

Supporting Information

Theoretical Insights into Unraveling the Mechanism, Selectivity Patterns, and Ligand Effects in Gold(I)-Catalyzed Annulations between Ynamides and Isoxazoles

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Cartesian Coordinates and Thermochemical Data (Energies in Hartree)

Pre

Number of imaginary frequencies: 0

C	-4.80421100	2.53721500	-3.70070500
C	-3.80612900	3.27966400	-3.92027900
C	-3.35382300	4.65502300	-3.84462700
C	-1.99734600	4.96041300	-4.01460700
C	-4.27313200	5.69132100	-3.62412100
C	-1.56633700	6.28007700	-3.97235500
H	-1.29050500	4.14824400	-4.18043700
C	-3.83864900	7.00897100	-3.59407000
H	-5.32668600	5.45067700	-3.49385500
C	-2.48710100	7.30535800	-3.77004100
H	-0.51163200	6.51002600	-4.10238400
H	-4.55646900	7.80962200	-3.43323200
H	-2.15174800	8.33946000	-3.74639300
N	-5.70071600	1.66188500	-3.35586000
S	-5.60857500	1.03714200	-1.70359400
O	-6.85353900	0.30981800	-1.53971500
O	-5.27274900	2.19684500	-0.89969500
C	-6.55985400	0.96280800	-4.32580300
H	-6.54692300	1.54012900	-5.25344400
H	-7.57908500	0.89999200	-3.94231000
Au	-2.78495500	1.83784800	-5.21505000
P	-1.56724700	0.41205900	-6.67430900
H	-6.16427200	-0.04259700	-4.51664600
C	-4.24815100	-0.07451100	-1.73544300
C	-4.48720000	-1.43275100	-1.95098900
C	-2.96097100	0.42588800	-1.53637700

C	-3.40628100	-2.29954200	-1.96313600
H	-5.50164900	-1.80013200	-2.08566200
C	-1.89459000	-0.46422600	-1.56146300
H	-2.79909800	1.48158800	-1.33202800
C	-2.09910900	-1.83034000	-1.77640300
H	-3.57175500	-3.36409900	-2.12195800
H	-0.88353800	-0.09350000	-1.40106500
C	-0.94920400	-2.78473600	-1.81405000
H	-0.95747600	-3.36942200	-2.74295800
H	-1.01053900	-3.50483600	-0.98870300
H	0.01165900	-2.26552800	-1.73960900
C	-2.34825300	-1.31462400	-6.62512600
C	-2.72881400	-1.63999800	-5.18098200
C	-1.46869400	-2.43944100	-7.16210100
C	-3.63081100	-1.22501100	-7.45550400
H	-3.42713000	-0.90130600	-4.76396800
H	-1.85831100	-1.69651300	-4.51795400
H	-3.22398700	-2.62132100	-5.16178100
H	-1.17569100	-2.29464900	-8.20703500
H	-2.04513900	-3.37398300	-7.11797900
H	-0.56703500	-2.58607000	-6.55623000
H	-4.18721600	-2.16460700	-7.33687300
H	-3.42856800	-1.08853300	-8.52456700
H	-4.28389100	-0.40670000	-7.11999500
C	0.22417600	0.51239400	-6.05745100
C	1.28276800	-0.22735900	-6.87204400
C	0.25372800	-0.00024800	-4.61765600
C	0.56677800	2.00492800	-6.07246100
H	1.43209300	0.22086900	-7.85938900
H	1.06743900	-1.29410400	-6.99538800

H	2.23734300	-0.14681900	-6.33413600
H	-0.52951500	0.46242200	-4.00099300
H	1.22672000	0.25048900	-4.17331200
H	0.14037200	-1.09045800	-4.56907800
H	1.59635200	2.13485400	-5.71199200
H	-0.09685600	2.58757200	-5.41814300
H	0.51237000	2.42857700	-7.08396200
C	-1.54823500	0.88802300	-8.45170900
C	-2.33098200	1.92948900	-8.99265100
C	-0.75130100	0.12973000	-9.32679500
C	-2.26831800	2.17802500	-10.37059400
C	-3.27882100	2.80006800	-8.24131900
C	-0.70341600	0.39045700	-10.68910500
H	-0.15273600	-0.69069700	-8.94444100
C	-1.46392100	1.42712800	-11.21534200
H	-2.87781000	2.98373900	-10.77631200
C	-2.84826000	3.98940900	-7.64347800
C	-4.64692000	2.50909200	-8.26650200
H	-0.07440000	-0.21962000	-11.33259600
H	-1.43879500	1.64718600	-12.27989100
C	-3.77034200	4.87114100	-7.08401100
H	-1.78439200	4.22914600	-7.63378300
C	-5.56677600	3.38648100	-7.69696200
H	-4.98865100	1.59705700	-8.75562600
C	-5.13026800	4.57158500	-7.10870600
H	-3.42357200	5.79757300	-6.62911200
H	-6.62912700	3.15342600	-7.73317300
H	-5.84852400	5.26617000	-6.67765100

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2476.248646

Electronic Energy (0K) + ZPE = -2475.556150

Enthalpy (298K) = -2475.511610

Free Energy (298K) = -2475.631981

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2476.663443

2a

Number of imaginary frequencies: 0

C	4.74513500	1.37410700	-0.40801700
C	3.34993500	1.36410700	-0.40801700
C	2.57746200	2.52204100	-0.40801700
C	3.28123900	3.71628400	-0.40801700
C	4.68965200	3.75360700	-0.40801700
C	5.43896300	2.59078100	-0.40801700
C	5.06979900	-0.01614900	-0.40801700
H	1.49234800	2.48527500	-0.40801700
H	2.72894400	4.65309300	-0.40801700
H	5.19138100	4.71792800	-0.40801700
H	6.52527000	2.61871600	-0.40801700
H	6.04625100	-0.48783100	-0.40801700
O	2.89988200	0.09179400	-0.40801700
N	4.00428100	-0.76600300	-0.40801700

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -399.415612

Electronic Energy (0K) + ZPE = -399.310375

Enthalpy (298K) = -399.303550

Free Energy (298K) = -399.340496

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -399.512212

TS_A

Number of imaginary frequencies: 1

C	-4.22990700	2.33823500	-2.68841300
C	-3.10417400	2.73907400	-3.21914100
C	-2.32862300	3.93450500	-2.89970500
C	-1.62994700	4.62397600	-3.90045200
C	-2.21125100	4.37229400	-1.57049600
C	-0.88867300	5.75785900	-3.59419100
H	-1.69213300	4.26411300	-4.92695300
C	-1.44462300	5.49027300	-1.26431000
H	-2.70962700	3.81652200	-0.77866200
C	-0.79344100	6.19443700	-2.27443000
H	-0.37106300	6.29373100	-4.38717800
H	-1.35495800	5.81338900	-0.22953300
H	-0.19993800	7.07285700	-2.03125800
N	-5.00433100	1.28907900	-2.43960300
S	-4.63379400	0.38421400	-0.99970800
O	-5.84738300	-0.36024700	-0.70284800
O	-4.09952900	1.35861300	-0.05634200
C	-6.30686500	1.11054800	-3.08864600
H	-7.06820000	1.76099700	-2.64172400
H	-6.61907600	0.06825100	-2.99362400
Au	-2.65547000	1.53264500	-4.91637200
P	-2.08666400	0.20653600	-6.82164000
H	-6.18266300	1.35080700	-4.14941800
C	-3.34622700	-0.71989700	-1.46718900
C	-3.67456400	-2.03774800	-1.78410200
C	-2.03110500	-0.25826000	-1.50501500
C	-2.65498900	-2.90542200	-2.14197800
H	-4.70723400	-2.37448000	-1.73514700

C	-1.02913900	-1.14451200	-1.88099700
H	-1.79227900	0.76653700	-1.22894400
C	-1.32461200	-2.47194000	-2.20548600
H	-2.88970000	-3.94008000	-2.38790800
H	0.00349900	-0.80154200	-1.91821900
C	-0.25027100	-3.42220000	-2.62906400
H	-0.50362100	-3.89461200	-3.58710300
H	-0.13292900	-4.23335000	-1.89960500
H	0.71687400	-2.92055400	-2.73556800
C	-3.06646000	-1.42156500	-6.73900500
C	-3.24573100	-1.79298400	-5.26581500
C	-2.43250600	-2.61179500	-7.45537400
C	-4.44836500	-1.13933600	-7.32946000
H	-3.79152300	-1.01659900	-4.71005400
H	-2.29183800	-1.96746600	-4.75547600
H	-3.82875700	-2.72343700	-5.20628100
H	-2.32628400	-2.46238300	-8.53454400
H	-3.08935400	-3.48219800	-7.31849800
H	-1.45349400	-2.87453200	-7.03781200
H	-5.07712300	-2.02921600	-7.18802800
H	-4.41267900	-0.92124900	-8.40295200
H	-4.94535900	-0.30158300	-6.82050800
C	-0.20612800	-0.01303200	-6.69864500
C	0.47794200	-0.73317600	-7.85787800
C	0.09825300	-0.75519300	-5.39729500
C	0.35973300	1.40847900	-6.61541100
H	0.41803800	-0.16495200	-8.79209800
H	0.08393900	-1.74030000	-8.03180300
H	1.54356500	-0.83612200	-7.61003400
H	-0.40134100	-0.29361100	-4.53417900

H	1.18185400	-0.72273200	-5.21574900
H	-0.19595400	-1.81112700	-5.44876200
H	1.45571900	1.35181700	-6.56046400
H	0.00340600	1.94188800	-5.72310000
H	0.10248500	2.00701400	-7.50022300
C	-2.37971700	0.90666800	-8.50553600
C	-2.88268600	2.20201400	-8.75711100
C	-2.00566400	0.11681800	-9.60598400
C	-2.93665500	2.65940400	-10.08274300
C	-3.40866900	3.15580500	-7.74556800
C	-2.09245700	0.57690600	-10.91225900
H	-1.62306800	-0.88561800	-9.44486300
C	-2.54868700	1.86715200	-11.15215400
H	-3.32015400	3.66179600	-10.26491400
C	-2.80353800	4.40910500	-7.60048300
C	-4.59156100	2.89302800	-7.04463200
H	-1.79567500	-0.07030400	-11.73383500
H	-2.61382800	2.25263100	-12.16684500
C	-3.36016100	5.37406400	-6.76618100
H	-1.89236700	4.62601700	-8.15737000
C	-5.15176600	3.86212800	-6.21584100
H	-5.08914300	1.93262100	-7.17736400
C	-4.53647800	5.10321300	-6.07268500
H	-2.87271500	6.34109200	-6.65782300
H	-6.07857300	3.64879700	-5.68560600
H	-4.97359900	5.85821000	-5.42304300
C	-6.73033900	5.03829800	-0.76111900
C	-6.35746400	5.62336800	-1.97355100
C	-6.90695300	6.80409200	-2.45951900
C	-7.87453400	7.38425900	-1.65548300

C	-8.27195900	6.81660100	-0.42747900
C	-7.71052200	5.64351700	0.03846900
C	-5.91437700	3.87505400	-0.69157900
H	-6.59563300	7.23818500	-3.40453600
H	-8.34356800	8.30913000	-1.98209700
H	-9.03632400	7.31776100	0.16025500
H	-8.01283600	5.20406000	0.98461900
H	-5.84607900	3.10615800	0.07174200
O	-5.40447200	4.87252600	-2.57463600
N	-5.14330500	3.80310800	-1.74308100

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2875.657538

Electronic Energy (0K) + ZPE = -2874.860629

Enthalpy (298K) = -2874.808567

Free Energy (298K) = -2874.948334

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2876.165287

A

Number of imaginary frequencies: 0

C	-1.37687600	0.73089900	1.84709200
C	-0.23397500	0.86394300	1.13833400
C	0.63687300	2.03194100	1.37232600
C	1.21511400	2.74599600	0.31298200
C	0.96576800	2.41055000	2.68548300
C	2.04578900	3.83321800	0.55465900
H	0.99222900	2.44260100	-0.70905600
C	1.82228000	3.47921000	2.92463000
H	0.56325200	1.84345200	3.52487200
C	2.35554400	4.20357700	1.86167500

H	2.46673900	4.38483600	-0.28353700
H	2.07390100	3.74696600	3.94861600
H	3.02034200	5.04336600	2.05055600
N	-2.19124000	-0.41216500	2.00149200
S	-1.80878500	-1.44324400	3.28153900
O	-3.01430200	-2.22059600	3.54147600
O	-1.25869800	-0.56395400	4.31432600
C	-2.92751900	-0.95615200	0.86170500
H	-3.56776400	-0.16711600	0.45317400
H	-3.56677100	-1.77502600	1.20124600
Au	0.30232100	-0.38440600	-0.46559000
P	1.19128800	-1.58791100	-2.36388500
H	-2.24672400	-1.31393000	0.07392600
C	-0.52872000	-2.57014000	2.80938200
C	-0.87064700	-3.88114900	2.47948200
C	0.80013400	-2.14843900	2.82818100
C	0.14060100	-4.77812900	2.16956300
H	-1.91210600	-4.19278400	2.49056400
C	1.79644200	-3.06131200	2.50366000
H	1.05483800	-1.13062400	3.11516300
C	1.48300700	-4.38161500	2.16777400
H	-0.11039800	-5.80719600	1.91539500
H	2.83855200	-2.74557800	2.51613500
C	2.54912000	-5.35534500	1.77700600
H	2.39924600	-5.69654900	0.74271700
H	2.52325800	-6.25039200	2.41020300
H	3.54818300	-4.91345600	1.84780000
C	0.52112000	-3.36681000	-2.40778400
C	0.26362000	-3.78705900	-0.96175200
C	1.43025400	-4.41508800	-3.04515900

C	-0.81914400	-3.32598400	-3.14145000
H	-0.47238500	-3.13588300	-0.47182700
H	1.17622300	-3.77551300	-0.35672700
H	-0.13046900	-4.81395900	-0.95207000
H	1.63940300	-4.23012300	-4.10336100
H	0.92068500	-5.38734200	-2.98867300
H	2.38185000	-4.51656800	-2.50934300
H	-1.29811000	-4.31089100	-3.05268500
H	-0.71007700	-3.10013700	-4.20833300
H	-1.50281700	-2.58774600	-2.69914700
C	3.07116900	-1.49580800	-2.09684800
C	3.95339200	-2.06448900	-3.20578600
C	3.39996300	-2.19957800	-0.77966200
C	3.38970800	-0.00375500	-1.95462600
H	3.87553300	-1.48634700	-4.13274600
H	3.74607100	-3.11599600	-3.43007900
H	4.99844400	-2.00035300	-2.87191500
H	2.77084500	-1.83680200	0.04506000
H	4.44731900	-1.99047600	-0.51984100
H	3.29009200	-3.28927700	-0.85164100
H	4.47659500	0.11767600	-1.84671200
H	2.91244000	0.43389600	-1.06787100
H	3.07755700	0.57333100	-2.83629800
C	0.93162300	-0.90120100	-4.06173300
C	0.25725300	0.30719100	-4.34243000
C	1.51372200	-1.59654600	-5.13535700
C	0.24904300	0.78661300	-5.66169300
C	-0.50947600	1.13356600	-3.37428500
C	1.47095600	-1.12104200	-6.43834700
H	2.02901300	-2.53424400	-4.95474000

C	0.84638600	0.09180900	-6.70183700
H	-0.27010300	1.72159800	-5.86539100
C	-0.16063300	2.47406200	-3.17828400
C	-1.67883100	0.64831100	-2.77664700
H	1.93241800	-1.69485800	-7.23822200
H	0.81101600	0.48940500	-7.71334800
C	-0.95370400	3.30848200	-2.39537500
H	0.73984800	2.86309500	-3.65315000
C	-2.47964100	1.48731200	-2.00672400
H	-1.97932600	-0.38441800	-2.95250400
C	-2.11730300	2.81802100	-1.80959500
H	-0.66237900	4.34659300	-2.24768300
H	-3.39738400	1.10035800	-1.56759100
H	-2.74617400	3.47138600	-1.20851600
C	-2.93097900	3.40702600	3.80263800
C	-2.64206200	3.95065300	2.54464200
C	-2.92261600	5.26169100	2.18627600
C	-3.52632000	6.02231400	3.17355400
C	-3.83132400	5.50508100	4.45172500
C	-3.54166300	4.20023500	4.78855200
C	-2.46042300	2.08098200	3.72696600
H	-2.68301000	5.65499200	1.20373000
H	-3.77388900	7.05835100	2.95711100
H	-4.30344100	6.15691800	5.18118600
H	-3.77006000	3.79538600	5.76956000
H	-2.42760400	1.27971000	4.45821900
O	-2.06752200	3.01761300	1.75175900
N	-1.94909000	1.88249000	2.52987900

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2875.678179

Electronic Energy (0K) + ZPE = -2874.878429

Enthalpy (298K) = -2874.827039

Free Energy (298K) = -2874.963314

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2876.184640

TS_B

Number of imaginary frequencies: 1

C	-1.12187100	0.97976100	1.79441500
C	-0.23754300	1.41247100	0.78984100
C	0.09249900	2.81274800	0.63793600
C	-0.83890100	3.86012000	0.81479000
C	1.41249600	3.14842200	0.26503600
C	-0.45154900	5.18099700	0.65282000
H	-1.87791600	3.62241400	1.03100700
C	1.80606500	4.47217100	0.15494700
H	2.12485400	2.34275500	0.09209300
C	0.87306000	5.49134100	0.34482500
H	-1.18447900	5.97552400	0.76924000
H	2.83523600	4.71308800	-0.09869600
H	1.17530700	6.53040000	0.23669000
N	-1.55587600	-0.36441200	1.84728200
S	-1.45230700	-1.19237400	3.31638900
O	-2.79075100	-1.61885200	3.70659800
O	-0.65099800	-0.35212600	4.19975900
C	-2.55338200	-0.83705900	0.88735000
H	-3.55992700	-0.47457100	1.13033000
H	-2.55883500	-1.93253500	0.86804000
Au	0.52184500	0.06345000	-0.61040500
P	1.49833000	-1.44342800	-2.22588500

H	-2.26230100	-0.48446200	-0.10986800
C	-0.50033200	-2.62890200	2.91777500
C	-1.13127900	-3.85233000	2.71715100
C	0.88699000	-2.50194700	2.84292100
C	-0.35309800	-4.96428100	2.41517900
H	-2.21185100	-3.93253200	2.80779300
C	1.64517700	-3.62509600	2.55171400
H	1.36282400	-1.53943100	3.02221200
C	1.03690600	-4.86499200	2.31704200
H	-0.83268400	-5.92760100	2.25029800
H	2.73016200	-3.54478700	2.49521200
C	1.86275300	-6.04044000	1.90321700
H	2.05784600	-6.00057700	0.82106500
H	1.35416800	-6.98791300	2.10783100
H	2.83625800	-6.04865300	2.40521400
C	0.61993900	-3.12723100	-2.17374900
C	0.20116500	-3.39401900	-0.72836700
C	1.44471300	-4.31734000	-2.65914300
C	-0.64809800	-2.99618200	-3.01732800
H	-0.44848700	-2.59857700	-0.33813400
H	1.05844100	-3.49126300	-0.05384400
H	-0.35849800	-4.33992200	-0.69382000
H	1.73589100	-4.24451200	-3.71217400
H	0.82883700	-5.22249400	-2.56075000
H	2.34595000	-4.47048100	-2.05382900
H	-1.22421400	-3.92746100	-2.92901200
H	-0.43638200	-2.83230900	-4.08025600
H	-1.29008100	-2.17923800	-2.65940100
C	3.33368200	-1.52576300	-1.74636900
C	4.25848200	-2.27881000	-2.69971500

C	3.43364400	-2.14861400	-0.35373000
C	3.80325100	-0.06869900	-1.68121200
H	4.35704100	-1.77238600	-3.66561000
H	3.95031400	-3.31462600	-2.87553500
H	5.25927500	-2.30688100	-2.24663200
H	2.75283800	-1.66950400	0.36333800
H	4.45913100	-2.01672800	0.01901900
H	3.22516600	-3.22646500	-0.36654400
H	4.87868700	-0.05245900	-1.45605300
H	3.28445400	0.49479500	-0.89416200
H	3.65559100	0.45657900	-2.63498800
C	1.48848400	-0.90046200	-3.99030200
C	0.95355300	0.32869600	-4.43295500
C	2.11768200	-1.72823700	-4.93540500
C	1.13156900	0.69877300	-5.77471300
C	0.14773700	1.28004000	-3.62348200
C	2.25703000	-1.35866100	-6.26579100
H	2.52290800	-2.68678100	-4.62812000
C	1.77596600	-0.12447100	-6.68539400
H	0.72162000	1.65168200	-6.10475000
C	0.58877900	2.59635700	-3.45019000
C	-1.13388300	0.93439600	-3.17650400
H	2.74749200	-2.03147500	-6.96488000
H	1.88705800	0.19108200	-7.72007000
C	-0.23305800	3.54622300	-2.85010500
H	1.57968800	2.87594800	-3.80760000
C	-1.95872300	1.88734200	-2.58249800
H	-1.49995100	-0.07889400	-3.33946200
C	-1.51164100	3.19656800	-2.42324000
H	0.12297200	4.56690700	-2.72474500

H	-2.96049900	1.60791600	-2.26136200
H	-2.16024700	3.94482000	-1.97268500
C	-2.20081100	3.48800200	4.17734800
C	-3.39578700	3.33864300	3.41015100
C	-4.52453800	4.11348700	3.76049400
C	-4.40690100	5.00145600	4.80810300
C	-3.21661300	5.15129400	5.55779500
C	-2.11332100	4.39227700	5.25342200
C	-1.25303000	2.56365100	3.71971200
H	-5.44554900	4.00781800	3.19502000
H	-5.26873200	5.61158000	5.07130300
H	-3.18697100	5.86153300	6.37893700
H	-1.18815500	4.47454500	5.81874700
H	-0.27067300	2.40078700	4.16521700
O	-3.34579400	2.48256700	2.44631400
N	-1.59804100	1.80431200	2.72476600

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2875.657886

Electronic Energy (0K) + ZPE = -2874.861555

Enthalpy (298K) = -2874.809967

Free Energy (298K) = -2874.947655

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2876.166470

B

Number of imaginary frequencies: 0

C	-0.28919300	1.13263000	2.50427500
C	0.90530700	1.29166800	1.65595400
C	1.80070300	2.36447900	1.86746200
C	2.83756300	2.58761700	0.92425700

C	1.70136800	3.23650400	2.98622000
C	3.71682700	3.64281900	1.07673700
H	2.92519700	1.90284200	0.08175300
C	2.57632500	4.29158400	3.12666200
H	0.92795200	3.07127200	3.73158400
C	3.58062100	4.49552600	2.17235900
H	4.50604800	3.80861300	0.34877900
H	2.49576200	4.95980700	3.97928300
H	4.27101200	5.32724900	2.29295000
N	-0.51243000	0.00923700	3.26215100
S	0.80443500	-0.75177700	4.07230400
O	0.32478000	-1.00342400	5.42074100
O	1.95090700	0.11377800	3.82962500
C	-1.86847900	-0.24758200	3.75671000
H	-2.53442500	-0.32835500	2.89458800
H	-2.19696100	0.54938800	4.43291500
Au	0.78030300	0.17446600	-0.09326600
P	0.72155700	-1.18791700	-2.08767200
H	-1.88040700	-1.18853100	4.30645300
C	1.06998100	-2.29391700	3.25861300
C	0.15040200	-3.33223100	3.41899300
C	2.24367500	-2.46255700	2.52975700
C	0.40222500	-4.54251300	2.79311100
H	-0.74165600	-3.20833100	4.02813300
C	2.48784800	-3.69514300	1.93706000
H	2.95817800	-1.64782700	2.44017600
C	1.56480700	-4.73790700	2.03574100
H	-0.31230000	-5.35763700	2.89343400
H	3.40745100	-3.84661600	1.37431800
C	1.77999200	-6.02014700	1.29945000

H	1.16324000	-6.03658100	0.38890900
H	1.48438200	-6.88790800	1.89927400
H	2.82425300	-6.14212400	0.99455700
C	-0.51606800	-2.60276800	-1.78447300
C	-0.48564700	-2.91860100	-0.28521800
C	-0.25678700	-3.90450900	-2.53978200
C	-1.90338800	-2.05734000	-2.12635100
H	-0.81589300	-2.06143500	0.31649700
H	0.50966200	-3.22542500	0.05888500
H	-1.17519200	-3.75352600	-0.09109200
H	-0.28356100	-3.79938900	-3.62876200
H	-1.05121700	-4.61463400	-2.26984700
H	0.69794300	-4.36357700	-2.25698000
H	-2.65502800	-2.78526500	-1.78893600
H	-2.04412300	-1.90446000	-3.20213400
H	-2.10037800	-1.11421900	-1.59806500
C	2.49211500	-1.77144500	-2.42735900
C	2.68284500	-2.58889800	-3.70195600
C	2.97199300	-2.57642800	-1.22318500
C	3.33079900	-0.49643500	-2.54049200
H	2.43642500	-2.01549400	-4.60221900
H	2.10146800	-3.51637600	-3.70803500
H	3.74402800	-2.86539400	-3.77323000
H	2.86885200	-2.00676400	-0.29005500
H	4.03647200	-2.81642100	-1.35574700
H	2.43015600	-3.52473200	-1.11079800
H	4.38202900	-0.77671800	-2.69492000
H	3.27240500	0.11458100	-1.62914800
H	3.02388700	0.12199900	-3.39411500
C	0.24243400	-0.35194600	-3.66300400

C	0.19469100	1.04893500	-3.82683400
C	0.02834300	-1.15908000	-4.79213300
C	-0.01926500	1.57345000	-5.11014600
C	0.30722700	2.06163500	-2.74458400
C	-0.21229700	-0.62280500	-6.04934800
H	0.06097200	-2.23992500	-4.69648600
C	-0.22259100	0.75714400	-6.21251900
H	-0.04936700	2.65560200	-5.22533200
C	1.35738400	2.98606300	-2.75173800
C	-0.71665800	2.21016000	-1.80090700
H	-0.38006900	-1.28438100	-6.89559300
H	-0.39723900	1.19809800	-7.19106600
C	1.39149000	4.02727300	-1.82799700
H	2.14501000	2.89003800	-3.49848300
C	-0.69527500	3.27031800	-0.89652100
H	-1.55183600	1.50907500	-1.79586700
C	0.36149500	4.17567500	-0.90124900
H	2.21761900	4.73550600	-1.84383900
H	-1.51546000	3.38500000	-0.18969600
H	0.38214900	4.99799000	-0.18775800
C	-3.39808000	2.05486700	1.45003800
C	-3.23319100	0.91348000	0.54651000
C	-4.34126400	0.66500800	-0.34754700
C	-5.47854700	1.41783100	-0.30935500
C	-5.63583000	2.50293800	0.60264600
C	-4.61358700	2.80924700	1.44942100
C	-2.38051200	2.49033900	2.29769700
H	-4.23848900	-0.16833800	-1.04104000
H	-6.29533900	1.18531900	-0.99132700
H	-6.55818800	3.07696500	0.60925100

H	-4.69871900	3.64229900	2.14746900
H	-2.59693800	3.37673700	2.90413600
O	-2.20735100	0.19455000	0.55282400
N	-1.13537200	2.08321500	2.38765000

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2875.690045

Electronic Energy (0K) + ZPE = -2874.892409

Enthalpy (298K) = -2874.840137

Free Energy (298K) = -2874.977773

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2876.196508

TS_c

Number of imaginary frequencies: 1

C	-0.14220800	1.16878100	2.60053100
C	0.85404100	1.40130300	1.52378000
C	1.76209400	2.48028600	1.71528600
C	2.60879800	2.85674900	0.64060400
C	1.90046500	3.17127200	2.95133000
C	3.52693000	3.88048400	0.78206400
H	2.51714400	2.32252900	-0.30378100
C	2.82451900	4.18425900	3.08818100
H	1.27593400	2.90140500	3.79879800
C	3.63479800	4.54196300	2.00454300
H	4.16226400	4.16372700	-0.05262000
H	2.92783000	4.70292100	4.03705700
H	4.36109300	5.34323300	2.12057500
N	0.12201300	0.42280600	3.71440600
S	1.45839000	-0.64857800	3.79754400
O	1.72117500	-0.79983800	5.21943700

O	2.47688100	-0.08094300	2.92253100
C	-0.88315800	0.41259400	4.78271700
H	-1.84872800	0.07985500	4.38627900
H	-0.98048500	1.42183800	5.19431900
Au	0.66693000	0.35069200	-0.26327100
P	0.79178800	-1.00744000	-2.24337000
H	-0.55436100	-0.25952600	5.57593300
C	0.92666400	-2.19039600	3.11577200
C	-0.37531200	-2.65075200	3.28035100
C	1.90756700	-2.96954200	2.50052900
C	-0.70302600	-3.90706800	2.78656200
H	-1.13536700	-2.03893700	3.75746600
C	1.56090500	-4.22735100	2.03159200
H	2.92245000	-2.59541700	2.38720000
C	0.25286300	-4.70914200	2.15708500
H	-1.72375100	-4.27164200	2.88764900
H	2.31416800	-4.84487800	1.54390700
C	-0.10720000	-6.04594900	1.59160100
H	0.07048700	-6.06754600	0.50801300
H	-1.15857700	-6.29215700	1.76886500
H	0.50994900	-6.84001600	2.02902900
C	-0.45563700	-2.43433900	-2.10999100
C	-0.54922500	-2.84015000	-0.63685800
C	-0.13319200	-3.68583200	-2.92289400
C	-1.80647300	-1.86546800	-2.54586600
H	-0.82626500	-2.00109400	0.01497900
H	0.38981600	-3.26429300	-0.26193600
H	-1.32274500	-3.61711000	-0.53857700
H	-0.08285500	-3.50761200	-4.00187700
H	-0.93917300	-4.41500000	-2.75784900

H	0.80199800	-4.15756700	-2.59878300
H	-2.58718100	-2.61140400	-2.34045700
H	-1.83738700	-1.63390400	-3.61684700
H	-2.06617400	-0.95630200	-1.98587100
C	2.59638700	-1.58076500	-2.33330900
C	2.99170100	-2.36689900	-3.58057100
C	2.88677300	-2.42022900	-1.08996300
C	3.44006700	-0.30440200	-2.28300300
H	2.93609000	-1.75635500	-4.48824200
H	2.39337700	-3.27180000	-3.72890100
H	4.03845500	-2.68116000	-3.46558400
H	2.58328600	-1.90374500	-0.16822500
H	3.96881800	-2.60407200	-1.03222700
H	2.38713100	-3.39630300	-1.12594500
H	4.50171800	-0.57859800	-2.35515800
H	3.29552000	0.24223800	-1.34190600
H	3.21544400	0.37250700	-3.11868800
C	0.47574600	-0.16473500	-3.85425300
C	0.23952900	1.22114400	-3.98114100
C	0.54642900	-0.93634900	-5.02599000
C	0.14067300	1.77511900	-5.26618200
C	0.03861500	2.18579300	-2.86668900
C	0.41684800	-0.37486400	-6.28852300
H	0.71521200	-2.00638400	-4.95822500
C	0.22775800	0.99651600	-6.41024300
H	-0.03441600	2.84612100	-5.35312200
C	0.93575700	3.24538800	-2.69598800
C	-1.12524600	2.15495000	-2.08619000
H	0.47208400	-1.00885300	-7.17001400
H	0.13570100	1.45793000	-7.39056800

C	0.68655300	4.24496400	-1.75894900
H	1.83161600	3.28622100	-3.31527900
C	-1.38262800	3.16753700	-1.16409100
H	-1.85155900	1.35389000	-2.22952000
C	-0.47683400	4.21129400	-0.99401800
H	1.39635700	5.06102300	-1.63892300
H	-2.30305400	3.14022900	-0.58366100
H	-0.68274200	5.00085200	-0.27399800
C	-2.96747800	1.51747200	1.53772200
C	-2.51130000	0.18050500	1.29626200
C	-3.40716700	-0.69825200	0.62352600
C	-4.63455600	-0.25336400	0.18789900
C	-5.06716600	1.07369900	0.40649500
C	-4.24044400	1.93569100	1.08521700
C	-2.15341900	2.42571800	2.25632500
H	-3.08500100	-1.72569500	0.46001800
H	-5.29236300	-0.94543100	-0.33593500
H	-6.04292300	1.39649700	0.05445300
H	-4.54723400	2.96279800	1.28557000
H	-2.57474200	3.41574300	2.46073000
O	-1.34488900	-0.20847000	1.66965800
N	-0.96156800	2.23043800	2.73778800

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2875.687439

Electronic Energy (0K) + ZPE = -2874.889909

Enthalpy (298K) = -2874.838785

Free Energy (298K) = -2874.972861

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2876.192921

C

Number of imaginary frequencies: 0

C	-0.64687700	0.71091700	2.39785600
C	0.40447900	1.11929000	1.37091800
C	1.33797200	2.15381900	1.69664100
C	2.16675500	2.64571200	0.65521000
C	1.49746500	2.72751200	2.98913400
C	3.09899500	3.64230300	0.88124300
H	2.04693500	2.23097700	-0.34420500
C	2.42745700	3.72280300	3.20816700
H	0.88664800	2.37532800	3.81287500
C	3.23128200	4.17971200	2.15950100
H	3.71918100	4.00396700	0.06536400
H	2.53849800	4.14899500	4.20150400
H	3.96416600	4.96185200	2.34422300
N	-0.11586800	0.28933700	3.68226200
S	1.07279800	-0.90439100	3.67904800
O	1.78287200	-0.76197100	4.94194400
O	1.77499800	-0.72698500	2.40553200
C	-1.07509200	0.21809400	4.78561800
H	-1.83939100	-0.55493300	4.62684500
H	-1.55815100	1.19401900	4.88177800
Au	0.31266600	0.29848100	-0.54179000
P	0.58421100	-0.90368600	-2.61974200
H	-0.53255900	0.01944400	5.71303000
C	0.28355100	-2.48935900	3.66863300
C	-0.05615600	-3.09457500	4.87519500
C	0.01321100	-3.10495000	2.44664200
C	-0.68575800	-4.33357600	4.84974300
H	0.18201100	-2.61337900	5.82071000

C	-0.61014800	-4.34225700	2.44321200
H	0.29942400	-2.62062000	1.51586300
C	-0.97429100	-4.97168100	3.64109400
H	-0.95185800	-4.81929400	5.78671000
H	-0.81599900	-4.83884200	1.49511400
C	-1.66030300	-6.30066500	3.61227500
H	-2.66608300	-6.21049800	3.18278700
H	-1.76046500	-6.72628800	4.61542700
H	-1.11161900	-7.01509000	2.98734300
C	-0.52507800	-2.44639500	-2.57922600
C	-0.52537500	-2.98813600	-1.14625800
C	-0.13650900	-3.59610200	-3.50573500
C	-1.93538600	-1.95949400	-2.91750700
H	-0.79535500	-2.21506600	-0.41629600
H	0.44543800	-3.40943000	-0.86044800
H	-1.27006100	-3.79484000	-1.07975300
H	-0.18443300	-3.33867900	-4.56795700
H	-0.85232800	-4.41502900	-3.34711000
H	0.86103000	-3.99053600	-3.28051500
H	-2.64456100	-2.78288100	-2.75160300
H	-2.02623700	-1.64368600	-3.96323100
H	-2.24600600	-1.12345200	-2.27487500
C	2.43264700	-1.30861300	-2.73749400
C	2.88696400	-1.94780800	-4.04732400
C	2.81006600	-2.22177200	-1.57195000
C	3.15695400	0.03054100	-2.58111300
H	2.76045100	-1.27393000	-4.90150900
H	2.37637100	-2.89142500	-4.26669400
H	3.96039400	-2.16741300	-3.96293600
H	2.46678500	-1.82707200	-0.60544400

H	3.90507700	-2.30110400	-1.52828200
H	2.41205300	-3.23597300	-1.69844700
H	4.23899100	-0.13957000	-2.66822300
H	2.96569600	0.48628100	-1.60061300
H	2.87014900	0.74657100	-3.36314100
C	0.20678200	0.00210100	-4.18221400
C	-0.08274300	1.38192800	-4.23460300
C	0.29166100	-0.70411800	-5.39368400
C	-0.23775500	1.99421200	-5.48705900
C	-0.26517200	2.29004500	-3.06958800
C	0.10883600	-0.08703600	-6.62301500
H	0.52117600	-1.76427400	-5.38449500
C	-0.14799600	1.27772300	-6.67090500
H	-0.45144600	3.06135800	-5.51526000
C	0.66538400	3.30824000	-2.83560800
C	-1.43806600	2.25791400	-2.30515100
H	0.17798300	-0.67209700	-7.53672100
H	-0.28296000	1.78310800	-7.62422300
C	0.43923200	4.26600400	-1.85072500
H	1.56711400	3.35281800	-3.44571400
C	-1.67271600	3.23223100	-1.33742200
H	-2.18682000	1.48785400	-2.49541300
C	-0.73482600	4.23389100	-1.10220600
H	1.17414300	5.05037400	-1.68128100
H	-2.60273600	3.21111200	-0.77306400
H	-0.92356500	4.99229900	-0.34525100
C	-3.10635200	1.07736600	1.11975700
C	-2.54910800	-0.20238900	1.20152600
C	-3.17725900	-1.28782800	0.60093700
C	-4.33436700	-1.06431400	-0.13796900

C	-4.88211900	0.21601900	-0.26537400
C	-4.27849000	1.28136100	0.38459900
C	-2.48332600	2.09028100	1.93450100
H	-2.75865300	-2.28470400	0.71939700
H	-4.82025500	-1.90757000	-0.62411400
H	-5.78798800	0.36720900	-0.84554500
H	-4.70644600	2.28234200	0.34365800
H	-3.00491500	3.04502500	2.05872800
O	-1.42558600	-0.41175000	1.92654600
N	-1.38731700	1.93675800	2.58956700

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2875.714925

Electronic Energy (0K) + ZPE = -2874.915150

Enthalpy (298K) = -2874.864057

Free Energy (298K) = -2874.998819

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2876.217711

TS_{C2}

Number of imaginary frequencies: 1

C	-0.34450100	0.73426300	2.95051200
C	0.07901300	1.13223400	1.57145000
C	0.77397300	2.39968700	1.51968600
C	0.85307000	3.09696000	0.29460900
C	1.47983400	2.92097900	2.63157900
C	1.57438800	4.27194500	0.18928000
H	0.31717900	2.70403300	-0.56693800
C	2.24317300	4.06967600	2.50575900
H	1.46733200	2.39787000	3.58446900
C	2.28051000	4.75415900	1.29229200

H	1.60424300	4.80603800	-0.75750300
H	2.80787200	4.43786600	3.35804500
H	2.86794700	5.66495300	1.20324300
N	-0.14099400	-0.53377500	3.46692200
S	1.39144400	-1.26752300	3.27587000
O	2.00627300	-1.36818800	4.59177300
O	2.08845200	-0.50086600	2.24824600
C	-0.81244700	-0.85518400	4.73504200
H	-1.88829900	-0.72935600	4.59435100
H	-0.46607100	-0.20491900	5.54452600
Au	0.21787800	0.00201400	-0.22812600
P	0.93372000	-1.24108500	-2.18074700
H	-0.60935600	-1.89644400	4.99344000
C	0.97941800	-2.89760000	2.73030700
C	-0.33100100	-3.29718000	2.48119600
C	2.04824700	-3.78727600	2.61715700
C	-0.56458600	-4.61570100	2.11533900
H	-1.15640800	-2.59401800	2.56601500
C	1.79215400	-5.09276100	2.22354200
H	3.06629000	-3.46527000	2.83066800
C	0.48619000	-5.52546700	1.96799400
H	-1.58501900	-4.94258800	1.92134400
H	2.61800700	-5.79407500	2.12059100
C	0.21378700	-6.92019600	1.50291700
H	0.05366900	-6.93398700	0.41598600
H	-0.69274500	-7.32632000	1.96481000
H	1.04938300	-7.59200300	1.72245000
C	-0.04597900	-2.87007900	-2.28859800
C	-0.40858100	-3.27744600	-0.86159200
C	0.67088600	-4.04929600	-2.94415300

C	-1.34184700	-2.56772100	-3.04019200
H	-1.00135800	-2.50344500	-0.35546700
H	0.47521600	-3.48743500	-0.24954600
H	-1.01298000	-4.19580100	-0.89807300
H	0.87071100	-3.90188900	-4.00970300
H	0.01602400	-4.92870800	-2.86634900
H	1.61090500	-4.29930600	-2.43864800
H	-1.97117500	-3.46842100	-3.02831300
H	-1.17111000	-2.29210800	-4.08716800
H	-1.91251900	-1.76426800	-2.55525500
C	2.79003700	-1.49008400	-1.82742100
C	3.62292400	-2.14418600	-2.92762100
C	2.93075100	-2.31520900	-0.54851400
C	3.34768800	-0.08164400	-1.58913600
H	3.69361000	-1.52075600	-3.82497400
H	3.25885100	-3.13638300	-3.21528300
H	4.64347300	-2.27137400	-2.54047700
H	2.31659400	-1.92133700	0.27007100
H	3.97957500	-2.27809800	-0.22010700
H	2.67441000	-3.36999300	-0.70926600
H	4.43456400	-0.15111900	-1.44316600
H	2.91882400	0.38795700	-0.69353500
H	3.16999300	0.58380800	-2.44588800
C	0.89928800	-0.51497200	-3.88557500
C	0.49006300	0.79459000	-4.22108300
C	1.41147700	-1.32555900	-4.91350400
C	0.67721300	1.24218500	-5.53967400
C	-0.22264900	1.75383300	-3.34246300
C	1.56060900	-0.87522000	-6.21714300
H	1.72031000	-2.34145400	-4.69608500

C	1.20842000	0.43133600	-6.52947700
H	0.35373900	2.25058200	-5.79018900
C	0.21779400	3.08067300	-3.25387800
C	-1.45254800	1.41573500	-2.76642800
H	1.95748400	-1.54400400	-6.97687700
H	1.32564100	0.81274400	-7.54100400
C	-0.55851400	4.04725900	-2.62143900
H	1.16923400	3.35659000	-3.70745200
C	-2.22713700	2.38354600	-2.13532100
H	-1.82832900	0.39854400	-2.86562300
C	-1.78576000	3.70182200	-2.06099700
H	-0.20568600	5.07548800	-2.57284600
H	-3.19074600	2.10749800	-1.71537300
H	-2.39960100	4.45714000	-1.57411900
C	-2.42486500	3.17628900	2.63376300
C	-2.79078200	2.32247900	1.52367000
C	-4.00081600	2.65197600	0.83182300
C	-4.67458700	3.80868100	1.11650700
C	-4.23479300	4.71180000	2.12493900
C	-3.14344000	4.38793400	2.87466400
C	-1.48275000	2.77272600	3.57311600
H	-4.35180200	1.96521700	0.06548000
H	-5.57534700	4.04876200	0.55414500
H	-4.78686600	5.62911700	2.30809700
H	-2.80859900	5.02768300	3.69065500
H	-1.26450900	3.47512600	4.38442900
O	-2.08323600	1.32100100	1.19070300
N	-0.92101700	1.58136500	3.73894300

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2875.672115

Electronic Energy (0K) + ZPE = -2874.873514

Enthalpy (298K) = -2874.822449

Free Energy (298K) = -2874.956209

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2876.178114

C2

Number of imaginary frequencies: 0

C	-0.03714400	0.62849800	3.13486300
C	-0.14237500	0.97545000	1.63597600
C	0.64566500	2.19781400	1.26801800
C	0.13838100	3.13523400	0.35956300
C	1.96717900	2.34707800	1.71264600
C	0.93010200	4.18162400	-0.09770000
H	-0.87831400	3.02546200	-0.01603100
C	2.75867400	3.39195000	1.24786600
H	2.38757200	1.62824800	2.41621800
C	2.24552500	4.31720600	0.34198700
H	0.51304900	4.89379500	-0.80779700
H	3.78248200	3.48507300	1.60392400
H	2.86394800	5.13709900	-0.01543700
N	-0.25616200	-0.59159900	3.67728700
S	0.57239100	-2.02801700	3.17196500
O	0.88710100	-2.74414900	4.39703900
O	1.66292800	-1.58436300	2.31998700
C	-0.86049200	-0.66098400	5.01818300
H	-1.69288700	0.04550300	5.05526100
H	-0.12878800	-0.42382900	5.79645100
Au	0.40179100	-0.25566500	-0.09410600
P	1.48358000	-1.23635100	-2.01938500

H	-1.24972200	-1.66874900	5.17685900
C	-0.67029200	-2.93430200	2.29992400
C	-1.67620100	-2.29810800	1.57258800
C	-0.52615900	-4.32064500	2.28824800
C	-2.53467300	-3.07782400	0.80889500
H	-1.80888700	-1.21866100	1.60706400
C	-1.39339500	-5.07737700	1.51243700
H	0.25520000	-4.80133800	2.87231600
C	-2.40011500	-4.47022800	0.75509200
H	-3.33403300	-2.59711700	0.24649400
H	-1.29155800	-6.16072200	1.49663900
C	-3.31052700	-5.28749800	-0.10448800
H	-2.93164500	-5.33162600	-1.13416800
H	-4.31511600	-4.85375200	-0.14970800
H	-3.38935900	-6.31702600	0.25878400
C	1.55803200	-3.13281300	-1.84068300
C	1.64207700	-3.45017400	-0.34871400
C	2.71825800	-3.85279100	-2.52521900
C	0.22345400	-3.66779400	-2.36373400
H	0.80686600	-3.00533500	0.20067600
H	2.57237500	-3.09577000	0.10787400
H	1.59828800	-4.54125100	-0.21896100
H	2.71567700	-3.76972000	-3.61560700
H	2.63309200	-4.92377500	-2.29277800
H	3.69091000	-3.51791500	-2.14700600
H	0.16046200	-4.74122600	-2.13513300
H	0.11584800	-3.54831300	-3.44781200
H	-0.63108800	-3.17705000	-1.87425000
C	3.19225400	-0.40158100	-1.99444200
C	4.13511100	-0.75882400	-3.14088200

C	3.87097800	-0.73060100	-0.66497700
C	2.91276300	1.10322100	-2.05924400
H	3.75326100	-0.42468100	-4.11142200
H	4.35662600	-1.82944100	-3.20091800
H	5.08733200	-0.23694400	-2.97103100
H	3.22234400	-0.52213200	0.19685800
H	4.77145600	-0.10794100	-0.56609700
H	4.18968700	-1.77915700	-0.61418500
H	3.86969600	1.64345400	-2.02794500
H	2.30394400	1.44638400	-1.21203000
H	2.40124400	1.38650200	-2.98919100
C	0.86777700	-0.90389500	-3.73293600
C	-0.16681800	0.00066800	-4.05395900
C	1.55142500	-1.52337700	-4.79279500
C	-0.43941500	0.26545900	-5.40584700
C	-1.05200500	0.70535900	-3.09361000
C	1.25175500	-1.26849500	-6.12344300
H	2.35650300	-2.21768300	-4.58071500
C	0.25249200	-0.35480300	-6.43390200
H	-1.24026900	0.96404900	-5.64094200
C	-1.14451800	2.10019700	-3.14771000
C	-1.92140500	0.00219200	-2.25124500
H	1.80553300	-1.77695800	-6.90884700
H	0.00574000	-0.13173000	-7.46920400
C	-2.09759200	2.77883900	-2.39513900
H	-0.47218400	2.65171600	-3.80404700
C	-2.87574500	0.68162200	-1.49957800
H	-1.87509700	-1.08651900	-2.22429600
C	-2.97236300	2.06953700	-1.57785600
H	-2.16199600	3.86364900	-2.45490200

H	-3.55766600	0.11991900	-0.86242600
H	-3.73013800	2.59939000	-1.00449000
C	-1.70965000	3.11153700	3.15090500
C	-2.24789400	2.21693700	2.19147000
C	-3.56752500	2.39107800	1.76576500
C	-4.29629800	3.48711400	2.19084200
C	-3.73836900	4.44042200	3.05618300
C	-2.46343800	4.24461900	3.53362000
C	-0.51377100	2.82674500	3.86809500
H	-3.98811800	1.66407000	1.07630900
H	-5.31481600	3.61524000	1.83203800
H	-4.31585600	5.30777700	3.36194800
H	-2.01779300	4.93677900	4.24510900
H	-0.07347100	3.61304300	4.48530600
O	-1.59132200	1.17878100	1.62192500
N	0.00700900	1.64023000	3.96326000

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2875.706220

Electronic Energy (0K) + ZPE = -2874.906793

Enthalpy (298K) = -2874.855495

Free Energy (298K) = -2874.989684

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2876.210629

TS_D

Number of imaginary frequencies: 1

C	-1.75155700	1.18399400	1.20905500
C	-0.34387300	1.17140100	0.72163200
C	0.70651200	1.96603700	1.32692300
C	2.03458400	1.49248900	1.23038400

C	0.49548700	3.23901100	1.89579000
C	3.09776100	2.23202800	1.71948000
H	2.21047200	0.51926200	0.77115700
C	1.56984800	4.00072800	2.33193200
H	-0.51526000	3.62127800	1.97974900
C	2.86606200	3.49607000	2.26247200
H	4.10913300	1.83849800	1.65812400
H	1.39329400	4.99030200	2.74598400
H	3.70075600	4.09153000	2.62543900
N	-1.35216200	-0.06321800	1.98614900
S	-1.14658800	-0.01605800	3.70696300
O	-2.44897200	-0.26228000	4.31468300
O	-0.39278500	1.17962700	4.03842700
C	-1.75040600	-1.38302700	1.47314400
H	-2.63363600	-1.75373700	2.00976100
H	-0.92315800	-2.09423700	1.56788500
Au	0.12528100	0.05460100	-0.99035900
P	0.71582000	-1.32265200	-2.84503700
H	-1.99906300	-1.28684900	0.41524400
C	-0.11522800	-1.43199800	3.92972300
C	-0.64326800	-2.58947600	4.49042500
C	1.21040400	-1.36000000	3.50355800
C	0.18252300	-3.69834200	4.62744200
H	-1.68335100	-2.62046200	4.80594500
C	2.01360000	-2.48154200	3.63941300
H	1.60311100	-0.44109800	3.07021500
C	1.51404600	-3.66311000	4.20335700
H	-0.21338600	-4.61245900	5.06604000
H	3.05039300	-2.44578400	3.30874200
C	2.40144900	-4.85508100	4.37044800

H	3.12530500	-4.93335100	3.55214000
H	1.82349600	-5.78359500	4.41720100
H	2.97591700	-4.77966600	5.30286400
C	-0.81349700	-2.29972700	-3.37822900
C	-1.21649300	-3.23442800	-2.23823200
C	-0.67202400	-3.10750100	-4.66624200
C	-1.91596100	-1.25820400	-3.58496900
H	-1.29485300	-2.70851000	-1.27677200
H	-0.51729200	-4.07106700	-2.12202300
H	-2.20297800	-3.66127900	-2.46675000
H	-0.52406800	-2.46477200	-5.54068500
H	-1.60809100	-3.66068200	-4.82561200
H	0.13992900	-3.84184500	-4.62835300
H	-2.84195400	-1.77412700	-3.87497700
H	-1.66470900	-0.55269100	-4.38809700
H	-2.11661900	-0.68444400	-2.66892900
C	2.16623400	-2.41206600	-2.27253200
C	2.41321500	-3.67391900	-3.09496100
C	1.91783700	-2.82982800	-0.81884900
C	3.40820600	-1.51856400	-2.30676200
H	2.65166100	-3.46514600	-4.14281900
H	1.56310800	-4.36516800	-3.05556100
H	3.28000800	-4.19858900	-2.66920900
H	1.82826700	-1.96298400	-0.15009500
H	2.77509500	-3.42820400	-0.47946300
H	1.01946300	-3.44601700	-0.70147800
H	4.23818400	-2.05034800	-1.82164200
H	3.25338500	-0.57620700	-1.76042100
H	3.71866000	-1.27424700	-3.32911300
C	1.32189200	-0.42269400	-4.33579300

C	1.45643900	0.98249100	-4.39469700
C	1.78320300	-1.18230800	-5.42373200
C	2.07348900	1.55373000	-5.51711600
C	0.98889200	1.95374500	-3.36841800
C	2.37483000	-0.59641800	-6.53399200
H	1.68974400	-2.26351600	-5.40414700
C	2.53011100	0.78388600	-6.57651100
H	2.17735300	2.63688400	-5.55189900
C	1.92304600	2.74686300	-2.69185700
C	-0.37456800	2.19214500	-3.15757200
H	2.71855900	-1.21994100	-7.35563000
H	2.99959300	1.26203600	-7.43292500
C	1.50600100	3.74833500	-1.81924700
H	2.98567100	2.57707800	-2.86422900
C	-0.79158000	3.20130600	-2.29095700
H	-1.11211900	1.59922100	-3.69696000
C	0.14728800	3.98212500	-1.62113500
H	2.24598200	4.35606700	-1.30223400
H	-1.85540200	3.38201200	-2.14903700
H	-0.17873300	4.77490800	-0.95102300
C	-4.44529500	1.38828800	1.58223800
C	-3.93721800	0.70600300	0.47515300
C	-4.74954900	-0.06987100	-0.33784700
C	-6.09702300	-0.17316000	-0.00923100
C	-6.62743300	0.49410600	1.09946200
C	-5.80620600	1.28471900	1.88752200
C	-3.50645900	2.24814300	2.26089600
H	-4.32523100	-0.58389700	-1.19808200
H	-6.74658600	-0.78833300	-0.62717500
H	-7.68360800	0.39764600	1.33509700

H	-6.19963200	1.82777600	2.74470200
H	-3.89349700	2.99889200	2.95590900
O	-2.61479800	0.84889300	0.15574100
N	-2.23535900	2.21116600	2.07014800

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2875.695543

Electronic Energy (0K) + ZPE = -2874.896790

Enthalpy (298K) = -2874.846288

Free Energy (298K) = -2874.979832

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2876.199823

D

Number of imaginary frequencies: 0

C	-1.74943900	1.21642100	1.44953100
C	-0.34782600	0.93396900	1.12589600
C	0.77372400	1.78807500	1.61283500
C	2.04844100	1.21840200	1.73973100
C	0.63348100	3.16157600	1.82407200
C	3.14168000	1.98850900	2.11547600
H	2.17756900	0.15505600	1.53240900
C	1.73431200	3.93791700	2.17732900
H	-0.34513600	3.62328100	1.72750600
C	2.98827500	3.35698000	2.33362500
H	4.11916700	1.52269400	2.22175500
H	1.60484800	5.00643300	2.33722000
H	3.84400100	3.96548600	2.61710900
N	-1.03774000	-0.03708500	2.13330700
S	-0.83969400	-0.00333700	3.94997900
O	-2.19094400	-0.22783900	4.43538400

O	-0.08683000	1.18503300	4.28645300
C	-1.43201900	-1.38628100	1.67469400
H	-2.20874800	-1.78410500	2.33538100
H	-0.55256600	-2.03845100	1.65981900
Au	0.19129600	0.02129700	-0.74048100
P	0.86988300	-1.27290300	-2.62541400
H	-1.83417200	-1.30669700	0.66398300
C	0.14892900	-1.43389600	4.22838200
C	-0.46505200	-2.63153800	4.59132200
C	1.53267200	-1.32726400	4.08919700
C	0.33270600	-3.74578700	4.80439700
H	-1.54439800	-2.68708600	4.70791900
C	2.30763400	-2.45734800	4.29970300
H	1.99278600	-0.37517600	3.83414400
C	1.72278400	-3.67830600	4.65810800
H	-0.12850500	-4.68880400	5.09118400
H	3.38934000	-2.39377700	4.19717800
C	2.57517900	-4.87847100	4.91526100
H	3.45834900	-4.88864200	4.26788900
H	2.01724700	-5.80818400	4.76568500
H	2.93518800	-4.87595700	5.95229900
C	-0.63717300	-2.26255400	-3.20635600
C	-1.06148500	-3.21159700	-2.08636000
C	-0.45743100	-3.06007600	-4.49605800
C	-1.74595300	-1.23178200	-3.43356300
H	-1.17290700	-2.69498400	-1.12315600
H	-0.35656300	-4.04179600	-1.95957100
H	-2.03652000	-3.64685400	-2.34611100
H	-0.29466200	-2.41039800	-5.36262400
H	-1.38403100	-3.62106000	-4.68168200

H	0.36035400	-3.78733700	-4.44345600
H	-2.65826100	-1.75565700	-3.75115000
H	-1.48313500	-0.51843500	-4.22604700
H	-1.97708900	-0.66686200	-2.51936000
C	2.31102100	-2.35859300	-2.01276200
C	2.61308600	-3.60021500	-2.84775300
C	2.01657400	-2.81378700	-0.57912100
C	3.53822400	-1.44422300	-1.97675900
H	2.90055300	-3.36854800	-3.87788600
H	1.77076300	-4.30221000	-2.86275000
H	3.46442300	-4.12348500	-2.39015400
H	1.87991800	-1.96397600	0.10289200
H	2.87621400	-3.39674600	-0.21976200
H	1.13211500	-3.45635500	-0.50997700
H	4.36018300	-1.97750500	-1.47970100
H	3.34774300	-0.52280200	-1.40608200
H	3.88021000	-1.16287800	-2.97951000
C	1.52657800	-0.38914300	-4.10419600
C	1.68452100	1.01266900	-4.15603100
C	2.01738000	-1.15374400	-5.17565700
C	2.35765900	1.57828700	-5.24838300
C	1.17553500	1.97511000	-3.14660700
C	2.66274400	-0.57406900	-6.25908400
H	1.90510000	-2.23284700	-5.16513100
C	2.84530000	0.80341700	-6.28991800
H	2.47811700	2.65993800	-5.27550500
C	2.07476500	2.79823800	-2.45946400
C	-0.19683000	2.16101600	-2.94995100
H	3.02746600	-1.20095800	-7.06907500
H	3.35784200	1.27523100	-7.12489900

C	1.61333600	3.78457600	-1.59362600
H	3.14440300	2.66286900	-2.61720400
C	-0.65898100	3.15777400	-2.09206000
H	-0.90681400	1.54675000	-3.50157000
C	0.24475900	3.97162400	-1.41355100
H	2.32515400	4.41550300	-1.06519500
H	-1.73011700	3.30169500	-1.96210500
H	-0.11566900	4.75460700	-0.74977600
C	-4.40741400	1.42248300	1.98099500
C	-3.96213100	0.71362800	0.86334200
C	-4.81845600	-0.05895200	0.09615500
C	-6.15297100	-0.12967600	0.48167300
C	-6.62417100	0.56520600	1.60021600
C	-5.75665200	1.34843000	2.34404700
C	-3.42129700	2.23942000	2.63974000
H	-4.44081700	-0.59025800	-0.77435800
H	-6.83982600	-0.73924900	-0.10020500
H	-7.67163800	0.49407800	1.87930000
H	-6.10263600	1.90718200	3.21135800
H	-3.75321300	2.96450900	3.38732500
O	-2.64915900	0.82855600	0.48185500
N	-2.15811300	2.17353800	2.39068300

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2875.704079

Electronic Energy (0K) + ZPE = -2874.903568

Enthalpy (298K) = -2874.853034

Free Energy (298K) = -2874.986235

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2876.208457

E

Number of imaginary frequencies: 0

C	-2.25456700	0.25608700	2.38112500
C	-0.86562600	0.06919700	2.18173400
C	0.16892500	0.99973500	2.74168600
C	1.48247500	0.86891300	2.26404000
C	-0.08318700	1.92892900	3.75591600
C	2.50523500	1.66633900	2.75818100
H	1.69788900	0.11066000	1.51071100
C	0.94465100	2.72441500	4.25085500
H	-1.08223800	2.02007000	4.17067500
C	2.23807300	2.60461200	3.75219900
H	3.51527400	1.54686300	2.37259600
H	0.73265700	3.43329300	5.04756400
H	3.03662900	3.22769700	4.14690000
N	-0.42379100	-1.29321900	2.09176500
S	-0.51163100	-2.19028300	3.54222900
O	-1.23746800	-3.42170600	3.25868300
O	-0.96742000	-1.25007000	4.55742100
C	-0.54384600	-2.07440400	0.87042500
H	-1.57670200	-2.38261500	0.65570100
H	0.07812700	-2.97255900	0.94854500
H	-0.15949700	-1.47785300	0.03316300
C	1.17948500	-2.60266500	3.86650800
C	1.66726200	-3.84990100	3.49541100
C	2.00023300	-1.64996700	4.46887200
C	3.00798900	-4.13939500	3.72100900
H	0.99747400	-4.58457100	3.05501400
C	3.33349000	-1.95766100	4.68142500
H	1.59079600	-0.68864200	4.77261900

C	3.85758000	-3.20218200	4.31013000
H	3.40192000	-5.11397400	3.43877300
H	3.98644500	-1.22299000	5.15076300
C	5.29851100	-3.51575700	4.56647200
H	5.95345800	-2.72166300	4.18951300
H	5.60189000	-4.45522100	4.09448200
H	5.49642300	-3.60631600	5.64176600
C	-4.96155700	0.38385600	2.79008100
C	-4.32953100	-0.84221100	2.55872600
C	-5.02005100	-2.04331200	2.55273000
C	-6.39163200	-1.99752300	2.76074300
C	-7.05794400	-0.78248900	2.97275000
C	-6.34842400	0.40393600	2.99461300
C	-4.10767500	1.53087700	2.79576200
H	-4.47236400	-2.97107800	2.40662800
H	-6.95808300	-2.92489400	2.76548500
H	-8.13199300	-0.77819500	3.13184100
H	-6.84747000	1.35407600	3.17319500
H	-4.53948000	2.51863300	2.97440600
O	-2.98659600	-0.87395000	2.35246600
N	-2.82393000	1.47329000	2.60188300
Au	-1.04217700	1.16657300	0.16275000
P	-0.68856300	2.81190800	-1.50725900
C	1.02010900	2.51584000	-2.26614900
C	2.08095800	2.65765700	-1.17575300
C	1.37658700	3.42684200	-3.43971300
C	1.00769500	1.07117700	-2.77096100
H	1.85408600	2.05912700	-0.28339600
H	2.22567100	3.69917900	-0.86555300
H	3.04278900	2.30609700	-1.57252100

H	0.72873700	3.26124900	-4.30675000
H	2.40108800	3.19207800	-3.75793200
H	1.35987900	4.49153200	-3.18293000
H	1.97959100	0.84332400	-3.22852000
H	0.24193500	0.91334500	-3.54152700
H	0.84447100	0.34751200	-1.96038700
C	-0.85855700	4.46299900	-0.57072600
C	-0.23768000	5.67238700	-1.26656000
C	-0.22115600	4.32227500	0.81586000
C	-2.36106800	4.68946100	-0.38378700
H	-0.67219300	5.88061500	-2.24884100
H	0.85023300	5.58648000	-1.36937700
H	-0.42664800	6.56078800	-0.64919900
H	-0.72669100	3.56758800	1.43112800
H	-0.31563300	5.28317500	1.33964000
H	0.84534400	4.07506200	0.78375900
H	-2.50652500	5.55361500	0.27796700
H	-2.85033400	3.82798300	0.09462500
H	-2.87887500	4.90151000	-1.32599200
C	-1.90507100	2.89596800	-2.88174700
C	-3.03042600	2.05018100	-2.97237300
C	-1.79006500	3.95493500	-3.79782100
C	-4.00674600	2.32908400	-3.93777100
C	-3.27397400	0.83111700	-2.15720200
C	-2.75722500	4.20151400	-4.76031400
H	-0.92904500	4.61376100	-3.75804400
C	-3.88281900	3.39027700	-4.82072200
H	-4.87182100	1.67163700	-3.99845000
C	-4.37437900	0.77019700	-1.29658900
C	-2.51604900	-0.32612400	-2.36721900

H	-2.63231300	5.02987300	-5.45235600
H	-4.65757300	3.57512000	-5.56015800
C	-4.71048200	-0.42246800	-0.66229800
H	-4.98281500	1.66217500	-1.14899900
C	-2.85620600	-1.51863000	-1.73784400
H	-1.67926000	-0.29831800	-3.06344700
C	-3.95525300	-1.56984600	-0.88580500
H	-5.58664400	-0.46327700	-0.01727900
H	-2.27322700	-2.41637300	-1.93232200
H	-4.23279100	-2.50860500	-0.41038100

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2875.707994

Electronic Energy (0K) + ZPE = -2874.906534

Enthalpy (298K) = -2874.854774

Free Energy (298K) = -2874.993177

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2876.260235

3a-Z

Number of imaginary frequencies: 0

C	-0.36650200	0.96522500	2.10955200
C	0.93410600	1.16843300	2.47419700
C	1.71905800	2.36934300	2.14659200
C	2.70143900	2.80832900	3.04791200
C	1.55336500	3.08397900	0.95105200
C	3.46381400	3.93826100	2.78049500
H	2.85967200	2.25117200	3.96956600
C	2.31844200	4.21308300	0.68546300
H	0.82531200	2.74243800	0.22131200
C	3.27417000	4.65059400	1.59878400

H	4.21275800	4.26326100	3.49989900
H	2.17540800	4.74735400	-0.25172600
H	3.87415500	5.53276400	1.38629100
N	1.56655800	0.20694100	3.31827400
S	2.55047800	-0.94638800	2.60779000
O	3.36990400	-1.50537900	3.67846700
O	3.17334800	-0.32017300	1.44886200
C	1.00895800	-0.11959500	4.63052300
H	0.25301100	-0.91631000	4.59136200
H	0.53970600	0.78705100	5.02365100
H	1.81579700	-0.41361400	5.30689700
C	1.47866500	-2.23419900	2.02166700
C	1.14357500	-3.28776100	2.86676200
C	0.94127700	-2.14052400	0.73775500
C	0.26170000	-4.26355900	2.41236700
H	1.58288700	-3.35371700	3.85950200
C	0.06087900	-3.11976900	0.30414800
H	1.22094100	-1.31424300	0.08828300
C	-0.29245400	-4.19286300	1.13233500
H	0.00150900	-5.09799800	3.06171700
H	-0.36254800	-3.05951300	-0.69765100
C	-1.26005000	-5.22621200	0.64710000
H	-2.23692100	-4.77403100	0.43147100
H	-1.40925600	-6.02063800	1.38507500
H	-0.91368500	-5.68733100	-0.28581400
C	-2.92134300	0.31941000	1.31062900
C	-2.16428800	-0.58233000	2.06467300
C	-2.65253900	-1.83879400	2.39371900
C	-3.92204100	-2.19108500	1.94672900
C	-4.69560300	-1.30706000	1.18857200

C	-4.19602600	-0.05200700	0.87446100
C	-2.31236000	1.60281900	1.06827200
H	-2.03558800	-2.51736200	2.97985500
H	-4.31605400	-3.17380800	2.19565300
H	-5.68519600	-1.60303100	0.85143800
H	-4.78059400	0.65726200	0.29110800
H	-2.89105700	2.36954900	0.54668400
O	-0.92786700	-0.23312000	2.50350000
N	-1.11437800	1.90235500	1.44475000

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -1620.931400

Electronic Energy (0K) + ZPE = -1620.549142

Enthalpy (298K) = -1620.523232

Free Energy (298K) = -1620.605115

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -1621.247929

TS_{A1}

Number of imaginary frequencies: 1

C	-4.21451700	2.56344000	-2.76048700
C	-3.06248300	2.81168400	-3.32745900
C	-2.19038500	3.95551900	-3.05702100
C	-1.59110200	4.69216500	-4.08793100
C	-1.91006000	4.29969200	-1.72482400
C	-0.78348100	5.78483600	-3.79385100
H	-1.78291500	4.41001600	-5.12235700
C	-1.07989100	5.37630500	-1.43711400
H	-2.35139100	3.71221400	-0.92091800
C	-0.52595500	6.13072300	-2.46887700
H	-0.34138600	6.36118700	-4.60356800

H	-0.86820100	5.63011900	-0.40079400
H	0.11646000	6.97825500	-2.24118100
N	-5.07378100	1.61732200	-2.41624800
S	-4.68619000	0.70320600	-0.99222700
O	-5.95499200	0.14943200	-0.54638400
O	-3.90971500	1.60344500	-0.15544100
C	-6.33952900	1.38460200	-3.11664900
H	-6.61259700	2.31302900	-3.62708700
H	-7.12412300	1.12351300	-2.40415100
Au	-2.66704500	1.49237300	-4.94050100
P	-1.93295500	0.19597900	-6.81166700
H	-6.21734800	0.58359000	-3.85845300
C	-3.63307700	-0.60220600	-1.53475200
C	-4.19142000	-1.84263200	-1.84177700
C	-2.25834100	-0.37881300	-1.60374500
C	-3.34628300	-2.87702500	-2.21421200
H	-5.26510800	-1.99682400	-1.76440800
C	-1.43297500	-1.42903500	-1.98650500
H	-1.84025000	0.58919800	-1.33599900
C	-1.96122400	-2.68564800	-2.29683400
H	-3.76337100	-3.85556000	-2.44774800
H	-0.35642200	-1.27388000	-2.03929500
C	-1.07452200	-3.80067200	-2.75197700
H	-1.21521900	-3.98838900	-3.82669400
H	-1.31078400	-4.73722900	-2.23404000
H	-0.01710900	-3.56969200	-2.58848700
C	-2.72861100	-1.52887500	-6.84000500
C	-3.02998000	-1.91302800	-5.39259100
C	-1.87461800	-2.62691200	-7.46880200
C	-4.05423700	-1.41746100	-7.59070000

H	-3.74508700	-1.21934600	-4.92843200
H	-2.12829700	-1.93133200	-4.77175900
H	-3.47203500	-2.92025800	-5.37365500
H	-1.62251800	-2.42891500	-8.51656900
H	-2.44992000	-3.56318300	-7.44729000
H	-0.94698800	-2.80217900	-6.91054400
H	-4.57579500	-2.38197800	-7.52116900
H	-3.92240800	-1.18247500	-8.65306300
H	-4.70972900	-0.65898800	-7.14256100
C	-0.04692600	0.16296900	-6.56942800
C	0.78687100	-0.48634000	-7.67227300
C	0.23951500	-0.53830800	-5.23955100
C	0.38038200	1.63112000	-6.45860100
H	0.75127000	0.08392400	-8.60633800
H	0.50284100	-1.52244200	-7.88087600
H	1.83448700	-0.49453600	-7.34095100
H	-0.33752200	-0.09897800	-4.41399500
H	1.30634200	-0.42118300	-5.00323300
H	0.02657500	-1.61470300	-5.27860400
H	1.47358400	1.67339400	-6.35562200
H	-0.05863700	2.12222900	-5.57980600
H	0.10838900	2.21073100	-7.35155600
C	-2.20550600	0.93471300	-8.47968100
C	-2.89122400	2.15004400	-8.69648900
C	-1.63044500	0.28858100	-9.58626800
C	-2.89426600	2.70262300	-9.98528000
C	-3.70050500	2.88584600	-7.68853500
C	-1.67312600	0.83440100	-10.86175500
H	-1.13026500	-0.66620200	-9.45298600
C	-2.28920400	2.06472800	-11.05814300

H	-3.41724200	3.64488200	-10.14062100
C	-3.36879900	4.19534100	-7.32849800
C	-4.89882300	2.33999500	-7.21175900
H	-1.21817200	0.30193700	-11.69328800
H	-2.31806700	2.51732800	-12.04645700
C	-4.20374000	4.93460800	-6.49292100
H	-2.44806900	4.63552900	-7.71210700
C	-5.73869100	3.08208000	-6.38833400
H	-5.18639500	1.33636300	-7.52112800
C	-5.39146900	4.38124500	-6.02217100
H	-3.92636600	5.95043700	-6.21687600
H	-6.67487300	2.64771200	-6.04250700
H	-6.05200800	4.96369300	-5.38225300
C	-6.11744900	6.02547300	-1.53844800
C	-6.72132300	4.96077900	-0.86535100
C	-7.86335900	5.09138200	-0.08417100
C	-8.38695400	6.37174100	-0.00964300
C	-7.79982000	7.46613500	-0.67811200
C	-6.66331000	7.31428200	-1.44799400
C	-5.00536700	5.41949500	-2.18331800
H	-8.30828100	4.24527500	0.42970400
H	-9.28090100	6.53982100	0.58584900
H	-8.25533900	8.44773800	-0.57921400
H	-6.20619900	8.15504600	-1.96165000
H	-4.24500000	5.85833200	-2.82186700
O	-6.02670900	3.82036800	-1.08957500
N	-4.95936800	4.14404000	-1.90042400

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2875.656972

Electronic Energy (0K) + ZPE = -2874.859452

Enthalpy (298K) = -2874.807888

Free Energy (298K) = -2874.945023

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2876.165333

A1

Number of imaginary frequencies: 0

C	-1.45237100	0.93653200	1.65465700
C	-0.24974600	1.00687300	1.04325600
C	0.61985500	2.17612400	1.27611200
C	1.25912800	2.85640700	0.22958800
C	0.87005200	2.59508800	2.59474400
C	2.08313500	3.94575400	0.48895800
H	1.09204600	2.52725600	-0.79572600
C	1.71552100	3.66808100	2.85151800
H	0.40591100	2.05688200	3.42163100
C	2.31778900	4.35434600	1.79998600
H	2.55635400	4.47065000	-0.33829000
H	1.90388800	3.96922800	3.87975500
H	2.97573700	5.19649500	2.00164300
N	-2.29346700	-0.18060900	1.82190100
S	-2.00937800	-1.15449900	3.17376900
O	-3.27744300	-1.82195700	3.44599700
O	-1.39405400	-0.28269900	4.16597900
C	-2.96672200	-0.77562800	0.67039600
H	-3.51772500	0.01247000	0.14601000
H	-3.68423600	-1.52443300	1.01600300
Au	0.39105600	-0.34865100	-0.42779100
P	1.43969700	-1.59324800	-2.21525100
H	-2.24847200	-1.23610300	-0.02711100

C	-0.82458900	-2.40992400	2.77169200
C	-1.26710700	-3.69227800	2.45172400
C	0.53524300	-2.11608000	2.86951300
C	-0.32874700	-4.69230000	2.23933200
H	-2.33216600	-3.90476000	2.39948300
C	1.45811200	-3.13132300	2.65104500
H	0.86506600	-1.11556800	3.14199500
C	1.04202300	-4.42955700	2.34002000
H	-0.66103300	-5.70044300	1.99497800
H	2.52297000	-2.91697800	2.73262500
C	2.03721500	-5.52445100	2.11733300
H	1.77787800	-6.12118200	1.23428500
H	2.05979400	-6.21355300	2.97135800
H	3.04961400	-5.12872500	1.98440000
C	0.78733400	-3.37465600	-2.31058800
C	0.46749600	-3.82567300	-0.88664200
C	1.73193000	-4.39768500	-2.93602300
C	-0.51976900	-3.32900800	-3.10148400
H	-0.25099000	-3.15479500	-0.39657300
H	1.36203600	-3.88156900	-0.25769500
H	0.02349000	-4.83135500	-0.92360700
H	1.96631000	-4.18626900	-3.98433700
H	1.23719400	-5.37882000	-2.91264100
H	2.66855000	-4.49339200	-2.37471100
H	-0.96652400	-4.33279600	-3.09822400
H	-0.37202200	-3.03145400	-4.14642100
H	-1.24650200	-2.64548400	-2.64161700
C	3.28584800	-1.48633900	-1.76057300
C	4.28990800	-2.03709700	-2.77120800
C	3.48492000	-2.20185900	-0.42335400

C	3.57625100	0.00743400	-1.57622400
H	4.32472700	-1.43905800	-3.68778600
H	4.11017000	-3.08318000	-3.03964200
H	5.28821500	-1.98374200	-2.31478800
H	2.75828400	-1.87271500	0.33247400
H	4.49026800	-1.96834400	-0.04560800
H	3.41682400	-3.29257100	-0.52559200
H	4.65120200	0.13880900	-1.38958900
H	3.03313900	0.42764700	-0.71978700
H	3.32058400	0.59422100	-2.47000000
C	1.33599000	-0.91324700	-3.93208900
C	0.62169500	0.25190000	-4.28779500
C	2.08176700	-1.55988900	-4.93222500
C	0.74664300	0.75059800	-5.59354400
C	-0.33818200	0.99525200	-3.42966200
C	2.16753700	-1.06970900	-6.22788000
H	2.62626600	-2.46803800	-4.69651700
C	1.51039900	0.10926500	-6.55664700
H	0.19649500	1.65312900	-5.85438600
C	-0.12687700	2.34861100	-3.14838600
C	-1.55219400	0.41006400	-3.05047300
H	2.75433400	-1.60522900	-6.97016400
H	1.57653100	0.51948600	-7.56152300
C	-1.10246000	3.09922200	-2.49669200
H	0.80883900	2.81580500	-3.45544800
C	-2.53369700	1.16332300	-2.41450100
H	-1.73973600	-0.63383800	-3.29822800
C	-2.31170400	2.51084500	-2.13520200
H	-0.92027300	4.15141000	-2.28486800
H	-3.48302300	0.69964200	-2.15354700

H	-3.08870500	3.10392200	-1.65618200
C	-2.77390300	4.22502600	2.49328100
C	-2.94592600	3.46065000	3.65569000
C	-3.49839300	3.95704300	4.82869100
C	-3.86888700	5.29000700	4.78456300
C	-3.70718500	6.08768400	3.62947900
C	-3.16495600	5.57509300	2.47151200
C	-2.21654300	3.32340900	1.56867600
H	-3.62140600	3.33983700	5.71235400
H	-4.30202200	5.74146100	5.67342500
H	-4.02154800	7.12683200	3.66293100
H	-3.03926000	6.17959500	1.57861600
H	-1.92248300	3.44903100	0.53165100
O	-2.50919200	2.19642800	3.46027900
N	-2.06225000	2.15339800	2.15382900

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2875.675517

Electronic Energy (0K) + ZPE = -2874.876301

Enthalpy (298K) = -2874.824683

Free Energy (298K) = -2874.962954

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2876.183068

TS_{B1}

Number of imaginary frequencies: 1

C	-1.23922600	0.86961500	1.63374100
C	-0.02862700	1.23449000	1.03906200
C	0.60315300	2.50204300	1.32552900
C	1.46355600	3.09016500	0.37547200
C	0.44163900	3.14587500	2.57353900

C	2.08414200	4.30191500	0.63193800
H	1.61230600	2.58311100	-0.57776300
C	1.09237200	4.34011200	2.83766600
H	-0.16656100	2.67666400	3.34402600
C	1.90143600	4.92765300	1.86480600
H	2.72538700	4.75377600	-0.12115600
H	0.97407200	4.81648200	3.80767100
H	2.40499600	5.86843000	2.07523500
N	-1.59812400	-0.48101800	1.83021300
S	-1.11512200	-1.11312400	3.34044600
O	-2.31725800	-1.49884000	4.07125700
O	-0.17752300	-0.14503800	3.89756600
C	-2.89121900	-0.93612200	1.32081800
H	-3.73941500	-0.47656200	1.84408000
H	-2.96221900	-2.02404900	1.41588500
Au	0.61808900	-0.04213600	-0.48521800
P	1.39850900	-1.50878000	-2.23287700
H	-2.93384300	-0.68652300	0.25358800
C	-0.21913100	-2.58445900	2.93825300
C	-0.89535300	-3.79629800	2.81837300
C	1.16124600	-2.50173200	2.76673400
C	-0.17230000	-4.93554400	2.48924900
H	-1.96724800	-3.84960500	2.99412500
C	1.86656500	-3.65498000	2.45184700
H	1.67409200	-1.55074400	2.89348900
C	1.21049500	-4.87957700	2.28765100
H	-0.68820300	-5.88867300	2.38566900
H	2.94696100	-3.60623400	2.32143500
C	1.96521700	-6.09100000	1.84170000
H	1.98652800	-6.13552100	0.74268300

H	1.49538200	-7.01526000	2.19365000
H	3.00461000	-6.07146300	2.18584300
C	0.41694000	-3.13695500	-2.18865100
C	0.02561600	-3.41502700	-0.73661000
C	1.15186200	-4.36191100	-2.72757900
C	-0.86725900	-2.90864600	-2.98654800
H	-0.58057000	-2.60080000	-0.31526100
H	0.89508500	-3.56195600	-0.08597500
H	-0.57315200	-4.33695800	-0.70673000
H	1.42121300	-4.27748700	-3.78558500
H	0.48301500	-5.22943700	-2.63759300
H	2.05685300	-4.58854000	-2.15149400
H	-1.49908500	-3.80284000	-2.89478300
H	-0.68108900	-2.73810800	-4.05302100
H	-1.44327600	-2.05961200	-2.59228300
C	3.24918700	-1.71308300	-1.86031600
C	4.07815800	-2.50544900	-2.86814100
C	3.37725800	-2.36150800	-0.48230200
C	3.80750000	-0.28728500	-1.79936700
H	4.14796300	-1.99865800	-3.83638900
H	3.70764300	-3.52315500	-3.02930800
H	5.10019200	-2.58797300	-2.47290300
H	2.78293900	-1.83501700	0.27741900
H	4.43046400	-2.32566100	-0.16976500
H	3.07091800	-3.41566000	-0.49168600
H	4.88817500	-0.33722700	-1.60654700
H	3.34754700	0.29973000	-0.99259200
H	3.66376600	0.25296400	-2.74530000
C	1.33139100	-0.90169300	-3.97655800
C	0.86485100	0.37618900	-4.35519200

C	1.85871200	-1.73656100	-4.97594300
C	1.01417500	0.78186300	-5.69016300
C	0.15220600	1.34338500	-3.48102500
C	1.96923000	-1.32966700	-6.29824100
H	2.20240800	-2.73356500	-4.71978100
C	1.56211200	-0.04990800	-6.65466200
H	0.65669100	1.77090500	-5.97138000
C	0.65390900	2.63889500	-3.31500800
C	-1.10555800	1.03478600	-2.94848900
H	2.37992600	-2.01002300	-7.04015900
H	1.65331200	0.29499200	-7.68186300
C	-0.08206900	3.60400900	-2.63345200
H	1.62573200	2.88997400	-3.73918600
C	-1.84600000	2.00278200	-2.27437100
H	-1.51951000	0.03877500	-3.10053500
C	-1.33705300	3.29051400	-2.11751300
H	0.32214100	4.60738700	-2.51529900
H	-2.83256400	1.75175300	-1.88680300
H	-1.92273600	4.05311600	-1.60637000
C	-3.32230800	3.71939700	2.37106600
C	-3.22368000	3.12699400	3.66170600
C	-3.87524000	3.73400000	4.75391400
C	-4.55067100	4.91303600	4.52087900
C	-4.63895100	5.50833700	3.23923100
C	-4.03713800	4.91523200	2.15741100
C	-2.68816000	2.86545100	1.46431400
H	-3.81610000	3.28618300	5.74106100
H	-5.04008400	5.40632000	5.35799400
H	-5.19404100	6.43411700	3.11946500
H	-4.09922500	5.34387300	1.16038500

H	-2.64160700	2.99363800	0.38286600
O	-2.53253200	2.02960900	3.71297700
N	-2.15341800	1.79062000	1.98610500

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2875.658790

Electronic Energy (0K) + ZPE = -2874.861908

Enthalpy (298K) = -2874.810507

Free Energy (298K) = -2874.946405

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2876.166077

B1

Number of imaginary frequencies: 0

C	-1.28862000	0.23238800	1.85943700
C	-0.01422200	0.88565600	1.51990900
C	0.36740400	2.10760100	2.09975300
C	1.61467500	2.67158100	1.72209700
C	-0.42836400	2.77203900	3.07469000
C	2.06017500	3.84072200	2.30514500
H	2.21331600	2.14036500	0.98298700
C	0.01209000	3.95664400	3.62486800
H	-1.40152000	2.36488300	3.35296800
C	1.25399300	4.48298200	3.24797400
H	3.02100000	4.26490000	2.02664100
H	-0.59813700	4.47876300	4.35635600
H	1.59693200	5.41149300	3.69894100
N	-1.31656700	-1.02202500	2.44378500
S	-0.20493800	-1.43056600	3.67595600
O	-0.99155800	-1.75265600	4.85499400
O	0.75847000	-0.33555000	3.68875800

C	-2.57129900	-1.77548300	2.40852900
H	-3.31021600	-1.36388200	3.10313300
H	-2.36912700	-2.81942700	2.66033000
Au	0.73498500	0.00203500	-0.20372300
P	1.16891200	-1.32797700	-2.16100800
H	-2.96525000	-1.74045300	1.38926200
C	0.59800300	-2.89602200	3.11184200
C	-0.00680900	-4.13694100	3.30647100
C	1.86066500	-2.78322500	2.53080200
C	0.65529700	-5.27746600	2.87146600
H	-0.96731400	-4.21760500	3.80978100
C	2.51509400	-3.93898900	2.13193400
H	2.32698800	-1.80718800	2.41181000
C	1.92020800	-5.19719700	2.28120600
H	0.19040300	-6.25185400	3.00872300
H	3.50982700	-3.86946200	1.69361300
C	2.64504900	-6.42520800	1.83161700
H	3.04781200	-6.29604900	0.81971800
H	1.99384100	-7.30445600	1.83621100
H	3.49845100	-6.63560400	2.48856000
C	-0.10349400	-2.74413800	-1.99590400
C	-0.18773400	-3.16889200	-0.52374500
C	0.18161100	-3.99667900	-2.82190900
C	-1.45748400	-2.15148200	-2.39356500
H	-0.51650500	-2.34754600	0.12755900
H	0.76168100	-3.55305200	-0.13315700
H	-0.93048600	-3.97526600	-0.44066600
H	0.21345000	-3.81329100	-3.89983500
H	-0.63260000	-4.71357300	-2.64656800
H	1.11497600	-4.48540200	-2.51879200

H	-2.24489300	-2.87615000	-2.14486000
H	-1.52548200	-1.93759600	-3.46631200
H	-1.67708400	-1.22318800	-1.84300300
C	2.96044400	-1.92281700	-2.23471000
C	3.33689100	-2.69561700	-3.49577200
C	3.23188400	-2.78421800	-1.00521200
C	3.82684400	-0.66491900	-2.16254700
H	3.26357300	-2.07654300	-4.39651500
H	2.73719000	-3.60055200	-3.64005300
H	4.38605600	-3.00847600	-3.40155100
H	2.95425000	-2.26835400	-0.07694000
H	4.30792600	-3.00289600	-0.95744600
H	2.70152000	-3.74404600	-1.04407700
H	4.88363200	-0.96489400	-2.15099600
H	3.63139600	-0.07830900	-1.25423400
H	3.67711300	-0.01923700	-3.03735600
C	0.81254300	-0.51163700	-3.77569900
C	0.46138800	0.85044300	-3.90327500
C	0.77432600	-1.31867900	-4.92506000
C	0.03769300	1.32286800	-5.15435200
C	0.54320700	1.88908600	-2.84059000
C	0.37314600	-0.82710500	-6.15907500
H	1.05443500	-2.36488900	-4.85987000
C	-0.01433600	0.50261000	-6.27118400
H	-0.23410700	2.37325600	-5.24335200
C	1.78459100	2.34916000	-2.38388500
C	-0.61497900	2.55667800	-2.42440000
H	0.35679600	-1.48610500	-7.02358000
H	-0.34407600	0.90473200	-7.22607600
C	1.86424100	3.44495600	-1.53038100

H	2.69349600	1.86125800	-2.73024400
C	-0.53434400	3.65161900	-1.56685800
H	-1.58313100	2.22124100	-2.79872200
C	0.70475400	4.10059200	-1.12070900
H	2.83794100	3.79850400	-1.19523500
H	-1.44262400	4.16508200	-1.25622300
H	0.76748200	4.96440600	-0.46231800
C	-3.55049800	2.76511500	0.81346400
C	-4.04043200	3.06825200	2.17160100
C	-4.96967700	4.18095100	2.25929500
C	-5.32341400	4.90996600	1.16699600
C	-4.82008400	4.61191000	-0.14065500
C	-3.96560400	3.56847400	-0.30219900
C	-2.71661800	1.69308500	0.57453100
H	-5.35610000	4.41384600	3.24953800
H	-6.01190700	5.74617000	1.28150000
H	-5.13660200	5.21199000	-0.98937500
H	-3.58789500	3.30438400	-1.29098200
H	-2.36595200	1.53532600	-0.45531800
O	-3.68480400	2.42870700	3.17511500
N	-2.39286600	0.74482200	1.45900800

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2875.684357

Electronic Energy (0K) + ZPE = -2874.886242

Enthalpy (298K) = -2874.833980

Free Energy (298K) = -2874.971876

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2876.195338

TS_{C1}

Number of imaginary frequencies: 1

C	-1.43204000	0.70870900	1.37487100
C	-0.05130200	1.20530200	1.15456700
C	0.50455300	2.43741300	1.55895200
C	1.90839700	2.58945700	1.38703900
C	-0.22892800	3.52377600	2.10423200
C	2.55536000	3.73425700	1.80619700
H	2.46726000	1.76328100	0.94812400
C	0.42094100	4.68802600	2.46632000
H	-1.30274600	3.44103200	2.20304900
C	1.80864300	4.78691000	2.34016500
H	3.63275100	3.82513400	1.70039700
H	-0.14878400	5.52510100	2.86021100
H	2.31212000	5.70020600	2.64904800
N	-1.62863700	-0.50005700	1.98071500
S	-0.67385200	-0.89510700	3.36295700
O	-1.60116500	-1.09846000	4.46081400
O	0.36003000	0.13240300	3.40341900
C	-2.93255900	-1.15364900	1.88866200
H	-3.65205300	-0.70861400	2.58370900
H	-2.81536800	-2.21847700	2.10690200
Au	0.74180800	0.04427200	-0.40877900
P	1.26722900	-1.40715400	-2.23424800
H	-3.29132600	-1.05976700	0.86040500
C	0.07613200	-2.44110600	2.96454000
C	-0.63648600	-3.62378600	3.15889900
C	1.40014100	-2.44940700	2.52743900
C	-0.01838700	-4.83087700	2.86188200
H	-1.64845900	-3.60601300	3.55621600
C	2.00588000	-3.66968100	2.26722100

H	1.94837000	-1.51657700	2.41168100
C	1.30385300	-4.87206000	2.40810400
H	-0.56465600	-5.76173200	3.00135100
H	3.04539600	-3.69550900	1.94336800
C	1.95870400	-6.16799500	2.05198100
H	1.98603400	-6.29241400	0.96053100
H	1.42039500	-7.02447300	2.46926500
H	2.99592600	-6.20119000	2.40308600
C	-0.02479700	-2.80582700	-2.13980300
C	-0.32102100	-3.09610400	-0.66372000
C	0.37007300	-4.12597500	-2.79939100
C	-1.30316000	-2.25812000	-2.77700500
H	-0.74826600	-2.22255200	-0.15119100
H	0.56686200	-3.41906900	-0.10663900
H	-1.05944300	-3.90901600	-0.61285300
H	0.56880000	-4.04339300	-3.87214600
H	-0.46914000	-4.82640900	-2.68620900
H	1.24096200	-4.58329000	-2.31494800
H	-2.12212600	-2.96412800	-2.58255000
H	-1.21483500	-2.13676800	-3.86224200
H	-1.59186500	-1.28857200	-2.34379400
C	3.05887400	-1.98971800	-2.10436500
C	3.54530700	-2.85921600	-3.26010000
C	3.22422500	-2.73986500	-0.78642100
C	3.90267300	-0.71342500	-2.06481900
H	3.53201800	-2.32189800	-4.21468400
H	2.97070300	-3.78446700	-3.37091900
H	4.58834500	-3.14055400	-3.05920000
H	2.88320100	-2.13801800	0.06618700
H	4.28922200	-2.96534900	-0.63506300

H	2.67888800	-3.69247700	-0.77740100
H	4.96061600	-0.99184000	-1.96310100
H	3.63848200	-0.07023700	-1.21356700
H	3.80070900	-0.12728400	-2.98750400
C	1.13791900	-0.65994900	-3.91494000
C	1.02481500	0.72591300	-4.14782800
C	1.19509800	-1.51890100	-5.02536400
C	0.98316000	1.18868600	-5.47094400
C	0.94359700	1.79473900	-3.11224600
C	1.13948300	-1.04440800	-6.32775300
H	1.29129400	-2.58956200	-4.87581400
C	1.03557800	0.32299300	-6.55325200
H	0.90101900	2.26128400	-5.63890400
C	2.08047300	2.54299500	-2.79007500
C	-0.29454500	2.18207500	-2.58612700
H	1.18244700	-1.74324200	-7.15947800
H	0.99503400	0.71548000	-7.56651700
C	1.98346100	3.65044800	-1.95205700
H	3.04223500	2.26336100	-3.21916800
C	-0.39239800	3.30121100	-1.76245000
H	-1.18766600	1.61193700	-2.84430200
C	0.74527400	4.03618800	-1.44325400
H	2.87547100	4.22476800	-1.70921000
H	-1.36213700	3.59941100	-1.36731500
H	0.66735300	4.91108200	-0.80073000
C	-3.98645800	2.38254800	1.50470700
C	-3.42911100	2.31094600	2.83418800
C	-4.19537300	2.90740200	3.88379300
C	-5.39433400	3.52173600	3.62405100
C	-5.92629300	3.60110600	2.31343200

C	-5.22361400	3.04001600	1.27977000
C	-3.33200200	1.79282700	0.40215400
H	-3.78828600	2.85587700	4.89134400
H	-5.95195500	3.96543300	4.44759200
H	-6.87632400	4.09845700	2.13878400
H	-5.60581700	3.07896000	0.25942300
H	-3.80466600	1.93332600	-0.57587500
O	-2.29906600	1.76823000	3.06287800
N	-2.23182900	1.08973500	0.37044200

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2875.678589

Electronic Energy (0K) + ZPE = -2874.881896

Enthalpy (298K) = -2874.830322

Free Energy (298K) = -2874.966455

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2876.185787

C1

Number of imaginary frequencies: 0

C	-1.59182700	0.95407500	1.47391700
C	-0.17501400	1.33526500	1.05047600
C	0.40589900	2.58847500	1.39931300
C	1.81652500	2.68314100	1.28228200
C	-0.30837700	3.74179900	1.81702300
C	2.48877400	3.83585200	1.64493400
H	2.36425900	1.80884800	0.93117000
C	0.36671600	4.91118200	2.11303800
H	-1.39232700	3.73380000	1.85265700
C	1.76175100	4.95319400	2.05413900
H	3.57286000	3.87794700	1.58626900

H	-0.19116400	5.79793500	2.40161500
H	2.28379900	5.87117800	2.31434500
N	-1.64681300	-0.48412900	1.78424700
S	-0.79577000	-0.85387900	3.20562300
O	-1.72001400	-0.91717800	4.33371900
O	0.32427600	0.09112400	3.22178700
C	-2.93159800	-1.17601900	1.66012200
H	-3.67163600	-0.85649200	2.40513500
H	-2.76408600	-2.25312700	1.76416200
Au	0.58718500	0.13994900	-0.47352000
P	1.16384900	-1.37210500	-2.24695500
H	-3.31878800	-1.01045200	0.65154700
C	-0.15065200	-2.47730600	2.93120100
C	-0.93395400	-3.59515100	3.20958800
C	1.16895500	-2.60500100	2.50113400
C	-0.39267700	-4.85921600	3.00977700
H	-1.94497200	-3.48136200	3.59351500
C	1.69764400	-3.87586300	2.33296700
H	1.77140100	-1.71766600	2.31703400
C	0.92421300	-5.01864900	2.56914300
H	-0.99686700	-5.74039900	3.21723800
H	2.73236300	-3.98948500	2.01115400
C	1.50982300	-6.37709600	2.34790000
H	1.73524500	-6.53349200	1.28503700
H	0.82744900	-7.17005700	2.66861100
H	2.45431100	-6.49364400	2.89234700
C	-0.14939700	-2.75144800	-2.17575100
C	-0.47507900	-3.03332400	-0.70440300
C	0.22571800	-4.08038400	-2.82852200
C	-1.40439300	-2.17505300	-2.83414300

H	-0.85205900	-2.14076300	-0.18810000
H	0.38765800	-3.41110400	-0.14281000
H	-1.25919800	-3.80336000	-0.66482900
H	0.42109300	-4.00734000	-3.90239700
H	-0.62216700	-4.76928600	-2.70845700
H	1.09172000	-4.54673400	-2.34418500
H	-2.23593200	-2.87681700	-2.68110000
H	-1.28429000	-2.02721200	-3.91339900
H	-1.69472200	-1.21442800	-2.38299800
C	2.93864700	-1.98144900	-2.01083600
C	3.48797200	-2.85375200	-3.13600400
C	3.01668600	-2.74119100	-0.68997900
C	3.79340900	-0.71548800	-1.91404400
H	3.55239400	-2.31226600	-4.08610700
H	2.90464600	-3.76729900	-3.29270200
H	4.50864400	-3.15764400	-2.86458000
H	2.60461600	-2.15431400	0.14136100
H	4.07122400	-2.95222900	-0.46271800
H	2.48921700	-3.70247400	-0.73262700
H	4.84219800	-1.00570200	-1.76179000
H	3.49099200	-0.07871000	-1.07096600
H	3.74458700	-0.11817600	-2.83411600
C	1.14245900	-0.68401900	-3.95915500
C	1.08743400	0.69617900	-4.24307200
C	1.25390100	-1.57855400	-5.03685900
C	1.16620200	1.11759200	-5.57854100
C	0.94248200	1.80012200	-3.25310800
C	1.31090000	-1.14509400	-6.35363400
H	1.31220100	-2.64554100	-4.84838000
C	1.27312100	0.21689900	-6.62746300

H	1.13084200	2.18630500	-5.78363600
C	2.04621900	2.59633100	-2.93140000
C	-0.32099300	2.16892800	-2.77714400
H	1.39339200	-1.87167400	-7.15824100
H	1.32526500	0.57777700	-7.65190800
C	1.89207500	3.73403500	-2.14380600
H	3.02780400	2.32959600	-3.32204200
C	-0.47631800	3.31804500	-2.00548400
H	-1.18822800	1.56133400	-3.03632200
C	0.62846200	4.10247100	-1.68797300
H	2.75910100	4.34523800	-1.90073500
H	-1.46620000	3.59967100	-1.65004300
H	0.50511100	5.00193500	-1.08784900
C	-4.10239500	2.14653300	1.65840500
C	-3.29036700	2.02488800	2.79159000
C	-3.77490400	2.32126600	4.05880900
C	-5.09462200	2.74199000	4.17742700
C	-5.92317000	2.87259100	3.05717700
C	-5.42624000	2.57764400	1.79826900
C	-3.49735300	1.78933000	0.40162200
H	-3.12101300	2.21557200	4.92057600
H	-5.48843400	2.97206300	5.16465100
H	-6.95084700	3.20363500	3.17758100
H	-6.04910400	2.66722600	0.90982400
H	-4.05254400	1.99269100	-0.51934500
O	-1.98726100	1.68502400	2.64475300
N	-2.34974800	1.21710100	0.27766400

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2875.705421

Electronic Energy (0K) + ZPE = -2874.906525

Enthalpy (298K) = -2874.855020

Free Energy (298K) = -2874.992442

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2876.208294

TS_{D1}

Number of imaginary frequencies: 1

C	-1.88882500	1.07400200	1.17190300
C	-0.46801000	1.05776200	0.74825700
C	0.57276900	1.86258200	1.37206500
C	1.90291700	1.39638000	1.29710300
C	0.35025200	3.14149100	1.92053200
C	2.95727100	2.14537100	1.79362800
H	2.08984400	0.42035000	0.84857000
C	1.41499400	3.91058200	2.36927900
H	-0.65494800	3.54217900	1.97398800
C	2.71410600	3.41150400	2.32504700
H	3.97087900	1.75527800	1.74685900
H	1.22701400	4.90373300	2.76954700
H	3.54076400	4.01345700	2.69537200
N	-1.45862100	-0.18587600	1.92877300
S	-1.23529400	-0.19987900	3.65863100
O	-2.50243900	-0.62199400	4.24088000
O	-0.62861700	1.06091200	4.04497400
C	-1.86096900	-1.49574900	1.39406600
H	-2.78535400	-1.83840200	1.87606000
H	-1.05885300	-2.22538600	1.54453000
Au	0.04295400	-0.03867300	-0.97381400
P	0.71579400	-1.40412500	-2.80747800
H	-2.03884900	-1.39489800	0.32280000

C	-0.05280700	-1.50032600	3.82994300
C	-0.47581700	-2.77553900	4.19155600
C	1.28917800	-1.21651000	3.57833100
C	0.47052500	-3.78790100	4.28965000
H	-1.52774700	-2.97095600	4.38575400
C	2.21526300	-2.24286400	3.67499900
H	1.60104000	-0.20598200	3.32222600
C	1.82111100	-3.54064100	4.02737100
H	0.15636900	-4.79093800	4.57203000
H	3.26780700	-2.03914900	3.48371400
C	2.84224500	-4.62740500	4.13852700
H	3.49904400	-4.64366200	3.26096800
H	2.37705300	-5.61229100	4.24219400
H	3.48496400	-4.46606500	5.01322700
C	-0.77379100	-2.41799400	-3.38406500
C	-1.17848600	-3.37328800	-2.26204100
C	-0.57985900	-3.21311100	-4.67313600
C	-1.89827100	-1.40386300	-3.61016800
H	-1.29144800	-2.86043200	-1.29746300
H	-0.46246700	-4.19472900	-2.14000300
H	-2.14943900	-3.82057700	-2.51630600
H	-0.43030400	-2.56118900	-5.54049200
H	-1.49589700	-3.79161600	-4.85712500
H	0.25154100	-3.92492700	-4.62048500
H	-2.79699400	-1.94030000	-3.94481800
H	-1.63841300	-0.67582900	-4.39029800
H	-2.15112700	-0.85476100	-2.69231700
C	2.17445200	-2.45961700	-2.19160900
C	2.48344400	-3.70921900	-3.01169200
C	1.88980400	-2.89182200	-0.74855900

C	3.39246500	-1.53299600	-2.18094400
H	2.75967000	-3.48619700	-4.04716000
H	1.64895400	-4.42033800	-3.01256300
H	3.34415100	-4.21727000	-2.55446700
H	1.73977900	-2.03046800	-0.08362700
H	2.75716200	-3.45633700	-0.37807100
H	1.01318900	-3.54377700	-0.66569900
H	4.22166200	-2.04656100	-1.67519500
H	3.19551600	-0.60009800	-1.63230200
H	3.72692300	-1.27175400	-3.19155100
C	1.34464700	-0.49476100	-4.28403100
C	1.45157700	0.91269300	-4.34333800
C	1.84818800	-1.24591000	-5.35928300
C	2.08067100	1.49504000	-5.45340700
C	0.94766900	1.87728000	-3.32789900
C	2.45197100	-0.64966700	-6.45740600
H	1.77812500	-2.32869400	-5.33978000
C	2.57719300	0.73360900	-6.50074900
H	2.16254200	2.58010200	-5.48783300
C	1.85789700	2.67892800	-2.62925400
C	-0.42258800	2.10229800	-3.15002300
H	2.82822800	-1.26750600	-7.26904000
H	3.05486000	1.22020700	-7.34783400
C	1.41081200	3.67539600	-1.76611400
H	2.92588800	2.51984900	-2.77687700
C	-0.86959700	3.10726600	-2.29369000
H	-1.14148800	1.50082800	-3.70514400
C	0.04554100	3.89603000	-1.60057200
H	2.13244500	4.29073800	-1.23249500
H	-1.93810500	3.27837500	-2.17819500

H	-0.30387500	4.68551800	-0.93832800
C	-4.52879600	1.35615000	1.75825800
C	-3.56089400	2.01345000	2.52083100
C	-3.87806000	2.65525800	3.70803600
C	-5.19550200	2.59821400	4.14675200
C	-6.18203900	1.93424300	3.40847600
C	-5.85438400	1.32763300	2.20780200
C	-4.07900600	0.87344500	0.47786200
H	-3.10126300	3.16396200	4.27235500
H	-5.46057900	3.07848100	5.08553300
H	-7.20450500	1.90610200	3.77450000
H	-6.60891300	0.82759800	1.60343400
H	-4.82862200	0.61322100	-0.27458400
O	-2.27884600	2.07834200	2.05032100
N	-2.83824000	0.77816000	0.14150700

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2875.695231

Electronic Energy (0K) + ZPE = -2874.896439

Enthalpy (298K) = -2874.845786

Free Energy (298K) = -2874.980244

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2876.198860

D1

Number of imaginary frequencies: 0

C	-1.84801400	1.00163800	1.25258300
C	-0.43593900	0.73351700	0.97046500
C	0.68198500	1.57544700	1.48408900
C	1.94764800	0.99030300	1.63227600
C	0.55583000	2.95100500	1.69545600

C	3.04563600	1.74808000	2.01894400
H	2.06398500	-0.07556600	1.43009100
C	1.66159500	3.71409400	2.06230000
H	-0.40973200	3.43317700	1.57458100
C	2.90687900	3.11899700	2.23239400
H	4.01569300	1.26998000	2.13870300
H	1.54280400	4.78437400	2.21879800
H	3.76693000	3.71779700	2.52315600
N	-1.12832800	-0.26463700	1.94199500
S	-0.97397800	-0.24438600	3.76153900
O	-2.31131700	-0.59962500	4.20780700
O	-0.35620600	1.01098100	4.13348300
C	-1.46508900	-1.62223700	1.46442100
H	-2.23477900	-2.05550800	2.11015300
H	-0.56091000	-2.24045900	1.45699900
Au	0.13401600	-0.13758300	-0.90941400
P	0.87750400	-1.37656900	-2.80289800
H	-1.86305300	-1.54347800	0.45231600
C	0.13656900	-1.57668700	4.06526100
C	-0.37321200	-2.84554700	4.33816000
C	1.50801300	-1.31942100	4.06138700
C	0.51860700	-3.87726600	4.59075600
H	-1.44600700	-3.01914500	4.35779300
C	2.37853300	-2.36829700	4.31197100
H	1.88356200	-0.31603500	3.87520300
C	1.90049400	-3.65783700	4.57688500
H	0.13842600	-4.87372900	4.80670500
H	3.45162600	-2.18597200	4.31487700
C	2.85562500	-4.76823500	4.87365300
H	3.74463500	-4.71025900	4.23639800

H	2.38967700	-5.74922800	4.73905400
H	3.20255900	-4.70665000	5.91324400
C	-0.57442800	-2.45849900	-3.36290900
C	-0.91466000	-3.43946100	-2.24174200
C	-0.37774000	-3.23862200	-4.66054900
C	-1.74767300	-1.49383100	-3.55866300
H	-1.01702500	-2.94113200	-1.26840500
H	-0.16710400	-4.23667200	-2.15154800
H	-1.87612800	-3.91817900	-2.47420100
H	-0.28062600	-2.57830200	-5.52882400
H	-1.27137200	-3.85713100	-4.82367700
H	0.48488100	-3.91378700	-4.63214500
H	-2.62607900	-2.06591700	-3.88842900
H	-1.53353500	-0.74253000	-4.33071000
H	-2.01123400	-0.97011700	-2.62884800
C	2.40267100	-2.35835500	-2.22599600
C	2.79495900	-3.54729800	-3.09836200
C	2.15753500	-2.86986000	-0.80240700
C	3.55358000	-1.35032400	-2.17452200
H	3.05296000	-3.26186300	-4.12279300
H	2.01152300	-4.31370600	-3.12977900
H	3.68947900	-4.01470800	-2.66309200
H	1.94792800	-2.04970500	-0.10256000
H	3.06722200	-3.38168300	-0.45823400
H	1.33419300	-3.59001700	-0.74596800
H	4.42523700	-1.83525500	-1.71371600
H	3.30118600	-0.47135600	-1.56294300
H	3.85184800	-1.00343300	-3.17090400
C	1.44198500	-0.43852600	-4.28778700
C	1.51343000	0.97085500	-4.33011000

C	1.93920300	-1.16193200	-5.38499800
C	2.10216200	1.58531400	-5.44483700
C	1.01196700	1.90139400	-3.28475700
C	2.50245000	-0.53514000	-6.48776900
H	1.89764800	-2.24603000	-5.38079900
C	2.59294600	0.85127800	-6.51417900
H	2.15658100	2.67248700	-5.46452100
C	1.92028300	2.71810000	-2.60170200
C	-0.35722600	2.07594900	-3.05733500
H	2.87476700	-1.13216000	-7.31666000
H	3.03906900	1.36095700	-7.36490300
C	1.47161500	3.68515500	-1.70802200
H	2.98699600	2.59468500	-2.78711800
C	-0.80706600	3.05269100	-2.17063700
H	-1.07392600	1.45981300	-3.59932500
C	0.10589200	3.85949400	-1.49614200
H	2.19045200	4.31190700	-1.18402700
H	-1.87599100	3.18648300	-2.01495500
H	-0.24565500	4.62893900	-0.81203300
C	-4.45268100	1.38684100	1.95143700
C	-3.42917800	2.00754500	2.66972100
C	-3.67153300	2.70918300	3.83910600
C	-4.98068800	2.76175100	4.30233200
C	-6.02658600	2.14248700	3.60716200
C	-5.76755000	1.46585600	2.42806800
C	-4.06671000	0.78643200	0.70462200
H	-2.84796200	3.18189200	4.36727200
H	-5.19293500	3.29430500	5.22614100
H	-7.04062200	2.20173900	3.99222700
H	-6.56591200	0.99051800	1.86164500

H	-4.85082500	0.47127900	0.01142100
O	-2.15222500	1.96615200	2.17839100
N	-2.83977400	0.62502100	0.32903700

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2875.704025

Electronic Energy (0K) + ZPE = -2874.904587

Enthalpy (298K) = -2874.853378

Free Energy (298K) = -2874.989725

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2876.207795

E1

Number of imaginary frequencies: 0

C	-2.17292400	0.28568400	2.36924200
C	-0.79609300	0.03456400	2.16399700
C	0.30374500	0.90159600	2.69817100
C	1.58377700	0.72747000	2.14854000
C	0.15240900	1.80197100	3.75830400
C	2.66872500	1.45597900	2.61413900
H	1.72341800	-0.01110100	1.35850900
C	1.24475500	2.52454100	4.22941100
H	-0.81048600	1.91708600	4.24468600
C	2.50165700	2.36497800	3.65623500
H	3.64982200	1.30452200	2.16993300
H	1.11057100	3.20827300	5.06410400
H	3.34968700	2.93397100	4.02866700
N	-0.42751900	-1.34477600	2.04624300
S	-0.53875600	-2.24369800	3.49320800
O	-1.21468900	-3.49405000	3.18455100
O	-1.04474600	-1.31312600	4.49435100

C	-0.55264700	-2.10888300	0.81552700
H	-1.59316000	-2.37421800	0.58573900
H	0.03721600	-3.02818300	0.89506400
H	-0.13327100	-1.51791900	-0.01012700
C	1.15273000	-2.61393800	3.87454000
C	1.68308100	-3.84549900	3.50134000
C	1.92935100	-1.65749300	4.52219700
C	3.01788800	-4.11035900	3.77303700
H	1.04494900	-4.58831800	3.02885100
C	3.26271200	-1.94063800	4.78092500
H	1.48855600	-0.71156500	4.83019200
C	3.82721200	-3.16371800	4.40807800
H	3.44292500	-5.07355000	3.49511700
H	3.87822700	-1.20020400	5.28944100
C	5.27108000	-3.45884900	4.67140400
H	5.86559800	-3.36742700	3.75350300
H	5.41119800	-4.48078600	5.04084700
H	5.69915700	-2.77172500	5.40801800
C	-4.81853600	0.95971600	2.38667300
C	-3.83947500	1.91039400	2.68976200
C	-4.14916600	3.24341700	2.90748000
C	-5.47992900	3.62552700	2.79800700
C	-6.48124600	2.69666500	2.49090800
C	-6.15535800	1.36757500	2.29158500
C	-4.34699000	-0.38215400	2.20389500
H	-3.35997500	3.94953500	3.15213700
H	-5.74687300	4.66663100	2.95844800
H	-7.51435400	3.02239600	2.41688300
H	-6.92224900	0.62950800	2.06374100
H	-5.07005200	-1.19284100	2.07997700

O	-2.53797900	1.51409200	2.80784500
N	-3.09159900	-0.69746700	2.16673200
Au	-1.07954200	1.09812800	0.12324100
P	-0.76832900	2.79778400	-1.51010900
C	0.99861600	2.61411700	-2.17009300
C	1.98453300	2.84455800	-1.02603700
C	1.36054900	3.53289800	-3.33610600
C	1.11441800	1.16585100	-2.65206900
H	1.75658600	2.24079100	-0.13809500
H	2.03642300	3.89750900	-0.72473800
H	2.98950100	2.56015600	-1.36558300
H	0.77799400	3.31405400	-4.23682200
H	2.41545800	3.36331600	-3.58961700
H	1.25989500	4.59740600	-3.09732800
H	2.12046800	1.00388600	-3.06125100
H	0.39946900	0.94104800	-3.45435100
H	0.96869800	0.44176200	-1.83797900
C	-1.08014800	4.41888500	-0.55723500
C	-0.48133700	5.66819200	-1.19979400
C	-0.51910600	4.28876400	0.86281900
C	-2.60109400	4.56648900	-0.46179600
H	-0.87554600	5.87088000	-2.20007300
H	0.61314600	5.63281400	-1.24902300
H	-0.74233300	6.53725100	-0.58116900
H	-1.00233700	3.48298800	1.43027600
H	-0.70900600	5.22875300	1.39902400
H	0.56193300	4.11382400	0.89086600
H	-2.83399200	5.39967400	0.21545900
H	-3.08065800	3.66624900	-0.04907500
H	-3.06588900	4.78600200	-1.42956400

C	-1.90919300	2.85089300	-2.94946700
C	-3.00254500	1.97297500	-3.10727200
C	-1.77667100	3.92105700	-3.85069800
C	-3.92707100	2.22717600	-4.12940700
C	-3.26896800	0.75186500	-2.30502800
C	-2.69244900	4.14325900	-4.86775300
H	-0.94331000	4.60878900	-3.75609400
C	-3.78441200	3.29548300	-5.00023500
H	-4.76545400	1.54323700	-4.24470500
C	-4.45998500	0.64453000	-1.58013700
C	-2.43479400	-0.36789700	-2.39957000
H	-2.55381500	4.98049400	-5.54630900
H	-4.51839300	3.45865000	-5.78493600
C	-4.81056800	-0.55572100	-0.97038800
H	-5.12454300	1.50608700	-1.51766400
C	-2.78828500	-1.56720100	-1.78959200
H	-1.52532500	-0.30968200	-2.99598500
C	-3.97753000	-1.66525800	-1.07335900
H	-5.75808700	-0.63102900	-0.43958500
H	-2.14223600	-2.43592900	-1.89588700
H	-4.25633800	-2.60713000	-0.60569600

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2875.702729

Electronic Energy (0K) + ZPE = -2874.900646

Enthalpy (298K) = -2874.849097

Free Energy (298K) = -2874.986951

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2876.257499

3a-E

Number of imaginary frequencies: 0

C	-2.04051400	0.72741800	2.42672500
C	-0.74071200	0.30622700	2.38618400
C	0.46836300	1.14143200	2.36459000
C	1.67298700	0.56964900	1.91462200
C	0.50752700	2.48031800	2.79409700
C	2.85335100	1.30029100	1.88147600
H	1.67606200	-0.47007700	1.59372800
C	1.69263300	3.20555000	2.76455300
H	-0.38992700	2.95609800	3.17384000
C	2.87203800	2.62659400	2.30447000
H	3.76525100	0.82641500	1.52339200
H	1.69244200	4.23630100	3.11348000
H	3.79590100	3.20018900	2.28263800
N	-0.53460200	-1.10060000	2.28668700
S	-0.58469800	-2.04651900	3.66452400
O	-1.58200600	-3.10251800	3.50462400
O	-0.65455300	-1.13448500	4.80087600
C	-0.79179000	-1.77868900	1.02244700
H	-1.86090800	-1.97201100	0.86504600
H	-0.24367000	-2.72807600	0.98367600
H	-0.41456500	-1.14363300	0.21440300
C	1.00761000	-2.83583100	3.67490500
C	1.13061000	-4.15822500	3.26513800
C	2.12137200	-2.10272700	4.08702800
C	2.38948900	-4.75200600	3.26446700
H	0.24862800	-4.71684600	2.96141200
C	3.36669200	-2.71016400	4.08043200
H	2.00831700	-1.07076400	4.41317800
C	3.52020100	-4.04132400	3.66890600

H	2.49482000	-5.78835100	2.94765400
H	4.24259100	-2.14905100	4.40380700
C	4.87528500	-4.67713300	3.67731100
H	5.58516100	-4.10260800	3.06982800
H	4.84424400	-5.70007700	3.28925300
H	5.28603200	-4.71320800	4.69404800
C	-4.63474100	1.65137200	2.53216700
C	-3.56503000	2.54769200	2.45839600
C	-3.76920100	3.91972800	2.44814700
C	-5.07619400	4.39135200	2.51416200
C	-6.16178300	3.51411600	2.58954700
C	-5.94028100	2.14528900	2.59767500
C	-4.28736400	0.25376600	2.52860800
H	-2.91729000	4.59207500	2.38804100
H	-5.25128400	5.46450000	2.50693200
H	-7.17394300	3.90575100	2.64068100
H	-6.76763400	1.44000500	2.65457700
H	-5.09031400	-0.48666100	2.57240200
O	-2.28924300	2.08013700	2.39296500
N	-3.07158100	-0.17692700	2.47767600

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -1620.928189

Electronic Energy (0K) + ZPE = -1620.546019

Enthalpy (298K) = -1620.519940

Free Energy (298K) = -1620.603145

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -1621.244294

Pre'

Number of imaginary frequencies: 0

C	-3.76044900	2.69223500	2.68129800
C	-2.97898700	3.66198200	2.90999400
C	-1.59463500	3.94415000	3.23796900
C	-1.15018100	5.26611700	3.38108500
C	-0.68348600	2.88944200	3.40205300
C	0.17971600	5.52676400	3.68706100
H	-1.86058700	6.08316600	3.24681400
C	0.64254100	3.15615800	3.70865100
H	-1.03035500	1.86387300	3.28476900
C	1.07594100	4.47412800	3.85222800
H	0.51568400	6.55556100	3.79573300
H	1.34442300	2.33555500	3.83570600
H	2.11668900	4.67950100	4.09177600
N	-4.62643400	1.79312700	2.34208300
S	-4.89099500	1.49717800	0.61133000
O	-6.33332700	1.49483500	0.44432700
O	-4.03876800	2.46124200	-0.05994700
C	-5.63308800	1.24631400	3.26763400
H	-5.20363300	1.24024900	4.27099700
H	-6.53680500	1.86761400	3.24600400
Au	-4.49079600	5.17346700	2.70343600
H	-5.87586300	0.22036900	2.97651400
C	-4.25322400	-0.13066600	0.43277900
C	-5.13679000	-1.19962300	0.31837300
C	-2.86860900	-0.30975400	0.43679300
C	-4.61207700	-2.47943200	0.19077700
H	-6.21056000	-1.03037500	0.32094200
C	-2.37106100	-1.59522000	0.31111300
H	-2.19842700	0.54281100	0.53163000
C	-3.23185600	-2.69537100	0.18321500

H	-5.28601600	-3.32833600	0.09524600
H	-1.29490000	-1.75862200	0.30925000
C	-2.66801600	-4.07085600	0.02836900
H	-3.43987200	-4.83864900	0.13747900
H	-2.21096700	-4.19193900	-0.96199000
H	-1.88042900	-4.26044900	0.76661000
C	-5.80298600	6.73716600	2.56027500
C	-6.60910500	8.83643200	2.47413900
C	-7.66337100	7.98873200	2.37619300
H	-6.55206100	9.91595100	2.47571100
H	-8.72389200	8.16868200	2.26525300
N	-7.14573700	6.70356500	2.43022500
N	-5.47629600	8.04629400	2.59009500
C	-4.12294500	8.50843000	2.74368300
C	-3.64996500	8.75347200	4.04168400
C	-3.32189900	8.62577500	1.59808500
C	-2.31533400	9.14193400	4.17248500
C	-1.99476900	9.01975800	1.78516300
C	-1.49758900	9.27700500	3.05658000
H	-1.90785200	9.33158900	5.16387200
H	-1.33960200	9.11932800	0.92136700
H	-0.46072700	9.58276800	3.17990700
C	-7.89457700	5.48035400	2.32979500
C	-8.26386300	4.81932600	3.50979100
C	-8.16084700	4.97275500	1.04910100
C	-8.93052500	3.59883100	3.37567900
C	-8.82773000	3.74939400	0.97140200
C	-9.20742000	3.06849300	2.12143100
H	-9.22993600	3.05219900	4.26869400
H	-9.03719700	3.31626800	-0.00493000

H	-9.72024400	2.11256400	2.03867300
C	-7.93597400	5.35699600	4.88729100
C	-9.18443700	5.49495200	5.75404700
C	-6.89394700	4.47421900	5.57410500
H	-7.50275600	6.36142000	4.77214900
H	-9.94447100	6.11987700	5.27026200
H	-8.92917900	5.95451400	6.71651800
H	-9.63699300	4.51820900	5.96659300
H	-5.97077600	4.40676500	4.97771700
H	-7.27924900	3.45660800	5.72586600
H	-6.63362200	4.88037000	6.55981200
C	-7.70158600	5.67673100	-0.21030300
C	-6.54817700	4.91239000	-0.85934400
C	-8.84442900	5.88361900	-1.20002800
H	-7.32772200	6.67193000	0.06676500
H	-5.73015500	4.72477500	-0.14859700
H	-6.14313800	5.47607100	-1.70968000
H	-6.88737900	3.93698000	-1.23237100
H	-9.67587800	6.43530200	-0.74470000
H	-9.23673200	4.92861500	-1.57261300
H	-8.49424100	6.45371200	-2.06905700
C	-4.50694400	8.53810000	5.27205200
C	-4.11496800	7.22848300	5.95869600
C	-4.42762900	9.70587200	6.25000900
H	-5.55531000	8.44729900	4.95399000
H	-4.22178800	6.36900200	5.27880000
H	-4.74584900	7.04918000	6.83859900
H	-3.06943900	7.26246600	6.29501200
H	-4.66873700	10.65814900	5.76300500
H	-3.42898800	9.79780500	6.69552200

H	-5.13734100	9.55609000	7.07233900
C	-3.82553500	8.29686400	0.20799100
C	-3.62181400	9.46016100	-0.75884100
C	-3.15209100	7.02899100	-0.31932900
H	-4.90578300	8.10123000	0.26583700
H	-4.08900400	10.38027600	-0.38789800
H	-4.06466300	9.22390400	-1.73388900
H	-2.55646700	9.66561000	-0.92430500
H	-3.32859600	6.17042200	0.34709200
H	-2.06629800	7.16825900	-0.40809200
H	-3.53986300	6.77117400	-1.31305300

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2516.335625

Electronic Energy (0K) + ZPE = -2515.490816

Enthalpy (298K) = -2515.438657

Free Energy (298K) = -2515.576711

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2516.808748

TS_A'

Number of imaginary frequencies: 1

C	-3.67905700	2.45005000	2.66816200
C	-3.19539500	3.58283600	3.08683200
C	-1.97310900	3.89991000	3.82387400
C	-1.22865800	5.03897800	3.48285100
C	-1.57450800	3.13478800	4.92856800
C	-0.09322500	5.38183900	4.20621600
H	-1.55175600	5.64829300	2.63784000
C	-0.45108300	3.49555700	5.66369200
H	-2.16193100	2.26613600	5.21789400

C	0.29590600	4.61381000	5.30198700
H	0.47862300	6.26306700	3.92330400
H	-0.15869100	2.90027300	6.52590100
H	1.17481000	4.89244000	5.87888200
N	-4.74192000	1.80089300	2.22354400
S	-4.91003000	1.52440900	0.51906000
O	-6.34398000	1.37426200	0.32470200
O	-4.14997500	2.56971000	-0.14505300
C	-5.88693400	1.50021700	3.09991900
H	-5.52596900	1.53555900	4.13081900
H	-6.68053700	2.24584700	2.96137400
Au	-4.55201400	5.14890700	2.69276800
H	-6.27670900	0.49938300	2.89249200
C	-4.10792600	-0.02387100	0.24444200
C	-4.77433900	-1.20276400	0.58067100
C	-2.81741900	-0.03614700	-0.27762000
C	-4.12221000	-2.41171800	0.39005000
H	-5.78986800	-1.17405000	0.96954900
C	-2.18731600	-1.25980900	-0.46783600
H	-2.31793700	0.89610000	-0.53044400
C	-2.82595100	-2.45917300	-0.13950400
H	-4.62788500	-3.34171500	0.64484200
H	-1.17901200	-1.28620400	-0.87788900
C	-2.15027300	-3.77446000	-0.36451700
H	-2.36122700	-4.47705300	0.44975900
H	-2.51259300	-4.24079500	-1.28993400
H	-1.06522400	-3.65993400	-0.45632900
C	-5.80860200	6.75656100	2.45960400
C	-6.54436100	8.88339300	2.32019900
C	-7.63256300	8.07447600	2.32503300

H	-6.44745100	9.95881000	2.26469200
H	-8.69064300	8.29159000	2.27347600
N	-7.15842400	6.77398500	2.40604300
N	-5.43693400	8.05445200	2.40711900
C	-4.06446600	8.47918700	2.44976100
C	-3.49359800	8.76103700	3.69959500
C	-3.34627300	8.53723600	1.24725900
C	-2.14594100	9.12500400	3.71984500
C	-2.00273300	8.91188600	1.32222800
C	-1.40905300	9.20342600	2.54401900
H	-1.66456900	9.34088700	4.67225100
H	-1.41219500	8.96446400	0.40896600
H	-0.36014600	9.49010000	2.58115200
C	-7.96168200	5.58339700	2.45535000
C	-8.26990500	5.03845400	3.70898300
C	-8.35327200	4.99528500	1.24346800
C	-9.00519000	3.85040900	3.72589800
C	-9.07293600	3.80159600	1.31525500
C	-9.39856700	3.23667300	2.54329700
H	-9.26492100	3.39797400	4.68195600
H	-9.37753900	3.30366700	0.39656900
H	-9.96409400	2.30787100	2.57722700
C	-7.81907400	5.66877400	5.01039000
C	-9.00904600	6.01835400	5.90002400
C	-6.83578200	4.75678300	5.74253500
H	-7.29247800	6.60668200	4.78030300
H	-9.71364900	6.68182300	5.38368000
H	-8.66872600	6.52635700	6.81054100
H	-9.55777000	5.11910600	6.20863100
H	-5.95223600	4.54330200	5.12116500

H	-7.30394500	3.79850400	6.00542400
H	-6.49469700	5.22676800	6.67357100
C	-7.95847000	5.58337300	-0.09473800
C	-6.74014800	4.84315500	-0.64552000
C	-9.09971400	5.56861100	-1.10607200
H	-7.67124300	6.63309000	0.06319400
H	-5.89666000	4.87292000	0.05956700
H	-6.41304100	5.28594600	-1.59520400
H	-6.98126000	3.78716400	-0.82719500
H	-10.00119700	6.05233600	-0.71147500
H	-9.36642400	4.54652700	-1.40350500
H	-8.79961700	6.10120000	-2.01643600
C	-4.26683200	8.61952900	4.99428200
C	-3.83094200	7.35442100	5.73516500
C	-4.12551500	9.84641600	5.88987800
H	-5.33349300	8.51022000	4.74980500
H	-3.99300000	6.45523200	5.12114200
H	-4.39702700	7.24040800	6.66863100
H	-2.76302900	7.39745100	5.99045800
H	-4.40547200	10.76650400	5.36303400
H	-3.09751400	9.96564200	6.25503400
H	-4.77328100	9.74822400	6.76926200
C	-3.95422800	8.15796300	-0.08692700
C	-3.80189400	9.27157900	-1.11897400
C	-3.33887600	6.85405900	-0.59605900
H	-5.03117400	7.98627600	0.05663400
H	-4.23793400	10.21282800	-0.76307100
H	-4.30626200	8.99515000	-2.05278900
H	-2.74711600	9.45776200	-1.35830300
H	-3.47343400	6.03498100	0.12707800

H	-2.26130400	6.97214700	-0.77279800
H	-3.80135800	6.55213600	-1.54422800
C	-1.43904700	-1.07491100	2.93659500
C	-0.52802200	-0.13380300	2.45101200
C	0.74999700	-0.45789800	2.00940200
C	1.07736000	-1.80275700	2.07307000
C	0.17723100	-2.77545000	2.55604500
C	-1.08754900	-2.43096000	2.99296100
C	-2.59232900	-0.29544600	3.22488900
H	1.43738000	0.29471300	1.63635100
H	2.06226400	-2.11983100	1.73895300
H	0.49026600	-3.81595400	2.57933000
H	-1.78737900	-3.17724500	3.35962500
H	-3.56281100	-0.59822400	3.60548900
O	-1.08765900	1.09909800	2.46050900
N	-2.36985900	0.96062700	2.95036300

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2915.748406

Electronic Energy (0K) + ZPE = -2914.797481

Enthalpy (298K) = -2914.738603

Free Energy (298K) = -2914.891233

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2916.317494

A'

Number of imaginary frequencies: 0

C	-3.58616900	2.22474400	2.73926500
C	-3.28404500	3.49304100	3.07822400
C	-2.00434500	3.84614600	3.72018100
C	-1.29680200	4.97218000	3.26882200

C	-1.49026300	3.13486500	4.81528000
C	-0.10129200	5.35083000	3.86603000
H	-1.69798000	5.54981500	2.43470800
C	-0.30730100	3.53343200	5.42964300
H	-2.03600300	2.27655300	5.20524700
C	0.39654300	4.63629300	4.95365000
H	0.43335000	6.22161400	3.49164700
H	0.06544000	2.97780800	6.28763100
H	1.32204900	4.94408700	5.43487100
N	-4.81669700	1.71708900	2.27314000
S	-4.95205200	1.49963500	0.59100900
O	-6.38066800	1.37247800	0.32286100
O	-4.15312400	2.50108900	-0.10734300
C	-6.05428600	1.99572200	3.01237700
H	-5.80643100	1.96222100	4.07732200
H	-6.47832500	2.98149300	2.77430200
Au	-4.60903900	5.06629600	2.76067900
H	-6.79542700	1.22129400	2.79639500
C	-4.16986500	-0.07430700	0.34358800
C	-4.76450300	-1.21312300	0.88979100
C	-2.97214900	-0.14843500	-0.35778000
C	-4.13681900	-2.43828200	0.72992500
H	-5.70258300	-1.13747100	1.43770100
C	-2.35670800	-1.38817300	-0.50664300
H	-2.52590500	0.75183000	-0.77336800
C	-2.92511500	-2.54413500	0.03200900
H	-4.58749800	-3.33518400	1.15230100
H	-1.41436900	-1.45805600	-1.04793200
C	-2.26867900	-3.87784600	-0.13815300
H	-2.30047500	-4.46044400	0.78997500

H	-2.78696600	-4.47052300	-0.90300700
H	-1.22422900	-3.77671300	-0.45074700
C	-5.83185600	6.71678600	2.51492200
C	-6.50492500	8.86546000	2.33928100
C	-7.61308500	8.08612800	2.29026700
H	-6.37611200	9.93779800	2.28761700
H	-8.66132300	8.33125800	2.18829800
N	-7.17764200	6.77366900	2.39522200
N	-5.42607800	8.00670300	2.48113200
C	-4.04627100	8.40021900	2.56359700
C	-3.50327100	8.67772100	3.82699800
C	-3.29415100	8.44159500	1.38125800
C	-2.15025000	9.01696300	3.88238800
C	-1.94469600	8.78567100	1.49171500
C	-1.37903400	9.07256100	2.72755900
H	-1.69140100	9.22993900	4.84636400
H	-1.32902400	8.82329000	0.59435300
H	-0.32586000	9.33821800	2.79262400
C	-8.01912400	5.60847900	2.40460800
C	-8.42515900	5.08872300	3.64142400
C	-8.35749400	5.02082700	1.17623500
C	-9.19328800	3.92180500	3.62398200
C	-9.11926400	3.85185300	1.21481700
C	-9.53362400	3.30828300	2.42513900
H	-9.52301000	3.48651100	4.56620800
H	-9.38597300	3.35633700	0.28315600
H	-10.12733500	2.39656400	2.43272000
C	-8.03615100	5.72025600	4.96242800
C	-9.26008400	6.03198100	5.81936600
C	-7.05385700	4.82730200	5.71963400

H	-7.52683600	6.67291900	4.75627100
H	-9.97477400	6.66822800	5.28347700
H	-8.95938200	6.55549400	6.73499400
H	-9.78502700	5.11663300	6.12156300
H	-6.13769300	4.65486400	5.13439200
H	-7.50298400	3.85011900	5.94452600
H	-6.76882600	5.29088100	6.67263600
C	-7.86582800	5.57991000	-0.14257600
C	-6.63954100	4.79872700	-0.61491900
C	-8.94576200	5.58769400	-1.21939800
H	-7.55710700	6.62256100	0.02213200
H	-5.83192200	4.82251400	0.13113000
H	-6.25362200	5.21587800	-1.55430300
H	-6.88938300	3.74306700	-0.78853500
H	-9.85520700	6.09961400	-0.88268700
H	-9.22285800	4.57086900	-1.52542800
H	-8.57754400	6.10376000	-2.11417000
C	-4.31199400	8.55251900	5.10124700
C	-3.93887600	7.26304800	5.83471700
C	-4.14761000	9.76069700	6.01800600
H	-5.37545400	8.48694100	4.82939500
H	-4.11671000	6.37821700	5.20490600
H	-4.52857000	7.15675600	6.75442600
H	-2.87552000	7.26648700	6.11269500
H	-4.37490300	10.69877900	5.49767600
H	-3.12729600	9.83345900	6.41555600
H	-4.82458200	9.67643700	6.87661600
C	-3.87480900	8.08697700	0.02811300
C	-3.68666200	9.21723000	-0.97993700
C	-3.26388900	6.78474000	-0.48918300

H	-4.95653600	7.92565800	0.14419900
H	-4.11896700	10.15703800	-0.61526500
H	-4.17404600	8.96490100	-1.92946500
H	-2.62466000	9.39480000	-1.19277600
H	-3.44205100	5.95194500	0.20800200
H	-2.17833700	6.88529300	-0.62307200
H	-3.69574200	6.51471200	-1.46107300
C	-1.48577200	-0.74993300	2.88818500
C	-0.74256900	0.20741400	2.18375100
C	0.50531600	-0.04011300	1.62873700
C	0.97856000	-1.33015100	1.80200400
C	0.25011500	-2.32101700	2.49720000
C	-0.98436700	-2.05266000	3.04881300
C	-2.66538900	-0.07450300	3.25257100
H	1.05836600	0.72367000	1.09218200
H	1.94728500	-1.59141000	1.38398100
H	0.67735000	-3.31524000	2.59286700
H	-1.55326700	-2.80931300	3.58112700
H	-3.54226800	-0.40144600	3.80088300
O	-1.42461600	1.37480100	2.11343100
N	-2.60011200	1.16124100	2.80057600

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2915.770847

Electronic Energy (0K) + ZPE = -2914.818473

Enthalpy (298K) = -2914.759606

Free Energy (298K) = -2914.913171

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2916.337810

TS_{B'}

Number of imaginary frequencies: 1

C	-3.25086100	2.34656500	2.71979100
C	-2.95700500	3.70241200	2.88354600
C	-1.62272600	4.16943500	3.21498300
C	-1.48230000	5.32830500	4.00998300
C	-0.45111500	3.55737700	2.72166100
C	-0.23100900	5.81188500	4.35449900
H	-2.37892200	5.83384900	4.36797500
C	0.79848300	4.07471200	3.03058000
H	-0.52850700	2.69989600	2.06057300
C	0.91431700	5.18869000	3.85954300
H	-0.14769300	6.68957400	4.99193100
H	1.69020500	3.60522400	2.62246700
H	1.89759800	5.58221100	4.10680600
N	-4.48529900	1.89203400	2.17634400
S	-4.60938600	1.73939000	0.51584900
O	-6.03935100	1.69109700	0.22534300
O	-3.75740200	2.73914900	-0.12085300
C	-5.68819000	1.87247300	3.01095600
H	-5.39079800	1.58280700	4.02575300
H	-6.17529500	2.85851000	3.04510900
Au	-4.46597600	5.11473300	2.72226200
H	-6.40239900	1.13552600	2.63555500
C	-3.90854200	0.14413900	0.17742100
C	-4.34351200	-0.95612700	0.91315100
C	-2.94130800	0.01446400	-0.81297400
C	-3.78311700	-2.19989300	0.65956300
H	-5.09537700	-0.83975100	1.69265200
C	-2.39825000	-1.24009200	-1.06031700
H	-2.60678800	0.88921200	-1.36434500

C	-2.80372700	-2.35941600	-0.32731700
H	-4.09701400	-3.06397000	1.24375400
H	-1.63073200	-1.35326200	-1.82474800
C	-2.20002000	-3.70228900	-0.59313800
H	-2.25458200	-4.34868900	0.28967000
H	-2.72977700	-4.21551800	-1.40636000
H	-1.15069500	-3.61525000	-0.89788800
C	-5.83744800	6.66662900	2.59600300
C	-6.63647700	8.77726000	2.50811000
C	-7.69016300	7.93560900	2.37035400
H	-6.57436100	9.85674500	2.52443600
H	-8.74728000	8.12134500	2.23836200
N	-7.17797800	6.64838300	2.42083800
N	-5.51366500	7.97972000	2.65340500
C	-4.16884200	8.45511200	2.82903800
C	-3.73994800	8.77763200	4.12540500
C	-3.33527400	8.52941200	1.70450400
C	-2.41523100	9.19135900	4.27615700
C	-2.02062300	8.95453000	1.90921300
C	-1.56495300	9.28106900	3.17991800
H	-2.04088800	9.43969800	5.26795100
H	-1.34584100	9.02715300	1.05766900
H	-0.53595100	9.60615400	3.31881200
C	-7.96027500	5.44522100	2.34184600
C	-8.35011200	4.82457500	3.53638300
C	-8.28073700	4.94170700	1.07143200
C	-9.08011800	3.63777700	3.43104400
C	-9.01101800	3.75392700	1.02306200
C	-9.40361000	3.10696200	2.18946800
H	-9.39767800	3.12456600	4.33758800

H	-9.27093100	3.32434200	0.05780000
H	-9.97146200	2.18099300	2.12808800
C	-7.99720300	5.37756100	4.90234600
C	-9.24245100	5.59122700	5.75859600
C	-6.99652400	4.46887100	5.61545000
H	-7.51871500	6.35861600	4.76703000
H	-9.96983500	6.23954000	5.25531900
H	-8.97220700	6.06012000	6.71252800
H	-9.74101600	4.64091100	5.98857500
H	-6.06443400	4.36941700	5.03903500
H	-7.41219600	3.46222400	5.76175300
H	-6.74658700	4.87317900	6.60450200
C	-7.80681900	5.62087900	-0.19729800
C	-6.47242900	5.02311200	-0.64662600
C	-8.82559800	5.54834300	-1.32909500
H	-7.64029400	6.68446300	0.02779800
H	-5.70585700	5.10413200	0.13772700
H	-6.10367800	5.53552100	-1.54490700
H	-6.58491100	3.95575900	-0.87977100
H	-9.81380000	5.90648600	-1.01642700
H	-8.93880800	4.52453300	-1.70782000
H	-8.49131500	6.16628200	-2.17083700
C	-4.63761200	8.61798300	5.33505800
C	-4.28699000	7.33028700	6.08159400
C	-4.57826700	9.81753300	6.27505300
H	-5.67530100	8.52627300	4.98485800
H	-4.37990700	6.44886100	5.42969700
H	-4.95090900	7.19066700	6.94435400
H	-3.25322800	7.36699300	6.45421900
H	-4.78651700	10.75626100	5.74821200

H	-3.59658000	9.91088700	6.75641900
H	-5.32058400	9.70502500	7.07433000
C	-3.80472800	8.16636600	0.31128600
C	-3.79938000	9.39062600	-0.60090300
C	-2.96404100	7.03458500	-0.27577300
H	-4.84229500	7.80781200	0.37441200
H	-4.42974100	10.19240900	-0.19585100
H	-4.17964600	9.12898500	-1.59593200
H	-2.78488500	9.79079600	-0.72657700
H	-2.97675500	6.14764900	0.37581200
H	-1.91802700	7.34022200	-0.40860100
H	-3.35049500	6.73961300	-1.25926400
C	-1.88023400	-0.83785100	3.52941200
C	-1.14064500	-0.53095300	2.34762700
C	-0.26538100	-1.49740300	1.80504100
C	-0.21494700	-2.72779200	2.41994600
C	-0.97223900	-3.04315800	3.57847700
C	-1.79655800	-2.10611300	4.14552400
C	-2.60072400	0.29787000	3.88186800
H	0.30944500	-1.26892400	0.91229600
H	0.43150500	-3.49493100	1.99808000
H	-0.88056000	-4.03195300	4.01819600
H	-2.37542800	-2.31818800	5.04063000
H	-3.27473700	0.38325900	4.73463600
O	-1.34002400	0.65224000	1.87479300
N	-2.41647100	1.37345500	3.14081600

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2915.745471

Electronic Energy (0K) + ZPE = -2914.796540

Enthalpy (298K) = -2914.737204

Free Energy (298K) = -2914.892491

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2916.312393

B'

Number of imaginary frequencies: 0

C	-5.22857100	3.47865300	2.90081700
C	-3.81618400	3.55519500	2.46609100
C	-2.80177600	3.16388600	3.37533000
C	-1.56811600	2.69652600	2.84863000
C	-2.98993600	3.14011300	4.78395700
C	-0.59559400	2.18309800	3.68242700
H	-1.42601200	2.70624700	1.76763800
C	-1.98957300	2.67388900	5.61413100
H	-3.91762200	3.51368600	5.21175800
C	-0.80491200	2.17724400	5.06408100
H	0.33044500	1.79571300	3.26549400
H	-2.12884700	2.67828600	6.69138300
H	-0.03312400	1.78459600	5.72204800
N	-6.09107200	4.49240100	2.57779100
S	-7.79411000	4.18944700	2.52897900
O	-8.34438400	5.43682100	2.01974400
O	-8.01461700	2.94467000	1.81497800
C	-5.60985000	5.83214100	2.22751500
H	-6.35322000	6.57000600	2.53548900
H	-4.68472600	6.03176900	2.77573700
H	-5.43585000	5.92850400	1.14743000
C	-8.25225900	4.00698800	4.22396300
C	-8.25175600	5.14304500	5.03236400
C	-8.61603600	2.75779000	4.71647700

C	-8.61928300	5.01306500	6.36249600
H	-7.97255000	6.11296800	4.62584600
C	-8.98858600	2.65213400	6.05019200
H	-8.60434700	1.88835300	4.06443000
C	-8.99581800	3.77087600	6.88875800
H	-8.62181600	5.88901200	7.00895700
H	-9.27955100	1.68291600	6.45115200
C	-9.42255900	3.65436700	8.31734500
H	-9.32372600	2.62812600	8.68517900
H	-8.83776400	4.31644000	8.96508000
H	-10.47563600	3.94329300	8.42976500
C	-2.99910000	4.79331800	-1.39494000
C	-2.05291000	4.97255400	-3.43414700
C	-3.02847000	5.91173000	-3.35166600
H	-1.36442000	4.71878200	-4.22835000
H	-3.37317500	6.65459500	-4.05756500
N	-2.05156300	4.30170900	-2.22319600
N	-3.59492600	5.78485400	-2.09323700
Au	-3.42244500	4.13496700	0.51434200
C	-4.38940200	0.30564200	3.23781000
C	-3.93756600	0.46982200	1.86067900
C	-3.03614000	-0.53456500	1.35940000
C	-2.66636500	-1.60263700	2.12589100
C	-3.14408600	-1.77403500	3.45795700
C	-3.98079900	-0.84077300	3.99149000
C	-5.14425500	1.26694700	3.90118000
H	-2.66627800	-0.40374800	0.34308800
H	-1.98422300	-2.34522500	1.71466700
H	-2.83012300	-2.63752100	4.03779800
H	-4.34395800	-0.93626300	5.01473300

H	-5.40501600	1.03175700	4.94063900
O	-4.30221900	1.44802400	1.16075400
N	-5.67031600	2.41774100	3.49159200
C	-4.66235600	6.59538800	-1.57207800
C	-5.98147400	6.14327400	-1.72211100
C	-4.32863000	7.78490300	-0.90764100
C	-6.99365400	6.93429000	-1.17326200
C	-5.37840400	8.53951400	-0.38012800
C	-6.69671600	8.11957400	-0.51257000
H	-8.02966900	6.61262300	-1.26173100
H	-5.15816000	9.46570900	0.14820600
H	-7.50109400	8.71906200	-0.09154600
C	-1.21981600	3.18786900	-1.86334200
C	-0.03096400	3.43883400	-1.16445100
C	-1.67922300	1.89792700	-2.16679200
C	0.71283800	2.33068200	-0.75213000
C	-0.89233300	0.82552000	-1.74188700
C	0.28567000	1.03871200	-1.03486500
H	1.63863300	2.48465300	-0.19969000
H	-1.20956400	-0.19177600	-1.96699400
H	0.88052700	0.18854800	-0.70769100
C	-2.89219200	8.21454300	-0.69157100
C	-2.46808800	7.91091300	0.74642100
C	-2.66574300	9.68637000	-1.02034300
H	-2.24896800	7.62393300	-1.35986200
H	-2.57312400	6.84011900	0.97832900
H	-1.42111000	8.19670900	0.90985800
H	-3.08625900	8.47397800	1.45976600
H	-2.99347100	9.92929300	-2.03798500
H	-3.20330800	10.34487000	-0.32657300

H	-1.59975000	9.93035400	-0.93928000
C	-6.32047200	4.82855200	-2.39326900
C	-7.41697800	4.98284100	-3.44314200
C	-6.72079700	3.78849400	-1.34595000
H	-5.42021700	4.46049300	-2.90648400
H	-7.16384200	5.74944700	-4.18525000
H	-7.56735900	4.03403100	-3.97194700
H	-8.37717300	5.25654300	-2.98763200
H	-5.91581700	3.61780900	-0.61465800
H	-7.61377900	4.11098800	-0.79290000
H	-6.94976100	2.82666700	-1.82269300
C	-2.95497500	1.65363700	-2.94613400
C	-3.89395700	0.68624400	-2.23198100
C	-2.62594800	1.16125400	-4.35432900
H	-3.48817300	2.61034000	-3.04501100
H	-4.13002000	1.02590000	-1.21336300
H	-4.83294600	0.59574800	-2.79261000
H	-3.45968400	-0.32050700	-2.16314100
H	-1.98606400	1.87232000	-4.89200900
H	-2.10035500	0.19765300	-4.31940300
H	-3.54412000	1.02053600	-4.93771800
C	0.43568800	4.83987000	-0.82605300
C	1.84888400	5.10077000	-1.33972900
C	0.34927600	5.09394000	0.67824400
H	-0.23408900	5.55691700	-1.32283900
H	1.92441400	4.92119900	-2.41888200
H	2.13672800	6.14137200	-1.14720400
H	2.58453900	4.45831800	-0.83914100
H	-0.67809400	4.95788800	1.04808200
H	1.00332200	4.40650600	1.23273300

H 0.66562500 6.11788800 0.91400900

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2915.773544

Electronic Energy (0K) + ZPE = -2914.824275

Enthalpy (298K) = -2914.763985

Free Energy (298K) = -2914.921226

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2916.341179

TS_{C2'}

Number of imaginary frequencies: 1

C	-5.23652200	3.44679800	2.90144600
C	-3.82515000	3.51025800	2.44816600
C	-2.80197400	3.13317400	3.35922200
C	-1.56541700	2.67732300	2.83168400
C	-2.98067300	3.12529300	4.76810200
C	-0.58089200	2.18772000	3.66560300
H	-1.42920200	2.67612800	1.74994300
C	-1.96768400	2.68443400	5.59863900
H	-3.90936600	3.49248500	5.19885400
C	-0.78078700	2.19589000	5.04882100
H	0.34802200	1.80864200	3.24722900
H	-2.10110100	2.70230100	6.67654800
H	0.00052300	1.82224900	5.70659800
N	-6.09376000	4.46156900	2.57208300
S	-7.79990000	4.16473800	2.53236100
O	-8.34549600	5.40729600	2.00684600
O	-8.02124100	2.91144900	1.83362400
C	-5.61278300	5.80043700	2.21767600
H	-6.35160500	6.53935900	2.53437200

H	-4.68196200	5.99860300	2.75634200
H	-5.45147300	5.89827600	1.13594600
C	-8.26219600	4.00611000	4.22843200
C	-8.26638900	5.15343900	5.02058700
C	-8.62767600	2.76368600	4.73702900
C	-8.63948900	5.04186800	6.35099000
H	-7.98740100	6.11813900	4.60184000
C	-9.00636400	2.67669300	6.07013200
H	-8.61282500	1.88504300	4.09754600
C	-9.01776400	3.80717500	6.89298600
H	-8.64538200	5.92697700	6.98477000
H	-9.29886000	1.71309000	6.48331100
C	-9.45171400	3.70941200	8.32078100
H	-9.33855300	2.69148500	8.70726300
H	-8.88238200	4.39247900	8.96030800
H	-10.51033200	3.98216400	8.42113700
C	-2.99225400	4.80426500	-1.39436000
C	-2.04731500	4.98454300	-3.43386700
C	-3.02499500	5.92156100	-3.35143500
H	-1.35838600	4.73219300	-4.22816600
H	-3.37140000	6.66352400	-4.05745000
N	-2.04395400	4.31421700	-2.22255600
N	-3.59053900	5.79418500	-2.09250800
Au	-3.42050600	4.13426000	0.50752500
C	-4.41539900	0.29104300	3.26950300
C	-3.95425600	0.46340400	1.90062700
C	-3.09536000	-0.56192400	1.37684200
C	-2.75969200	-1.65494100	2.12617100
C	-3.23445400	-1.82807900	3.45742900
C	-4.03851300	-0.87466000	4.00745200

C	-5.16550900	1.25552400	3.93758500
H	-2.72347500	-0.42695700	0.36193600
H	-2.10463300	-2.41342800	1.70036900
H	-2.94548000	-2.70851400	4.02455600
H	-4.40128500	-0.97172700	5.03061600
H	-5.43265900	1.01277600	4.97358400
O	-4.27817900	1.47446900	1.21999200
N	-5.68395400	2.41063600	3.53455500
C	-4.66036200	6.60113300	-1.57076600
C	-5.97798400	6.14322200	-1.71625700
C	-4.33003200	7.79302800	-0.90876400
C	-6.99232700	6.93277800	-1.16924300
C	-5.38168400	8.54507200	-0.38149100
C	-6.69884500	8.12088000	-0.51223800
H	-8.02726600	6.60725900	-1.25613800
H	-5.16398700	9.47279300	0.14516300
H	-7.50478100	8.71909500	-0.09241300
C	-1.21041200	3.20201500	-1.86160800
C	-0.02058100	3.45561000	-1.16536400
C	-1.66996000	1.91076200	-2.15908500
C	0.72549300	2.34917600	-0.75255700
C	-0.88228600	0.83995500	-1.73163500
C	0.29833400	1.05603100	-1.02992200
H	1.65253700	2.50536200	-0.20286200
H	-1.20080900	-0.17814500	-1.95117200
H	0.89467800	0.20732100	-0.70172100
C	-2.89465200	8.22595200	-0.69247800
C	-2.46918500	7.91560800	0.74378200
C	-2.67195200	9.70006400	-1.01326300
H	-2.25036900	7.64047800	-1.36428500

H	-2.57028000	6.84315100	0.96974100
H	-1.42331600	8.20442000	0.90896800
H	-3.08961400	8.47227900	1.46019500
H	-3.00242900	9.94832400	-2.02872000
H	-3.20900700	10.35362500	-0.31442600
H	-1.60625500	9.94559500	-0.93316300
C	-6.31448500	4.82458300	-2.38095100
C	-7.40019600	4.97575800	-3.44251600
C	-6.72828600	3.79245100	-1.33078800
H	-5.41067500	4.45026400	-2.88306500
H	-7.13505300	5.73394100	-4.18909300
H	-7.55176600	4.02317100	-3.96417800
H	-8.36269700	5.26003800	-2.99843500
H	-5.93341200	3.62812700	-0.58698100
H	-7.62913600	4.11804100	-0.79262600
H	-6.95058200	2.82709000	-1.80344300
C	-2.94881000	1.66260000	-2.93186300
C	-3.89017800	0.71083400	-2.19995300
C	-2.62714900	1.14852600	-4.33389100
H	-3.47715000	2.62048400	-3.04305600
H	-4.12008300	1.06657100	-1.18529400
H	-4.83214100	0.61677300	-2.75488700
H	-3.46051500	-0.29689000	-2.11781700
H	-1.98559200	1.84907700	-4.88323800
H	-2.10645500	0.18276000	-4.28759100
H	-3.54801000	1.00461300	-4.91223800
C	0.44284200	4.85760400	-0.82678200
C	1.85541800	5.12278400	-1.33977900
C	0.35532000	5.10938500	0.67792900
H	-0.22887600	5.57334300	-1.32289200

H	1.93163100	4.94500100	-2.41917700
H	2.14063100	6.16381500	-1.14565900
H	2.59260700	4.48147400	-0.83998000
H	-0.67106000	4.96677300	1.04817400
H	1.01344100	4.42487500	1.23114900
H	0.66607800	6.13472200	0.91505100

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2915.773521

Electronic Energy (0K) + ZPE = -2914.824445

Enthalpy (298K) = -2914.764948

Free Energy (298K) = -2914.919935

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2916.341072

C2'

Number of imaginary frequencies: 0

C	-5.39029400	2.95260800	2.83840400
C	-4.10767300	2.65331600	2.05821100
C	-2.87797800	2.56634800	2.90451200
C	-1.77397900	1.81532000	2.46831800
C	-2.74566100	3.33587700	4.06623200
C	-0.58556100	1.82710700	3.18458500
H	-1.84598900	1.23342100	1.54799100
C	-1.54060900	3.36716800	4.76537700
H	-3.58862200	3.92285800	4.43109900
C	-0.45914600	2.60756400	4.33486900
H	0.25496800	1.22831900	2.83956900
H	-1.45909400	3.97781000	5.66191600
H	0.47581700	2.61899200	4.88993600
N	-6.24431200	3.93358400	2.48406200

S	-7.95801500	3.74984200	2.81362000
O	-8.55423900	4.80613900	2.01377400
O	-8.26852900	2.35475700	2.56333700
C	-5.82917900	5.21784300	1.90939700
H	-6.37931100	6.01595000	2.41758600
H	-4.76520900	5.36604500	2.10524900
H	-6.03409100	5.26490100	0.83576500
C	-8.15218800	4.12718200	4.52213200
C	-8.13693700	5.46357100	4.91854900
C	-8.33141200	3.09187900	5.43874600
C	-8.29213200	5.75772500	6.26593500
H	-8.01982700	6.26116000	4.18834500
C	-8.49503100	3.41129400	6.77700700
H	-8.34986900	2.05915500	5.10207600
C	-8.47407500	4.74271300	7.21039500
H	-8.28161200	6.79533800	6.59347600
H	-8.64323200	2.61649200	7.50604400
C	-8.66778400	5.06548900	8.65709900
H	-9.70703700	4.88171700	8.95797700
H	-8.03696100	4.43323900	9.29240500
H	-8.43777400	6.11361000	8.87158500
C	-2.94176400	4.78408600	-1.36764600
C	-1.77806300	5.29473200	-3.23304100
C	-2.84171200	6.13351800	-3.17317100
H	-0.97833500	5.19462600	-3.95442000
H	-3.16680600	6.93160300	-3.82624600
N	-1.86170000	4.47624900	-2.11881700
N	-3.53976700	5.80643000	-2.01977300
Au	-3.54544600	3.81758400	0.34414500
C	-4.77055500	-0.01559700	3.39678700

C	-4.47055500	0.18439600	2.02967000
C	-4.17191500	-0.91323800	1.22038400
C	-4.10992900	-2.17942200	1.77324200
C	-4.34498300	-2.39090700	3.14232500
C	-4.67091300	-1.32004400	3.93927500
C	-5.27337000	1.02013100	4.22267100
H	-3.95988800	-0.73965500	0.16844900
H	-3.85391400	-3.02313700	1.13679300
H	-4.27483100	-3.39077000	3.56021600
H	-4.87890400	-1.45109000	4.99958900
H	-5.39039200	0.78424000	5.28510400
O	-4.47930000	1.38649300	1.42166200
N	-5.71343200	2.19549100	3.86673400
C	-4.73123700	6.46139700	-1.55502800
C	-5.97580100	5.89539900	-1.86431500
C	-4.58674100	7.62074800	-0.77685100
C	-7.11335000	6.55139500	-1.38437500
C	-5.75401200	8.23310500	-0.31763000
C	-7.00479800	7.70846900	-0.62457000
H	-8.09770200	6.14204200	-1.60705500
H	-5.68416300	9.13163300	0.29246800
H	-7.90309300	8.20228800	-0.26029000
C	-0.96695800	3.40716900	-1.78138000
C	0.08298200	3.67011900	-0.89117300
C	-1.23643800	2.13286300	-2.29917800
C	0.89565000	2.59430000	-0.52796900
C	-0.39398400	1.09135800	-1.90563600
C	0.66094400	1.31966100	-1.02928100
H	1.71862000	2.75853200	0.16631400
H	-0.57036700	0.08683800	-2.28729700

H	1.30508000	0.49449700	-0.73270600
C	-3.22432500	8.13957800	-0.36526900
C	-2.87487800	7.61493800	1.02997300
C	-3.12590100	9.66039900	-0.40234300
H	-2.47700200	7.74375100	-1.06790900
H	-2.90074700	6.51466900	1.06986900
H	-1.87273900	7.94708500	1.33026200
H	-3.59282100	7.99638000	1.77031500
H	-3.43511800	10.06532200	-1.37314100
H	-3.74461600	10.12992600	0.37283300
H	-2.09087400	9.97241300	-0.21888700
C	-6.12480300	4.60356500	-2.64228700
C	-7.00014400	4.79142200	-3.87881900
C	-6.68311200	3.49919200	-1.74271800
H	-5.13055100	4.28213000	-2.98655500
H	-6.61579900	5.58818000	-4.52717000
H	-7.03450600	3.86473000	-4.46442700
H	-8.03225800	5.04636100	-3.60654100
H	-6.00771500	3.28735100	-0.89882600
H	-7.66057600	3.78243100	-1.32862700
H	-6.81931600	2.57107100	-2.31179500
C	-2.41493300	1.86073000	-3.21012400
C	-3.44210000	0.97390300	-2.50870100
C	-1.97099000	1.24833800	-4.53517000
H	-2.90825600	2.81659600	-3.43639800
H	-3.78193900	1.42686800	-1.56466200
H	-4.31852300	0.81915000	-3.15039400
H	-3.01707600	-0.01286600	-2.28007400
H	-1.24485600	1.89017500	-5.04916800
H	-1.50680300	0.26470100	-4.38790500

H	-2.83201600	1.11035700	-5.20022300
C	0.33383700	5.04555800	-0.30984300
C	1.69120200	5.58616500	-0.75123800
C	0.21569100	5.02182100	1.21255500
H	-0.43729100	5.73188000	-0.68995200
H	1.76456300	5.63508900	-1.84492800
H	1.85079100	6.59592300	-0.35362500
H	2.50945700	4.95119900	-0.38685300
H	-0.76536600	4.63612500	1.52838700
H	0.98675800	4.38233700	1.66242800
H	0.34043300	6.03117800	1.62441400

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2915.805502

Electronic Energy (0K) + ZPE = -2914.850304

Enthalpy (298K) = -2914.792273

Free Energy (298K) = -2914.941871

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2916.369665

TS_c

Number of imaginary frequencies: 1

C	-6.22630600	3.09526200	2.51946500
C	-4.78608400	3.31074100	2.22313000
C	-3.92793700	3.37440600	3.35474100
C	-2.52276400	3.33041400	3.14149000
C	-4.39844000	3.53478300	4.69043900
C	-1.63813600	3.43525900	4.19546200
H	-2.16107200	3.19034800	2.12310300
C	-3.50773700	3.66676800	5.73409900
H	-5.46547900	3.57137700	4.89487300

C	-2.13105600	3.61152000	5.48984600
H	-0.56733500	3.38572800	4.01827300
H	-3.87583200	3.80801000	6.74699600
H	-1.43575100	3.70667600	6.32069800
N	-7.00878000	4.18610700	2.71144200
S	-8.59634400	4.00279300	3.40785400
O	-9.21857800	5.30122400	3.20659100
O	-9.20395000	2.79611800	2.88060600
C	-6.58901700	5.48980200	2.18580100
H	-7.44076800	6.17016000	2.20869900
H	-5.77703300	5.90637300	2.79446100
H	-6.26515900	5.37299900	1.14349200
C	-8.20584500	3.80142900	5.11654900
C	-7.70676600	4.90629000	5.80841500
C	-8.33845600	2.55592900	5.71976500
C	-7.33033200	4.74560800	7.13212500
H	-7.61117600	5.87240900	5.31568700
C	-7.96077000	2.42002700	7.05002600
H	-8.72340400	1.71053000	5.15539500
C	-7.45003900	3.50293700	7.77027300
H	-6.93705200	5.59497300	7.68827300
H	-8.05897100	1.45293700	7.53939000
C	-7.05106700	3.35284700	9.20370200
H	-6.95576700	2.30021500	9.48741000
H	-6.09887800	3.85665100	9.40618100
H	-7.79958400	3.80954100	9.86378800
C	-3.31819200	4.33871100	-1.49127900
C	-1.94890800	4.57393100	-3.26953400
C	-2.85113400	5.58479500	-3.31268600
H	-1.12485100	4.31664700	-3.92070500

H	-2.98758100	6.39896500	-4.01121700
N	-2.24986000	3.82641600	-2.14276800
N	-3.68522800	5.41763700	-2.21768600
Au	-4.11222500	3.67700100	0.31327900
C	-6.95327300	0.38772100	1.37078200
C	-7.13714500	1.39898100	0.36345600
C	-7.67841600	0.96407800	-0.88402200
C	-7.91876000	-0.36716400	-1.12636400
C	-7.67670700	-1.36112800	-0.14990800
C	-7.21822800	-0.97327500	1.08354300
C	-6.64422100	0.75365300	2.69903900
H	-7.86650600	1.71797200	-1.64557400
H	-8.30858100	-0.66516000	-2.09878900
H	-7.87630100	-2.40620000	-0.37005800
H	-7.05858000	-1.70486100	1.87612600
H	-6.64227700	-0.04733000	3.44591400
O	-6.83412300	2.62374700	0.57569100
N	-6.44180800	1.94744100	3.17780700
C	-4.73628600	6.31281500	-1.81960100
C	-5.99684200	6.16992500	-2.41837600
C	-4.45713900	7.26212500	-0.82639500
C	-7.01769400	7.00433900	-1.96188000
C	-5.51368500	8.07634600	-0.40903400
C	-6.77984100	7.94398400	-0.96434900
H	-8.01416000	6.91671900	-2.38976000
H	-5.33698900	8.82706600	0.35996100
H	-7.59015400	8.58441700	-0.62260400
C	-1.47687100	2.73718400	-1.61432800
C	-0.35477200	3.05230200	-0.83298900
C	-1.91786200	1.42564600	-1.83678800

C	0.32756800	1.98858900	-0.23926200
C	-1.20449200	0.39941300	-1.21348400
C	-0.09848600	0.67761500	-0.41911100
H	1.20416100	2.19242900	0.37409500
H	-1.52193600	-0.63255600	-1.35411200
H	0.44268000	-0.13678900	0.05762300
C	-3.07824400	7.44237800	-0.22288700
C	-3.09053800	7.21708900	1.28727700
C	-2.51294200	8.81823700	-0.56745600
H	-2.40295300	6.69223400	-0.65951700
H	-3.44553100	6.20490700	1.53193300
H	-2.08026500	7.33454900	1.69998800
H	-3.74092600	7.93991900	1.79765100
H	-2.48031700	8.97622800	-1.65268600
H	-3.11919300	9.62121600	-0.12828300
H	-1.49235200	8.91988800	-0.17784300
C	-6.25679900	5.11170400	-3.47024200
C	-7.22707500	5.56903000	-4.55297300
C	-6.76302700	3.83231700	-2.80498000
H	-5.30200900	4.87607600	-3.96151200
H	-6.91875000	6.51941000	-5.00461100
H	-7.27882500	4.81618400	-5.34829100
H	-8.24476600	5.69362700	-4.16176200
H	-6.06710400	3.46101700	-2.03951800
H	-7.72626700	4.01852800	-2.30870400
H	-6.90980500	3.03986800	-3.55137900
C	-3.12358100	1.10861900	-2.69615000
C	-4.29224100	0.60842900	-1.84843600
C	-2.78414400	0.10059400	-3.79099200
H	-3.44639500	2.03679600	-3.19071300

H	-4.56918200	1.33665300	-1.07059800
H	-5.17434800	0.43661700	-2.47824200
H	-4.04622700	-0.33903600	-1.34860000
H	-1.94333200	0.43951600	-4.40779600
H	-2.52086700	-0.87781300	-3.36943000
H	-3.64936800	-0.04857900	-4.44811500
C	0.12838000	4.47538300	-0.63236900
C	1.51584800	4.66336500	-1.24226500
C	0.12108700	4.88376300	0.83813300
H	-0.55760700	5.15486300	-1.15699100
H	1.52896700	4.38958900	-2.30451500
H	1.83382700	5.70950500	-1.15647300
H	2.26364500	4.04564900	-0.72810300
H	-0.89014000	4.83472500	1.26449600
H	0.77778000	4.24080000	1.43951700
H	0.47974400	5.91573400	0.94460800

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2915.767869

Electronic Energy (0K) + ZPE = -2914.819177

Enthalpy (298K) = -2914.759639

Free Energy (298K) = -2914.915117

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2916.334872

C'

Number of imaginary frequencies: 0

C	-1.60147800	-0.69162000	1.47400600
C	-0.10515900	-0.42317900	1.28868700
C	0.71179100	-0.25914300	2.44082200
C	2.12259900	-0.33896600	2.26726900

C	0.21890600	0.00404500	3.75232900
C	2.98751200	-0.17848500	3.33105100
H	2.51089500	-0.56299200	1.27385300
C	1.09102600	0.19045900	4.80437800
H	-0.84927800	0.08864300	3.91847600
C	2.47085100	0.09446200	4.59870700
H	4.06062800	-0.25915500	3.18085900
H	0.70249400	0.41054300	5.79541000
H	3.14972000	0.23609700	5.43663100
N	-2.26787200	0.50160800	1.95176900
S	-3.82504700	0.30860300	2.62501700
O	-4.50364200	1.58002800	2.39959700
O	-4.43208500	-0.93163100	2.15976100
C	-2.02427000	1.72713500	1.17866600
H	-2.55564800	2.55841100	1.64352900
H	-0.95250600	1.95746300	1.21173500
H	-2.34702200	1.63682600	0.13199300
C	-3.47967200	0.16838300	4.35678300
C	-3.02912100	1.30148700	5.03411800
C	-3.61495300	-1.05569400	4.99897500
C	-2.70416400	1.19275900	6.37740800
H	-2.92886700	2.25198400	4.51312600
C	-3.28760600	-1.14359900	6.34733400
H	-3.96311800	-1.92560400	4.44805400
C	-2.82676400	-0.02933500	7.05228200
H	-2.35000100	2.06806600	6.91997900
H	-3.38918300	-2.09662300	6.86346800
C	-2.48757500	-0.12254600	8.50656600
H	-2.38897800	-1.16267600	8.83248600
H	-1.55185800	0.40205700	8.73184900

H	-3.26955000	0.34485800	9.11872200
C	1.45347000	0.64190100	-2.37353900
C	2.82122900	0.93563200	-4.14452300
C	1.91943900	1.94771500	-4.15311700
H	3.64563900	0.69944400	-4.80339000
H	1.78340800	2.78569100	-4.82292900
N	2.52073100	0.15193700	-3.04282300
N	1.08731800	1.74571900	-3.06245500
Au	0.64646000	-0.07215000	-0.58967400
C	-2.03473600	-3.32672800	0.65335800
C	-2.31821500	-2.27015400	-0.22043100
C	-2.78478500	-2.53072100	-1.50548100
C	-2.89948900	-3.85064600	-1.92466200
C	-2.57334000	-4.91596700	-1.07941100
C	-2.16287400	-4.64965600	0.21629000
C	-1.79435000	-2.95982400	2.02496200
H	-3.04844200	-1.70327400	-2.15794100
H	-3.25036600	-4.05284200	-2.93441700
H	-2.66782200	-5.94030300	-1.42884700
H	-1.94942100	-5.45579300	0.91654400
H	-1.78776500	-3.75263900	2.78008300
O	-2.19032400	-0.98690100	0.18230500
N	-1.67142000	-1.75307400	2.44382200
C	0.04833500	2.64165900	-2.63403400
C	-1.22258400	2.51705100	-3.21435100
C	0.35161100	3.58170100	-1.63973000
C	-2.22412500	3.36918400	-2.74878500
C	-0.68721000	4.41147400	-1.20858000
C	-1.95992000	4.30448500	-1.75349700
H	-3.22617900	3.29918400	-3.16638900

H	-0.49096900	5.15354700	-0.43602200
H	-2.75529600	4.95893400	-1.40346700
C	3.28816700	-0.96222600	-2.56118600
C	4.41118300	-0.68804600	-1.76630100
C	2.84300400	-2.26007100	-2.84511600
C	5.08818900	-1.78098600	-1.22168500
C	3.55285000	-3.31735000	-2.27213200
C	4.65868700	-3.08069300	-1.46423300
H	5.96485600	-1.60883000	-0.59902600
H	3.23186500	-4.34012700	-2.46284300
H	5.19701200	-3.91828800	-1.02605100
C	1.73288200	3.72420500	-1.03288800
C	1.70678900	3.44013900	0.46748000
C	2.31912700	5.10311100	-1.32386500
H	2.39891100	2.98129300	-1.49544800
H	1.32574400	2.42756800	0.66846600
H	2.71591300	3.51763400	0.89244600
H	1.06683100	4.15590200	1.00053100
H	2.35854500	5.29993100	-2.40249800
H	1.72392800	5.89884700	-0.85760900
H	3.33959300	5.17515100	-0.92751400
C	-1.51708000	1.44442000	-4.24113800
C	-2.53832200	1.87140700	-5.28814100
C	-1.98706500	0.17781400	-3.52551900
H	-0.58145200	1.20529000	-4.76719400
H	-2.26734400	2.82267000	-5.76114500
H	-2.60660000	1.10938200	-6.07330700
H	-3.54206400	1.97935400	-4.85756600
H	-1.23910400	-0.18731700	-2.80607000
H	-2.91267200	0.38490100	-2.96781500

H	-2.19198300	-0.62640000	-4.24514600
C	1.63482000	-2.53187100	-3.71599200
C	0.47526000	-3.08604300	-2.89041600
C	1.97457200	-3.47379000	-4.86811500
H	1.30446500	-1.57839000	-4.15440900
H	0.20446000	-2.40830300	-2.06587600
H	-0.41242300	-3.22247500	-3.52165900
H	0.72931300	-4.06146800	-2.45288800
H	2.80696700	-3.09183500	-5.47099100
H	2.25206800	-4.47095200	-4.50317300
H	1.10595100	-3.59556100	-5.52644900
C	4.90156200	0.72202100	-1.50249300
C	6.30274700	0.92055900	-2.07646500
C	4.86555300	1.07484400	-0.01795100
H	4.23247400	1.42658600	-2.01587600
H	6.33437800	0.68618600	-3.14780300
H	6.62622600	1.96031700	-1.94575700
H	7.03592400	0.27883100	-1.57063200
H	3.84272800	1.03240400	0.38046200
H	5.49240500	0.39465900	0.57436200
H	5.24277100	2.09398300	0.13681600

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2915.789201

Electronic Energy (0K) + ZPE = -2914.838269

Enthalpy (298K) = -2914.778984

Free Energy (298K) = -2914.933873

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2916.353726

Number of imaginary frequencies: 0

C	-5.49551900	1.05110300	-2.84630300
C	-4.16983600	1.28362500	-3.01155900
C	-3.52444100	2.42479300	-3.67112000
C	-4.05606200	3.03225800	-4.81810200
C	-2.31123100	2.90254200	-3.15552700
C	-3.39908300	4.09874900	-5.41768000
H	-4.98369500	2.65921600	-5.24514000
C	-1.66568300	3.98056800	-3.74939000
H	-1.88140700	2.42620100	-2.27786700
C	-2.20809800	4.58395700	-4.88086300
H	-3.82196900	4.55507800	-6.31022700
H	-0.73251100	4.34817600	-3.32854500
H	-1.69947600	5.42280500	-5.35082000
N	-6.41894200	2.05144300	-3.26395300
S	-6.95320000	3.09138200	-2.03444300
O	-5.86355300	3.19201900	-1.07105600
O	-8.28812600	2.69847300	-1.58574600
C	-7.48302300	1.60871000	-4.16551800
H	-7.01351200	1.10897700	-5.01881400
H	-8.03121100	2.47906300	-4.54339500
H	-8.18599500	0.91936500	-3.68153500
C	-7.09669300	4.62812000	-2.90443400
C	-5.93338200	5.33879300	-3.20098000
C	-8.34877700	5.10363700	-3.27637100
C	-6.03749300	6.53870200	-3.88564500
H	-4.96135900	4.95348300	-2.89733800
C	-8.43308300	6.31022400	-3.96381500
H	-9.24270800	4.53803200	-3.02498400
C	-7.28589600	7.04076900	-4.27838800

H	-5.13628200	7.10247100	-4.12501900
H	-9.40742700	6.69343900	-4.26203300
C	-7.37421800	8.34104800	-5.01326900
H	-6.75245700	8.32832500	-5.91670100
H	-7.01119400	9.16859200	-4.39106000
H	-8.40327100	8.56767700	-5.30923000
C	-4.34759100	-1.67009200	-2.91750300
C	-3.24747500	-0.81359900	-3.05445600
C	-2.10438600	-1.19850000	-3.73705300
C	-2.03952700	-2.48254400	-4.27111300
C	-3.10691600	-3.36756800	-4.11800800
C	-4.24874500	-2.96601900	-3.43854400
C	-5.56993000	-1.22909900	-2.25579100
H	-1.27503000	-0.49939400	-3.81690200
H	-1.14193800	-2.79957800	-4.79671100
H	-3.04176500	-4.37333600	-4.52497100
H	-5.08807500	-3.64846900	-3.31375900
H	-6.16239500	-2.02121600	-1.78440500
O	-3.28192700	0.40550800	-2.40824100
N	-6.07309200	-0.04463000	-2.22033800

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -1620.912834

Electronic Energy (0K) + ZPE = -1620.530760

Enthalpy (298K) = -1620.504930

Free Energy (298K) = -1620.586798

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -1621.230465

TS_{A1'}

Number of imaginary frequencies: 1

C	-3.51706600	2.55759800	2.82612900
C	-3.06734900	3.77069900	2.97033600
C	-1.70589700	4.25071300	3.21151600
C	-0.74173200	4.09988000	2.20601500
C	-1.37542700	4.94584600	4.38043500
C	0.53924900	4.61414000	2.38239700
H	-1.01327900	3.57914500	1.28674500
C	-0.08825200	5.44047800	4.55783000
H	-2.13510700	5.09135600	5.14767500
C	0.87175200	5.27829900	3.56081400
H	1.28017400	4.49459900	1.59487200
H	0.16229800	5.96800500	5.47587100
H	1.87383700	5.67788100	3.69756500
N	-4.55576900	1.82953700	2.45552400
S	-4.75634800	1.47681500	0.76804200
O	-6.19335400	1.35290700	0.58116100
O	-3.97126800	2.46700700	0.05022000
C	-5.57253200	1.32901700	3.38880000
H	-5.20107600	1.49300000	4.40279900
H	-6.50899500	1.88091900	3.24712000
Au	-4.55764000	5.22363600	2.74109300
H	-5.74053700	0.25681000	3.24227700
C	-3.99205100	-0.10419700	0.60188400
C	-4.74185600	-1.25398900	0.84250500
C	-2.62338200	-0.16279200	0.34455900
C	-4.09822400	-2.48360000	0.82181500
H	-5.81009200	-1.18635800	1.03460900
C	-2.00056300	-1.40273500	0.33309600
H	-2.05720000	0.74863200	0.16341100
C	-2.72402300	-2.57599000	0.57462900

H	-4.66819800	-3.39237400	1.00790300
H	-0.93010300	-1.46616900	0.14225100
C	-2.04160000	-3.90674300	0.56458300
H	-2.50585900	-4.59888300	1.27596100
H	-2.10812900	-4.37028600	-0.42835400
H	-0.97848000	-3.81259000	0.81131000
C	-5.88066400	6.78494000	2.57403400
C	-6.63579500	8.90500400	2.44285600
C	-7.70904400	8.08098800	2.34714300
H	-6.55365100	9.98300900	2.42709900
H	-8.76404900	8.28548700	2.22688000
N	-7.22229000	6.78443100	2.42590400
N	-5.52547800	8.08922500	2.58679400
C	-4.15750100	8.50814400	2.73255800
C	-3.67782500	8.77545500	4.02334900
C	-3.34359500	8.53494600	1.59152700
C	-2.32219900	9.08225900	4.15172800
C	-1.99572600	8.85175800	1.77445900
C	-1.48927800	9.11948700	3.03979600
H	-1.91022500	9.28331800	5.13926200
H	-1.33352500	8.88146300	0.91064700
H	-0.43442500	9.35654800	3.16152100
C	-8.00952600	5.58310300	2.36884200
C	-8.42534200	4.99877300	3.57290600
C	-8.28390600	5.02658800	1.11082700
C	-9.15448000	3.81011400	3.48916000
C	-9.00654400	3.83293100	1.08283300
C	-9.44024500	3.23209200	2.25866700
H	-9.49576000	3.32838100	4.40423400
H	-9.22599000	3.36304600	0.12586900

H	-10.00480500	2.30317100	2.21498500
C	-8.08034900	5.57979600	4.92821700
C	-9.32998100	5.84001200	5.76442300
C	-7.10843200	4.66233800	5.66991200
H	-7.57683200	6.54568500	4.77587200
H	-10.03289700	6.49992200	5.24167800
H	-9.06034700	6.31552600	6.71522800
H	-9.85641000	4.90636400	6.00056700
H	-6.18782400	4.50082500	5.08841900
H	-7.56219400	3.68038500	5.86133200
H	-6.83128300	5.09578900	6.63917200
C	-7.76346900	5.63971800	-0.17200400
C	-6.53485500	4.86665300	-0.65226900
C	-8.82416400	5.70223000	-1.26612800
H	-7.44954900	6.67161600	0.04129000
H	-5.74660500	4.84293100	0.11484200
H	-6.11996600	5.32273000	-1.56056400
H	-6.80044500	3.82647600	-0.88450300
H	-9.72875200	6.22080700	-0.92666300
H	-9.11644500	4.70101100	-1.60735200
H	-8.43232000	6.23914600	-2.13831600
C	-4.55765000	8.66834300	5.25137800
C	-4.24259500	7.38263200	6.01701600
C	-4.43114400	9.88342100	6.16499700
H	-5.60485600	8.61187900	4.92209400
H	-4.36879200	6.49352200	5.38059100
H	-4.90345600	7.28078800	6.88736800
H	-3.20566500	7.39291800	6.38101100
H	-4.62745000	10.81776300	5.62580900
H	-3.43065500	9.95444600	6.61029500

H	-5.14945600	9.81076400	6.99048400
C	-3.85982300	8.21046800	0.20532900
C	-3.70639400	9.40577900	-0.73184500
C	-3.16272400	6.97468200	-0.36243400
H	-4.93346900	7.98396000	0.27727200
H	-4.22438000	10.29006200	-0.34028400
H	-4.12648700	9.17501700	-1.71841900
H	-2.65054000	9.67005500	-0.87466100
H	-3.28875700	6.10309900	0.29878200
H	-2.08579600	7.14883300	-0.48726000
H	-3.57378300	6.72015600	-1.34734400
C	-0.61804600	-0.39970700	3.55357100
C	-1.89488600	-0.93974500	3.71475100
C	-2.13680300	-2.27897400	3.99933300
C	-1.00826300	-3.07540000	4.10130200
C	0.29469000	-2.56114000	3.93059100
C	0.51190100	-1.22465500	3.65840700
C	-0.87241300	0.96856600	3.26446800
H	-3.14375800	-2.66776500	4.11751600
H	-1.12979000	-4.13464000	4.31538400
H	1.14120200	-3.23666700	4.01947600
H	1.51363500	-0.82490400	3.53011100
H	-0.17885600	1.77552900	3.05590000
O	-2.82748500	0.02335300	3.54188300
N	-2.15969000	1.19806300	3.25270200

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2915.746890

Electronic Energy (0K) + ZPE = -2914.796346

Enthalpy (298K) = -2914.737353

Free Energy (298K) = -2914.890872

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2916.316174

A1'

Number of imaginary frequencies: 0

C	-3.56490600	2.27608600	2.75338600
C	-3.29223800	3.52787200	3.17374200
C	-2.07095400	3.84046100	3.93898900
C	-1.67331000	3.06893300	5.04285700
C	-1.30946500	4.97405100	3.61246000
C	-0.55044000	3.41647400	5.78612900
H	-2.26566700	2.20238700	5.33584300
C	-0.17442600	5.30540600	4.34267600
H	-1.62175100	5.59483100	2.77134100
C	0.20745700	4.53088000	5.43631700
H	-0.26859000	2.81338800	6.64666400
H	0.40429300	6.18440700	4.06582700
H	1.08492800	4.80120200	6.01921100
N	-4.77217700	1.77502700	2.23076600
S	-4.80895200	1.41297800	0.57616300
O	-6.22042300	1.34078300	0.21451400
O	-3.90311100	2.31537600	-0.12948600
C	-6.05020900	2.07829700	2.88466700
H	-5.85812500	2.13688000	3.95953200
H	-6.48082300	3.02882300	2.54224400
Au	-4.58655200	5.11324700	2.79803800
H	-6.76456000	1.27161600	2.69710800
C	-4.11355500	-0.21810900	0.50367600
C	-4.76423300	-1.25231400	1.17676400
C	-2.93183300	-0.43968300	-0.19465400

C	-4.20508600	-2.52011900	1.15752700
H	-5.68728900	-1.06186300	1.72166400
C	-2.38683000	-1.71960500	-0.20401400
H	-2.44116000	0.38270000	-0.71023400
C	-3.00820300	-2.77166600	0.47228700
H	-4.69560500	-3.33440300	1.68860200
H	-1.45468700	-1.90322800	-0.73639000
C	-2.41753400	-4.14634800	0.46145200
H	-2.60901900	-4.67055100	1.40463400
H	-2.86013700	-4.75352400	-0.33899800
H	-1.33593800	-4.11893900	0.28988700
C	-5.80185500	6.75743300	2.48733100
C	-6.48866100	8.89611700	2.25675000
C	-7.58999100	8.10704200	2.20829200
H	-6.36721600	9.96808700	2.18319900
H	-8.63853900	8.34149800	2.08637400
N	-7.14607800	6.80078700	2.34725900
N	-5.40561200	8.04900000	2.43189900
C	-4.03035400	8.45475600	2.52148000
C	-3.49524600	8.73568300	3.78716300
C	-3.27481200	8.50459000	1.34162800
C	-2.14544700	9.08809200	3.84705500
C	-1.93155700	8.86995200	1.45549700
C	-1.37280000	9.15948300	2.69404900
H	-1.69153500	9.30301400	4.81303600
H	-1.31420300	8.91770100	0.55972700
H	-0.32359600	9.43937600	2.76256400
C	-7.97926600	5.62971500	2.37422700
C	-8.41372900	5.14999600	3.61766600
C	-8.28178700	4.99766700	1.15848300

C	-9.17838100	3.98076500	3.62072700
C	-9.04110100	3.82772200	1.21792300
C	-9.48707700	3.32600500	2.43515600
H	-9.52975400	3.57612200	4.56867200
H	-9.28019300	3.29780700	0.29766000
H	-10.07875200	2.41325300	2.45883100
C	-8.05058300	5.82220300	4.92586800
C	-9.28754700	6.14443400	5.75957800
C	-7.06914300	4.95894200	5.71833000
H	-7.54756900	6.77397600	4.70082200
H	-10.00216200	6.75895900	5.19886000
H	-9.00243200	6.69522000	6.66411700
H	-9.80689800	5.23248600	6.08100700
H	-6.14808000	4.77182400	5.14516000
H	-7.51521200	3.98714600	5.97066000
H	-6.79307200	5.45411700	6.65801700
C	-7.75901500	5.51267000	-0.16658500
C	-6.52930400	4.71044500	-0.59395900
C	-8.81814700	5.49198000	-1.26409900
H	-7.44882000	6.55861000	-0.02869300
H	-5.73079300	4.75497800	0.16167300
H	-6.12777500	5.09558900	-1.54037400
H	-6.78396400	3.65188600	-0.73830700
H	-9.73119000	6.01786700	-0.96028500
H	-9.09430300	4.46740900	-1.54383800
H	-8.43057000	5.97874300	-2.16705000
C	-4.30910100	8.60952000	5.05820600
C	-3.90437200	7.34816100	5.82264100
C	-4.18704600	9.84277200	5.94809400
H	-5.36819600	8.50568900	4.78060700

H	-4.05439700	6.44486900	5.21190000
H	-4.49788500	7.24623000	6.74032200
H	-2.84402400	7.38638700	6.10853600
H	-4.44423600	10.76069200	5.40607400
H	-3.17001300	9.95792700	6.34406000
H	-4.86237900	9.75577600	6.80773100
C	-3.84508600	8.13003800	-0.01034900
C	-3.67898300	9.25617200	-1.02642900
C	-3.20596700	6.83628200	-0.51484400
H	-4.92304100	7.94536100	0.10403400
H	-4.13736400	10.18737900	-0.67157900
H	-4.15407600	8.98443200	-1.97683100
H	-2.62050200	9.45906400	-1.23409100
H	-3.35918300	6.00937100	0.19540700
H	-2.12420800	6.96150300	-0.65761200
H	-3.63767100	6.54248800	-1.47981200
C	-0.77853700	-0.05705000	2.56428900
C	-1.77659800	-0.72364600	3.28992600
C	-1.65891600	-2.03104200	3.73958000
C	-0.46192000	-2.65433100	3.42675800
C	0.56179600	-2.01200100	2.69559300
C	0.42385800	-0.71403200	2.25257900
C	-1.34783300	1.19330000	2.25684400
H	-2.45343900	-2.52388000	4.29048800
H	-0.30710900	-3.68051800	3.75057900
H	1.47435800	-2.56018900	2.47965800
H	1.20339400	-0.21452600	1.68583000
H	-0.97548200	2.03178000	1.67735400
O	-2.85792900	0.07447200	3.45005600
N	-2.55234600	1.24933900	2.78590900

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2915.773465

Electronic Energy (0K) + ZPE = -2914.820015

Enthalpy (298K) = -2914.761592

Free Energy (298K) = -2914.911944

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2916.34114

TS_{B1}'

Number of imaginary frequencies: 1

C	-3.15205900	2.54813100	2.59309700
C	-2.99578500	3.86823800	3.05489900
C	-1.71359900	4.35026000	3.54170900
C	-1.71227900	5.25802200	4.62290200
C	-0.47833000	4.02746800	2.94359800
C	-0.52589500	5.76149700	5.13115000
H	-2.66520200	5.53241700	5.07363500
C	0.70132200	4.57879700	3.42151800
H	-0.45239000	3.39622400	2.06034400
C	0.68512000	5.42934800	4.52541500
H	-0.54698200	6.43523400	5.98479300
H	1.64165000	4.34526600	2.92818200
H	1.61525600	5.84797600	4.90219900
N	-4.42478900	2.06160900	2.18987700
S	-4.57592200	1.33884400	0.69164600
O	-6.00268100	1.29758700	0.39712500
O	-3.64822800	2.02042100	-0.20638400
C	-5.57323100	2.11050800	3.10447400
H	-5.21452600	1.95847500	4.12869000
H	-6.09922900	3.07187000	3.03547500

Au	-4.49078100	5.27610300	2.89795500
H	-6.28006000	1.31463000	2.85770000
C	-3.98053800	-0.32403600	0.90267000
C	-4.32433900	-1.04941300	2.04295500
C	-3.17600400	-0.87920100	-0.09021000
C	-3.82079700	-2.33243700	2.19862700
H	-4.94587000	-0.61316000	2.82237100
C	-2.69226300	-2.17025200	0.07890900
H	-2.91430000	-0.29703200	-0.97045800
C	-2.99725700	-2.91016000	1.22468900
H	-4.05849600	-2.89736600	3.09871500
H	-2.05029000	-2.60829700	-0.68374100
C	-2.45790000	-4.29272000	1.41046000
H	-2.27112600	-4.50819200	2.46847800
H	-3.17358800	-5.04222200	1.04816500
H	-1.52462000	-4.43647500	0.85538600
C	-5.85475800	6.81380400	2.66466800
C	-6.67591800	8.89941700	2.41229200
C	-7.70461700	8.03112900	2.24351500
H	-6.63285500	9.97936800	2.37713600
H	-8.75202000	8.19033400	2.02732600
N	-7.17774200	6.75943100	2.39963200
N	-5.55421700	8.13252400	2.67654700
C	-4.22399300	8.62567400	2.90697900
C	-3.86884800	8.99924600	4.21166900
C	-3.32672000	8.64764500	1.83035300
C	-2.55164400	9.40973900	4.42277600
C	-2.02102400	9.06703900	2.09550700
C	-1.63690200	9.44218100	3.37642100
H	-2.23329100	9.69720600	5.42333100

H	-1.29668000	9.09836500	1.28311300
H	-0.61398400	9.76258400	3.56231000
C	-7.91725600	5.53191200	2.29193400
C	-8.44607700	4.96747600	3.46103200
C	-8.04585500	4.94229900	1.02584400
C	-9.14125900	3.76316700	3.33001500
C	-8.75151800	3.74033700	0.95008800
C	-9.29622400	3.15882300	2.08861200
H	-9.56264300	3.29052500	4.21571200
H	-8.86570200	3.24649500	-0.01320600
H	-9.84173600	2.22103700	2.00787200
C	-8.23594900	5.58149100	4.83009200
C	-9.54390700	5.73221000	5.60093600
C	-7.22926000	4.75247400	5.62899700
H	-7.81059600	6.58799200	4.69958600
H	-10.28424100	6.30715200	5.03202800
H	-9.36562300	6.25257400	6.54965900
H	-9.98646500	4.75730200	5.84178700
H	-6.25894100	4.69221400	5.11288500
H	-7.59622400	3.72704500	5.77547400
H	-7.06459000	5.19382300	6.62012800
C	-7.38813700	5.52613700	-0.20710200
C	-6.12526500	4.73207900	-0.54478800
C	-8.32973300	5.57534400	-1.40591500
H	-7.08519000	6.55921200	0.01721100
H	-5.41606900	4.72616600	0.29826200
H	-5.61780200	5.16400700	-1.41719800
H	-6.37341100	3.68758900	-0.77591700
H	-9.25851100	6.10917400	-1.17166400
H	-8.59595100	4.56921300	-1.75362000

H	-7.84447000	6.08959100	-2.24412900
C	-4.83907900	8.89026100	5.36992800
C	-4.56898400	7.60730500	6.15738900
C	-4.79815200	10.10386100	6.29236200
H	-5.85759400	8.82033700	4.96163600
H	-4.64732200	6.71753900	5.51516900
H	-5.28546900	7.50086300	6.98198900
H	-3.55758900	7.62409800	6.58861000
H	-4.93997100	11.04008300	5.73972800
H	-3.84631900	10.17181300	6.83419100
H	-5.59279400	10.02980000	7.04431800
C	-3.71749100	8.23545600	0.42611600
C	-3.61243700	9.41618800	-0.53605900
C	-2.87830400	7.05476500	-0.05886100
H	-4.76855600	7.91205700	0.43693400
H	-4.23356600	10.25781900	-0.20467600
H	-3.94401600	9.12334500	-1.53975700
H	-2.57769900	9.77334300	-0.61894300
H	-2.97819400	6.18921600	0.61403400
H	-1.81367100	7.31719100	-0.11472700
H	-3.19658600	6.74545400	-1.06235600
C	-0.91671800	-0.28664800	2.70938000
C	-1.47443700	-0.31091500	4.02504700
C	-1.11940900	-1.37430700	4.88875600
C	-0.26902800	-2.34604900	4.40918700
C	0.27164500	-2.32081200	3.09975800
C	-0.04921400	-1.29640900	2.24452700
C	-1.41615300	0.83021100	2.03771100
H	-1.52685500	-1.40975000	5.89461000
H	-0.00092700	-3.17132100	5.06599800

H	0.93723000	-3.11774400	2.78088300
H	0.34484400	-1.24920700	1.23174800
H	-1.19203200	1.08807600	0.99981700
O	-2.27051500	0.65661100	4.31344000
N	-2.17206000	1.65615400	2.70914200

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2915.742453

Electronic Energy (0K) + ZPE = -2914.792613

Enthalpy (298K) = -2914.733728

Free Energy (298K) = -2914.886585

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2916.311516

BI'

Number of imaginary frequencies: 0

C	0.36059700	-1.94871300	0.59716100
C	0.77439200	-0.67557300	1.20253000
C	1.96233600	-0.59472400	1.95064500
C	2.71445200	-1.75507400	2.29295100
C	2.42761000	0.68156300	2.38088400
C	3.86854700	-1.63301900	3.03746600
H	2.40166500	-2.73250800	1.92666500
C	3.58183700	0.78944100	3.12494600
H	1.85142200	1.56603500	2.10712300
C	4.29696200	-0.36792900	3.45343400
H	4.44857000	-2.51484900	3.29413900
H	3.93747100	1.76223500	3.45243900
H	5.20954200	-0.28134300	4.03885000
N	-0.77669500	-2.57113000	1.04369900
S	-1.67715900	-3.54293300	-0.06447900

O	-2.85863200	-3.91304700	0.70123300
O	-1.81380500	-2.81060800	-1.31433600
C	-1.46046400	-2.12306900	2.25881700
H	-0.72438800	-1.63997300	2.90898400
H	-2.26998200	-1.41688200	2.03679100
Au	-0.35854400	0.90346200	0.56466900
H	-1.86521900	-2.98703300	2.79013700
C	-0.66177000	-4.96307600	-0.31282800
C	-0.42979600	-5.81071200	0.76827000
C	-0.14558300	-5.22650400	-1.57751800
C	0.34698900	-6.94168400	0.56948300
H	-0.85089300	-5.59110400	1.74772400
C	0.61964500	-6.37057800	-1.75631500
H	-0.33882600	-4.54321200	-2.40032900
C	0.88323600	-7.23619400	-0.69005100
H	0.54219500	-7.61466800	1.40244100
H	1.02802000	-6.59581200	-2.73986500
C	1.75091000	-8.43880900	-0.88280700
H	2.79785000	-8.19361900	-0.66045700
H	1.46049800	-9.25631200	-0.21453500
H	1.71353500	-8.80040100	-1.91559300
C	-1.37987500	2.54455800	-0.16851100
C	-1.83094600	4.64540400	-0.84271100
C	-2.92174300	3.88437000	-1.11464900
H	-1.62849300	5.69550300	-1.00303500
H	-3.87525500	4.12867900	-1.56238500
N	-2.61976300	2.59886000	-0.69893500
N	-0.90012300	3.80436800	-0.25726400
C	0.41742900	4.17583200	0.18286400
C	0.57082700	4.66491600	1.48894500

C	1.49363800	3.98032300	-0.69400200
C	1.86620100	4.97257300	1.90898400
C	2.76805200	4.31097800	-0.22707300
C	2.95287700	4.80280400	1.05855200
H	2.02658800	5.34607600	2.91866500
H	3.62738000	4.17546600	-0.88181900
H	3.95383200	5.05330500	1.40336100
C	-3.48368100	1.45182100	-0.77700800
C	-4.25187900	1.12337400	0.34768500
C	-3.46611500	0.68357400	-1.95083700
C	-5.02354000	-0.03908900	0.27549700
C	-4.25647600	-0.46593400	-1.97074100
C	-5.02281600	-0.82655800	-0.86845100
H	-5.63066700	-0.32934800	1.13159000
H	-4.25663200	-1.10091900	-2.85439900
H	-5.62305800	-1.73314000	-0.90144700
C	-4.25742300	1.95924400	1.61105300
C	-5.66446200	2.44861100	1.94403300
C	-3.65675500	1.18424300	2.78227200
H	-3.63059500	2.84766000	1.44566600
H	-6.09964600	3.01336000	1.11057500
H	-5.64318200	3.10298500	2.82394200
H	-6.33680400	1.61133000	2.17093500
H	-2.61973900	0.88072700	2.57208600
H	-4.23714300	0.27685700	2.99704900
H	-3.65580900	1.79949500	3.69082300
C	-2.57630500	1.03246800	-3.12635900
C	-1.29759100	0.19297800	-3.08467100
C	-3.27850900	0.86598900	-4.46998200
H	-2.28698600	2.08949200	-3.03616100

H	-0.74762200	0.34758300	-2.14320200
H	-0.63602300	0.45512900	-3.92077500
H	-1.53517500	-0.87675500	-3.15631800
H	-4.22696100	1.41489800	-4.50482100
H	-3.48817500	-0.18784600	-4.69238700
H	-2.63784000	1.24378100	-5.27575600
C	-0.59642700	4.77761600	2.44677700
C	-0.60021700	3.58005500	3.39874900
C	-0.59675900	6.08607300	3.22999400
H	-1.52657800	4.74401500	1.86197500
H	-0.63926600	2.62714500	2.84845600
H	-1.46395500	3.62398200	4.07419100
H	0.30964600	3.57487100	4.01546100
H	-0.54812100	6.95666000	2.56545400
H	0.24838600	6.14473300	3.92742000
H	-1.51350400	6.16486700	3.82630400
C	1.32622900	3.39901000	-2.08221800
C	1.79490400	4.37566800	-3.15685100
C	2.05837900	2.06140700	-2.19278200
H	0.25723000	3.20629400	-2.25390500
H	1.25335600	5.32761500	-3.09437300
H	1.62792900	3.95433000	-4.15555000
H	2.86706600	4.59082300	-3.06283700
H	1.71812600	1.35990500	-1.41459100
H	3.14300200	2.18958400	-2.07844500
H	1.87993500	1.60212900	-3.17386200
C	3.21375200	-2.41621100	-1.43367100
C	3.70760900	-3.60180200	-0.70475700
C	4.99614100	-4.10437100	-1.14879000
C	5.71568100	-3.48269300	-2.12127500

C	5.23904800	-2.30519600	-2.78331800
C	4.02474200	-1.79910700	-2.44580200
C	1.97099200	-1.87512300	-1.18081000
H	5.36858000	-4.99413300	-0.64471900
H	6.68633000	-3.88483400	-2.40888800
H	5.84635100	-1.83666200	-3.55293800
H	3.62993000	-0.91269500	-2.94393700
H	1.68070200	-0.97860100	-1.74819700
O	3.08567600	-4.13326100	0.22939500
N	1.02870400	-2.40690700	-0.39581600

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2915.773420

Electronic Energy (0K) + ZPE = -2914.823782

Enthalpy (298K) = -2914.763401

Free Energy (298K) = -2914.920224

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2916.34545

TS_{Cl}'

Number of imaginary frequencies: 1

C	0.92048900	-1.65900400	0.06840600
C	1.31323800	-0.37716000	0.71819200
C	2.53560600	-0.06412800	1.35242500
C	3.69490300	-0.89141300	1.38778900
C	2.61395100	1.20580800	2.00515100
C	4.83073200	-0.48040000	2.05641500
H	3.70286100	-1.82816400	0.85264000
C	3.73772200	1.58798000	2.70348400
H	1.75185800	1.87023700	1.96127100
C	4.84995700	0.74232900	2.73016300

H	5.71327900	-1.11385200	2.05765900
H	3.76178400	2.54810400	3.21218600
H	5.74579900	1.04642100	3.26675200
N	-0.29080000	-2.17346100	0.41441900
S	-1.24587500	-3.15882100	-0.64472300
O	-2.46653300	-3.35657200	0.11967700
O	-1.27392400	-2.50880100	-1.94171800
C	-0.74248200	-2.06349700	1.80407300
H	-0.09623500	-1.35049500	2.32648400
H	-1.77274700	-1.70272200	1.84270300
Au	-0.10514600	1.07754700	0.29057300
H	-0.65430700	-3.03064100	2.30954100
C	-0.39666400	-4.69751700	-0.76687100
C	-0.39223400	-5.54582100	0.34124900
C	0.23035100	-5.04537800	-1.95907300
C	0.27040100	-6.75824800	0.24471700
H	-0.90095100	-5.26232300	1.26009600
C	0.87599700	-6.27292800	-2.03748400
H	0.20731300	-4.36734600	-2.80906100
C	0.91299600	-7.13829800	-0.94122000
H	0.29472500	-7.42861000	1.10219400
H	1.37537700	-6.55984800	-2.96143500
C	1.61862800	-8.45377900	-1.02912300
H	2.07275900	-8.72571500	-0.06979800
H	0.91695400	-9.25573300	-1.29322600
H	2.40187600	-8.43770900	-1.79443700
C	-1.38266800	2.63469300	-0.16149700
C	-2.12729000	4.73250200	-0.51421800
C	-3.13697700	3.88106500	-0.82581200
H	-2.06194500	5.81150400	-0.54020200

H	-4.14376300	4.05686100	-1.17931600
N	-2.65636600	2.60140100	-0.60649000
N	-1.06372100	3.94758500	-0.10193300
C	0.22777700	4.42747200	0.31016400
C	0.41003100	4.78192700	1.65557500
C	1.25707300	4.47070600	-0.64086400
C	1.68612700	5.19799700	2.03971700
C	2.51385300	4.89733500	-0.20483100
C	2.72637200	5.25850300	1.11927500
H	1.86855400	5.47442500	3.07662400
H	3.33691300	4.94520000	-0.91621700
H	3.71276800	5.58804800	1.43895800
C	-3.39600200	1.38127500	-0.77851200
C	-4.06231100	0.84985800	0.33437300
C	-3.37371300	0.75895700	-2.03454800
C	-4.72020800	-0.36951200	0.16014300
C	-4.04950300	-0.45632700	-2.15493800
C	-4.71232300	-1.01565800	-1.06970600
H	-5.24371500	-0.81900300	1.00264200
H	-4.03853400	-0.98193400	-3.10795500
H	-5.22155200	-1.97027300	-1.18154300
C	-4.08642100	1.54332600	1.68117900
C	-5.51597300	1.86866000	2.10697200
C	-3.37305100	0.71164700	2.74445700
H	-3.54693700	2.49749100	1.59248300
H	-6.02868400	2.47706200	1.35167300
H	-5.51609200	2.42734500	3.05083300
H	-6.10637900	0.95648200	2.26219800
H	-2.32415500	0.52708500	2.46920800
H	-3.86285100	-0.26150500	2.88391400

H	-3.38603000	1.23092300	3.71107700
C	-2.60113200	1.33319500	-3.20352400
C	-1.27711400	0.58853800	-3.38019500
C	-3.40414100	1.31147800	-4.50028300
H	-2.36886700	2.38433800	-2.97891300
H	-0.67199600	0.61517300	-2.46088300
H	-0.69106400	1.03370400	-4.19477000
H	-1.45492300	-0.46767800	-3.62009200
H	-4.37378600	1.81072000	-4.38669700
H	-3.59006600	0.28623300	-4.84432000
H	-2.84914800	1.82421900	-5.29511100
C	-0.69614000	4.64692400	2.68129500
C	-0.52767300	3.34112100	3.46079300
C	-0.76429000	5.83318600	3.63716500
H	-1.65613500	4.59706600	2.14812500
H	-0.53991500	2.46565000	2.79361900
H	-1.33401600	3.22383800	4.19591600
H	0.42720200	3.33800300	4.00619600
H	-0.83177000	6.78589400	3.09889800
H	0.11321600	5.87712800	4.29467300
H	-1.64645700	5.74405900	4.28204300
C	1.05946000	4.05484200	-2.08356300
C	1.37133600	5.20250000	-3.04051400
C	1.90052100	2.82206100	-2.41375200
H	0.00317500	3.78540800	-2.22711600
H	0.76342800	6.08748700	-2.81566900
H	1.16530100	4.90255700	-4.07508900
H	2.42752200	5.49616200	-2.98596700
H	1.66023000	1.98047700	-1.74473300
H	2.97294800	3.03587500	-2.31475600

H	1.72050600	2.49958700	-3.44693400
C	3.02496500	-3.54742600	-1.02946300
C	2.75160800	-3.90872300	0.34224500
C	3.36240800	-5.10898900	0.82218500
C	4.20231000	-5.84555300	0.02435800
C	4.48574500	-5.46778600	-1.31094300
C	3.89676800	-4.33848600	-1.81880600
C	2.35264200	-2.47136800	-1.65499700
H	3.15102200	-5.40118900	1.84895800
H	4.66382900	-6.74579400	0.42818100
H	5.15501700	-6.07061900	-1.91868600
H	4.07848100	-4.03049100	-2.84880500
H	2.61446400	-2.27127300	-2.69856900
O	2.03782200	-3.17714600	1.10564100
N	1.40488400	-1.71474500	-1.17612000

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2915.763736

Electronic Energy (0K) + ZPE = -2914.813256

Enthalpy (298K) = -2914.754562

Free Energy (298K) = -2914.905819

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2916.332219

C1'

Number of imaginary frequencies: 0

C	1.31810900	-1.69848800	0.04786600
C	1.66743100	-0.23572600	0.34193500
C	3.00197700	0.18777300	0.59531900
C	4.17499100	-0.59048700	0.38279400
C	3.17331100	1.51388400	1.08812400

C	5.42348800	-0.07002400	0.65519500
H	4.10881600	-1.58469200	-0.04019100
C	4.42357300	2.01030100	1.39975400
H	2.28860000	2.13265500	1.24246600
C	5.55080500	1.21987200	1.17746700
H	6.31068400	-0.66685200	0.46306200
H	4.52595000	3.01675900	1.79720200
H	6.53946600	1.61407000	1.40103500
N	-0.02217100	-1.94437900	0.58664500
S	-1.19391500	-2.91598800	-0.14526100
O	-2.37338300	-2.75494300	0.69613200
O	-1.24883700	-2.57840700	-1.55800400
C	-0.05986300	-1.89258800	2.05311400
H	0.56078600	-1.04994100	2.38371500
H	-1.08110600	-1.70632300	2.38876300
Au	0.11379900	1.09593800	0.09487600
H	0.33229000	-2.80749200	2.51638800
C	-0.65837100	-4.60056300	0.01462900
C	-0.73830800	-5.22283500	1.26009100
C	-0.16895000	-5.27904500	-1.09918600
C	-0.29567300	-6.53287700	1.38790500
H	-1.15818600	-4.69782500	2.11488600
C	0.25618600	-6.59203600	-0.95362900
H	-0.13300100	-4.78305900	-2.06651600
C	0.20898200	-7.23387600	0.28852200
H	-0.34929000	-7.02657000	2.35665200
H	0.64000600	-7.13212800	-1.81829900
C	0.68142200	-8.64710300	0.42274400
H	0.80044700	-8.93524500	1.47199500
H	-0.03154100	-9.34424000	-0.03575700

H	1.64098200	-8.79281300	-0.08815200
C	-1.32317200	2.55746300	-0.18682800
C	-2.25479300	4.61349400	-0.23652000
C	-3.16960700	3.73645700	-0.71866000
H	-2.29088300	5.68390900	-0.08807200
H	-4.17820800	3.87539400	-1.08299300
N	-2.58045400	2.48302700	-0.67425600
N	-1.13041400	3.87077900	0.07848500
C	0.09332300	4.39819900	0.61497200
C	0.26887600	4.39334600	2.00569000
C	1.07106900	4.85418000	-0.28179500
C	1.48227700	4.87943200	2.49875900
C	2.26457700	5.33198800	0.26237600
C	2.46684500	5.34876100	1.63769100
H	1.65556800	4.88938800	3.57371700
H	3.04940500	5.68980200	-0.40190900
H	3.40269700	5.72927000	2.04204900
C	-3.21819700	1.27355000	-1.11896600
C	-4.05218100	0.59448300	-0.21815400
C	-2.98931400	0.84244300	-2.43187100
C	-4.68433200	-0.55915200	-0.68120400
C	-3.64345700	-0.32102300	-2.84291000
C	-4.48711600	-1.00858000	-1.98160500
H	-5.33083400	-1.12122300	-0.01037600
H	-3.48470100	-0.69286300	-3.85384700
H	-4.98757300	-1.91257900	-2.32196200
C	-4.19930500	1.04292900	1.22105700
C	-5.61209200	0.86446800	1.76455000
C	-3.19282800	0.29297100	2.09721100
H	-3.95821200	2.11500800	1.27418800

H	-6.36108400	1.34179400	1.12147300
H	-5.68835200	1.31068300	2.76330900
H	-5.87767400	-0.19562800	1.86470400
H	-2.16203600	0.43316000	1.73664700
H	-3.40192100	-0.78523500	2.07854600
H	-3.24953400	0.64093100	3.13719600
C	-2.05280700	1.56392100	-3.37858400
C	-0.79243200	0.73245800	-3.61571900
C	-2.73418000	1.91009800	-4.69940100
H	-1.74339700	2.51017400	-2.91004000
H	-0.26910000	0.51797900	-2.67206700
H	-0.10033500	1.26239400	-4.28308300
H	-1.03959100	-0.23021300	-4.08369800
H	-3.64581600	2.49887500	-4.54039300
H	-3.00955600	1.00770700	-5.26013000
H	-2.05787800	2.49597300	-5.33380200
C	-0.77445900	3.84948700	2.95987300
C	-0.27665300	2.56279800	3.61859600
C	-1.16980400	4.88197200	4.01170300
H	-1.67830100	3.60191800	2.38392400
H	-0.04044000	1.79297500	2.86750400
H	-1.03760100	2.15730600	4.29721200
H	0.63142600	2.74908000	4.20809700
H	-1.52481900	5.81074600	3.54903000
H	-0.32623100	5.13264900	4.66750200
H	-1.97371800	4.48938100	4.64596000
C	0.89381700	4.77093300	-1.78368400
C	1.25495600	6.07599100	-2.48571600
C	1.71711700	3.61014000	-2.34430500
H	-0.16436000	4.56197000	-1.99703700

H	0.69393400	6.92484100	-2.07706900
H	1.02850600	6.00292300	-3.55614600
H	2.32481900	6.30265800	-2.39480600
H	1.43445100	2.65296400	-1.87977600
H	2.78872300	3.76954200	-2.15953400
H	1.57129100	3.52168000	-3.42847100
C	2.66010100	-3.72266600	-1.32753200
C	2.66748500	-3.69423400	0.07220100
C	3.20327800	-4.74454900	0.80585900
C	3.73812800	-5.82825000	0.11727100
C	3.74836600	-5.87131600	-1.28123600
C	3.21047400	-4.81718900	-2.00212300
C	2.04422300	-2.59888000	-1.98658700
H	3.19781900	-4.69958100	1.89198400
H	4.15856000	-6.65691600	0.68267500
H	4.17562000	-6.72785600	-1.79547600
H	3.19712700	-4.82585800	-3.09098900
H	2.11677700	-2.53028200	-3.07596700
O	2.22262200	-2.59165700	0.72468800
N	1.38377000	-1.67578400	-1.38186900

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2915.788908

Electronic Energy (0K) + ZPE = -2914.837158

Enthalpy (298K) = -2914.778356

Free Energy (298K) = -2914.930151

SMD-M06/6-311+G(d,p)/SDD

Electronic Energy (0K) = -2916.353689