14403600	-1. 50350200
H	5. 32409300	0. 37939200	0. 61298400
H	4. 34477600	-0. 08039400	-3. 54479300
H	6. 05235600	0. 11466700	-1. 74758000
C	-3. 30106000	2. 64930000	2. 08129800
H	-3. 81016300	1. 67462200	2. 06015000
H	-4. 05456000	3. 38188600	2. 39168200
N	-1. 33633200	1. 44519700	3. 02531400
H	-0. 77239700	1. 35313900	3. 86763300
H	-1. 89470900	0. 59477100	2. 96820800
C	-2. 84886400	3. 00134200	0. 65942500
H	-3. 74663200	3. 06849400	0. 03585800

H	-2.39733700	4.00249800	0.64692600
C	-1.88904400	1.99230300	0.01603800
H	-2.12420400	0.98962400	0.38424300
H	-2.01046800	1.97539600	-1.06753200
C	-0.42339000	2.30152200	0.32567800
H	-0.36029900	2.90514800	1.23624600
N	0.37857900	1.07385600	0.63789400
H	1.22835900	1.35472600	1.13219200
H	-0.20484400	0.55286000	1.31894200
C	-2.22895000	2.60413800	3.16994700
H	-1.62161100	3.51815800	3.12453000
H	-2.73562800	2.61232600	4.14583800
C	0.25067400	3.10006300	-0.77607500
O	-0.32893700	3.77206300	-1.59153300
O	1.57982200	3.03177200	-0.65968100
C	2.33315800	3.65579100	-1.70448000
H	2.16016100	4.73390700	-1.70511900
H	3.37810400	3.43748900	-1.48875600
H	2.04743400	3.23752300	-2.67193000

c-TS-gas

Sum of electronic and thermal Free Energies= -1378.396944

Imaginary frequency= -217.78

0 1

C	-6.56053800	0.69313700	-0.75811300
C	-6.17340500	1.54728800	0.46831900
C	-4.63882100	1.43952400	0.57427300
H	-7.52007100	0.18218700	-0.62756900
H	-6.65305800	1.30575400	-1.66591400
H	-6.62336700	1.10684800	1.36343100
H	-6.52442700	2.57938900	0.39722700
H	-4.12852500	2.27594600	0.07913900
H	-4.27576000	1.42659000	1.60431500
C	-5.39571100	-0.25477900	-0.88504600
H	-5.39587000	-1.13198700	-1.52305100
C	-4.34093600	0.15188600	-0.16854200
C	-0.81658300	-1.01961800	0.30128100
C	-1.88956800	-0.08465300	0.68270800
O	-1.76452900	0.91860300	1.41353300
C	-3.03034500	-0.48704600	-0.12583500
N	-1.48476200	-1.94258000	-0.55570300
H	-0.99073200	-2.39017900	-1.31897600
N	-2.70305600	-1.50155700	-0.89191600
C	0.12383100	-1.55969600	1.31213000

C	0. 70417800	-2. 82367300	1. 13643300
C	0. 51115000	-0. 79822600	2. 42474700
C	1. 66564300	-3. 29627100	2. 02097800
H	0. 40413300	-3. 43753700	0. 29298500
C	1. 47767900	-1. 27497600	3. 30599800
H	0. 02637900	0. 15626400	2. 60379300
C	2. 06956800	-2. 51907000	3. 10452900
H	2. 10438600	-4. 27598100	1. 85984800
H	1. 75884100	-0. 67283800	4. 16559500
H	2. 82413800	-2. 88674400	3. 79220900
C	0. 10029200	0. 09942600	-1. 00598500
O	-0. 68833100	0. 50377600	-1. 86878400
C	1. 28419100	-0. 75850800	-1. 42310000
C	2. 42870400	-0. 99733500	-0. 65520300
C	1. 17226300	-1. 35332500	-2. 68313100
C	3. 44268000	-1. 81571500	-1. 14803000
H	2. 54107200	-0. 57591500	0. 34150200
C	2. 17966300	-2. 18256400	-3. 16570700
H	0. 28706800	-1. 12533900	-3. 26906600
C	3. 31978300	-2. 41338600	-2. 39915800
H	4. 32424500	-1. 99649600	-0. 54115900
H	2. 08010700	-2. 63965600	-4. 14505900
H	4. 10974500	-3. 05566600	-2. 77504800
N	0. 56032200	1. 20461800	-0. 00985200
H	-0. 27717100	1. 43996300	0. 56746600
H	1. 29732100	0. 91040300	0. 65390800
C	1. 69489800	3. 40335100	0. 21057300
H	0. 97299900	3. 68715100	0. 98785800
H	1. 91256800	4. 31839800	-0. 34903800
N	2. 65593100	1. 77796400	1. 76994800
H	3. 50165300	1. 34135200	2. 12724400
H	2. 12756700	2. 09681700	2. 57916000
C	2. 98592000	2. 90755800	0. 88276500
H	3. 40575400	3. 75857500	1. 44356000
C	1. 04581200	2. 40340000	-0. 74112800
H	1. 75106600	2. 05157500	-1. 50058900
H	0. 18524400	2. 82241600	-1. 26309000
C	4. 05149900	2. 43949000	-0. 11162800
H	4. 94675100	2. 16759100	0. 46191000
H	3. 71308900	1. 51648500	-0. 59882900
C	4. 41930500	3. 48964700	-1. 15566800
H	5. 27418900	3. 16147900	-1. 75028300
H	3. 59325600	3. 67916800	-1. 84728700
H	4. 68431500	4. 44063800	-0. 68226600

c-TS-DCM

Sum of electronic and thermal Free Energies= -1378.441372

Imaginary frequency=-198.96

O 1

C	-6.57777200	0.76775600	-0.79285400
C	-6.22235800	1.55728200	0.48469600
C	-4.68887900	1.45926000	0.61295300
H	-7.53236800	0.23817000	-0.70813800
H	-6.66164900	1.42711000	-1.66813700
H	-6.68354400	1.06544700	1.34692600
H	-6.58126000	2.58871700	0.46121200
H	-4.18046900	2.32908200	0.17670600
H	-4.34886200	1.39074000	1.64891800
C	-5.40044000	-0.15980700	-0.95063800
H	-5.38795300	-1.00049200	-1.63758200
C	-4.36031200	0.21598100	-0.19281600
C	-0.81577800	-0.94270000	0.26474100
C	-1.90258300	-0.01457500	0.66200700
O	-1.79844000	0.96019600	1.42327400
C	-3.04328000	-0.41279000	-0.15314900
N	-1.49527800	-1.86241200	-0.59248800
H	-1.01167300	-2.36705400	-1.32761500
N	-2.70998300	-1.42628300	-0.92084500
C	0.07892900	-1.52399200	1.30412700
C	0.59260200	-2.81972900	1.14929700
C	0.47546400	-0.77662500	2.42185000
C	1.48928400	-3.34475100	2.07352100
H	0.29193700	-3.42062300	0.29608900
C	1.37679700	-1.30546600	3.34344200
H	0.06159000	0.21423800	2.57614800
C	1.89386600	-2.58719900	3.17192400
H	1.87549500	-4.34966100	1.93260700
H	1.67022200	-0.70970900	4.20303900
H	2.59809200	-2.99546500	3.88984400
C	0.11231500	0.12135200	-0.99509700
O	-0.66947800	0.55061200	-1.86876300
C	1.27362800	-0.76660500	-1.43061200
C	2.42802200	-1.01184100	-0.67891700
C	1.13162600	-1.38299100	-2.67724000
C	3.42175000	-1.85467300	-1.17432600
H	2.57095200	-0.56204100	0.30073800
C	2.11746800	-2.23722700	-3.16380100

H	0.23902000	-1.16345200	-3.25473000
C	3.26778100	-2.47323100	-2.41311200
H	4.31466400	-2.03303500	-0.58303500
H	1.99171500	-2.71125900	-4.13240600
H	4.04138500	-3.13387100	-2.79196000
N	0.62449000	1.22652100	-0.03101500
H	-0.18906200	1.54284400	0.52320500
H	1.34592900	0.92947500	0.65964900
C	1.85024100	3.36991300	0.18813400
H	1.11771900	3.68215500	0.94394600
H	2.11621900	4.26985200	-0.37436300
N	2.70207700	1.69771200	1.76195100
H	3.52952300	1.24518300	2.14567900
H	2.17309000	2.04397200	2.56126400
C	3.09967900	2.82690200	0.89812500
H	3.52112800	3.65536800	1.48807900
C	1.19156100	2.38875600	-0.77487100
H	1.90892300	1.98990300	-1.49770200
H	0.36997100	2.84415500	-1.32728800
C	4.18819200	2.34211000	-0.06218800
H	5.05030000	2.03261100	0.54170500
H	3.83905300	1.44037200	-0.58090300
C	4.62530300	3.39515700	-1.07498300
H	5.49098300	3.04812000	-1.64481100
H	3.82940700	3.62256300	-1.79078500
H	4.90510500	4.32975200	-0.57690100

c-TS[‡] -gas

Sum of electronic and thermal Free Energies= -1378.391026

Imaginary frequency= -239.78

0 1

C	-5.74566300	-1.23597800	-1.51679100
C	-5.78864700	-0.83989400	-0.02527100
C	-4.33083300	-0.50859900	0.35312100
H	-6.46209700	-2.02688000	-1.76113300
H	-5.98436100	-0.38479900	-2.16967300
H	-6.12022100	-1.70165600	0.56183100
H	-6.47886700	-0.01798800	0.17810700
H	-4.12021800	0.56817400	0.28473400
H	-4.07097000	-0.80951300	1.37061900
C	-4.31105900	-1.65449100	-1.71066700
H	-3.94562100	-2.17177300	-2.59119600
C	-3.53179600	-1.25249000	-0.69969100
C	0.13267600	-1.29870600	0.04597600

C	-1. 23477700	-1. 00390200	0. 49796200
O	-1. 54253100	-0. 39543500	1. 54166400
C	-2. 08508800	-1. 41331800	-0. 60709400
N	-0. 08020900	-2. 00461100	-1. 17370400
H	0. 59436500	-1. 95007300	-1. 92820700
N	-1. 35060700	-1. 89811500	-1. 58161700
C	1. 16147400	-1. 80280400	0. 98597800
C	2. 16830900	-2. 66636400	0. 53535300
C	1. 20176800	-1. 36763700	2. 32060400
C	3. 20574000	-3. 05214900	1. 37630800
H	2. 14166100	-3. 03228000	-0. 48607700
C	2. 24598500	-1. 75375800	3. 15619900
H	0. 39499100	-0. 75262700	2. 70658300
C	3. 26020900	-2. 58577100	2. 68721000
H	3. 97795000	-3. 71672200	1. 00179500
H	2. 25922400	-1. 40829900	4. 18538900
H	4. 07437700	-2. 88039200	3. 34103700
C	0. 59458100	0. 46766500	-0. 65771800
O	-0. 25300300	0. 82866700	-1. 48304200
C	2. 03336500	0. 27214700	-1. 11866900
C	3. 15437800	0. 13168000	-0. 29350700
C	2. 20227400	0. 21228300	-2. 50551700
C	4. 41741800	-0. 05160300	-0. 84956300
H	3. 06965500	0. 12049800	0. 79101800
C	3. 46365700	0. 01639600	-3. 05865200
H	1. 32116000	0. 34548300	-3. 12528200
C	4. 57625600	-0. 11161300	-2. 23117100
H	5. 27593300	-0. 16197300	-0. 19516300
H	3. 57866300	-0. 02584300	-4. 13701600
H	5. 56238800	-0. 25931400	-2. 65930200
N	0. 55544800	1. 26116700	0. 70871300
H	-0. 21613000	0. 88360500	1. 29807500
H	1. 41929100	1. 09808100	1. 22644200
C	-1. 18673300	2. 98911600	0. 34728200
H	-1. 63049500	2. 09929700	-0. 10954600
H	-1. 33381500	3. 80134100	-0. 37062500
N	-1. 58280600	2. 28803600	2. 65132100
H	-1. 89908700	2. 56789100	3. 57372800
H	-2. 07081600	1. 42674000	2. 41091200
C	0. 31621700	2. 74561300	0. 55402500
H	0. 59754200	3. 15651800	1. 53159900
C	-1. 87847400	3. 32789500	1. 66641800
H	-2. 95229900	3. 48672100	1. 48589200
H	-1. 47446000	4. 27564000	2. 04477500

C	1. 22524200	3. 34797900	-0. 51539700
H	2. 24281800	2. 95990500	-0. 38529400
H	0. 88243500	3. 02096400	-1. 50129200
C	1. 25604300	4. 87173400	-0. 41838000
H	1. 91407800	5. 29171100	-1. 18185200
H	0. 26397600	5. 30879400	-0. 56245500
H	1. 62529400	5. 19699800	0. 55952600

c-TS[‡] -DCM

Sum of electronic and thermal Free Energies= -1378.431810

Imaginary frequency= -225.11

0 1

C	-5. 78887700	-1. 13496400	-1. 55359700
C	-5. 84094900	-0. 82794800	-0. 04211100
C	-4. 38920900	-0. 49548100	0. 35730700
H	-6. 49434300	-1. 91848000	-1. 84833400
H	-6. 03312300	-0. 24949400	-2. 15698200
H	-6. 15938600	-1. 72806200	0. 49290500
H	-6. 54268600	-0. 02870900	0. 20686200
H	-4. 19589300	0. 58612600	0. 34575100
H	-4. 12931800	-0. 84610900	1. 35888100
C	-4. 34915000	-1. 52651900	-1. 76589200
H	-3. 98194900	-1. 99117300	-2. 67584600
C	-3. 57549000	-1. 17327800	-0. 72992100
C	0. 10239900	-1. 23239900	0. 02159900
C	-1. 27466800	-0. 94077400	0. 47930100
O	-1. 58805800	-0. 37407000	1. 53841200
C	-2. 12717200	-1. 32961400	-0. 63496900
N	-0. 12409000	-1. 92541800	-1. 20699800
H	0. 56099200	-1. 92278800	-1. 95540100
N	-1. 38892900	-1. 80947600	-1. 61083500
C	1. 08895200	-1. 82477800	0. 96692400
C	2. 03997700	-2. 74562100	0. 50637000
C	1. 13083000	-1. 43500400	2. 31408400
C	3. 01807800	-3. 24573000	1. 36002400
H	2. 01824000	-3. 07098800	-0. 52934800
C	2. 11378700	-1. 93718800	3. 16386100
H	0. 38031100	-0. 75430200	2. 70205500
C	3. 06654600	-2. 83746300	2. 69149900
H	3. 74652700	-3. 95560000	0. 98025700
H	2. 12893400	-1. 62467700	4. 20360000
H	3. 83310900	-3. 22337000	3. 35586300
C	0. 62225900	0. 47499600	-0. 62990500
O	-0. 20766100	0. 88238500	-1. 46619600

C	2.06014100	0.24308300	-1.09623000
C	3.18146100	0.08785900	-0.27254400
C	2.22603600	0.15652400	-2.48220100
C	4.43891800	-0.13452300	-0.82982800
H	3.10515800	0.11293400	0.81170200
C	3.48066600	-0.07952900	-3.03780000
H	1.35062200	0.29488800	-3.10836700
C	4.59302900	-0.22169300	-2.21161000
H	5.29801100	-0.24928000	-0.17643200
H	3.58961100	-0.14293200	-4.11603000
H	5.57426700	-0.39965900	-2.64022500
N	0.61048200	1.27972100	0.72753600
H	-0.17342200	0.95179900	1.32077600
H	1.46252000	1.09699600	1.26105300
C	-1.04391100	3.10324100	0.36158500
H	-1.53068100	2.24564300	-0.11272100
H	-1.13972300	3.93716100	-0.34001800
N	-1.54896000	2.36620200	2.63726500
H	-1.89766500	2.64549900	3.55028100
H	-2.10122700	1.55948000	2.35066900
C	0.44167000	2.77753200	0.57509700
H	0.74459300	3.16627400	1.55446700
C	-1.73587800	3.45532100	1.67529100
H	-2.79082500	3.69675900	1.47967500
H	-1.27107300	4.35728000	2.09160400
C	1.38939400	3.34358200	-0.47965300
H	2.38501800	2.90818500	-0.33688200
H	1.04432700	3.04431900	-1.47382100
C	1.49291200	4.86262100	-0.36928300
H	2.18678700	5.25383000	-1.11749100
H	0.52713200	5.35153900	-0.52766800
H	1.86090300	5.15967200	0.61826300

d-TS-gas

Sum of electronic and thermal Free Energies= -1417.658782

Imaginary frequency=-219.83

0 1

C	-5.08483000	-2.65769900	-1.24342800
C	-5.23862200	-2.02602600	0.15673500
C	-3.89821200	-1.31625100	0.43182800
H	-5.60576200	-3.61672900	-1.33026300
H	-5.49468900	-2.00646600	-2.02825300
H	-5.37562700	-2.82322900	0.89372200
H	-6.09904100	-1.35679000	0.23135500

H	-3. 93024200	-0. 25361800	0. 15339900
H	-3. 59178200	-1. 35395300	1. 47988800
C	-3. 58992800	-2. 77741500	-1. 39308100
H	-3. 10398900	-3. 34985300	-2. 17576700
C	-2. 93574800	-2. 03952300	-0. 48790200
C	0. 64826200	-1. 21618500	0. 19454600
C	-0. 75454400	-1. 14295400	0. 63476000
O	-1. 20001800	-0. 51083700	1. 60809500
C	-1. 49113800	-1. 85887200	-0. 40306700
N	0. 59570000	-2. 09552700	-0. 92468400
H	1. 25078500	-1. 99889700	-1. 69185000
N	-0. 66728300	-2. 30389600	-1. 32126700
C	1. 75701300	-1. 36559700	1. 15762900
C	2. 93416200	-2. 03701300	0. 79502500
C	1. 69542400	-0. 77396200	2. 43158300
C	4. 02274200	-2. 08370100	1. 65706400
H	2. 99539200	-2. 52152100	-0. 17432100
C	2. 79273300	-0. 81900600	3. 28824700
H	0. 76385200	-0. 31539200	2. 75076900
C	3. 96590900	-1. 46229900	2. 90312400
H	4. 92397400	-2. 60552000	1. 35049300
H	2. 72270100	-0. 35812800	4. 26890400
H	4. 82011300	-1. 49312600	3. 57123500
C	0. 74940700	0. 54132700	-0. 77641900
O	-0. 18752100	0. 62692900	-1. 57773600
C	2. 17496700	0. 51001500	-1. 29156500
C	3. 32397500	0. 71842300	-0. 52148800
C	2. 31202200	0. 21899400	-2. 65270400
C	4. 58470200	0. 63666300	-1. 10639500
H	3. 26417100	0. 92123600	0. 54553300
C	3. 57316500	0. 12413900	-3. 23160400
H	1. 40420300	0. 08732200	-3. 23334000
C	4. 71320200	0. 33542100	-2. 45927000
H	5. 46721400	0. 79756600	-0. 49589800
H	3. 66577500	-0. 10445800	-4. 28844400
H	5. 69815100	0. 26701500	-2. 90952600
C	-1. 59644800	3. 77466600	-0. 10908600
H	-2. 12152600	4. 46494000	-0. 77927600
H	-1. 47402900	4. 31675700	0. 83925600
C	-2. 71563400	2. 24577000	1. 59529400
H	-3. 36541700	3. 03276900	2. 00406900
H	-3. 25060100	1. 29703200	1. 69767600
N	-1. 45034300	2. 16621100	2. 35189800
H	-1. 43312500	1. 29990100	2. 88048700

H	-1.37189300	2.93551000	3.00736100
C	0.83249600	2.90885300	0.20155200
H	1.83149300	3.00906500	-0.22973700
H	0.81522000	3.39831000	1.17988200
N	0.63584200	1.44989000	0.47364900
H	1.31724500	1.14573700	1.17577400
H	-0.28441400	1.32681300	0.94424800
C	-2.48459100	2.52468500	0.10673300
H	-1.98618600	1.64898800	-0.33307600
C	-0.21113800	3.53231900	-0.72146800
H	-0.29800600	2.93011200	-1.62966500
H	0.20953000	4.50134200	-1.01471300
C	-3.83318400	2.69124400	-0.59568800
H	-4.48614100	1.82946200	-0.42644000
H	-4.35235600	3.58296300	-0.22437200
H	-3.69907700	2.80327600	-1.67488500

d-TS-DCM

Sum of electronic and thermal Free Energies= -1417.700057

Imaginary frequency= -240.19

O 1

C	-5.08878100	-2.66282400	-1.35574700
C	-5.25937200	-2.04715000	0.04923400
C	-3.93081200	-1.32047300	0.33778200
H	-5.59677200	-3.62745300	-1.45706700
H	-5.49932200	-2.00800600	-2.13727900
H	-5.38893600	-2.85354100	0.77802900
H	-6.12859500	-1.38968300	0.12437200
H	-3.97713000	-0.25543300	0.06899300
H	-3.63093600	-1.36524800	1.38732800
C	-3.59132700	-2.76422700	-1.49592900
H	-3.09916000	-3.33016500	-2.28104100
C	-2.95006500	-2.02367600	-0.58053300
C	0.63602600	-1.18130000	0.13469500
C	-0.76777200	-1.18141200	0.60317300
O	-1.20976900	-0.69160300	1.64959900
C	-1.50746900	-1.82005500	-0.48783400
N	0.57829800	-1.98720100	-1.04267400
H	1.24216300	-1.86353400	-1.79986800
N	-0.68228900	-2.18149400	-1.44213300
C	1.74300100	-1.43674400	1.08580200
C	2.88729700	-2.13978500	0.67899900
C	1.70091500	-0.93285600	2.39650800
C	3.96061000	-2.31564300	1.54572900

H	2. 93635600	-2. 55065500	-0. 32498500
C	2. 78126000	-1. 10813700	3. 25877200
H	0. 80329500	-0. 42759900	2. 74017800
C	3. 91886000	-1. 79323200	2. 83793000
H	4. 83597500	-2. 86235300	1. 20811400
H	2. 72715600	-0. 71228800	4. 26857600
H	4. 75968000	-1. 92669100	3. 51096500
C	0. 74495400	0. 59663800	-0. 70089600
O	-0. 20119300	0. 73525100	-1. 49884900
C	2. 16474600	0. 58536900	-1. 25484900
C	3. 33195300	0. 74910900	-0. 49921200
C	2. 27635100	0. 37329700	-2. 63287900
C	4. 58068200	0. 70403700	-1. 11547800
H	3. 29490400	0. 90554000	0. 57622000
C	3. 52502600	0. 31406700	-3. 24545100
H	1. 36156100	0. 26759300	-3. 20736300
C	4. 68179300	0. 48212400	-2. 48720200
H	5. 47647200	0. 83711100	-0. 51703500
H	3. 59354100	0. 14558900	-4. 31571100
H	5. 65720700	0. 44306200	-2. 96184300
C	-1. 54632000	3. 84805700	0. 08241200
H	-2. 05445400	4. 58164400	-0. 55429100
H	-1. 42568600	4. 33975000	1. 05849300
C	-2. 64921400	2. 17605100	1. 67295300
H	-3. 30492000	2. 89938800	2. 18073300
H	-3. 15207200	1. 20502300	1. 69391300
N	-1. 36043400	2. 02942300	2. 36730800
H	-1. 42201800	1. 29118700	3. 06163800
H	-1. 11719100	2. 88788800	2. 85393900
C	0. 88784200	2. 93100900	0. 33063000
H	1. 87531300	3. 03279500	-0. 12401500
H	0. 91848300	3. 38770300	1. 32444100
N	0. 66861700	1. 46468200	0. 56870300
H	1. 37577200	1. 15398800	1. 24170900
H	-0. 24363900	1. 38893600	1. 10903400
C	-2. 45631700	2. 60123400	0. 21492600
H	-1. 97597800	1. 76623800	-0. 31386600
C	-0. 16177900	3. 61673900	-0. 53930800
H	-0. 26130800	3. 07270000	-1. 48236000
H	0. 27124700	4. 59513400	-0. 77772900
C	-3. 82303400	2. 84891900	-0. 42375700
H	-4. 48412700	1. 98336900	-0. 30652400
H	-4. 31660800	3. 71105900	0. 04100800
H	-3. 72624400	3. 05507700	-1. 49394700

d-TS' -gas

Sum of electronic and thermal Free Energies= -1417.657735

Imaginary frequency= -218.71

0 1

C	5.48667700	-1.98544200	-1.50140200
C	5.59511900	-1.39337300	-0.08007600
C	4.18582800	-0.85983700	0.24515700
H	6.12120700	-2.86698600	-1.63844500
H	5.79120600	-1.25775800	-2.26678400
H	5.84121900	-2.19644300	0.62139900
H	6.37135000	-0.62956100	0.00691800
H	4.08642000	0.20807100	0.00266200
H	3.91090300	-0.97031300	1.29686300
C	4.01522300	-2.28736200	-1.62418000
H	3.58517600	-2.89185000	-2.41546900
C	3.29702000	-1.66842200	-0.67924400
C	-0.34608500	-1.35512800	0.11183200
C	1.04629600	-1.14632600	0.54112000
O	1.43136700	-0.54305300	1.55805500
C	1.84308000	-1.67931200	-0.55954800
N	-0.21001500	-2.13578700	-1.07201000
H	-0.88736300	-2.05956500	-1.82214100
N	1.06020600	-2.15234200	-1.49957000
C	-1.41132900	-1.70743600	1.07188900
C	-2.50533700	-2.48776700	0.67035000
C	-1.39890200	-1.20608900	2.38510300
C	-3.56530400	-2.72827800	1.53582200
H	-2.52530400	-2.90394100	-0.33191000
C	-2.46747800	-1.44579400	3.24562000
H	-0.52493200	-0.66061400	2.72899900
C	-3.56136200	-2.19695200	2.82406000
H	-4.40283500	-3.33117800	1.19893100
H	-2.43628600	-1.05177500	4.25694100
H	-4.39373500	-2.37948900	3.49550600
C	-0.67559900	0.43686400	-0.72111000
O	0.21909600	0.68282800	-1.53767200
C	-2.10643100	0.28876700	-1.20258700
C	-3.24640700	0.31287200	-0.39223600
C	-2.25489400	0.08947100	-2.57887700
C	-4.50912500	0.14063600	-0.95245000
H	-3.17593500	0.43782200	0.68600500
C	-3.51660500	-0.09601900	-3.13431200

H	-1.35718600	0.10212300	-3.18923300
C	-4.64768400	-0.06845600	-2.32164200
H	-5.38398900	0.15824700	-0.31078800
H	-3.61767700	-0.25165700	-4.20357500
H	-5.63359800	-0.20817400	-2.75293500
C	1.36938800	3.79674000	0.15117400
H	1.85772100	4.54413800	-0.48335400
H	1.20228100	4.29225300	1.11953800
C	2.60823000	2.28453400	1.80555800
H	3.16870200	3.12034200	2.24286900
H	3.24302000	1.39686700	1.86749900
N	1.36398100	2.04988700	2.56933000
H	1.41791300	1.13805400	3.01184600
H	1.25206900	2.74413400	3.29921100
C	-0.95500400	2.71676800	0.41647400
H	-1.96957000	2.74863700	0.00914700
H	-0.96191900	3.14543700	1.42412700
N	-0.62285100	1.26814700	0.58854400
H	-1.26521300	0.85990600	1.27415400
H	0.30757100	1.18847700	1.04235500
C	-0.00398300	3.51553600	-0.48061700
H	0.13980000	2.95752100	-1.41066000
C	2.31927500	2.59361600	0.33648900
H	1.91984300	1.70370300	-0.16622700
H	3.27518800	2.79900400	-0.15849500
C	-0.70482300	4.84181000	-0.79347500
H	-1.66273500	4.68251500	-1.29683700
H	-0.08119200	5.46023300	-1.44344100
H	-0.89377700	5.41056700	0.12486100

d-TS[‡] -DCM

Sum of electronic and thermal Free Energies= -1417.699477

Imaginary frequency= -242.87

0 1

C	5.54703200	-1.85763200	-1.54207000
C	5.65524900	-1.31242900	-0.10240500
C	4.24157100	-0.80566900	0.24625100
H	6.18855100	-2.72834100	-1.71224700
H	5.84032000	-1.10163100	-2.28419000
H	5.91460500	-2.13523300	0.57135700
H	6.42161300	-0.54125800	0.00493900
H	4.12951200	0.26900400	0.04374000
H	3.97333100	-0.95623100	1.29444800
C	4.07821400	-2.17071800	-1.67017900

H	3. 65822300	-2. 75564600	-2. 48278600
C	3. 35470400	-1. 59077100	-0. 70171400
C	-0. 29990400	-1. 31739100	0. 10268200
C	1. 09793800	-1. 13024700	0. 54925200
O	1. 48622300	-0. 61907800	1. 60682900
C	1. 90029200	-1. 61350700	-0. 57653100
N	-0. 15008300	-2. 06996500	-1. 10146600
H	-0. 83976700	-2. 02398700	-1. 84419300
N	1. 11694100	-2. 06491800	-1. 52758500
C	-1. 34417400	-1. 74847000	1. 06089700
C	-2. 40011000	-2. 57406100	0. 64509600
C	-1. 33779300	-1. 29165700	2. 38984200
C	-3. 42228800	-2. 91921700	1. 52269800
H	-2. 42198200	-2. 94730300	-0. 37454500
C	-2. 36692700	-1. 63795700	3. 26296000
H	-0. 50695100	-0. 68437300	2. 73632800
C	-3. 41707900	-2. 44693500	2. 83464300
H	-4. 22916600	-3. 55860100	1. 17731800
H	-2. 34140300	-1. 27666900	4. 28674800
H	-4. 21862800	-2. 71292400	3. 51627300
C	-0. 67386100	0. 45596300	-0. 67036100
O	0. 23029600	0. 75440900	-1. 47242500
C	-2. 08509300	0. 25981900	-1. 20999900
C	-3. 25597100	0. 25834500	-0. 44322400
C	-2. 18027000	0. 04314000	-2. 58866400
C	-4. 49283300	0. 04247200	-1. 04745700
H	-3. 22977500	0. 41741500	0. 63221000
C	-3. 41453300	-0. 18723500	-3. 18949500
H	-1. 26562300	0. 06852100	-3. 17237900
C	-4. 57574900	-0. 18631400	-2. 41906000
H	-5. 39210800	0. 04774100	-0. 43960100
H	-3. 47006500	-0. 35831300	-4. 26005300
H	-5. 54076000	-0. 35963300	-2. 88488200
C	1. 17650000	3. 91167200	0. 23560500
H	1. 62064500	4. 70498700	-0. 37522500
H	0. 99119900	4. 36806000	1. 21984700
C	2. 46548400	2. 33984400	1. 80934300
H	3. 02650000	3. 13052800	2. 32562400
H	3. 08216400	1. 43797300	1. 81346200
N	1. 20782900	2. 02664000	2. 51096300
H	1. 36441500	1. 28547600	3. 18680900
H	0. 87422700	2. 83861100	3. 02307400
C	-1. 11093100	2. 71245800	0. 44963000
H	-2. 11162300	2. 69848500	0. 01083600

H	-1.18609400	3.13059300	1.45910000
N	-0.70426900	1.27965500	0.63280000
H	-1.36863200	0.85414700	1.28686000
H	0.20277600	1.29203400	1.18054000
C	-0.18225700	3.57978100	-0.40683300
H	-0.00612500	3.05995900	-1.35348200
C	2.19019600	2.75293400	0.36458700
H	1.83176800	1.88282000	-0.19937300
H	3.14270300	3.04261900	-0.09270200
C	-0.94143300	4.88041300	-0.68822700
H	-1.89029800	4.68992800	-1.19864400
H	-0.34454300	5.54313900	-1.32072600
H	-1.15989900	5.41576600	0.24370400