

Supporting Information

Insights into the Gold(I)-Catalyzed Intermolecular Annulations of Alkynes with *N*-allenamides: A Mechanistic DFT Study

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Author Contributions

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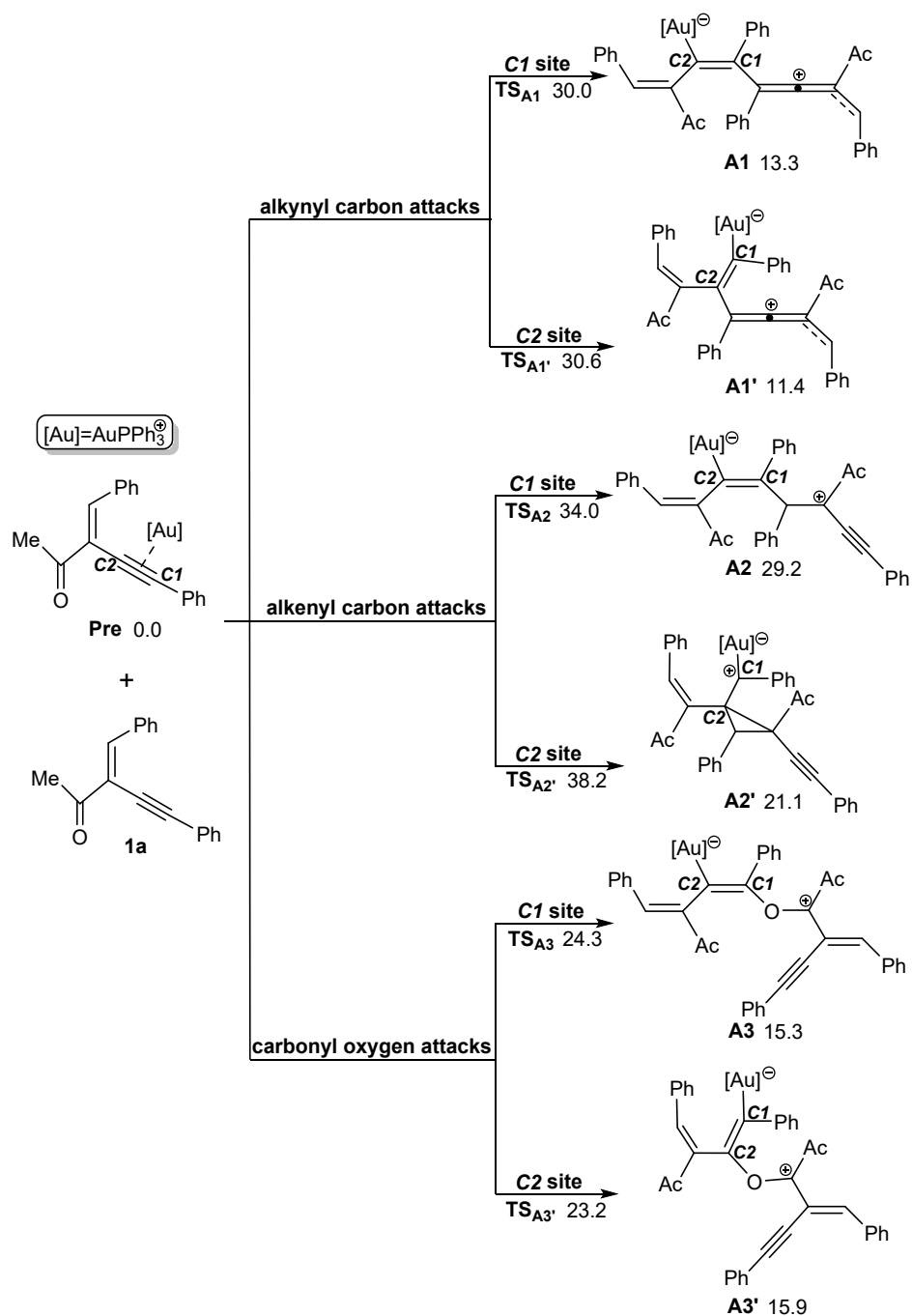


Figure S1. The cases that the unactivated alkyne **1a** competitively nucleophilic attacks the **C1/C2** site within activated alkyne **Pre**, and relative Gibbs free energy ΔG of key intermediates and transition states are shown.

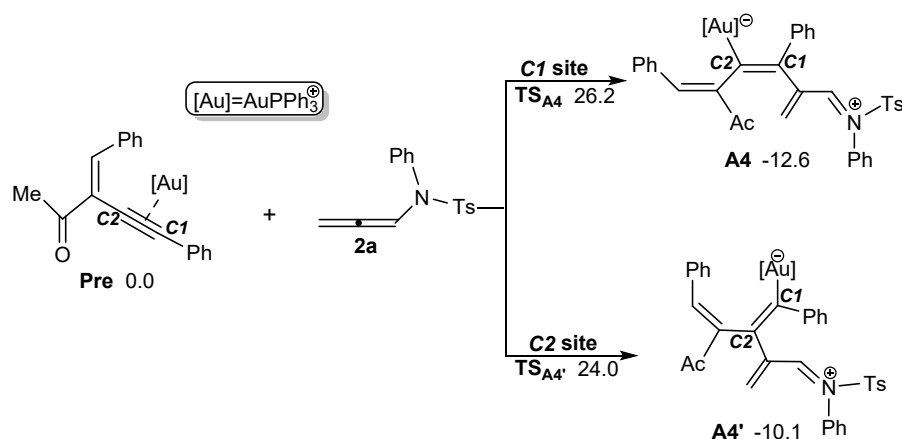


Figure S2. The cases that the unactivated *N*-allenamides **2a** competitively nucleophilic attacks the **C1/C2** site within activated alkyne **Pre**, and relative Gibbs free energy ΔG of key intermediates and transition states are shown.

Cartesian Coordinates and Thermochemical Data (Energies in Hartree)

AuPPh₃⁺

Number of imaginary frequencies: 0

Au	7.29835900	4.48443700	-1.37418800
P	8.64616700	2.96793100	-0.31869600
C	9.36803800	1.79837400	-1.50022600
C	8.56249100	1.29588400	-2.52790200
C	10.69010300	1.36558900	-1.36591800
C	9.07969800	0.36207100	-3.41654900
H	7.53377000	1.64295800	-2.62957400
C	11.20184900	0.43352500	-2.26356200
H	11.31804600	1.75190700	-0.56460100
C	10.39969100	-0.06544400	-3.28566700
H	8.45525800	-0.02666800	-4.21706700
H	12.23120200	0.09841600	-2.16389100
H	10.80533400	-0.78970100	-3.98810600
C	10.01893300	3.78755000	0.53566800
C	10.43701700	3.36726300	1.80087300
C	10.69547100	4.82054800	-0.12258200
C	11.52984800	3.98395200	2.40337100

H	9.91580500	2.56177500	2.31529700
C	11.78769800	5.42735200	0.48373300
H	10.36374000	5.14664800	-1.10886600
C	12.20241500	5.01018300	1.74730700
H	11.85479500	3.65936800	3.38880100
H	12.31242700	6.23113500	-0.02674800
H	13.05326000	5.49139000	2.22378900
C	7.72610200	2.00965200	0.91389600
C	8.03664800	0.66810700	1.15551600
C	6.74084500	2.65151200	1.67120800
C	7.35973800	-0.02461000	2.15430200
H	8.80647900	0.16600900	0.57186900
C	6.07207500	1.95356800	2.66915700
H	6.50032600	3.69656200	1.47515000
C	6.38058200	0.61611500	2.90823500
H	7.59885600	-1.06827700	2.34277600
H	5.30445900	2.45188400	3.25594900
H	5.85232000	0.07010000	3.68621800

Electronic Energy (0K) = -1171.3817704

Electronic Energy (0K) + ZPE = -1171.107591

Enthalpy (298K) = -1171.088638

Free Energy (298K) = -1171.157742

1a

Number of imaginary frequencies: 0

C	-3.76836500	1.36392300	-0.41869200
H	-2.99007300	2.11578200	-0.24583500
H	-4.22524600	1.58105600	-1.39151000
H	-4.53063900	1.44957700	0.35893100
C	-3.20722300	-0.03130200	-0.38433100

O	-3.64107800	-0.86007200	0.39840100
C	-2.10093200	-0.39654200	-1.32743200
C	-1.62768800	0.51721600	-2.21911100
H	-2.12083200	1.48899100	-2.20852200
C	-0.57605500	0.42081600	-3.21601500
C	-0.47787800	1.47020200	-4.14759900
C	0.35161500	-0.63220200	-3.30020200
C	0.48953000	1.45901200	-5.14172800
H	-1.18225100	2.29856300	-4.08345700
C	1.32398100	-0.63607100	-4.29009900
H	0.31563800	-1.43921000	-2.57524300
C	1.39402400	0.40241300	-5.21720300
H	0.54251000	2.27725700	-5.85612400
H	2.03715800	-1.45613800	-4.33769800
H	2.15676200	0.39070200	-5.99252000
C	-1.64777800	-1.73877300	-1.21588800
C	-1.31672100	-2.90207700	-1.08502400
C	-0.91220000	-4.25995100	-0.94725400
C	-1.39770500	-5.03547600	0.11829000
C	-0.02649900	-4.83893700	-1.87077400
C	-1.00183200	-6.35893800	0.25402700
H	-2.08532500	-4.58493800	0.83060600
C	0.36384500	-6.16332100	-1.72601900
H	0.34400000	-4.24063000	-2.70101400
C	-0.12106000	-6.92561000	-0.66507200
H	-1.38207700	-6.95260900	1.08215000
H	1.05031400	-6.60391100	-2.44546700
H	0.18681100	-7.96298200	-0.55565800

Electronic Energy (0K) = -768.9520093

Electronic Energy (0K) + ZPE = -768.689970

Enthalpy (298K) = -768.672375

Free Energy (298K) = -768.736774

Pre

Number of imaginary frequencies: 0

C	-2.80218000	1.63028300	0.77971200
H	-2.26685800	2.57637900	0.63676200
H	-3.56226700	1.55903100	-0.00617200
H	-3.29032700	1.64443200	1.75631100
C	-1.85393800	0.46899400	0.73655700
O	-1.65915300	-0.22746900	1.72134800
C	-1.12030000	0.17650500	-0.53349200
C	-1.17593500	1.01678300	-1.60369200
H	-1.85771600	1.86090000	-1.49864600
C	-0.47920700	0.99358100	-2.87490400
C	-0.90484300	1.91875900	-3.84571800
C	0.59556700	0.13992300	-3.18934400
C	-0.29858900	1.97824800	-5.09159500
H	-1.72709300	2.59149900	-3.60725800
C	1.20743400	0.21178000	-4.43212700
H	0.96406400	-0.57368500	-2.45727500
C	0.75997600	1.12357900	-5.38767500
H	-0.64868500	2.69419800	-5.83090900
H	2.04071500	-0.44869400	-4.65990400
H	1.24162200	1.17048100	-6.36150800
C	-0.36339300	-1.03476500	-0.51611300
C	0.15368100	-2.15754500	-0.49321900
C	0.63232400	-3.49197500	-0.69690200
C	1.07541600	-4.27167200	0.38253200
C	0.66480000	-4.01045200	-2.00036900

C	1.54635000	-5.55699600	0.15422900
H	1.04427100	-3.85811000	1.38940800
C	1.13772300	-5.29791700	-2.21426800
H	0.31698000	-3.39831400	-2.82997000
C	1.57827600	-6.07007400	-1.14135800
H	1.88932500	-6.16093600	0.99065200
H	1.16207300	-5.70148500	-3.22331200
H	1.94873400	-7.07745900	-1.31516200
Au	1.61686900	-0.81093200	0.69276000
P	3.45343100	0.00570400	1.85748600
C	4.32576100	-1.33870100	2.71313900
C	4.48185000	-2.55422400	2.03646600
C	4.85134600	-1.18299300	3.99752500
C	5.15827700	-3.60549100	2.64231500
H	4.06895800	-2.67380600	1.03351100
C	5.52499600	-2.24188200	4.60044100
H	4.73632000	-0.24032200	4.53023600
C	5.67781300	-3.44959300	3.92584800
H	5.27573100	-4.54942800	2.11519400
H	5.93088800	-2.12073800	5.60192500
H	6.20045200	-4.27470900	4.40388700
C	2.98432700	1.23074100	3.11309500
C	3.80844100	2.31679600	3.42062300
C	1.78265700	1.04463700	3.80564500
C	3.42844700	3.20995500	4.41768900
H	4.74478100	2.46789500	2.88538100
C	1.41261800	1.93745600	4.80436800
H	1.13847200	0.19983800	3.55901700
C	2.23418300	3.02078600	5.10773300
H	4.06697200	4.05741400	4.65497000

H	0.47761100	1.79128900	5.33972800
H	1.93937600	3.72266800	5.88424000
C	4.65144000	0.80177400	0.74875100
C	6.02403300	0.77234800	1.01161700
C	4.16795100	1.48958800	-0.36956600
C	6.90414500	1.43150100	0.15895800
H	6.40540800	0.23802800	1.88070700
C	5.05234500	2.14888400	-1.21557500
H	3.09683700	1.50309800	-0.57658400
C	6.41954000	2.11809800	-0.95117400
H	7.97178300	1.40709600	0.36301700
H	4.67466300	2.67996600	-2.08603800
H	7.11186600	2.62774000	-1.61710000

Electronic Energy (0K) = -1940.3798258

Electronic Energy (0K) + ZPE = -1939.842684

Enthalpy (298K) = -1939.805225

Free Energy (298K) = -1939.917599

Pre1

Number of imaginary frequencies: 0

C	-4.62612100	1.44721100	0.26155400
H	-4.56055400	2.33686100	-0.37615700
H	-5.36167800	0.77166300	-0.18628600
H	-4.96312700	1.75415300	1.25330000
C	-3.28880600	0.79411700	0.38126400
O	-2.74467500	0.80721000	1.49988700
C	-2.65689700	0.15295700	-0.78373000
C	-3.17735900	0.37881500	-2.02969200
H	-4.04381500	1.03802800	-2.06868100
C	-2.75217500	-0.07613700	-3.33392900

C	-3.37783700	0.52422300	-4.44391200
C	-1.77675700	-1.06408900	-3.56893400
C	-3.02925700	0.17311900	-5.73846500
H	-4.14143300	1.28144900	-4.27291400
C	-1.43920000	-1.41973500	-4.86554800
H	-1.29821100	-1.56596200	-2.73440200
C	-2.05623000	-0.80042100	-5.95191000
H	-3.51808100	0.65401500	-6.58192600
H	-0.68906900	-2.18915100	-5.03185200
H	-1.78196500	-1.08236300	-6.96580500
C	-1.50485600	-0.63637600	-0.52687200
C	-0.53877800	-1.33513300	-0.27749100
C	0.62613200	-2.12687400	-0.06650000
C	1.62626600	-2.17110400	-1.05191000
C	0.80820100	-2.82158200	1.13899200
C	2.79538500	-2.88350100	-0.81887600
H	1.47996500	-1.63086000	-1.98545800
C	1.98386700	-3.52561200	1.36378100
H	0.02535000	-2.79290300	1.89509700
C	2.98057100	-3.55245600	0.39039200
H	3.56986400	-2.91238100	-1.58176100
H	2.12466000	-4.04407500	2.31053300
H	3.90254900	-4.09957200	0.57257500
Au	-0.68626600	0.45288700	2.22414800
P	1.27388100	0.50082800	3.42434700
C	2.70827000	1.03632700	2.44522800
C	3.65605200	1.92878600	2.95132600
C	2.88372100	0.47784700	1.17476100
C	4.77134700	2.25826100	2.18534700
H	3.52952500	2.36660500	3.94011300

C	4.00328500	0.80288300	0.41957300
H	2.14586000	-0.22173900	0.78173400
C	4.94637100	1.69567100	0.92451100
H	5.50611800	2.95658100	2.57887100
H	4.13425300	0.35896900	-0.56516300
H	5.82051500	1.95532900	0.33182000
C	1.14121000	1.65765500	4.82232000
C	1.80658600	1.41812100	6.02804600
C	0.40326800	2.83454900	4.65504000
C	1.72870800	2.35077500	7.05770400
H	2.38552000	0.50596000	6.16518000
C	0.33573900	3.76571100	5.68459500
H	-0.12123200	3.01612200	3.71601400
C	0.99755700	3.52293500	6.88600700
H	2.24327500	2.16042800	7.99660000
H	-0.23886200	4.67901800	5.55089300
H	0.93830900	4.24880300	7.69364100
C	1.71857600	-1.10890900	4.14488300
C	3.03513400	-1.57404600	4.15227500
C	0.70412500	-1.87133300	4.73481500
C	3.33168300	-2.79964300	4.74381100
H	3.82986700	-0.98661600	3.69524300
C	1.00609600	-3.09298300	5.32420400
H	-0.32365600	-1.50655000	4.72709700
C	2.32051800	-3.55802200	5.32633500
H	4.35712700	-3.16102000	4.74758500
H	0.21557500	-3.68386400	5.78043000
H	2.55545400	-4.51557000	5.78528100

Electronic Energy (0K) = -1940.3838608

Electronic Energy (0K) + ZPE = -1939.844975

Enthalpy (298K) = -1939.808226

Free Energy (298K) = -1939.916978

Pre2

Number of imaginary frequencies: 0

C	-3.68751500	1.70513500	-0.30182500
H	-3.01497000	2.57164600	-0.33341900
H	-4.26502400	1.69687400	-1.23332900
H	-4.36890400	1.81608200	0.54411800
C	-2.92018700	0.42859300	-0.12734900
O	-3.08307200	-0.29503000	0.83524900
C	-1.90473000	0.01963700	-1.18718300
C	-1.66843100	0.83483200	-2.29507000
H	-2.24897200	1.75778800	-2.32526900
C	-0.86726900	0.60701500	-3.48945200
C	-1.02286400	1.52767300	-4.54118100
C	0.05930100	-0.44188100	-3.63951000
C	-0.29646800	1.39379400	-5.71527300
H	-1.73210900	2.34597300	-4.42878900
C	0.78961000	-0.56414100	-4.81142300
H	0.20887900	-1.15411500	-2.83320500
C	0.61334100	0.34827400	-5.85178900
H	-0.43491800	2.10933400	-6.52166600
H	1.50520800	-1.37621400	-4.91592600
H	1.18780600	0.24430000	-6.76912200
C	-1.40032100	-1.30442400	-1.04252100
C	-1.00146300	-2.44349500	-0.89053800
C	-0.50326600	-3.76948900	-0.76802400
C	-0.63962700	-4.47390800	0.43878800
C	0.13286100	-4.38050400	-1.86145100

C	-0.14115600	-5.76454300	0.54617000
H	-1.13703500	-3.99690300	1.28020100
C	0.62645700	-5.67160900	-1.74293700
H	0.22749700	-3.83277500	-2.79732400
C	0.49115700	-6.36453800	-0.54112300
H	-0.24730800	-6.30659200	1.48271900
H	1.11770500	-6.14229100	-2.59112700
H	0.87938700	-7.37648400	-0.45200700
Au	-0.10310300	1.34743000	-0.51983200
P	1.69077300	2.39903000	0.53970900
C	3.25961200	1.57734400	0.13177000
C	4.17952900	1.20422400	1.11323800
C	3.53189400	1.32211100	-1.21829000
C	5.36644700	0.57646700	0.74263000
H	3.97292000	1.39798800	2.16435300
C	4.72164300	0.70462000	-1.58062400
H	2.81211600	1.61274600	-1.98528700
C	5.63741400	0.32822300	-0.59876900
H	6.07993500	0.28119200	1.50796900
H	4.93249200	0.50925800	-2.62931800
H	6.56440900	-0.16438800	-0.88254700
C	1.50754400	2.37846800	2.34405100
C	2.09476700	3.36569100	3.14172700
C	0.79861700	1.32819500	2.93666500
C	1.97217900	3.29685900	4.52528300
H	2.64593700	4.18676700	2.68545700
C	0.68339200	1.26399000	4.32077700
H	0.33570400	0.56384900	2.31046400
C	1.26875100	2.24828000	5.11308900
H	2.42639200	4.06551600	5.14569200

H	0.13086600	0.44835900	4.78059200
H	1.17256400	2.20031000	6.19513900
C	1.85122200	4.13383500	0.02685100
C	3.10056400	4.75083000	-0.08519500
C	0.68407500	4.86359700	-0.22263800
C	3.17590500	6.09331100	-0.44371300
H	4.01164900	4.18607400	0.10875400
C	0.76671200	6.20483700	-0.57689000
H	-0.28882000	4.37711300	-0.13704800
C	2.01266400	6.81749100	-0.69025000
H	4.14735400	6.57332900	-0.53336400
H	-0.14103100	6.77037400	-0.77287800
H	2.07686600	7.86503000	-0.97486500

Electronic Energy (0K) = -1940.3712537

Electronic Energy (0K) + ZPE = -1939.834724

Enthalpy (298K) = -1939.797139

Free Energy (298K) = -1939.912476

2a

Number of imaginary frequencies: 0

C	7.30590400	6.21156000	-1.66540500
C	6.00304300	6.18991000	-1.61786800
C	4.69261300	6.20390400	-1.58814900
H	4.13107900	7.01245000	-2.05393700
N	3.87752000	5.16634500	-1.06379500
C	4.48641200	4.06107900	-0.37725600
C	5.27680100	4.27158100	0.75407700
C	4.27121800	2.77374500	-0.86290700
C	5.85930300	3.18268400	1.39306600
H	5.43057900	5.28297100	1.12767000

C	4.85294500	1.68928600	-0.21521600
H	3.64653700	2.64018400	-1.74264200
C	5.64802600	1.89338800	0.90967700
H	6.47710200	3.34211300	2.27357600
H	4.68746300	0.68307700	-0.59282600
H	6.10587200	1.04441300	1.41238000
O	1.88283100	6.66370300	-1.44722800
O	1.57210000	4.36269200	-0.43659300
S	2.31937500	5.60561500	-0.54545300
C	2.53481200	6.28232000	1.07352400
C	2.34318100	5.46686400	2.18489200
C	2.98934500	7.59541800	1.20536100
C	2.60404800	5.98258100	3.44877100
H	1.99096200	4.44599100	2.05929000
C	3.24907500	8.08806400	2.47467400
H	3.12603200	8.22382100	0.32827600
C	3.06273100	7.29160600	3.61265200
H	2.45015000	5.35721100	4.32628600
H	3.60019000	9.11212200	2.59336900
C	3.34391300	7.84891800	4.97236400
H	2.67491200	8.68871400	5.19784900
H	3.21287400	7.09328400	5.75322200
H	4.36849100	8.23488300	5.03660600
H	7.89950500	6.68193900	-0.87981200
H	7.86024300	5.75765900	-2.48835000

Electronic Energy (0K) = -1221.4098203

Electronic Energy (0K) + ZPE = -1221.137969

Enthalpy (298K) = -1221.118516

Free Energy (298K) = -1221.185763

B

Number of imaginary frequencies: 0

C	4.53068600	3.98825200	3.90100800
C	4.74571000	3.77668600	2.57596800
C	3.81974600	4.52443500	1.78212900
H	3.19221100	5.28284200	2.26475300
N	3.63204200	4.42737900	0.48501100
C	4.21185700	3.43989300	-0.38603600
C	5.25418500	3.79784900	-1.23612300
C	3.65329500	2.16262700	-0.40225200
C	5.75379100	2.84241600	-2.11633200
H	5.65971400	4.80647100	-1.20202300
C	4.15743700	1.22213400	-1.29227700
H	2.82918800	1.92478400	0.26850700
C	5.20273100	1.56334800	-2.14837200
H	6.57486600	3.10108900	-2.78079100
H	3.73137100	0.22235100	-1.32017900
H	5.58942400	0.82531000	-2.84772900
O	3.13066700	6.07701500	-1.44128500
O	1.95637300	6.37088700	0.78758200
S	2.42882600	5.53199700	-0.29789000
C	1.21590800	4.37686500	-0.80053600
C	0.30348900	3.91408300	0.14727800
C	1.25851000	3.87546800	-2.10177900
C	-0.58980800	2.92395200	-0.23085400
H	0.29102300	4.32025500	1.15650600
C	0.35231500	2.88824000	-2.45382700
H	1.99192500	4.24903000	-2.81264500
C	-0.57693200	2.39692900	-1.52817000
H	-1.31329300	2.54766100	0.48943200

H	0.36497500	2.48293100	-3.46376400
C	-1.54620500	1.33452700	-1.93328200
H	-2.29741400	1.74129400	-2.62208600
H	-2.07287200	0.91686500	-1.07005100
H	-1.03957300	0.51927000	-2.46232000
H	5.13585400	3.50528100	4.66666600
H	3.73207400	4.63898000	4.26972800
Au	6.29908600	2.57486400	1.86330400
P	8.12654500	1.24844300	1.15446400
C	9.46910100	2.23284000	0.41434700
C	9.17379500	3.49527900	-0.10959600
C	10.77468800	1.73699700	0.33148100
C	10.17226000	4.25018600	-0.71790900
H	8.15855800	3.88715400	-0.03400900
C	11.76968500	2.49539600	-0.27446600
H	11.01335600	0.75484500	0.73742200
C	11.46844900	3.75042400	-0.79981200
H	9.93863800	5.23260700	-1.12154100
H	12.78325600	2.10642000	-0.33627600
H	12.24972500	4.34192500	-1.27150000
C	8.89830900	0.33603700	2.53278400
C	9.41914500	-0.95277300	2.39134600
C	9.00229500	0.99392400	3.76367500
C	10.03651600	-1.57445000	3.47311500
H	9.34721500	-1.47337900	1.43747600
C	9.62605100	0.37162900	4.83892000
H	8.59236700	1.99869200	3.87457000
C	10.14126800	-0.91413700	4.69422700
H	10.43937300	-2.57818900	3.35919500
H	9.70466700	0.88851500	5.79248900

H	10.62428800	-1.40412900	5.53649000
C	7.68140600	-0.01196600	-0.08597400
C	8.34434400	-0.12944700	-1.30886500
C	6.62549300	-0.88021400	0.21688500
C	7.95826200	-1.11339300	-2.21692000
H	9.16281600	0.54429600	-1.55698600
C	6.25237300	-1.86795200	-0.68641200
H	6.09836200	-0.78338500	1.16718800
C	6.91765000	-1.98308300	-1.90649800
H	8.47811300	-1.20165500	-3.16809900
H	5.43704800	-2.54477700	-0.44147000
H	6.62260100	-2.75345300	-2.61512400

Electronic Energy (0K) = -2392.8451548

Electronic Energy (0K) + ZPE = -2392.296662

Enthalpy (298K) = -2392.257890

Free Energy (298K) = -2392.372344

B1

Number of imaginary frequencies: 0

C	6.15832100	6.49584700	0.26055100
C	4.97789200	6.51326600	-0.34306400
C	3.83693200	7.30841400	-0.40543000
H	2.96513600	7.05522500	0.20433200
N	3.67007900	8.33439500	-1.25120500
C	4.74077800	8.81274300	-2.08581300
C	4.90957100	8.29122900	-3.36638100
C	5.60776800	9.76788500	-1.56590900
C	5.97543100	8.74002800	-4.13963200
H	4.21731600	7.54223000	-3.74817200
C	6.67096500	10.20555500	-2.34737600

H	5.44331800	10.15203000	-0.56149700
C	6.85387900	9.69256000	-3.62977600
H	6.11846700	8.33854000	-5.14004000
H	7.35844600	10.94975000	-1.95385200
H	7.68751800	10.03782200	-4.23636500
O	1.32893100	8.60518700	-0.29168000
O	2.25824900	10.34993300	-1.89001500
S	2.04654000	8.97117400	-1.50021400
C	1.44476300	8.03350100	-2.85897300
C	1.51294500	8.57368200	-4.14045000
C	0.93366800	6.75385900	-2.62259900
C	1.04971700	7.81162400	-5.20540500
H	1.91024500	9.57364400	-4.29572900
C	0.48157900	6.01107200	-3.70238500
H	0.86651900	6.35579900	-1.61158400
C	0.53283500	6.52775200	-5.00558900
H	1.08315400	8.22087600	-6.21326000
H	0.07833400	5.01135200	-3.53734300
C	0.06996200	5.70326800	-6.16258200
H	-0.92336200	5.27731700	-5.97843400
H	0.03071200	6.29081500	-7.08513800
H	0.75281100	4.85866600	-6.32994300
H	6.87626400	5.69593700	0.09328700
H	6.44984100	7.28467600	0.95551300
Au	4.30950100	5.00340600	-1.71212200
P	3.81178600	3.31594100	-3.28350500
C	4.74614800	1.79260900	-2.96160100
C	5.95961900	1.88356900	-2.27222600
C	4.29357100	0.55043800	-3.41724900
C	6.71782500	0.73998500	-2.04504100

H	6.30255200	2.85260900	-1.90610700
C	5.05331800	-0.59033900	-3.18237300
H	3.34817600	0.47413000	-3.95335100
C	6.26378400	-0.49517000	-2.49948100
H	7.65961600	0.81271800	-1.50654400
H	4.69887100	-1.55621700	-3.53398300
H	6.85245600	-1.39053000	-2.31416400
C	4.23169400	3.85595000	-4.97080200
C	5.02505400	3.09284100	-5.82858700
C	3.74353900	5.09863500	-5.39443500
C	5.32926000	3.57421900	-7.10029400
H	5.40993700	2.12644000	-5.50776700
C	4.04152300	5.56904700	-6.66697700
H	3.11696600	5.69440600	-4.72657000
C	4.84013700	4.80703000	-7.51932100
H	5.95120900	2.97907600	-7.76458700
H	3.65418600	6.53267500	-6.99316200
H	5.08204000	5.17738700	-8.51272500
C	2.05218700	2.85610500	-3.31287800
C	1.36375800	2.81723200	-2.09498000
C	1.38618700	2.53913100	-4.49963700
C	0.01927600	2.46509100	-2.06548700
H	1.88520100	3.06683000	-1.16988200
C	0.03792700	2.19294500	-4.46514600
H	1.91648200	2.56438100	-5.45124500
C	-0.64505000	2.15888800	-3.25197700
H	-0.51250800	2.43600800	-1.11752300
H	-0.48042300	1.95114000	-5.39035700
H	-1.69879300	1.89145100	-3.23033700

Electronic Energy (0K) = -2392.851772

Electronic Energy (0K) + ZPE = -2392.301675

Enthalpy (298K) = -2392.263880

Free Energy (298K) = -2392.371621

B1'

Number of imaginary frequencies: 0

C	7.33004400	6.51129100	-1.47770900
C	6.08422600	6.11597800	-1.26444100
C	4.81434300	6.15363200	-1.82204700
H	4.49123200	5.28555700	-2.40408900
N	3.84493200	7.07409500	-1.64894000
C	2.47195700	6.70684700	-1.88420900
C	1.92336500	5.66693200	-1.13720800
C	1.72932400	7.37747100	-2.85114700
C	0.60749800	5.28413400	-1.37191400
H	2.53182700	5.16987500	-0.38143200
C	0.41257500	6.99148700	-3.07146300
H	2.18513900	8.18260700	-3.42137400
C	-0.14658700	5.94841200	-2.33600500
H	0.17131300	4.46713400	-0.80151200
H	-0.17722800	7.50435800	-3.82668300
H	-1.17640800	5.65099700	-2.51802300
O	5.39347300	9.12357400	-1.43857800
O	2.92245000	9.32371200	-0.92741200
S	4.18003900	8.60825800	-0.83417900
C	4.47420100	8.14447100	0.83796700
C	3.39498400	7.72616000	1.61712600
C	5.76024600	8.26150100	1.36458400
C	3.61993400	7.42339700	2.95353300
H	2.39472800	7.65329400	1.19337000

C	5.95691900	7.96287600	2.70516400
H	6.58167100	8.59418000	0.73539700
C	4.89585200	7.54382600	3.51759300
H	2.78797500	7.09923200	3.57711100
H	6.95117700	8.06469000	3.13861800
C	5.13882900	7.22995100	4.95919400
H	5.60016200	8.08187700	5.47305500
H	4.21075200	6.97446600	5.48016600
H	5.83529700	6.38450600	5.06294800
H	8.13754800	6.25632400	-0.79405000
H	7.58979400	7.11155900	-2.35037600
Au	5.54243900	4.84057100	0.38804600
P	5.17414100	3.48132500	2.28840100
C	5.16373100	1.70061000	1.90861000
C	6.11766200	1.22234100	1.00348900
C	4.26748200	0.81362000	2.51059000
C	6.17776900	-0.13434900	0.70824300
H	6.81231400	1.91820100	0.53110700
C	4.32748700	-0.54266400	2.20411300
H	3.52115000	1.17809800	3.21500300
C	5.27982500	-1.01606000	1.30599800
H	6.91950800	-0.50332700	0.00401200
H	3.62642400	-1.23150000	2.66937900
H	5.32007100	-2.07618100	1.06725100
C	6.46267400	3.72733100	3.54683400
C	6.50849800	2.93125500	4.69790300
C	7.41905900	4.72965700	3.35747700
C	7.48648900	3.15852200	5.65862100
H	5.77812200	2.13559200	4.84333000
C	8.40101500	4.94908400	4.31966200

H	7.39391600	5.33810800	2.45172000
C	8.43017800	4.16757500	5.47054400
H	7.51617700	2.54314300	6.55437600
H	9.14315000	5.72955300	4.16831000
H	9.19580200	4.33769900	6.22377200
C	3.56028700	3.84531600	3.05365600
C	2.43111200	3.77401200	2.22644000
C	3.41601700	4.24313200	4.38323100
C	1.17677900	4.10302400	2.72331900
H	2.53620200	3.45075200	1.18938400
C	2.15477700	4.57040800	4.87835500
H	4.28355000	4.30701500	5.03781400
C	1.03819700	4.50633000	4.05127600
H	0.30464900	4.04580800	2.07595800
H	2.05059500	4.88058100	5.91574100
H	0.05708400	4.76905200	4.43953200

Electronic Energy (0K) = -2392.8484224

Electronic Energy (0K) + ZPE = -2392.298297

Enthalpy (298K) = -2392.260464

Free Energy (298K) = -2392.368490

B2

Number of imaginary frequencies: 0

C	1.63752500	2.85189800	-0.07726700
C	0.30554700	2.73263600	-0.18465900
C	-0.98813600	2.97061100	-0.25190100
H	-1.28569900	4.01589400	-0.35118000
N	-2.03333100	2.04452500	-0.28355300
C	-1.91194400	0.76704300	0.35909200
C	-1.51690300	0.69080000	1.69851900

C	-2.24835000	-0.38500400	-0.34976400
C	-1.44921400	-0.55001100	2.32113600
H	-1.27846400	1.60287000	2.24442300
C	-2.18463200	-1.62209100	0.28531600
H	-2.56943900	-0.29688700	-1.38486700
C	-1.78413000	-1.70520900	1.61610500
H	-1.14592500	-0.61468600	3.36357400
H	-2.44432100	-2.52330900	-0.26630900
H	-1.73381600	-2.67399000	2.10891800
O	-3.47497400	3.94665700	-1.11275700
O	-4.44393900	1.61101800	-0.91309000
S	-3.62507800	2.69101700	-0.39242300
C	-4.08650200	3.01628000	1.27795200
C	-4.75496700	2.03421300	2.00563900
C	-3.69357000	4.22020000	1.86379100
C	-5.03715700	2.27354300	3.34408100
H	-5.05033000	1.10194200	1.53013600
C	-3.98439900	4.43593900	3.20206600
H	-3.18316000	4.98188000	1.27863200
C	-4.65772100	3.46966100	3.96008400
H	-5.56207000	1.51750000	3.92499300
H	-3.69037900	5.37238400	3.67301700
C	-4.98804200	3.73007000	5.39500000
H	-4.18399200	4.27783600	5.89844900
H	-5.89481300	4.34318000	5.47746000
H	-5.17184600	2.79917600	5.94099400
H	2.27208500	2.95554100	-0.96152700
H	2.11835900	3.00833200	0.89127000
Au	1.25411900	0.59322800	-0.26481100
P	1.92561500	-1.64259600	-0.61558700

C	3.73375400	-1.72932100	-0.81897500
C	4.36917100	-0.69454300	-1.51389100
C	4.48082200	-2.80917500	-0.34055200
C	5.74108300	-0.74180000	-1.73085200
H	3.78468900	0.14904500	-1.88343900
C	5.85513300	-2.84777200	-0.55607600
H	3.99274500	-3.61925600	0.19929700
C	6.48415500	-1.81701400	-1.24856200
H	6.23224700	0.06489800	-2.26962900
H	6.43552600	-3.68751000	-0.18149000
H	7.55868200	-1.85007200	-1.41207000
C	1.20880000	-2.31942800	-2.14170900
C	1.69547500	-3.50602000	-2.70312400
C	0.15782500	-1.63709300	-2.76081700
C	1.11784400	-4.01013600	-3.86214300
H	2.52373200	-4.03554300	-2.23354300
C	-0.41781500	-2.14647400	-3.92079400
H	-0.20510400	-0.70176100	-2.33136100
C	0.06063400	-3.33305400	-4.46775500
H	1.49604900	-4.93296900	-4.29525400
H	-1.23530200	-1.61312100	-4.40006800
H	-0.38602900	-3.73130700	-5.37586000
C	1.51502600	-2.76625800	0.75504700
C	0.81147100	-3.95704700	0.56762500
C	1.91678300	-2.38878000	2.04240600
C	0.51531600	-4.76636300	1.66210200
H	0.48628100	-4.25549200	-0.42738700
C	1.62120300	-3.20127000	3.12942200
H	2.46001300	-1.45472700	2.19222600
C	0.91940800	-4.39108300	2.93930500

H	-0.03213100	-5.69374600	1.51173400
H	1.93617400	-2.90540800	4.12728900
H	0.68491800	-5.02419900	3.79181700

Electronic Energy (0K) = -2392.8402831

Electronic Energy (0K) + ZPE = -2392.291920

Enthalpy (298K) = -2392.253362

Free Energy (298K) = -2392.365055

B2'

Number of imaginary frequencies: 0

C	6.70914600	6.65816400	-3.55195100
C	5.71172200	6.51391200	-2.66512100
C	4.71791000	6.57838900	-1.79994000
H	4.41366100	5.69827000	-1.23472100
N	4.02342400	7.74670200	-1.47776900
C	4.25073600	8.95685900	-2.21862100
C	3.98216600	9.00167400	-3.58781500
C	4.73031800	10.07675400	-1.54520100
C	4.21203100	10.18076100	-4.28747000
H	3.58764100	8.11863500	-4.09016000
C	4.95016900	11.25406100	-2.25251000
H	4.92146900	10.01215300	-0.47691300
C	4.69494400	11.30461700	-3.62041700
H	4.00564000	10.22417600	-5.35403800
H	5.32368300	12.13316300	-1.73326600
H	4.87101700	12.22637200	-4.17004500
O	2.53929300	6.28758100	-0.04281300
O	2.22615300	8.80418400	-0.05049700
S	2.47811700	7.55827800	-0.75177100
C	1.36998300	7.42510100	-2.11682500

C	0.74717000	8.57203500	-2.60296300
C	1.22757400	6.19115300	-2.75261500
C	-0.03536700	8.47305800	-3.74592200
H	0.87674200	9.52451900	-2.09485500
C	0.44105600	6.11589700	-3.89222300
H	1.71232800	5.30221400	-2.35444600
C	-0.19735800	7.25175100	-4.40656100
H	-0.52854500	9.36108700	-4.13695500
H	0.31289700	5.15919400	-4.39596100
C	-1.06220500	7.15004300	-5.62237700
H	-2.07099900	6.81245300	-5.35131500
H	-1.16635900	8.11751300	-6.12400100
H	-0.66358800	6.42499600	-6.34023000
H	7.69249100	7.02180900	-3.24445200
Au	6.71606700	4.46063900	-2.87969500
P	7.16837000	2.17266700	-2.58662700
H	6.52315200	6.58354800	-4.62626400
C	8.33095800	1.57265100	-3.84895200
C	8.05411500	1.87819900	-5.18746900
C	9.46162900	0.82129600	-3.52391000
C	8.90143000	1.42828400	-6.19159800
H	7.16963400	2.46419700	-5.44093700
C	10.31110100	0.38024400	-4.53579700
H	9.68368200	0.57956900	-2.48602200
C	10.03225300	0.68138600	-5.86471400
H	8.68288700	1.66430500	-7.23024900
H	11.19291900	-0.20266100	-4.28103200
H	10.69893300	0.33494000	-6.65082000
C	7.88821300	1.82315800	-0.95797500
C	7.77727100	0.55779100	-0.37212000

C	8.58723700	2.83974600	-0.30017000
C	8.36590900	0.31691300	0.86438400
H	7.23356000	-0.23786800	-0.87994400
C	9.17478400	2.59181100	0.93592100
H	8.66620600	3.82673900	-0.75767300
C	9.06114000	1.33206100	1.51745800
H	8.27718700	-0.66563600	1.32142100
H	9.71391300	3.38509000	1.44782700
H	9.51465800	1.14072700	2.48724900
C	5.66795600	1.15851700	-2.73873000
C	5.69239200	-0.10503700	-3.33588400
C	4.47434700	1.65845000	-2.20733800
C	4.52590800	-0.86144200	-3.39622700
H	6.61919700	-0.49838900	-3.75132100
C	3.31383100	0.89637000	-2.26720900
H	4.45759800	2.64711600	-1.74679200
C	3.34021300	-0.36212400	-2.86464600
H	4.54451300	-1.84369600	-3.86200600
H	2.38676400	1.28736700	-1.85478500
H	2.43061400	-0.95569200	-2.91702900

Electronic Energy (0K) = -2392.8332695

Electronic Energy (0K) + ZPE = -2392.284996

Enthalpy (298K) = -2392.246042

Free Energy (298K) = -2392.361493

TS_A

Number of imaginary frequencies: 1

C	-3.42321100	0.57809100	-2.50711300
C	-2.55917500	1.13390600	-1.73499900
C	-1.23655800	1.44933200	-2.24718300

C	-1.17947500	1.11430900	-3.69113800
O	-2.17837400	0.57987500	-4.18171200
C	-4.62710200	-0.06076500	-2.91232500
C	-5.21275700	-1.01660200	-2.06177600
C	-5.24792400	0.27068300	-4.12779400
C	-6.41722400	-1.60648000	-2.41599200
H	-4.71507800	-1.27411200	-1.12862100
C	-6.43888700	-0.34445300	-4.48053100
H	-4.78013100	0.99994700	-4.78369300
C	-7.02686400	-1.27562100	-3.62471300
H	-6.87487000	-2.33709500	-1.75399200
H	-6.91746200	-0.09461300	-5.42388600
H	-7.96438900	-1.75024700	-3.90415300
H	0.29542100	2.44654200	-4.47774600
C	0.02646100	1.38514600	-4.52218200
H	-0.16780500	1.10187300	-5.55803900
H	0.88232000	0.81440200	-4.14456000
C	-0.18349600	2.00831800	-1.60110400
C	-0.06031300	2.30826500	-0.18296900
C	0.58285900	3.49587500	0.19969000
C	-0.53781700	1.44164100	0.81490700
C	0.68128900	3.84410500	1.54073000
H	0.98630500	4.15323900	-0.56891600
C	-0.41139500	1.78135500	2.15803700
H	-0.95757000	0.47641700	0.53654900
C	0.17925000	2.98978500	2.52153200
H	1.16316500	4.77692500	1.82329600
H	-0.78005100	1.09919000	2.92306700
H	0.26655900	3.25580700	3.57285600
Au	-3.49249300	1.66657500	0.09395700

P	-4.54756500	2.25861600	2.10300700
H	0.67315300	2.29649000	-2.21383500
C	-6.26421600	1.66166200	2.18326400
C	-6.96828300	1.51622500	0.98318600
C	-6.88702900	1.35280800	3.39695500
C	-8.28514100	1.07060800	0.99638200
H	-6.47738300	1.75115200	0.03751500
C	-8.20529500	0.90867200	3.40444900
H	-6.34147900	1.45451400	4.33457400
C	-8.90247400	0.76635100	2.20695100
H	-8.82513200	0.95237100	0.05973400
H	-8.68869100	0.66866800	4.34854800
H	-9.93055000	0.41211300	2.21787900
C	-4.56903500	4.05520200	2.37569500
C	-5.53129100	4.67079400	3.18175100
C	-3.54732400	4.81884600	1.80193400
C	-5.46738900	6.04115900	3.41003500
H	-6.32995100	4.08306000	3.63212700
C	-3.48386700	6.18760200	2.03963000
H	-2.80652500	4.33443100	1.16302100
C	-4.44481200	6.79749600	2.84204400
H	-6.21864500	6.51977800	4.03360900
H	-2.68872400	6.77839000	1.59118900
H	-4.39971600	7.86890800	3.02295200
C	-3.69057400	1.53889500	3.54175500
C	-3.46803700	0.15596000	3.54424200
C	-3.21036900	2.32073100	4.59338600
C	-2.77674300	-0.43665500	4.59317500
H	-3.83636000	-0.45718000	2.72043400
C	-2.51008800	1.72213300	5.63910600

H	-3.37424200	3.39709800	4.59692700
C	-2.29341400	0.34830900	5.64023800
H	-2.60875600	-1.51101200	4.59267700
H	-2.13590100	2.33511600	6.45575600
H	-1.74673200	-0.11568800	6.45782800

Electronic Energy (0K) = -1940.3753494

Electronic Energy (0K) + ZPE = -1939.838128

Enthalpy (298K) = -1939.802102

Free Energy (298K) = -1939.908545

A

Number of imaginary frequencies: 0

C	-0.14089400	-1.24843800	-1.81156300
C	0.28190200	-0.45307400	-0.79843100
C	1.50546000	0.16137500	-1.30919700
C	1.69160700	-0.31625800	-2.63632500
O	0.74564300	-1.16352100	-2.92934400
C	-1.29046400	-2.10818900	-2.04855100
C	-2.09510000	-2.53236100	-0.97917000
C	-1.62642700	-2.51816700	-3.34708900
C	-3.21774700	-3.31573100	-1.20837100
H	-1.82864700	-2.24953900	0.03929200
C	-2.74651400	-3.31029800	-3.56853300
H	-1.01165100	-2.20606500	-4.18746800
C	-3.55027500	-3.70734900	-2.50372000
H	-3.83057800	-3.63210000	-0.36676200
H	-2.99463300	-3.61444700	-4.58280700
H	-4.42767700	-4.32471900	-2.68120400
H	3.25149100	0.86440200	-3.47743500
C	2.74877500	-0.09413900	-3.62808300

H	2.33328700	-0.14130100	-4.63895600
H	3.50536600	-0.88630400	-3.54521200
C	2.38756900	1.07657300	-0.76724800
C	2.49641900	1.51236400	0.59212600
C	2.97225500	2.81705300	0.83872100
C	2.16805300	0.68318700	1.68603700
C	3.03026100	3.30778200	2.13248200
H	3.26036700	3.44199300	-0.00443600
C	2.27456900	1.16691300	2.98118400
H	1.89311700	-0.35434100	1.51151600
C	2.67712200	2.48392500	3.20328300
H	3.36514500	4.32550800	2.31404400
H	2.03667100	0.51804000	3.82204300
H	2.73791100	2.86266900	4.22129300
Au	-0.76869600	0.04167300	0.92879800
P	-1.92943200	0.65059800	2.88992700
H	3.07726800	1.55643800	-1.46593500
C	-3.49463800	-0.25256700	3.11593600
C	-3.97986300	-0.60448000	4.37894600
C	-4.23273800	-0.57824500	1.97282500
C	-5.19437900	-1.27365600	4.49292900
H	-3.41023300	-0.35545900	5.27353500
C	-5.44906800	-1.24123400	2.09234600
H	-3.84774800	-0.31048800	0.98764100
C	-5.92769900	-1.59140900	3.35248800
H	-5.56801100	-1.54942000	5.47625200
H	-6.01840200	-1.49236500	1.20042600
H	-6.87519800	-2.11694700	3.44686000
C	-2.33181000	2.42369200	2.96513100
C	-3.45714800	2.90389200	3.64042600

C	-1.44432300	3.32412000	2.36518000
C	-3.69050700	4.27358600	3.71286000
H	-4.15347300	2.21015700	4.10932100
C	-1.67756700	4.69242300	2.44748900
H	-0.57076600	2.94790200	1.83002200
C	-2.80184800	5.16637200	3.11914600
H	-4.56988200	4.64414500	4.23433700
H	-0.98528000	5.38898000	1.98037600
H	-2.98924000	6.23614900	3.17599900
C	-0.93552500	0.30914200	4.38106600
C	-0.36535900	-0.96456400	4.49992300
C	-0.70059200	1.26881900	5.36714900
C	0.42594000	-1.27556700	5.59881200
H	-0.54524600	-1.71350900	3.72706400
C	0.10185900	0.95528900	6.46237400
H	-1.14040000	2.26139800	5.28280400
C	0.66352100	-0.31218900	6.57919500
H	0.86263000	-2.26734600	5.68972400
H	0.28303200	1.70583600	7.22827000
H	1.28742400	-0.55311300	7.43676300

Electronic Energy (0K) = -1940.402576

Electronic Energy (0K) + ZPE = -1939.862004

Enthalpy (298K) = -1939.826519

Free Energy (298K) = -1939.931035

TS_B

Number of imaginary frequencies: 1

C	8.33632500	6.51580400	-0.62678200
C	7.13574900	6.10220800	-1.07550000
C	5.82826300	6.46121400	-1.08679000

H	5.57382700	7.47237700	-1.41005700
N	4.75114800	5.64326100	-0.90939300
C	4.85498900	4.36004000	-0.28324000
C	5.26472800	4.27358500	1.04943700
C	4.50731600	3.21793800	-1.00634400
C	5.33582000	3.02549400	1.65771500
H	5.50682200	5.18434600	1.59638100
C	4.57441500	1.97509000	-0.38378500
H	4.17440200	3.31897600	-2.03650100
C	4.99223100	1.87970300	0.94163500
H	5.65139100	2.94742400	2.69535700
H	4.30768100	1.07976000	-0.94107800
H	5.05538400	0.90440200	1.42037800
O	3.34621900	7.55568300	-1.81689800
O	2.35007300	5.22938900	-1.65539300
S	3.15415200	6.30370400	-1.10385600
C	2.66850400	6.61340300	0.55861100
C	1.96547500	5.63455600	1.25685900
C	3.08093400	7.79950000	1.16605700
C	1.66485900	5.86174100	2.59320800
H	1.66209500	4.71507600	0.76185700
C	2.76813800	8.00345800	2.50065400
H	3.62642100	8.55279600	0.60150300
C	2.05906400	7.04139800	3.23175500
H	1.11559700	5.10872500	3.15504400
H	3.07567200	8.92502900	2.99159100
C	1.70959600	7.28843800	4.66418500
H	2.50888200	7.82714500	5.18451900
H	0.80449200	7.90497600	4.73917000
H	1.51278600	6.35286700	5.19739400

H	9.26331100	6.29001600	-1.15577600
H	8.44721400	7.06002800	0.31486000
Au	7.78919000	4.01328900	-1.25648300
P	8.59938300	1.82489400	-1.55141900
C	10.41698300	1.80629200	-1.68761500
C	11.03214700	2.84271600	-2.39852900
C	11.19382100	0.77983100	-1.14363400
C	12.41160800	2.84812600	-2.56831700
H	10.42571800	3.64598300	-2.81940700
C	12.57544100	0.79434800	-1.31082200
H	10.72259500	-0.03104600	-0.59030000
C	13.18338000	1.82550100	-2.02114800
H	12.88619500	3.65564400	-3.12065600
H	13.17784700	-0.00378700	-0.88361600
H	14.26343300	1.83442500	-2.14717800
C	7.98047000	1.04931200	-3.07413300
C	8.57190300	-0.11362900	-3.58202100
C	6.90140600	1.63054400	-3.74497300
C	8.07313700	-0.69246300	-4.74265400
H	9.42021000	-0.56725200	-3.07004300
C	6.40597100	1.04735400	-4.90733500
H	6.46187200	2.55016600	-3.35700100
C	6.99061800	-0.11371900	-5.40333000
H	8.53178200	-1.59625900	-5.13654900
H	5.56876200	1.50606200	-5.42787600
H	6.60594800	-0.56732800	-6.31385200
C	8.18941600	0.71955300	-0.16304600
C	7.52216800	-0.49380700	-0.33800400
C	8.54828000	1.13651300	1.12488100
C	7.22017400	-1.28552900	0.76804000

H	7.23218500	-0.82481500	-1.33356900
C	8.25371800	0.33884500	2.22300000
H	9.06189000	2.08865300	1.26577700
C	7.58739400	-0.87311500	2.04492700
H	6.70023700	-2.23007100	0.62663100
H	8.54037800	0.66403500	3.22037300
H	7.35225400	-1.49451300	2.90588900

Electronic Energy (0K) = -2392.8344297

Electronic Energy (0K) + ZPE = -2392.286971

Enthalpy (298K) = -2392.248767

Free Energy (298K) = -2392.360648

TS_c

Number of imaginary frequencies: 1

C	-0.68908400	4.05779300	-3.73505200
C	-0.85241200	4.15261800	-2.43501000
C	-1.23063700	4.85497800	-1.34499500
H	-0.50280300	5.09417400	-0.56788700
N	-2.52211300	5.14116500	-1.01463800
C	-3.56914500	5.20675300	-1.99537100
C	-4.66435000	4.35343100	-1.89419400
C	-3.47847700	6.14662400	-3.02193600
C	-5.68228100	4.44039100	-2.83772100
H	-4.69539300	3.62448700	-1.08561000
C	-4.49874800	6.22213100	-3.96268500
H	-2.61797500	6.81390700	-3.06377300
C	-5.59850000	5.37093100	-3.87059100
H	-6.53748900	3.77156600	-2.76719800
H	-4.43706200	6.95111200	-4.76682000
H	-6.39449900	5.43524800	-4.60868000

O	-4.11792700	5.45714700	0.95361200
O	-1.61066900	5.67332900	1.30040300
S	-2.81260400	5.91747900	0.51848200
C	-2.91097300	7.61327500	0.05475300
C	-1.72547200	8.31357200	-0.17576900
C	-4.15866600	8.18363300	-0.17892300
C	-1.80649200	9.61236100	-0.64809100
H	-0.75950600	7.85169700	0.01752600
C	-4.21451600	9.49052800	-0.64705600
H	-5.06624800	7.61383700	0.00522900
C	-3.04746400	10.21695500	-0.89577200
H	-0.89382000	10.17740900	-0.82986500
H	-5.18178000	9.95562700	-0.82716800
C	-3.10564500	11.61558300	-1.42033600
H	-4.13273800	11.99080400	-1.45677600
H	-2.51093800	12.29445900	-0.79800200
H	-2.68979700	11.66979300	-2.43429000
H	-0.75761900	4.93414400	-4.38177600
H	-0.44774000	3.11338600	-4.22460900
C	-3.23660600	0.41373800	-2.26175500
C	-2.57330400	1.21432800	-1.37741000
C	-1.25737800	1.38638400	-1.97561500
C	-1.24152700	0.66691700	-3.17235300
O	-2.41068000	0.06475700	-3.34107700
C	-4.57351100	-0.16910100	-2.33858500
C	-4.83620900	-1.21712600	-3.23395800
C	-5.62740700	0.29143700	-1.53135800
C	-6.09932600	-1.79293000	-3.30458800
H	-4.03958400	-1.58769000	-3.87399100
C	-6.88662900	-0.28998400	-1.60252300

H	-5.45837800	1.12128200	-0.84502700
C	-7.13046900	-1.33776600	-2.48775800
H	-6.27609900	-2.60752500	-4.00367400
H	-7.68463300	0.08759000	-0.96505800
H	-8.11716600	-1.79160400	-2.54423900
H	-0.57228200	0.56863300	-5.18720700
C	-0.19948700	0.37557200	-4.17473800
H	0.08189900	-0.68436300	-4.13014700
H	0.70118300	0.97111200	-4.00589800
C	-0.15451500	2.17741900	-1.56493200
C	0.28331100	2.41337500	-0.19407000
C	-0.19620000	1.65384400	0.88392800
C	1.29261500	3.36229000	0.04528700
C	0.28001100	1.88070100	2.17100100
H	-0.91738800	0.86012900	0.70901400
C	1.75363600	3.59797700	1.33051000
H	1.69619300	3.92686500	-0.79560800
C	1.23753600	2.86416300	2.40037400
H	-0.09797300	1.27950000	2.99591100
H	2.52262200	4.34711700	1.50186200
H	1.60092500	3.04570000	3.40922400
Au	-3.37489800	1.88865400	0.42513000
P	-4.59942800	2.21906000	2.42806900
H	0.64905700	2.27448500	-2.29639400
C	-4.51604900	0.72103300	3.46754000
C	-4.14737100	-0.49082500	2.87299100
C	-4.86970100	0.74701000	4.82041900
C	-4.13352100	-1.66268800	3.62310800
H	-3.87434100	-0.51214800	1.81628600
C	-4.84985900	-0.42555700	5.56768600

H	-5.16391600	1.68508100	5.29018900
C	-4.48247600	-1.62956200	4.97007800
H	-3.84593600	-2.60114500	3.15474300
H	-5.12358500	-0.39979100	6.61986400
H	-4.46746900	-2.54435800	5.55818000
C	-6.36511400	2.38406500	1.97903000
C	-6.76071900	3.48819800	1.20982600
C	-7.29229600	1.37984500	2.26723500
C	-8.06556200	3.57950600	0.74062300
H	-6.04586800	4.27839400	0.97969800
C	-8.59936400	1.47750500	1.79276300
H	-6.99994500	0.51461700	2.85994400
C	-8.98621900	2.57241700	1.02748900
H	-8.36314000	4.44065800	0.14596000
H	-9.31446000	0.69119000	2.02327400
H	-10.00535800	2.64383400	0.65446900
C	-4.19256000	3.59749900	3.54183300
C	-2.84014000	3.89810900	3.72292900
C	-5.16673800	4.34099900	4.21215400
C	-2.46337300	4.93661600	4.56610000
H	-2.07986400	3.33070500	3.18415200
C	-4.78526000	5.38394000	5.05087800
H	-6.22295800	4.11180700	4.07612500
C	-3.43633200	5.68301500	5.22628200
H	-1.40906800	5.17329300	4.69287700
H	-5.54526100	5.96552600	5.56772300
H	-3.14324500	6.50442800	5.87630100

Electronic Energy (0K) = -3161.8144996

Electronic Energy (0K) + ZPE = -3161.000327

Enthalpy (298K) = -3160.945772

Free Energy (298K) = -3161.091737

C

Number of imaginary frequencies: 0

C	3.05507500	1.17807300	-2.00952000
C	2.36337800	0.53393700	-1.06124700
C	1.34228300	1.23442700	-0.29634100
H	1.34771800	1.14880200	0.79664800
N	0.39752200	1.97552500	-0.79624700
C	0.04619800	2.06298200	-2.19393300
C	-0.59295100	0.96932900	-2.77061500
C	0.31291900	3.22836700	-2.90661400
C	-0.94984700	1.03955100	-4.11147200
H	-0.80140700	0.08719000	-2.16523200
C	-0.05596900	3.28274400	-4.24636000
H	0.81012300	4.06706200	-2.42251300
C	-0.68101200	2.19214500	-4.84647100
H	-1.44224400	0.18997600	-4.57842100
H	0.15310500	4.17980000	-4.82315900
H	-0.96264900	2.24200000	-5.89533900
O	-2.06960300	2.00798900	0.01467100
O	-0.20961500	2.48572900	1.67667200
S	-0.83430400	2.66999000	0.38102600
C	-0.84093800	4.34905700	-0.09703500
C	0.22473800	5.15831400	0.30713700
C	-1.87492500	4.82157800	-0.90176500
C	0.24023100	6.47565200	-0.11396100
H	1.01812800	4.76425800	0.93849300
C	-1.83799700	6.14976000	-1.30184400
H	-2.68632800	4.16585400	-1.20674600

C	-0.78716000	6.98954400	-0.92074900
H	1.05690000	7.12840800	0.18867900
H	-2.63822500	6.54388900	-1.92422100
C	-0.74738700	8.41768400	-1.35550700
H	-1.59551400	8.66949300	-1.99864100
H	-0.76418300	9.08903500	-0.48833400
H	0.17782300	8.63441300	-1.90301400
H	2.86326700	2.21593200	-2.27038800
H	3.87740100	0.68023500	-2.52030300
C	-0.81571200	-2.24404100	-1.25139400
C	0.06978500	-1.65685200	-0.37808700
C	1.32235700	-1.64662100	-1.09581400
C	1.10303900	-2.18730100	-2.33108900
O	-0.19084400	-2.57318000	-2.43694900
C	-2.23519000	-2.57608200	-1.19637200
C	-2.81403100	-3.40737200	-2.16771300
C	-3.06550000	-2.06274200	-0.18674900
C	-4.16796300	-3.71926000	-2.12146100
H	-2.19231000	-3.81457200	-2.96118800
C	-4.41647400	-2.37929400	-0.14275100
H	-2.64063500	-1.40217600	0.56922500
C	-4.97817000	-3.21128900	-1.10937700
H	-4.59208900	-4.36990100	-2.88365700
H	-5.03535800	-1.96655800	0.65210700
H	-6.03674200	-3.45849000	-1.07564000
H	1.69687800	-1.59388100	-4.29943700
C	1.94272700	-2.34692600	-3.53717200
H	1.80050800	-3.33328700	-3.99371800
H	3.00347100	-2.23530000	-3.29130700
C	2.58921900	-0.92985000	-0.71126000

C	3.11116700	-1.15791000	0.69680000
C	2.80470100	-2.32369800	1.40637800
C	3.99210800	-0.23813000	1.27418800
C	3.35183200	-2.55355300	2.66659200
H	2.13462400	-3.06042500	0.96784300
C	4.54633700	-0.47016800	2.53065800
H	4.26312900	0.66445500	0.72599200
C	4.22101000	-1.62602300	3.23573900
H	3.10116300	-3.46650100	3.20372000
H	5.23898800	0.25343700	2.95588400
H	4.64745600	-1.80665700	4.22008700
Au	-0.24933600	-1.08041300	1.58747300
P	-0.57928900	-0.65808900	3.89595400
H	3.38326900	-1.25912900	-1.40000300
C	0.05138600	-2.06553100	4.87221100
C	0.79174100	-1.90548800	6.04535500
C	-0.22431900	-3.35414200	4.39755900
C	1.25762800	-3.02424000	6.73198200
H	1.00941400	-0.90838200	6.42527700
C	0.23241400	-4.46792200	5.09276900
H	-0.79215400	-3.48121200	3.47449700
C	0.97946400	-4.30255500	6.25752700
H	1.83707300	-2.89397700	7.64307800
H	0.01418900	-5.46581400	4.71942200
H	1.34587300	-5.17380300	6.79572400
C	0.28193300	0.81651800	4.52960800
C	-0.37881200	1.84552200	5.20034800
C	1.64915800	0.93419400	4.25206400
C	0.32308400	2.98570000	5.58641900
H	-1.44285900	1.76658100	5.41659900

C	2.34676400	2.06757400	4.64811700
H	2.16983300	0.13022800	3.72715100
C	1.68168900	3.09844600	5.31141400
H	-0.19695500	3.78749300	6.10563900
H	3.41098300	2.14987500	4.43609600
H	2.22639400	3.98993800	5.61420600
C	-2.32482900	-0.46694000	4.37957300
C	-2.76246600	-0.77352800	5.67219200
C	-3.23031700	0.04050900	3.44239800
C	-4.09413500	-0.57466900	6.01975300
H	-2.06016300	-1.16498600	6.40749500
C	-4.56161300	0.23968400	3.79511000
H	-2.88962100	0.28248200	2.43480900
C	-4.99272300	-0.07024100	5.08210100
H	-4.43139200	-0.81597300	7.02512000
H	-5.26278200	0.63337100	3.06281700
H	-6.03448400	0.08041100	5.35612100

Electronic Energy (0K) = -3161.8709528

Electronic Energy (0K) + ZPE = -3161.053769

Enthalpy (298K) = -3160.999263

Free Energy (298K) = -3161.145690

C1

Number of imaginary frequencies: 0

C	-3.46687100	4.18868200	-1.53624900
C	-4.28405600	3.66517600	-0.41397900
C	-4.85797900	4.29174000	0.62133000
H	-5.34211000	3.73875000	1.41829100
N	-4.94836000	5.66674700	0.84991800
C	-4.82124500	6.66934000	-0.16558800

C	-5.80986200	6.76749600	-1.14356400
C	-3.72089100	7.52468000	-0.16785900
C	-5.67901200	7.71625900	-2.14993200
H	-6.66409000	6.09273000	-1.10625100
C	-3.60503700	8.48066600	-1.17299800
H	-2.95566500	7.41713800	0.60091200
C	-4.57878600	8.57231500	-2.16382300
H	-6.44175700	7.79602700	-2.92062800
H	-2.74749500	9.14877900	-1.18505300
H	-4.48091900	9.31574800	-2.95135100
O	-6.60233700	7.20444300	2.04942300
O	-5.98095300	4.96925100	3.06338800
S	-5.61166000	6.18369800	2.34891000
C	-4.23476500	6.93020000	3.15840700
C	-3.21763400	6.10331900	3.63179200
C	-4.18287600	8.31363800	3.29907100
C	-2.13228000	6.68617500	4.26880700
H	-3.27802300	5.02056100	3.51228400
C	-3.08607300	8.87514500	3.93835400
H	-4.99106600	8.93201100	2.91633900
C	-2.04871700	8.07492100	4.42931400
H	-1.33265600	6.05394200	4.65317100
H	-3.03170600	9.95493500	4.06514700
C	-0.86311400	8.69695800	5.09607600
H	-0.14131900	9.05461900	4.35021000
H	-1.15358000	9.56299900	5.70059300
H	-0.34221300	7.98165900	5.74043200
H	-3.34752600	5.26258500	-1.33845600
C	-3.23493400	0.21888700	-2.61002100
C	-3.29504700	1.33068300	-1.81036400

C	-2.25283800	2.19985800	-2.23614200
C	-1.61618200	1.56846800	-3.26439300
O	-2.20572600	0.35959500	-3.49996800
C	-4.06719600	-0.96532500	-2.70451600
C	-4.23457900	-1.63638100	-3.92426900
C	-4.76195600	-1.43610500	-1.57842400
C	-5.10304600	-2.71593400	-4.01789300
H	-3.69540900	-1.29065700	-4.80328300
C	-5.65255200	-2.49845300	-1.68318400
H	-4.55885600	-1.01601000	-0.58776700
C	-5.82665800	-3.14200500	-2.90497300
H	-5.22738000	-3.22169200	-4.97282900
H	-6.18394200	-2.84134600	-0.79660900
H	-6.50998800	-3.98385600	-2.98617800
H	-0.71213300	1.84975500	-5.17599200
C	-0.45888400	1.91744500	-4.11104100
H	0.39031500	1.24648500	-3.93089300
H	-0.13427100	2.94031700	-3.89698200
C	-2.06027300	3.56511000	-1.66787000
C	-1.33918800	3.62189200	-0.33258500
C	-0.95992900	2.47773900	0.37010100
C	-1.09827800	4.87124100	0.25095600
C	-0.38047100	2.57630300	1.63519900
H	-1.11942600	1.49631700	-0.07385500
C	-0.51968900	4.97404800	1.51030400
H	-1.36298200	5.77878900	-0.29356200
C	-0.16742100	3.82301700	2.21484100
H	-0.09508800	1.67127900	2.16842500
H	-0.33594000	5.95752000	1.93964100
H	0.28745500	3.90060600	3.20074400

Au	-4.60125400	1.56237000	-0.26783900
P	-6.08410200	1.27623700	1.67068500
H	-1.50558000	4.18170800	-2.39062200
H	-3.99017100	4.09763800	-2.49832000
C	-5.18779400	1.51185600	3.23851800
C	-5.72529100	1.06390000	4.45192600
C	-3.92326800	2.11199200	3.22327300
C	-5.01951900	1.24769000	5.63508700
H	-6.69004900	0.55771000	4.47064300
C	-3.21783700	2.28584500	4.41039100
H	-3.48056800	2.43895700	2.28010700
C	-3.76863300	1.86160800	5.61564900
H	-5.44277200	0.90122000	6.57468400
H	-2.23145300	2.74719700	4.38485400
H	-3.21835100	1.99844500	6.54351400
C	-6.67122600	-0.45041500	1.71350600
C	-7.99868700	-0.77691300	1.42690500
C	-5.74981400	-1.46691300	1.99964500
C	-8.40468000	-2.10897000	1.44343600
H	-8.72212900	0.00579200	1.20590900
C	-6.16325900	-2.79368400	2.01810900
H	-4.71093400	-1.22154900	2.22368200
C	-7.49226500	-3.11530800	1.74344600
H	-9.44167300	-2.35660800	1.22972000
H	-5.44712100	-3.57858500	2.24904900
H	-7.81421800	-4.15368800	1.76299400
C	-7.56467900	2.32994400	1.64118700
C	-8.22866300	2.73137200	2.80277300
C	-8.03436500	2.74882600	0.39062200
C	-9.35160800	3.54580400	2.71176600

H	-7.85854000	2.43110500	3.78075200
C	-9.15839200	3.56261800	0.30549800
H	-7.51339900	2.44175600	-0.51718700
C	-9.81384800	3.96382700	1.46699700
H	-9.86146900	3.86302400	3.61812500
H	-9.51825600	3.88911500	-0.66729100
H	-10.68684700	4.60892400	1.40227500

Electronic Energy (0K) = -3161.8305515

Electronic Energy (0K) + ZPE = -3161.011439

Enthalpy (298K) = -3160.957896

Free Energy (298K) = -3161.099773

TS_D

Number of imaginary frequencies: 1

C	2.65214300	2.14904200	-0.74315300
C	2.21580200	0.91327100	-0.49742700
C	0.82293300	0.73103900	-0.00385300
H	0.67043900	0.59954100	1.06625100
N	-0.20763200	1.32276800	-0.62342000
C	-0.26371900	1.61645500	-2.03602900
C	-0.47452800	0.57355500	-2.93267700
C	-0.13112900	2.93259600	-2.47330100
C	-0.52115000	0.85090300	-4.29417600
H	-0.61196300	-0.43794700	-2.55874800
C	-0.19081700	3.19888700	-3.83680800
H	0.02111500	3.73546300	-1.75414600
C	-0.37744300	2.16034600	-4.74539400
H	-0.67882000	0.04162000	-5.00263600
H	-0.08347300	4.22164600	-4.18880100
H	-0.41582700	2.37419000	-5.81073900

O	-2.76079700	0.95025900	-0.55911400
O	-1.43573700	0.99879400	1.60248600
S	-1.72185100	1.52157600	0.27529900
C	-1.86301100	3.27019700	0.31651400
C	-0.98416100	3.99120200	1.12733800
C	-2.79714500	3.89656100	-0.50318500
C	-1.05554400	5.37386500	1.10759300
H	-0.26166100	3.47934800	1.76148300
C	-2.85218900	5.28382900	-0.50108200
H	-3.46079000	3.30810000	-1.13198000
C	-1.98765800	6.03867000	0.29713900
H	-0.38199400	5.95794200	1.73198500
H	-3.57651900	5.79313900	-1.13360000
C	-2.06647300	7.53086400	0.31185100
H	-2.55029900	7.91772400	-0.59033500
H	-2.65265500	7.87491600	1.17385900
H	-1.07293700	7.98356700	0.40026700
H	2.02079700	3.02767900	-0.62935500
H	3.68658100	2.31481800	-1.03881400
C	0.07198800	-2.30692900	-1.20598800
C	0.85634400	-1.51738000	-0.37063000
C	2.08604500	-1.35921600	-1.10912700
C	1.98308800	-2.02474000	-2.28291500
O	0.75071300	-2.63321000	-2.33880300
C	-1.28637600	-2.81767800	-1.11079500
C	-1.77929200	-3.73851600	-2.04707600
C	-2.14447200	-2.35967200	-0.09820500
C	-3.08749000	-4.19734600	-1.95934000
H	-1.13025500	-4.09624400	-2.84233800
C	-3.45070200	-2.82016900	-0.01652300

H	-1.77664200	-1.63275500	0.62634800
C	-3.92766700	-3.74403500	-0.94496900
H	-3.45435300	-4.91519900	-2.68946500
H	-4.10090400	-2.45120100	0.77435100
H	-4.95109700	-4.10595200	-0.88014100
H	2.40290100	-1.77158400	-4.36328000
C	2.85868200	-2.19324600	-3.45816100
H	3.06715000	-3.25177000	-3.65630200
H	3.81319700	-1.68599700	-3.28497200
C	3.06617800	-0.32955800	-0.64309800
C	3.79673500	-0.75438000	0.62368000
C	4.43353600	-2.00010300	0.63667500
C	3.86659300	0.04561700	1.76365000
C	5.11798800	-2.43756700	1.76378500
H	4.38661200	-2.62930500	-0.25287200
C	4.54517300	-0.39652100	2.90021900
H	3.38901700	1.02495900	1.76963500
C	5.16917800	-1.63865500	2.90609200
H	5.60719400	-3.40984400	1.75657600
H	4.58205600	0.23589800	3.78590700
H	5.68727800	-1.98830600	3.79703300
Au	0.75147300	-1.87514900	1.72180700
P	0.55956500	-2.16410600	4.04166100
H	3.81675100	-0.13090000	-1.42312000
C	0.13556800	-0.55786800	4.79656300
C	-1.06446000	-0.35024800	5.47833000
C	1.00933100	0.51810300	4.58931800
C	-1.38636600	0.92153000	5.94837200
H	-1.75604600	-1.17502200	5.64016400
C	0.68992500	1.78051600	5.07211800

H	1.94587400	0.35965600	4.05215000
C	-0.51259900	1.98410800	5.74841200
H	-2.32514600	1.07761900	6.47461400
H	1.37841300	2.60846500	4.91820800
H	-0.76753900	2.97487200	6.11744500
C	-0.76615600	-3.31111900	4.52583900
C	-0.80863000	-3.87074000	5.80725900
C	-1.78704400	-3.58693400	3.61223700
C	-1.86734900	-4.69691600	6.16688200
H	-0.01667400	-3.65662400	6.52432300
C	-2.84638600	-4.41148200	3.97785700
H	-1.74610900	-3.15478800	2.61118500
C	-2.88528900	-4.96616900	5.25388200
H	-1.89871900	-5.13262900	7.16267500
H	-3.63690400	-4.62551900	3.26201900
H	-3.71134900	-5.61369100	5.53874300
C	2.06346200	-2.76849800	4.87150800
C	2.72900000	-3.84966900	4.28318900
C	2.54833300	-2.21871400	6.06068600
C	3.86326100	-4.38210400	4.88440900
H	2.35654300	-4.26942200	3.34777800
C	3.69257300	-2.74761300	6.65228100
H	2.03495300	-1.38074600	6.52991200
C	4.34731500	-3.82849400	6.06810600
H	4.37675000	-5.22123800	4.42031800
H	4.06982100	-2.31714400	7.57707300
H	5.23963900	-4.24020800	6.53430600

Electronic Energy (0K) = -3161.8557019

Electronic Energy (0K) + ZPE = -3161.038959

Enthalpy (298K) = -3160.985207

Free Energy (298K) = -3161.130285

D

Number of imaginary frequencies: 0

C	2.13128500	2.25441800	-0.12071800
C	1.51138400	1.10241400	-0.35337000
C	0.05082300	0.83763600	0.04505900
H	-0.11789100	1.09557800	1.09616100
N	-0.93286000	1.61556200	-0.72921800
C	-1.00392200	1.45129600	-2.15056500
C	-1.96152200	0.59726300	-2.70247900
C	-0.08740400	2.10798300	-2.97514200
C	-1.98537200	0.38586600	-4.07670100
H	-2.68307500	0.11161400	-2.04772500
C	-0.11529100	1.88832600	-4.34889200
H	0.64192200	2.78225500	-2.53113100
C	-1.05964300	1.02539800	-4.89832200
H	-2.72926800	-0.28062300	-4.50663700
H	0.59979300	2.39682100	-4.99122200
H	-1.07874700	0.85444600	-5.97223800
O	-3.25679500	2.60336700	-0.64199300
O	-1.83226800	2.47561400	1.44665400
S	-1.95786600	2.71077500	0.00911100
C	-1.30850600	4.31789800	-0.35032900
C	-0.40444400	4.89938300	0.53791100
C	-1.68442600	4.96217800	-1.52549500
C	0.13201800	6.14106300	0.23280100
H	-0.14352000	4.38761400	1.46199100
C	-1.13468200	6.20602400	-1.81321600
H	-2.40448800	4.50314100	-2.19864300

C	-0.22205700	6.81093900	-0.94510000
H	0.83247500	6.60930400	0.92265700
H	-1.42221100	6.72236500	-2.72727000
C	0.35530200	8.15807000	-1.24583600
H	0.09936100	8.49019500	-2.25680500
H	-0.02094700	8.90981200	-0.54047400
H	1.44740600	8.15230800	-1.15050100
H	1.62519200	3.08591300	0.36878900
H	3.16735800	2.41244000	-0.41673300
C	-1.08499500	-1.61080200	-0.40822300
C	-0.08223200	-0.64122300	-0.25724900
C	1.00056200	-1.06317300	-1.11187400
C	0.63898200	-2.22651800	-1.69879900
O	-0.63105600	-2.55643100	-1.25848300
C	-2.42938200	-1.76327900	0.12300100
C	-3.19377500	-2.89710700	-0.18080500
C	-2.95058900	-0.78533000	0.98339900
C	-4.45527800	-3.05184500	0.38077000
H	-2.79499700	-3.65455900	-0.85096700
C	-4.21362700	-0.94574800	1.53406700
H	-2.36105100	0.09512100	1.23637500
C	-4.96744500	-2.08126200	1.23847700
H	-5.04271500	-3.93573400	0.14415700
H	-4.61044000	-0.18168400	2.19792400
H	-5.95569700	-2.20682300	1.67462200
H	0.58637800	-3.57009200	-3.34977600
C	1.28942900	-3.19712400	-2.59716000
H	1.67560300	-4.06213200	-2.03990400
H	2.13086600	-2.72236000	-3.11094300
C	2.15409900	-0.10599000	-1.03610000

C	3.31267700	-0.73990100	-0.27566000
C	4.13379000	-1.65282900	-0.94284600
C	3.52087600	-0.52263400	1.08847200
C	5.13161800	-2.34306100	-0.26140400
H	3.98432500	-1.82146500	-2.00980100
C	4.51914700	-1.21446700	1.77397800
H	2.90833900	0.20619100	1.61810600
C	5.32231800	-2.13175600	1.10332300
H	5.76557200	-3.04540700	-0.79864000
H	4.66518000	-1.03366400	2.83834800
H	6.10016600	-2.67281300	1.63749500
Au	0.49600400	-1.80537800	1.64659800
P	1.07459500	-3.08544500	3.49488400
H	2.50486500	0.17217600	-2.04158900
C	-0.39423100	-3.50498500	4.47837400
C	-0.31836000	-3.76840600	5.84932400
C	-1.62886800	-3.57248900	3.82299800
C	-1.47214900	-4.10160400	6.55233100
H	0.63816300	-3.70779700	6.36740000
C	-2.77767900	-3.90668100	4.52994900
H	-1.68841900	-3.35153100	2.75583100
C	-2.69853300	-4.17027500	5.89495000
H	-1.41346900	-4.30402900	7.61902700
H	-3.73428600	-3.94598800	4.01332500
H	-3.59730000	-4.42365200	6.45243900
C	2.25594600	-2.27607000	4.61317700
C	3.41703800	-2.91267700	5.05560000
C	1.97944000	-0.96408600	5.01788200
C	4.29471100	-2.23906400	5.90217100
H	3.64159100	-3.93056500	4.74128100

C	2.85750500	-0.29917700	5.86417800
H	1.07424100	-0.46520300	4.66905300
C	4.01678700	-0.93653200	6.30468500
H	5.19839000	-2.73624300	6.24622500
H	2.63984700	0.71907900	6.17727400
H	4.70595600	-0.41324600	6.96325800
C	1.84015500	-4.63252600	2.92864700
C	1.77292100	-5.80967800	3.67915700
C	2.54650800	-4.61457200	1.72066700
C	2.41218500	-6.95752700	3.22127800
H	1.22120400	-5.83047200	4.61808400
C	3.19072700	-5.76190700	1.27287500
H	2.58476100	-3.69596600	1.13102200
C	3.12166000	-6.93338200	2.02274400
H	2.35608100	-7.87418000	3.80330500
H	3.74153700	-5.74045800	0.33485100
H	3.61860500	-7.83401200	1.66974800

Electronic Energy (0K) = -3161.9078824

Electronic Energy (0K) + ZPE = -3161.088115

Enthalpy (298K) = -3161.034570

Free Energy (298K) = -3161.179512

3a

Number of imaginary frequencies: 0

C	1.34061700	2.19506700	0.69603900
C	1.01979300	1.10354500	0.00930600
C	-0.42369200	0.62096900	-0.19474100
H	-0.98422200	0.69642300	0.74447000
N	-1.19464400	1.40797600	-1.18616800
C	-0.73112200	1.49441400	-2.53860000

C	-1.28364100	0.65450800	-3.50594800
C	0.28224300	2.39189200	-2.88111700
C	-0.81722200	0.70788700	-4.81438600
H	-2.07914500	-0.02885400	-3.21561600
C	0.74697500	2.43869200	-4.19255200
H	0.70228100	3.04084000	-2.11493700
C	0.19896100	1.59754000	-5.15720800
H	-1.24668500	0.05174300	-5.56783000
H	1.53754800	3.13585400	-4.46040600
H	0.56348900	1.63636300	-6.18132800
O	-3.45392900	2.29266700	-1.85287400
O	-2.90700000	1.87908800	0.58437700
S	-2.50677600	2.33497700	-0.74531300
C	-1.93670800	4.00787100	-0.59749000
C	-1.50133200	4.46906000	0.64427900
C	-1.89164800	4.82347200	-1.72489200
C	-1.00353500	5.75913500	0.74755200
H	-1.56880300	3.82467700	1.51826100
C	-1.38866400	6.11348900	-1.60150300
H	-2.25246000	4.45665500	-2.68296700
C	-0.93391700	6.59720700	-0.37231000
H	-0.66678000	6.13176400	1.71401200
H	-1.35343400	6.76121000	-2.47580500
C	-0.38351600	7.98257800	-0.24090400
H	-0.47000000	8.54180300	-1.17772200
H	-0.90699500	8.54328000	0.54276200
H	0.67646200	7.95829900	0.04152400
H	0.57530100	2.83323100	1.13572400
H	2.37794300	2.49340600	0.84241800
C	-0.90584900	-1.93135800	-0.95409400

C	-0.21634100	-0.78966000	-0.64947900
C	1.15781000	-1.05498500	-0.88811300
C	1.25796400	-2.34337000	-1.30610600
O	0.00126100	-2.87968300	-1.34940000
C	-2.30534400	-2.31263100	-0.97061000
C	-2.70803800	-3.55747700	-1.47576200
C	-3.28401300	-1.42821600	-0.49232800
C	-4.05308000	-3.90318800	-1.50370000
H	-1.95861300	-4.25066100	-1.84990000
C	-4.62717200	-1.77980700	-0.52773300
H	-2.99557500	-0.46499500	-0.07524900
C	-5.01960500	-3.01681100	-1.03402500
H	-4.34922300	-4.87266400	-1.89896100
H	-5.37097800	-1.07966100	-0.15339500
H	-6.07218700	-3.28932400	-1.06003200
H	2.29359900	-3.57666600	-2.71647100
C	2.38274000	-3.22171000	-1.68213100
H	2.43747600	-4.10564400	-1.03432100
H	3.32316400	-2.66982700	-1.58741600
C	2.02794900	0.13620600	-0.62535000
C	3.25331100	-0.12426700	0.21706900
C	4.50828800	0.31073300	-0.20733000
C	3.15009800	-0.79344700	1.44099700
C	5.64242200	0.08106000	0.57021600
H	4.59688300	0.83209600	-1.16032600
C	4.27857500	-1.02396600	2.21792800
H	2.17237700	-1.13341800	1.78306700
C	5.53018600	-0.58675700	1.78443100
H	6.61423800	0.42572200	0.22267300
H	4.18307200	-1.54658900	3.16758300

H	6.41332600	-0.77000700	2.39259900
H	2.36429800	0.56562200	-1.58442800

Electronic Energy (0K) = -1990.4787328

Electronic Energy (0K) + ZPE = -1989.936363

Enthalpy (298K) = -1989.901527

Free Energy (298K) = -1990.004957

TS_{A1}

Number of imaginary frequencies: 1

C	-0.93984700	3.70811500	4.68145400
H	-2.03018200	3.68737000	4.62060700
H	-0.59539300	2.95756800	5.40259900
H	-0.62717400	4.69199900	5.05316700
C	-0.38134800	3.45177700	3.31100600
O	-1.10225100	3.40202900	2.33104400
C	1.10458800	3.24522200	3.16911900
C	1.95297000	3.53856900	4.20899200
H	1.47440100	3.93922000	5.10323900
C	3.38533800	3.43840500	4.32334800
C	3.98477900	4.06390900	5.43534700
C	4.20737300	2.74605400	3.41437000
C	5.35796500	4.02647200	5.61609300
H	3.35355500	4.58929600	6.15043300
C	5.57841000	2.69965500	3.60746600
H	3.78185500	2.21689600	2.56694800
C	6.15804800	3.34460600	4.70046500
H	5.80780300	4.52246300	6.47248900
H	6.18714300	2.15081300	2.89316700
H	7.23551100	3.30792200	4.84427100
C	1.51199200	2.79570400	1.90796500

C	1.69632200	2.23594700	0.81305500
C	1.96102900	2.35204300	-0.60425000
C	1.09306500	1.77513200	-1.53737200
C	3.09413000	3.04915400	-1.04304100
C	1.36331700	1.88427800	-2.89514300
H	0.21262700	1.23669000	-1.19034600
C	3.35758600	3.15291400	-2.40399400
H	3.76310000	3.49602200	-0.30938000
C	2.49964400	2.56401900	-3.33051000
H	0.68727000	1.43058000	-3.61638900
H	4.23919800	3.69381600	-2.74090300
H	2.71157800	2.64231500	-4.39431300
C	5.82668400	0.69606500	-1.11854600
H	6.31925300	-0.24928700	-1.37662900
H	5.39399800	1.10850500	-2.03669900
H	6.57698700	1.38665600	-0.72670400
C	4.78380400	0.47696300	-0.05803500
O	4.95060000	0.90790000	1.07443000
C	3.55089100	-0.29588300	-0.39074000
C	3.43788600	-0.91881100	-1.59685700
H	4.26727000	-0.79045900	-2.29201800
C	2.39655000	-1.80878100	-2.08363400
C	2.74206900	-2.70885800	-3.10809800
C	1.08345300	-1.85358200	-1.57594200
C	1.83751800	-3.65746300	-3.56385800
H	3.74490500	-2.66385100	-3.53128000
C	0.17954100	-2.80604900	-2.03503200
H	0.75353500	-1.11260800	-0.85247000
C	0.55628600	-3.71877200	-3.01723500
H	2.13081800	-4.35349200	-4.34658500

H	-0.83246300	-2.82183200	-1.63524500
H	-0.15376900	-4.46194900	-3.37296400
C	2.57417500	-0.41946300	0.67519000
C	1.77673300	0.26969200	1.41475100
C	0.85838700	0.11689000	2.53664400
C	1.34326900	-0.25324100	3.79902100
C	-0.51599000	0.30159500	2.35059900
C	0.45697900	-0.45960700	4.85088600
H	2.41486500	-0.39203000	3.93842500
C	-1.39628700	0.09782200	3.40681700
H	-0.88500800	0.62854200	1.37995100
C	-0.91273000	-0.28796500	4.65582000
H	0.83800900	-0.75303600	5.82631800
H	-2.46276700	0.24879200	3.25543000
H	-1.60398600	-0.44753200	5.48002000
Au	2.17670100	-2.46395800	1.31471900
P	1.72353800	-4.68684400	1.86374900
C	2.84753100	-5.41447600	3.09523500
C	3.15041600	-4.64770600	4.22653000
C	3.38286900	-6.69680800	2.95830300
C	3.97948400	-5.16406500	5.21426200
H	2.73235200	-3.64488600	4.32992400
C	4.22064500	-7.20513500	3.94785300
H	3.14770200	-7.30042200	2.08287600
C	4.51819500	-6.44157600	5.07249600
H	4.21415500	-4.56643900	6.09191400
H	4.64025700	-8.20236800	3.83783400
H	5.17562900	-6.84138100	5.84102600
C	1.80345200	-5.74529500	0.38688500
C	0.82475600	-6.69432300	0.08421200

C	2.90263900	-5.58162400	-0.46451800
C	0.94441400	-7.46828700	-1.06762100
H	-0.03276200	-6.82995000	0.74069600
C	3.02049000	-6.36204400	-1.60771900
H	3.66272000	-4.83462500	-0.23056300
C	2.03822600	-7.30334000	-1.91168500
H	0.17812100	-8.20303500	-1.30297600
H	3.87148400	-6.22462800	-2.27115100
H	2.12447100	-7.90736300	-2.81195200
C	0.05307400	-4.84562100	2.56619200
C	-0.29822300	-5.93623100	3.36848700
C	-0.89374200	-3.85490900	2.28610300
C	-1.58795900	-6.03399100	3.87909500
H	0.43706000	-6.70813700	3.59392500
C	-2.18233200	-3.95700700	2.80028700
H	-0.61320000	-2.99965800	1.66741200
C	-2.52786200	-5.04519100	3.59653100
H	-1.85875900	-6.88287700	4.50237500
H	-2.91364700	-3.18089000	2.58679200
H	-3.53344800	-5.12225700	4.00355500

Electronic Energy (0K) = -2709.3192347

Electronic Energy (0K) + ZPE = -2708.516733

Enthalpy (298K) = -2708.463414

Free Energy (298K) = -2708.606495

A1

Number of imaginary frequencies: 0

C	-2.53933300	4.80821300	3.28269200
H	-3.62505700	4.85676500	3.38637000
H	-2.08951400	4.59640400	4.26038600

H	-2.16503800	5.78522600	2.95271300
C	-2.19713500	3.74042800	2.28954400
O	-3.04896000	3.08652400	1.72344600
C	-0.72984100	3.48490400	1.98251300
C	0.28097700	4.24329300	2.60594000
H	-0.07323200	5.06082200	3.23660000
C	1.69074500	4.14160800	2.55144100
C	2.41528900	5.21549300	3.13086000
C	2.40730700	3.07779900	1.94757200
C	3.79380900	5.25143500	3.06606700
H	1.86533200	6.02290800	3.60968400
C	3.78466400	3.12541500	1.88661300
H	1.89464100	2.21258500	1.53719200
C	4.47687400	4.20808300	2.43943300
H	4.34148600	6.08175900	3.50214500
H	4.32417800	2.31438700	1.40653900
H	5.56296800	4.23084400	2.39052300
C	-0.46419700	2.53514200	1.05399400
C	-0.37380300	1.61623500	0.13530300
C	-0.47655500	2.06247200	-1.28190000
C	-1.48171500	1.51553500	-2.08394800
C	0.40463900	3.00943500	-1.80681300
C	-1.57095300	1.88035800	-3.42018000
H	-2.17361100	0.78939100	-1.65894400
C	0.30716200	3.37350700	-3.14683700
H	1.18680600	3.42461300	-1.17244800
C	-0.67103300	2.80222100	-3.95552000
H	-2.34211500	1.44122700	-4.04885100
H	1.00550200	4.09734400	-3.56075600
H	-0.73840500	3.07965200	-5.00486100

C	3.15777600	0.89937700	-2.62300200
H	3.72029600	0.03106700	-2.98725200
H	2.51471500	1.24334700	-3.44025000
H	3.86563000	1.68807300	-2.35703600
C	2.36497400	0.53823700	-1.39445300
O	2.69740500	0.99036100	-0.30505000
C	1.19529000	-0.38592500	-1.50937100
C	0.95391900	-0.99517900	-2.70361000
H	1.62210600	-0.76727600	-3.53348400
C	-0.05000100	-1.99983300	-3.01557500
C	0.21375300	-2.88093500	-4.08118200
C	-1.24503900	-2.17814300	-2.29291900
C	-0.64580400	-3.92960600	-4.37619000
H	1.12181200	-2.73960800	-4.66664200
C	-2.10892500	-3.22714900	-2.59520100
H	-1.51355600	-1.47369000	-1.51068000
C	-1.80662900	-4.11479400	-3.62362000
H	-0.41388500	-4.60484400	-5.19703400
H	-3.02964100	-3.34153000	-2.02592200
H	-2.48162900	-4.93665900	-3.85198400
C	0.48514400	-0.69771600	-0.26338700
C	-0.17367600	0.18880000	0.51870800
C	-0.74860200	-0.20114000	1.83587300
C	0.04037600	-0.81048100	2.82115300
C	-2.11253100	-0.01218700	2.08966000
C	-0.52804800	-1.25106500	4.01378500
H	1.10894500	-0.93449900	2.64444700
C	-2.68094600	-0.45332300	3.28101500
H	-2.73022200	0.48826000	1.34464200
C	-1.89209300	-1.08189800	4.24271100

H	0.09843000	-1.72147800	4.76906100
H	-3.74484000	-0.30772000	3.45681900
H	-2.33623200	-1.42766600	5.17360400
Au	0.48361900	-2.72315900	0.31068000
P	0.20439400	-4.99493700	0.88377200
C	0.77159800	-5.45841300	2.55091500
C	0.17081500	-6.49251400	3.27723400
C	1.84249600	-4.75175200	3.10719300
C	0.64656200	-6.82033900	4.54234100
H	-0.67126900	-7.03892300	2.85351100
C	2.31647200	-5.08464200	4.37219600
H	2.29937200	-3.93465200	2.54734800
C	1.71828600	-6.11790500	5.08849900
H	0.17633300	-7.62395600	5.10421300
H	3.14851000	-4.53192600	4.80210000
H	2.08464700	-6.37391900	6.08007400
C	-1.59263300	-5.31803900	0.87444200
C	-2.17863900	-6.34431700	0.13240400
C	-2.40188200	-4.44382600	1.61289000
C	-3.56414000	-6.49512400	0.13035300
H	-1.55912500	-7.02414700	-0.45089500
C	-3.78148100	-4.60389700	1.61362100
H	-1.94544500	-3.63634600	2.19007800
C	-4.36405200	-5.62894100	0.86837600
H	-4.01768600	-7.29527300	-0.45018300
H	-4.40332900	-3.92457700	2.19262000
H	-5.44485700	-5.74981200	0.86283900
C	0.93522200	-6.18012300	-0.28837100
C	1.29306200	-7.48077000	0.07789200
C	1.08911200	-5.76685800	-1.61664600

C	1.79836600	-8.35681800	-0.87746300
H	1.17929500	-7.81200400	1.10922800
C	1.58895600	-6.64830500	-2.56891100
H	0.81456600	-4.75011000	-1.90478800
C	1.94538000	-7.94240800	-2.19915900
H	2.07863300	-9.36709100	-0.58835000
H	1.70697700	-6.31923000	-3.59917300
H	2.34313000	-8.63068700	-2.94152700

Electronic Energy (0K) = -2709.3454111

Electronic Energy (0K) + ZPE = -2708.541520

Enthalpy (298K) = -2708.488060

Free Energy (298K) = -2708.633127

TS_{A1'}

Number of imaginary frequencies: 1

C	-1.23346000	2.43544100	3.31347900
H	-2.17125500	1.88269600	3.22713500
H	-0.82298200	2.29245300	4.32036800
H	-1.43266600	3.50634300	3.18854100
C	-0.28624700	1.93740800	2.26168600
O	-0.61908300	1.06206700	1.47993300
C	1.08874600	2.53328100	2.17266100
C	1.49477300	3.48933600	3.07382400
H	0.76070900	3.74948900	3.83659300
C	2.72886400	4.22691700	3.19357200
C	2.90029200	4.98782400	4.36714600
C	3.76947400	4.20964000	2.24632300
C	4.08066900	5.67310600	4.60597500
H	2.09697700	5.01120700	5.10271900
C	4.94669900	4.90017400	2.48699800

H	3.64763700	3.66391200	1.31578400
C	5.11009000	5.62501200	3.66747000
H	4.20139900	6.24561300	5.52208100
H	5.74273500	4.87934200	1.74627900
H	6.03784200	6.16215900	3.85048800
C	1.87416200	2.06920100	1.11068800
C	2.52242100	1.62158300	0.14491600
C	2.96185200	2.01012900	-1.19046300
C	2.09082400	1.88745200	-2.27927500
C	4.24606000	2.53111900	-1.38197500
C	2.49972600	2.30001900	-3.54241500
H	1.09341400	1.47933300	-2.12409100
C	4.64469200	2.94591300	-2.64811400
H	4.92730900	2.60002300	-0.53512800
C	3.77447300	2.83178500	-3.72937800
H	1.81558100	2.21204000	-4.38329100
H	5.64140400	3.35763900	-2.78895000
H	4.08957000	3.15582600	-4.71852400
C	4.94129300	-0.82862100	-2.89496800
H	4.96175800	-1.90324200	-3.11690500
H	4.14164000	-0.38275700	-3.49695500
H	5.90699400	-0.40363800	-3.17865800
C	4.72627000	-0.60546200	-1.42530100
O	5.64241600	-0.27100600	-0.69153000
C	3.36304600	-0.84287500	-0.85222800
C	2.48655200	-1.66905500	-1.48000600
H	2.81960700	-2.10592600	-2.42373300
C	1.21743000	-2.18352700	-0.99181800
C	0.88366300	-3.50647200	-1.32999300
C	0.33775800	-1.44402500	-0.18521600

C	-0.28019700	-4.08751900	-0.84319800
H	1.56614300	-4.08497600	-1.95501100
C	-0.83883000	-2.02159300	0.27550500
H	0.54815100	-0.40602900	0.06570600
C	-1.14625800	-3.34411600	-0.04280600
H	-0.51423300	-5.11986300	-1.09421300
H	-1.51623700	-1.42505100	0.88240900
H	-2.06648100	-3.79306900	0.32513800
C	3.14383900	-0.34900400	0.48848500
C	3.20323900	-0.68539500	1.72723300
C	2.90104300	-0.05615100	2.99532300
C	3.78890000	0.86972400	3.56061400
C	1.70566800	-0.37485000	3.66260500
C	3.45461700	1.50973300	4.74619000
H	4.71938600	1.10090700	3.04419400
C	1.38170300	0.26979700	4.84698100
H	1.03088800	-1.11059900	3.22424000
C	2.24801000	1.22408100	5.38460700
H	4.13199700	2.25265500	5.16384500
H	0.44856100	0.03310500	5.35398200
H	1.99047600	1.73422300	6.31074200
Au	3.59200500	-2.79242000	1.76550300
P	3.62801000	-5.13348900	1.73147000
C	2.21407100	-5.79437200	2.66651600
C	2.28776900	-6.99448300	3.37715500
C	1.01072700	-5.07926700	2.62860300
C	1.16394600	-7.47358100	4.04487600
H	3.22022000	-7.55625100	3.41114300
C	-0.11090500	-5.56841700	3.28746600
H	0.95459700	-4.13706200	2.07856200

C	-0.03255300	-6.76383500	3.99901500
H	1.22459800	-8.40528100	4.60227700
H	-1.04395300	-5.00993900	3.25416900
H	-0.90744500	-7.14143000	4.52325100
C	5.12243500	-5.93873000	2.37859200
C	5.56831500	-7.16516000	1.87596800
C	5.81381400	-5.31911200	3.42431400
C	6.69802900	-7.76580000	2.42147800
H	5.03375600	-7.65221400	1.06122400
C	6.93913800	-5.92756500	3.96932200
H	5.46854200	-4.35756200	3.80488400
C	7.38153200	-7.14846700	3.46601500
H	7.04662100	-8.71798700	2.02863800
H	7.47606900	-5.44287700	4.78116700
H	8.26673000	-7.61932500	3.88740100
C	3.42405000	-5.72776600	0.02007600
C	2.51510600	-6.73276300	-0.31675600
C	4.21513800	-5.14122400	-0.97524000
C	2.39336800	-7.14219400	-1.64270900
H	1.89833800	-7.19536200	0.45257800
C	4.09701200	-5.56048900	-2.29515300
H	4.92144600	-4.35111900	-0.71305600
C	3.18118500	-6.55745600	-2.62984500
H	1.68247200	-7.92315900	-1.90193800
H	4.71748300	-5.10853200	-3.06548500
H	3.08449500	-6.88027300	-3.66381500

Electronic Energy (0K) = -2709.3164045

Electronic Energy (0K) + ZPE = -2708.515122

Enthalpy (298K) = -2708.461620

Free Energy (298K) = -2708.605648

A1'

Number of imaginary frequencies: 0

C	-4.66094600	2.82246100	1.66456100
H	-5.60381700	2.48398700	1.22994400
H	-4.60449400	2.49771700	2.71062900
H	-4.63862700	3.91915700	1.65791000
C	-3.53050500	2.26413700	0.85415500
O	-3.73019800	1.62497700	-0.16235000
C	-2.10728500	2.52085900	1.31015600
C	-1.84888900	3.35308700	2.39989900
H	-2.72964300	3.73050500	2.92213400
C	-0.61471400	3.83394500	2.93495300
C	-0.68147400	4.49736900	4.18083800
C	0.64513800	3.66557300	2.31969300
C	0.46946200	4.93456300	4.81141300
H	-1.65340700	4.64065500	4.65055100
C	1.79032600	4.11313900	2.95171700
H	0.71648300	3.20374700	1.33922000
C	1.70675900	4.73744400	4.19857400
H	0.40880600	5.43222200	5.77533500
H	2.75690200	3.98563000	2.47171000
H	2.61332000	5.08478600	4.68844900
C	-1.13981100	1.81842200	0.64372700
C	-0.39833900	1.24831200	-0.27175400
C	-0.08140100	2.17067400	-1.40999300
C	-1.11019000	2.67997900	-2.20622600
C	1.24773000	2.52345400	-1.66454900
C	-0.80430700	3.52282600	-3.27048400
H	-2.14037900	2.40211500	-1.98907100

C	1.54196700	3.37026500	-2.72636800
H	2.03966300	2.12111000	-1.03466400
C	0.51842800	3.86769200	-3.53153700
H	-1.60408400	3.91066900	-3.89698900
H	2.57567200	3.64174100	-2.92779800
H	0.75474600	4.52634100	-4.36408200
C	3.14916800	-1.46570500	-2.32776200
H	2.89103300	-2.53305900	-2.27701000
H	2.97043800	-1.13316200	-3.35642000
H	4.20942800	-1.34126900	-2.09585900
C	2.34255800	-0.67647700	-1.33033000
O	2.90741300	-0.07145800	-0.42655400
C	0.85472200	-0.66752500	-1.42538000
C	0.24509000	-1.23419200	-2.49348900
H	0.90024100	-1.66012700	-3.25457400
C	-1.16629500	-1.44373500	-2.79699500
C	-1.45895600	-2.34692500	-3.83523000
C	-2.24445800	-0.82772200	-2.13765000
C	-2.76894000	-2.64633600	-4.18397700
H	-0.63498300	-2.82098800	-4.36895000
C	-3.55435700	-1.11742300	-2.49724900
H	-2.07586300	-0.10028400	-1.35063800
C	-3.82370100	-2.03111700	-3.51381200
H	-2.96693500	-3.35504300	-4.98512700
H	-4.36830300	-0.61631700	-1.97729100
H	-4.85168500	-2.25677200	-3.78816700
C	0.12927200	-0.13758900	-0.23525300
C	-0.07171700	-0.92160600	0.84608900
C	-0.83190400	-0.40476800	1.97963700
C	-0.18722500	0.28763700	3.02437100

C	-2.22729400	-0.60455500	2.05287000
C	-0.92256900	0.81145000	4.07595800
H	0.89340700	0.41958600	2.97965200
C	-2.95495300	-0.07572200	3.10684500
H	-2.72239700	-1.16787500	1.26235600
C	-2.30990400	0.65368400	4.10958100
H	-0.41601500	1.36181700	4.86667300
H	-4.03212600	-0.22354400	3.14795100
H	-2.88481300	1.06947200	4.93471100
Au	0.69173700	-2.85578600	0.83582100
P	1.65372300	-4.99827900	0.53779200
C	1.81970400	-6.03828200	2.02091900
C	2.85937000	-6.96210500	2.16582300
C	0.85113700	-5.91706100	3.02239400
C	2.92032500	-7.76367500	3.30115200
H	3.61855000	-7.05879100	1.39030500
C	0.91532400	-6.72284900	4.15420200
H	0.04921500	-5.18664300	2.91100700
C	1.94983900	-7.64455700	4.29311900
H	3.72827900	-8.48300500	3.41231700
H	0.16091200	-6.62494600	4.93130500
H	2.00165500	-8.27065300	5.18092800
C	3.33774200	-4.82416400	-0.14460900
C	3.78361100	-5.55377800	-1.24904500
C	4.19508200	-3.90387500	0.47193800
C	5.07610700	-5.36174600	-1.73208900
H	3.12467800	-6.27170800	-1.73502500
C	5.48817300	-3.72672700	-0.00538100
H	3.84471400	-3.32276000	1.32623500
C	5.92715800	-4.45246400	-1.11157000

H	5.41712500	-5.92888900	-2.59507000
H	6.15041000	-3.01240400	0.47809900
H	6.93541200	-4.30621500	-1.49214800
C	0.72985000	-5.98207500	-0.68740400
C	0.67290500	-7.37747700	-0.64126800
C	0.09706100	-5.29732100	-1.73168000
C	-0.00786500	-8.07804000	-1.63268700
H	1.16111900	-7.91975200	0.16710400
C	-0.57712100	-6.00169500	-2.72223500
H	0.12940300	-4.20578900	-1.76192000
C	-0.63078400	-7.39264700	-2.67192600
H	-0.05184200	-9.16376800	-1.59128200
H	-1.07274900	-5.46254400	-3.52708100
H	-1.16380300	-7.94356600	-3.44338200

Electronic Energy (0K) = -2709.3499387

Electronic Energy (0K) + ZPE = -2708.545634

Enthalpy (298K) = -2708.492490

Free Energy (298K) = -2708.636270

TS_{A2}

Number of imaginary frequencies: 1

C	0.57432900	2.97740100	2.06196000
H	0.91030800	2.40497600	2.93591300
H	1.12828100	3.92376100	2.06404600
H	-0.49608800	3.17140300	2.16000600
C	0.81252500	2.23137600	0.78521000
O	-0.09618300	1.85757200	0.06838700
C	2.24471900	1.98317400	0.34502300
C	3.26742700	1.86055200	1.29676600
H	2.97189400	2.17989200	2.29652200

C	4.72366000	1.98117300	1.09846800
C	5.51566900	2.00177200	2.25622500
C	5.35179400	2.11931800	-0.14474300
C	6.89158600	2.15488000	2.17980700
H	5.03375800	1.89689200	3.22855100
C	6.73257000	2.28208000	-0.21940200
H	4.75951200	2.12952600	-1.05546000
C	7.50611100	2.29697700	0.93681900
H	7.48669900	2.16912700	3.08976600
H	7.20419000	2.40282100	-1.19276400
H	8.58430700	2.42316900	0.87087900
C	2.38911400	1.79370400	-1.02592800
C	2.42071900	1.61780100	-2.23570300
C	2.58314900	1.37812100	-3.61769600
C	1.46805200	1.27878000	-4.46864500
C	3.87936900	1.19745900	-4.13672900
C	1.65365700	1.00576300	-5.81562900
H	0.47117900	1.40976400	-4.05343600
C	4.05142400	0.92388200	-5.48386800
H	4.73376000	1.26925800	-3.46592600
C	2.94039000	0.82757700	-6.32250900
H	0.79314900	0.92976800	-6.47553700
H	5.05157500	0.78596000	-5.88714800
H	3.07952500	0.61494200	-7.37996800
C	6.92745000	-1.11863200	-0.88908100
H	7.01542600	-2.12194700	-1.32571800
H	6.72149900	-0.41725400	-1.70304900
H	7.88093300	-0.86587400	-0.41857800
C	5.86423100	-1.12310500	0.17630300
O	6.17108600	-1.21265700	1.35481700

C	4.41909000	-1.06706300	-0.22640400
C	4.07051700	-1.40084200	-1.50203200
H	4.89658200	-1.59103800	-2.18685300
C	2.76789100	-1.61586100	-2.09836900
C	2.73031000	-2.10959700	-3.41698300
C	1.54443300	-1.34915400	-1.45724400
C	1.52649100	-2.32411500	-4.06841600
H	3.67049400	-2.31670500	-3.92763700
C	0.33794700	-1.56233600	-2.11209100
H	1.53917900	-0.95291000	-0.44681200
C	0.32301400	-2.04891700	-3.41690800
H	1.52170300	-2.69817700	-5.08957000
H	-0.59538700	-1.33110300	-1.60182600
H	-0.62357500	-2.21099600	-3.92764700
C	3.51013000	-0.92037900	0.88929800
C	2.87301600	-0.06956700	1.62559300
C	1.90196400	-0.12335000	2.72353900
C	2.28016500	0.25538000	4.01767200
C	0.60655300	-0.61097700	2.49819900
C	1.37962700	0.13800600	5.07099100
H	3.28953200	0.62647500	4.19065500
C	-0.28944800	-0.72479700	3.55495900
H	0.31148900	-0.91297100	1.49358700
C	0.09403500	-0.34937000	4.84110500
H	1.68308400	0.42536800	6.07503600
H	-1.28843100	-1.11475600	3.37330800
H	-0.60961500	-0.43788200	5.66534300
Au	3.11885900	-2.83453900	1.82755400
P	2.37403200	-4.82490900	2.79361200
C	2.67285700	-4.85576100	4.58722600

C	2.96596600	-6.03569100	5.27477800
C	2.55324400	-3.65030800	5.28884000
C	3.14012800	-6.00560200	6.65568700
H	3.05757700	-6.97832800	4.73718100
C	2.71871300	-3.62854100	6.66793500
H	2.33006800	-2.72602300	4.75166700
C	3.01649100	-4.80605500	7.35106300
H	3.37330100	-6.92410400	7.18913600
H	2.62344700	-2.68909000	7.20832500
H	3.15585900	-4.78765700	8.42939700
C	3.06369700	-6.35612100	2.10364100
C	2.30111100	-7.52249500	1.99467300
C	4.40560300	-6.35702600	1.70894200
C	2.88219400	-8.68232800	1.49173600
H	1.25637500	-7.52596900	2.30266600
C	4.98174500	-7.52079400	1.21297300
H	4.99342800	-5.44222900	1.78837400
C	4.21927600	-8.68115900	1.10267900
H	2.28852300	-9.58913600	1.40485000
H	6.02442100	-7.52038600	0.90488200
H	4.66822700	-9.58929600	0.70698600
C	0.56688100	-4.91718800	2.58666300
C	-0.27992900	-5.32875100	3.61812900
C	0.02893900	-4.54963300	1.34730200
C	-1.65632000	-5.36694600	3.41027700
H	0.13207100	-5.61663800	4.58429400
C	-1.34495500	-4.59624400	1.14366400
H	0.69052600	-4.22086400	0.54404600
C	-2.18790000	-5.00038700	2.17739500
H	-2.31389300	-5.68306000	4.21660300

H	-1.75922800	-4.30836300	0.18019300
H	-3.26372300	-5.02690300	2.02063800

Electronic Energy (0K) = -2709.3127089

Electronic Energy (0K) + ZPE = -2708.511044

Enthalpy (298K) = -2708.457715

Free Energy (298K) = -2708.600240

A2

Number of imaginary frequencies: 0

C	-2.34523800	3.65875900	1.50031100
H	-2.18569600	3.19934600	2.48603900
H	-1.64886300	4.49995600	1.41266600
H	-3.37786100	4.01139500	1.44740300
C	-2.12572500	2.64416800	0.42727500
O	-3.02388700	2.06797400	-0.14877200
C	-0.68496300	2.36141700	-0.00336600
C	0.38035900	2.23717700	0.99284500
H	0.11775800	2.83376700	1.87574400
C	1.81686100	2.52259700	0.64308500
C	2.79834700	2.14907900	1.56651900
C	2.19986200	3.25297400	-0.48354400
C	4.13256400	2.47702600	1.35959600
H	2.51185000	1.57885500	2.44999100
C	3.53783500	3.57999300	-0.69319000
H	1.45565000	3.59732700	-1.19705300
C	4.50843800	3.19157100	0.22444600
H	4.88068200	2.16655800	2.08568800
H	3.81658800	4.15175000	-1.57575300
H	5.55258100	3.44704800	0.05883900
C	-0.54013200	2.15673600	-1.34261200

C	-0.48085700	1.99653100	-2.56236500
C	-0.26800400	1.82737400	-3.93285400
C	-1.35555000	1.73248600	-4.82553400
C	1.05808200	1.71304000	-4.40753800
C	-1.11285700	1.52875700	-6.17298500
H	-2.36824000	1.81252800	-4.43756100
C	1.28296300	1.51204900	-5.75630100
H	1.87850100	1.77670000	-3.69360900
C	0.19968200	1.41953700	-6.63487100
H	-1.94277300	1.45205000	-6.87004000
H	2.29803600	1.42362800	-6.13376500
H	0.38283500	1.25950200	-7.69481000
C	4.05839400	-0.29846600	-0.75485900
H	4.27315200	-1.18009500	-1.37165700
H	3.80649100	0.53107200	-1.42359900
H	4.95972000	-0.05813800	-0.18488300
C	2.95405700	-0.60722500	0.22164600
O	3.21583200	-0.95829600	1.36077800
C	1.52590900	-0.49543900	-0.24938900
C	1.29482300	-0.82472400	-1.55097900
H	2.17805900	-1.00251300	-2.16533600
C	0.04946600	-1.09408700	-2.24499700
C	0.12373300	-1.55243700	-3.57464300
C	-1.22609900	-0.93464900	-1.67441800
C	-1.02184100	-1.81645400	-4.30745900
H	1.10437900	-1.68642000	-4.03106500
C	-2.37592000	-1.20319900	-2.40870900
H	-1.31328300	-0.58992200	-0.64674600
C	-2.27977000	-1.64151800	-3.72643700
H	-0.93956700	-2.15800000	-5.33701800

H	-3.35146100	-1.06458400	-1.94605200
H	-3.17979200	-1.85152500	-4.29997800
C	0.55100100	-0.35773000	0.82753500
C	0.00351600	0.74789800	1.38482300
C	-0.99461500	0.66370800	2.48747600
C	-0.72172900	1.26404800	3.72178300
C	-2.20395100	-0.02440200	2.32634000
C	-1.62604500	1.16232500	4.77521000
H	0.21486000	1.80421600	3.86187400
C	-3.11104600	-0.12196500	3.37705600
H	-2.43873400	-0.47745000	1.36300500
C	-2.82348200	0.47053300	4.60486700
H	-1.39457100	1.62560100	5.73174000
H	-4.04617500	-0.65958000	3.23143700
H	-3.53344200	0.39799800	5.42549400
Au	0.06923500	-2.21980500	1.69132900
P	-0.83578500	-4.20786200	2.59199600
C	-0.61328500	-4.34261700	4.39198400
C	-0.64362900	-5.57110500	5.05824900
C	-0.47005500	-3.15817200	5.12188400
C	-0.53267300	-5.60799600	6.44466800
H	-0.75688100	-6.49765400	4.49670100
C	-0.36823800	-3.19975900	6.50758300
H	-0.43291300	-2.20319300	4.59560900
C	-0.39816900	-4.42540300	7.16822700
H	-0.55269900	-6.56428100	6.96208100
H	-0.25767300	-2.27532000	7.06966200
H	-0.31131400	-4.46066700	8.25169600
C	-0.28243200	-5.78451800	1.87624700
C	-1.16444400	-6.84168000	1.63632400

C	1.07901400	-5.93334700	1.59008100
C	-0.68454600	-8.03896200	1.11382000
H	-2.22510100	-6.73215000	1.85887400
C	1.55363800	-7.13432700	1.07522200
H	1.76492100	-5.10531900	1.77148700
C	0.67150000	-8.18535700	0.83459300
H	-1.37314600	-8.85928600	0.92555300
H	2.61240000	-7.24750800	0.85430300
H	1.04295500	-9.12193300	0.42500300
C	-2.63817700	-4.11711200	2.32088100
C	-3.56394800	-4.28854300	3.35122700
C	-3.08515400	-3.80153900	1.03093500
C	-4.92505900	-4.13603300	3.09408700
H	-3.22824100	-4.53413400	4.35767900
C	-4.44304200	-3.65474100	0.77871100
H	-2.36066000	-3.66533600	0.22665300
C	-5.36433800	-3.81705200	1.81321500
H	-5.64333800	-4.26727900	3.90001900
H	-4.78218500	-3.40689400	-0.22486500
H	-6.42718500	-3.69348500	1.61820700

Electronic Energy (0K) = -2709.3217998

Electronic Energy (0K) + ZPE = -2708.518615

Enthalpy (298K) = -2708.465356

Free Energy (298K) = -2708.607789

TS_{A2'}

Number of imaginary frequencies: 1

C	2.20409300	3.69927600	0.91551100
H	2.42591100	3.44632700	1.95857800
H	2.85963600	4.53633300	0.64257300

H	1.15981400	4.00934900	0.83343300
C	2.45021100	2.55544300	-0.01762400
O	1.60627300	2.13168200	-0.78102400
C	3.87242000	2.00014400	-0.08252100
C	4.64069800	1.85677100	1.08401200
H	4.15302000	2.24614000	1.97811500
C	6.10918000	1.87724800	1.21120100
C	6.62193400	2.06015900	2.50237100
C	7.00351800	1.72968100	0.14453300
C	7.98986800	2.09687400	2.72681200
H	5.92774600	2.16341300	3.33614300
C	8.37505800	1.77295500	0.37072300
H	6.63104900	1.58738600	-0.86698500
C	8.87274500	1.95080900	1.65870900
H	8.37025800	2.23714700	3.73573400
H	9.06003600	1.66237000	-0.46713400
H	9.94628100	1.97720000	1.83018000
C	4.26053800	1.60466500	-1.35738400
C	4.46941000	1.13331700	-2.46654600
C	4.67161600	0.49091700	-3.70615600
C	3.60511000	0.39137200	-4.61830200
C	5.89992900	-0.13446500	-3.99074400
C	3.76976800	-0.32563700	-5.79333900
H	2.66049300	0.87661300	-4.38392200
C	6.05196400	-0.84644300	-5.16949500
H	6.71730000	-0.05201700	-3.27664400
C	4.98858900	-0.94493800	-6.06751000
H	2.94657900	-0.40636900	-6.49846400
H	6.99933000	-1.33083700	-5.39213000
H	5.11248700	-1.50784200	-6.98960000

C	7.43974600	-1.64171200	0.25605400
H	7.33937000	-2.72272400	0.09353600
H	7.46420600	-1.15414200	-0.72384200
H	8.38255400	-1.46697300	0.78130200
C	6.31413300	-1.14552800	1.12488100
O	6.46223500	-1.03880300	2.33130900
C	4.97203900	-0.86836200	0.50931800
C	4.62904000	-1.57358500	-0.60502800
H	5.43281600	-2.18133300	-1.02571900
C	3.36231600	-1.79504200	-1.28480300
C	3.33468000	-2.81096900	-2.25843100
C	2.17672800	-1.07992600	-1.03646100
C	2.16439500	-3.11851800	-2.94036400
H	4.25024300	-3.35914800	-2.48001300
C	1.01319900	-1.37638400	-1.73133400
H	2.17754100	-0.26294700	-0.32527500
C	0.99967500	-2.40047700	-2.67901900
H	2.16471500	-3.90976600	-3.68608700
H	0.11291900	-0.79686400	-1.53520800
H	0.08564100	-2.62927200	-3.22271800
C	4.07369500	-0.03538500	1.29305000
C	3.10675700	-0.18851300	2.15398500
C	2.20226100	0.72346300	2.84742300
C	2.63992100	1.45136500	3.96322800
C	0.87135200	0.85065900	2.42290700
C	1.76799800	2.31607900	4.61734400
H	3.66492200	1.32868100	4.31154100
C	0.00804200	1.71799500	3.08191200
H	0.52228900	0.26261500	1.57419800
C	0.45335800	2.45552000	4.17711200

H	2.11700700	2.88091200	5.47887200
H	-1.01950800	1.81597200	2.73905000
H	-0.22571300	3.13026400	4.69270100
Au	2.76214400	-2.27054400	2.43944200
P	2.31081900	-4.57292400	2.42297000
C	0.63897800	-4.92976200	1.80008700
C	-0.18674700	-5.89536100	2.37835900
C	0.19843500	-4.21461900	0.67970600
C	-1.44625400	-6.14186100	1.83677200
H	0.14867900	-6.45551000	3.25003800
C	-1.05397000	-4.47276200	0.13757400
H	0.84374200	-3.45710700	0.22934300
C	-1.87822200	-5.43530800	0.71877800
H	-2.09034700	-6.89095100	2.29114700
H	-1.38867000	-3.91620300	-0.73533200
H	-2.86223100	-5.63141500	0.29915600
C	2.47640100	-5.43840800	4.01003200
C	2.87039200	-6.77836800	4.07410600
C	2.15785900	-4.74617300	5.18227100
C	2.94236400	-7.41891600	5.30671600
H	3.12028800	-7.32098100	3.16285500
C	2.22648000	-5.39374900	6.41104600
H	1.85918300	-3.69901400	5.12735600
C	2.62038000	-6.72803600	6.47241100
H	3.25207800	-8.46003100	5.35657600
H	1.97986300	-4.85330600	7.32183500
H	2.68198600	-7.23108600	7.43466600
C	3.44968100	-5.38746500	1.25637200
C	4.79791300	-5.01107400	1.28553900
C	3.01522500	-6.34438800	0.33645200

C	5.70168500	-5.59002500	0.40245100
H	5.13546800	-4.25484300	1.99683700
C	3.92294500	-6.91330400	-0.55292300
H	1.96835000	-6.64292300	0.31064700
C	5.26208500	-6.53617100	-0.52226100
H	6.74992200	-5.30060000	0.43208000
H	3.57961600	-7.65340100	-1.27187500
H	5.96753000	-6.98025800	-1.22082700

Electronic Energy (0K) = -2709.3096381

Electronic Energy (0K) + ZPE = -2708.505740

Enthalpy (298K) = -2708.452826

Free Energy (298K) = -2708.593480

A2'

Number of imaginary frequencies: 0

C	-1.96209900	3.86001300	-1.90181700
H	-1.39331500	4.72025400	-2.27139900
H	-2.03584600	3.14733700	-2.73526100
H	-2.96321300	4.16167000	-1.58855000
C	-1.24701800	3.19251000	-0.78119000
O	-1.80118200	2.86865800	0.26042100
C	0.21032300	2.88171100	-0.94879900
C	1.12932200	3.52238700	0.10510300
H	0.54891300	4.13141100	0.79593900
C	2.45136500	4.12614900	-0.19530700
C	2.74744200	5.34325700	0.43036500
C	3.42050400	3.55055000	-1.02669800
C	3.97152700	5.97113600	0.23073800
H	2.00523300	5.79788000	1.08612200
C	4.64469000	4.17938000	-1.22552100

H	3.22491100	2.60230500	-1.52095800
C	4.92502000	5.39141300	-0.60035500
H	4.17973600	6.91555000	0.72864200
H	5.38402300	3.71666500	-1.87587100
H	5.88398000	5.87988800	-0.75760300
C	0.68792200	2.73137300	-2.28844700
C	1.03323700	2.56078900	-3.43870900
C	1.42209700	2.25605800	-4.77386700
C	0.49759700	2.36718700	-5.82331400
C	2.72052900	1.79346400	-5.03862600
C	0.87327200	2.02797800	-7.11600400
H	-0.51122300	2.71544500	-5.60994500
C	3.08487300	1.45474500	-6.33471000
H	3.42989300	1.69523600	-4.21824400
C	2.16499800	1.57336300	-7.37442500
H	0.15349000	2.11616100	-7.92638700
H	4.09164300	1.09591800	-6.53552800
H	2.45428200	1.30771400	-8.38856200
C	4.22528600	0.19130700	0.35966300
H	4.07675600	-0.89478800	0.41829000
H	4.52038400	0.43348100	-0.66721100
H	5.02839900	0.46267600	1.04859900
C	2.97579200	0.91606700	0.78093800
O	2.90600900	1.43351900	1.88696100
C	1.80060800	0.98383700	-0.13452200
C	1.69115200	0.02251000	-1.08680600
H	2.57312900	-0.61475600	-1.16828500
C	0.67107900	-0.38941500	-2.04522700
C	1.09858000	-1.26873300	-3.05492200
C	-0.67911700	0.00618500	-2.04715000

C	0.23294100	-1.70366600	-4.05055500
H	2.13433600	-1.60625200	-3.05601000
C	-1.54740100	-0.43794400	-3.03445500
H	-1.05685200	0.66617500	-1.27208200
C	-1.09394400	-1.28519400	-4.04523400
H	0.59473300	-2.37435900	-4.82618600
H	-2.58787300	-0.11878800	-3.01655900
H	-1.77820300	-1.62509900	-4.81907300
C	0.80086500	2.05438200	0.22622400
C	-0.13248400	1.61224600	1.30818800
C	-0.25628700	2.30396500	2.57629500
C	0.71937400	3.17961500	3.09987600
C	-1.41143300	2.05629400	3.35296700
C	0.53880800	3.77636600	4.33833600
H	1.64984800	3.33114100	2.56363200
C	-1.60808900	2.69188100	4.56636300
H	-2.16748100	1.37611200	2.96061400
C	-0.62750100	3.54925800	5.06589500
H	1.31353000	4.42445200	4.74031400
H	-2.51631500	2.50740700	5.13442500
H	-0.76792700	4.03080800	6.03101500
Au	-0.83898600	-0.34715800	1.22703600
P	-1.47531500	-2.62873200	1.12766300
C	-3.12681500	-2.88323300	0.41083600
C	-3.78936500	-4.11095400	0.51698200
C	-3.73146500	-1.82468300	-0.27323500
C	-5.03994600	-4.27597800	-0.06635700
H	-3.32502700	-4.93692800	1.05480600
C	-4.98248400	-1.99485600	-0.85825100
H	-3.21640100	-0.86495200	-0.34066100

C	-5.63528300	-3.21951300	-0.75371700
H	-5.55350600	-5.23071300	0.01819400
H	-5.45051300	-1.16841900	-1.38821700
H	-6.61542200	-3.35211600	-1.20628900
C	-1.48124500	-3.47291500	2.74120000
C	-1.16984200	-4.83026600	2.86821400
C	-1.83913200	-2.73293600	3.87292000
C	-1.22385600	-5.43976600	4.11741500
H	-0.88076800	-5.41077000	1.99288700
C	-1.89497500	-3.34821500	5.11920600
H	-2.06951300	-1.67110400	3.77443900
C	-1.58613000	-4.70053300	5.24060600
H	-0.97949600	-6.49502500	4.21373600
H	-2.17089900	-2.76868500	5.99698900
H	-1.62355900	-5.17981800	6.21610400
C	-0.29365400	-3.55400200	0.09125100
C	1.05637300	-3.52380900	0.46760500
C	-0.67497300	-4.24161500	-1.06154000
C	2.00763200	-4.19200500	-0.29262000
H	1.35901400	-2.97717700	1.36263300
C	0.28438100	-4.90869700	-1.82148500
H	-1.71762700	-4.25835200	-1.37427700
C	1.62095100	-4.88681600	-1.43859000
H	3.05279100	-4.17030100	0.00817800
H	-0.01840200	-5.44736900	-2.71650300
H	2.36602700	-5.41025700	-2.03328400

Electronic Energy (0K) = -2709.3372944

Electronic Energy (0K) + ZPE = -2708.531929

Enthalpy (298K) = -2708.479066

Free Energy (298K) = -2708.620811

TS_{A3}

Number of imaginary frequencies: 1

C	4.62451000	2.24462100	2.76614500
H	4.28363200	1.27600600	3.13501000
H	5.71537500	2.27766100	2.80570400
H	4.23166100	3.02423500	3.43265900
C	4.11101800	2.47767600	1.38709600
O	3.11642200	1.87567100	0.94078000
C	4.74604400	3.46411500	0.48831000
C	5.64098500	4.36365100	0.99465800
H	5.85235400	4.27581800	2.06002200
C	6.35261500	5.44980700	0.35858700
C	7.19766700	6.22261400	1.17795400
C	6.25499200	5.78213700	-1.00571800
C	7.91701900	7.28824900	0.65985500
H	7.27944400	5.97267600	2.23478000
C	6.97775100	6.84752300	-1.51975800
H	5.61026900	5.20180400	-1.65879400
C	7.80815200	7.60335000	-0.69275600
H	8.56250100	7.87521800	1.30851900
H	6.89365700	7.09391900	-2.57553900
H	8.37006800	8.43853400	-1.10441300
C	4.31515800	3.37627800	-0.86340000
C	3.89749500	3.15710800	-1.98453600
C	3.38394600	2.83389900	-3.27159800
C	2.31996800	1.92094600	-3.36362700
C	3.93394800	3.37238000	-4.44476200
C	1.82606600	1.54443800	-4.60458000
H	1.89665400	1.51290800	-2.44711900

C	3.42802400	2.99579900	-5.68212800
H	4.75861400	4.07878600	-4.37399100
C	2.37927800	2.08114200	-5.76587100
H	1.00810400	0.82796900	-4.66290300
H	3.85715500	3.41494800	-6.58922600
H	1.99296100	1.78629000	-6.73879100
C	5.97986200	-0.04404800	-1.53051500
H	6.15112400	-1.01760900	-2.00513300
H	5.57716000	0.62940900	-2.29590800
H	6.93415700	0.34531700	-1.16872200
C	5.04664700	-0.17389400	-0.35748600
O	5.44700700	0.05046800	0.77631700
C	3.63020200	-0.58643500	-0.59528100
C	3.22529200	-0.95327900	-1.83648900
H	3.96893100	-0.94999100	-2.63343600
C	1.90206700	-1.39805700	-2.25148900
C	1.81046600	-2.31705700	-3.30920300
C	0.71481800	-0.92995600	-1.66179300
C	0.57607100	-2.78822000	-3.73598000
H	2.72537800	-2.66533900	-3.78661800
C	-0.52171800	-1.37987200	-2.11279100
H	0.76431800	-0.17488500	-0.88011600
C	-0.59342100	-2.31627700	-3.14125700
H	0.52149600	-3.51559500	-4.54302000
H	-1.43289500	-0.99201600	-1.66246300
H	-1.56082900	-2.67334000	-3.48784400
C	2.77315000	-0.66397800	0.58719300
C	2.46782600	0.16926200	1.51682500
C	1.82196500	0.43722400	2.77873800
C	1.98750900	-0.48173800	3.82761000

C	1.02916400	1.57577800	2.97695700
C	1.34327400	-0.27724700	5.04124800
H	2.62496200	-1.35169000	3.67522800
C	0.39939700	1.77740000	4.19772800
H	0.91680900	2.29775100	2.17230100
C	0.54935300	0.85174900	5.22872100
H	1.47521000	-0.99592100	5.84693400
H	-0.21466000	2.66225500	4.34554000
H	0.05334500	1.01525100	6.18256700
Au	1.85297700	-2.55259300	1.00616300
P	0.96313700	-4.69822700	1.34625300
C	2.24037300	-5.90677800	1.82335100
C	1.89968100	-7.21104600	2.20120900
C	3.58244500	-5.51623800	1.81589000
C	2.89394300	-8.10847300	2.56959600
H	0.85715500	-7.52624400	2.20695900
C	4.57560700	-6.41933600	2.18565700
H	3.84650600	-4.49926200	1.52412700
C	4.23090300	-7.71235400	2.56338100
H	2.62620400	-9.12058700	2.86353800
H	5.61769000	-6.10912100	2.18095000
H	5.00557000	-8.41723000	2.85625200
C	-0.30367900	-4.74613500	2.65477200
C	-1.29382900	-5.73418100	2.69309800
C	-0.24700200	-3.78354900	3.66774700
C	-2.21060700	-5.75781500	3.73821100
H	-1.35765800	-6.47888300	1.90100400
C	-1.16500200	-3.81338500	4.71258700
H	0.51575700	-3.00427000	3.63208200
C	-2.14584500	-4.80015400	4.74778800

H	-2.98020100	-6.52568400	3.76311700
H	-1.11875300	-3.05980600	5.49549800
H	-2.86688600	-4.82052200	5.56169500
C	0.16125400	-5.34829000	-0.15672900
C	0.78233400	-6.30420900	-0.96432700
C	-1.06997700	-4.80696900	-0.54648100
C	0.16835700	-6.72452900	-2.14132700
H	1.74287200	-6.72732200	-0.67567100
C	-1.68470200	-5.24265100	-1.71357800
H	-1.55577000	-4.04909200	0.06866200
C	-1.06604400	-6.20170700	-2.51335000
H	0.65555500	-7.47163800	-2.76348400
H	-2.64860500	-4.82908600	-2.00187700
H	-1.54730600	-6.54041100	-3.42797700

Electronic Energy (0K) = -2709.326053

Electronic Energy (0K) + ZPE = -2708.523670

Enthalpy (298K) = -2708.470201

Free Energy (298K) = -2708.615658

A3

Number of imaginary frequencies: 0

C	1.13073900	1.83439500	2.82235500
H	1.08072200	0.76929100	3.05943700
H	2.10721400	2.21491200	3.12147800
H	0.35179300	2.34755500	3.40385100
C	0.87338400	2.03985500	1.38443200
O	0.05564700	1.28181100	0.73648500
C	1.44277200	3.09682500	0.58474500
C	2.12642900	4.11195700	1.21611800
H	2.18608000	4.03924700	2.30096000

C	2.76469600	5.28228400	0.68458100
C	3.36207300	6.15511600	1.61878100
C	2.83572200	5.60780800	-0.68585100
C	4.00544800	7.30847000	1.20434600
H	3.31046600	5.90720000	2.67758600
C	3.48256600	6.76166200	-1.09355400
H	2.38462300	4.95197000	-1.42381000
C	4.06650100	7.61302300	-0.15448700
H	4.45960500	7.97215500	1.93530200
H	3.53362900	7.00472800	-2.15178900
H	4.57192400	8.51747500	-0.48491500
C	1.22845400	2.97438200	-0.81633200
C	0.99797900	2.72731800	-1.98383200
C	0.69960000	2.38265000	-3.33121900
C	-0.23439900	1.36244000	-3.57217000
C	1.32892500	3.01430900	-4.41397200
C	-0.52566500	0.97263800	-4.87144700
H	-0.72163100	0.88052600	-2.72641500
C	1.02521700	2.62330700	-5.71155400
H	2.05453100	3.80334000	-4.22720800
C	0.10331200	1.60338700	-5.94333600
H	-1.24507100	0.17256600	-5.03918100
H	1.51411000	3.11477700	-6.54937000
H	-0.12444400	1.30114400	-6.96290600
C	3.43980600	-0.49795200	-1.22273400
H	3.62009200	-1.52523000	-1.55819000
H	3.19169000	0.09801500	-2.10912300
H	4.35183000	-0.10001100	-0.77239100
C	2.33867000	-0.43277900	-0.19816600
O	2.56425000	0.07110400	0.89747700

C	0.98455000	-0.97344400	-0.52453000
C	0.75043400	-1.41205300	-1.78924800
H	1.58261000	-1.40731700	-2.49352100
C	-0.49573000	-1.90696100	-2.35981200
C	-0.41942200	-2.80870700	-3.43497200
C	-1.76668600	-1.47994400	-1.93584100
C	-1.56854300	-3.29043600	-4.04739300
H	0.56135200	-3.12746500	-3.78609400
C	-2.91602800	-1.94040300	-2.57092900
H	-1.84813600	-0.74477200	-1.13831200
C	-2.82144700	-2.84843500	-3.62332700
H	-1.48812200	-3.99406600	-4.87271700
H	-3.89003000	-1.58092600	-2.24578900
H	-3.72108000	-3.19875000	-4.12485400
C	-0.01209500	-1.06472000	0.55965500
C	-0.42728600	0.01080800	1.23961500
C	-1.43663500	0.14578200	2.30097600
C	-1.52785100	-0.80669200	3.32550600
C	-2.33753900	1.21897500	2.29998200
C	-2.52607200	-0.71994800	4.28793900
H	-0.79714900	-1.61391400	3.36759800
C	-3.32573400	1.31183400	3.27509000
H	-2.27415600	1.97791600	1.52194800
C	-3.43187900	0.33840500	4.26460000
H	-2.58940800	-1.48069300	5.06472400
H	-4.02216500	2.14710100	3.25411700
H	-4.20983200	0.41070500	5.02107500
Au	-0.75205200	-2.97914900	0.99823600
P	-1.59208900	-5.09356300	1.62914800
C	-2.87385000	-5.77638800	0.53035500

C	-3.25801500	-5.05283700	-0.60127000
C	-3.45591000	-7.02353100	0.78831500
C	-4.22489600	-5.56775500	-1.46135200
H	-2.79395400	-4.08659700	-0.81171900
C	-4.41931100	-7.53263800	-0.07248000
H	-3.15701200	-7.59739300	1.66517700
C	-4.80482500	-6.80375100	-1.19711600
H	-4.52062000	-4.99954900	-2.34088600
H	-4.87006100	-8.50122000	0.13087400
H	-5.55769400	-7.20561700	-1.87143700
C	-0.32397700	-6.39805500	1.75368500
C	-0.38066400	-7.42233500	2.70374300
C	0.71313200	-6.38077900	0.81489300
C	0.59172800	-8.41720400	2.71071800
H	-1.17854300	-7.44120900	3.44450400
C	1.67882400	-7.38179400	0.82147300
H	0.76155600	-5.57696200	0.07914300
C	1.61916200	-8.39848600	1.77080900
H	0.54579700	-9.20989600	3.45390100
H	2.48320600	-7.36269200	0.08989900
H	2.37839800	-9.17715800	1.78158500
C	-2.33480100	-4.94548300	3.28909800
C	-1.47988200	-4.71842400	4.37611800
C	-3.71713800	-4.91853500	3.48409600
C	-2.00353000	-4.49934500	5.64437300
H	-0.39945600	-4.71712800	4.22900400
C	-4.23728700	-4.68630300	4.75562200
H	-4.39341400	-5.07994100	2.64645000
C	-3.38470400	-4.48366200	5.83580400
H	-1.33215900	-4.33683900	6.48437000

H	-5.31501300	-4.66971800	4.89991200
H	-3.79512100	-4.31134500	6.82813500

Electronic Energy (0K) = -2709.342712

Electronic Energy (0K) + ZPE = -2708.537956

Enthalpy (298K) = -2708.484776

Free Energy (298K) = -2708.629920

TS_{A3'}

Number of imaginary frequencies: 1

C	4.18571700	2.14794200	2.14016600
H	3.86938500	1.15431600	2.46277700
H	5.21732200	2.31649800	2.45630700
H	3.54264100	2.88926100	2.63485300
C	4.01664700	2.27579300	0.66871100
O	3.19649400	1.56909300	0.03798300
C	4.76756900	3.26911500	-0.11704800
C	5.40849400	4.29365600	0.52144600
H	5.32600700	4.30031300	1.60794800
C	6.17209500	5.40054300	-0.00518900
C	6.70851400	6.30607000	0.93039900
C	6.41176700	5.62780100	-1.37383800
C	7.45747600	7.39740300	0.51965300
H	6.52649000	6.13670400	1.99070600
C	7.16104200	6.72089400	-1.77952800
H	6.00945000	4.94391900	-2.11555400
C	7.68511200	7.60713500	-0.83869100
H	7.86392100	8.08653300	1.25573500
H	7.33966200	6.88664400	-2.83927100
H	8.27156900	8.46266200	-1.16579700
C	4.73211100	3.02827900	-1.51702400

C	4.63814900	2.64366900	-2.66680900
C	4.46545900	2.09674400	-3.96842400
C	3.48812000	1.10147900	-4.14595700
C	5.25376900	2.49245700	-5.05871900
C	3.31280900	0.50874600	-5.38817500
H	2.87414500	0.81140700	-3.29349900
C	5.06686800	1.89664200	-6.29933300
H	6.01037400	3.26197300	-4.92023300
C	4.10193200	0.90493000	-6.46689400
H	2.55566100	-0.26256800	-5.51568200
H	5.68019000	2.20539400	-7.14263700
H	3.96397700	0.44146800	-7.44108800
C	6.17426100	-0.92475300	-1.66784600
H	6.13156900	-2.01411700	-1.79023700
H	5.90276100	-0.47432000	-2.63121000
H	7.19424600	-0.63484800	-1.40709100
C	5.24948000	-0.46504800	-0.57826700
O	5.68022100	0.11768500	0.40827200
C	3.78582800	-0.70941400	-0.71340500
C	3.28828000	-1.40978000	-1.76871000
H	4.01963000	-1.83968900	-2.45620500
C	1.91192600	-1.73962700	-2.09848500
C	1.68305100	-2.92886200	-2.81086800
C	0.81575800	-0.92371500	-1.77072300
C	0.39195800	-3.32281200	-3.13591300
H	2.53441100	-3.54825300	-3.09265600
C	-0.47094000	-1.30810000	-2.12014400
H	0.98250900	0.02777000	-1.27084700
C	-0.68699500	-2.51308600	-2.78894500
H	0.22776900	-4.25569800	-3.67017800

H	-1.31079600	-0.66108400	-1.87880700
H	-1.69842400	-2.81093600	-3.05686500
C	2.94738700	-0.23167900	0.36676800
C	2.09647000	-0.56059500	1.28228200
C	1.22614500	0.21104000	2.16793200
C	0.93862900	-0.26851500	3.45437500
C	0.65060800	1.42186800	1.75345000
C	0.12420400	0.45729200	4.31503200
H	1.36963200	-1.21869500	3.77068700
C	-0.18119400	2.13327900	2.61055700
H	0.85609700	1.80089900	0.75520100
C	-0.44123300	1.65831500	3.89408700
H	-0.07955300	0.07740800	5.31359700
H	-0.62777800	3.06619700	2.27346900
H	-1.08910100	2.22089500	4.56240100
Au	1.92687700	-2.68722600	1.23382000
P	1.68892500	-5.01886400	1.13472700
C	0.43410000	-5.54304600	-0.07742200
C	-0.82735600	-4.93848000	-0.00827300
C	0.68338000	-6.51916300	-1.04442300
C	-1.83302100	-5.32308600	-0.88612400
H	-1.02085700	-4.17082600	0.74238600
C	-0.32526500	-6.89132400	-1.93076500
H	1.66096600	-6.99432900	-1.10807500
C	-1.58185500	-6.29935500	-1.84931300
H	-2.81312700	-4.85574100	-0.82284300
H	-0.12812800	-7.65280400	-2.68175000
H	-2.36875700	-6.59709900	-2.53847600
C	3.24483000	-5.83802200	0.66379000
C	3.48186800	-7.18332600	0.96538700

C	4.20875300	-5.10431300	-0.03560700
C	4.66725700	-7.78746400	0.56137500
H	2.73910200	-7.75930200	1.51654900
C	5.39224500	-5.71385400	-0.43937100
H	4.03315800	-4.04812200	-0.25054500
C	5.62088300	-7.05413200	-0.14114400
H	4.84878300	-8.83297600	0.79881700
H	6.14227400	-5.13961300	-0.97825900
H	6.54889900	-7.52869900	-0.45148800
C	1.18718200	-5.75454700	2.72279900
C	1.71585400	-5.19999600	3.89377200
C	0.32729700	-6.85326400	2.80085500
C	1.39341000	-5.74537900	5.13102100
H	2.37909200	-4.33600900	3.83162200
C	0.00236200	-7.39090800	4.04294500
H	-0.09023500	-7.28956100	1.89428000
C	0.53449900	-6.83949900	5.20515700
H	1.80588900	-5.31107300	6.03861700
H	-0.66950300	-8.24399800	4.10106500
H	0.27549100	-7.26149400	6.17345400

Electronic Energy (0K) = -2709.3260964

Electronic Energy (0K) + ZPE = -2708.524402

Enthalpy (298K) = -2708.470661

Free Energy (298K) = -2708.617454

A3'

Number of imaginary frequencies: 0

C	3.04401900	0.55170500	1.13876300
H	2.85872100	-0.50615600	1.31884400
H	4.08439800	0.67934000	0.82099000

H	2.90293500	1.11596700	2.06934600
C	2.13914500	1.07246500	0.09442300
O	1.19720900	0.35984900	-0.41809700
C	2.21138100	2.40711400	-0.44684400
C	3.16413700	3.26717900	0.05605700
H	3.80052900	2.86250900	0.84180400
C	3.46359000	4.63237200	-0.26847600
C	4.44612000	5.26635600	0.52215900
C	2.85880700	5.36524300	-1.31094800
C	4.80131900	6.58442100	0.29257000
H	4.92277500	4.70368700	1.32308700
C	3.22402600	6.68067400	-1.53957500
H	2.11343700	4.89336400	-1.94253900
C	4.18905700	7.29381000	-0.73923300
H	5.55619200	7.06121500	0.91207400
H	2.75550000	7.23618600	-2.34794100
H	4.46677600	8.32871900	-0.92495400
C	1.23871100	2.73803400	-1.43229800
C	0.36484100	2.93900400	-2.25266200
C	-0.64780000	3.20514900	-3.21705100
C	-1.29580800	2.14535600	-3.87141400
C	-1.00720000	4.52831400	-3.51899700
C	-2.28586900	2.40968600	-4.80756700
H	-1.00907400	1.12129100	-3.64047600
C	-1.99724200	4.78132000	-4.45817200
H	-0.50592900	5.34745600	-3.00726700
C	-2.63815200	3.72522600	-5.10262200
H	-2.78498500	1.58540500	-5.31141300
H	-2.27156000	5.80806300	-4.68848600
H	-3.41414600	3.92720500	-5.83722200

C	2.45279400	-3.24184400	-2.61091500
H	1.99673000	-4.21179000	-2.37767900
H	2.00999700	-2.89007500	-3.54971200
H	3.52812700	-3.37551500	-2.74797200
C	2.22753000	-2.25679700	-1.49893600
O	3.17516800	-1.74769500	-0.91286600
C	0.84261400	-1.89089000	-1.10057500
C	-0.22750400	-2.44347800	-1.71890300
H	-0.02256200	-3.22260500	-2.45588700
C	-1.65153700	-2.18843000	-1.52395800
C	-2.54520400	-3.23853400	-1.78458400
C	-2.17013400	-0.94589800	-1.12598800
C	-3.91294800	-3.07113800	-1.60206200
H	-2.14970900	-4.19903700	-2.11720200
C	-3.53852400	-0.77242900	-0.96937800
H	-1.49618100	-0.10700400	-0.96601900
C	-4.41246500	-1.83649900	-1.19474000
H	-4.59033200	-3.90194600	-1.78959400
H	-3.92752400	0.20003800	-0.67646000
H	-5.48370900	-1.69693500	-1.06691800
C	0.75020500	-0.94351900	0.03077000
C	0.23680800	-1.12745000	1.25082900
C	0.14841300	-0.05953600	2.26114900
C	0.60315700	-0.30764600	3.56581000
C	-0.37146800	1.21203900	1.97010900
C	0.58793000	0.69202100	4.53062200
H	0.98754700	-1.29909300	3.80668200
C	-0.40367500	2.20586300	2.94374400
H	-0.75501300	1.42499800	0.97236600
C	0.08664800	1.95563700	4.22257200

H	0.96074200	0.48229500	5.53101500
H	-0.81368300	3.18355400	2.69888000
H	0.06633800	2.73661900	4.97922900
Au	-0.60325000	-2.99637200	1.66919000
P	-1.64560400	-5.09552700	1.96731300
C	-0.86731600	-6.18728700	3.19949300
C	-0.38061300	-5.60058700	4.37278200
C	-0.76569500	-7.56966100	3.02038700
C	0.19708000	-6.39128000	5.35981200
H	-0.45418600	-4.52078600	4.50771800
C	-0.17802000	-8.35544200	4.00762900
H	-1.14524800	-8.03446200	2.11133900
C	0.30203000	-7.76792100	5.17490300
H	0.57470700	-5.93156300	6.27012800
H	-0.09616200	-9.43023200	3.86363200
H	0.76310500	-8.38484000	5.94276300
C	-3.39899800	-4.96475300	2.43639700
C	-4.06205800	-5.98273400	3.12794700
C	-4.10306100	-3.82507500	2.03383200
C	-5.41877000	-5.85928900	3.40998900
H	-3.52062100	-6.87345700	3.44433300
C	-5.46127000	-3.71031200	2.31021200
H	-3.58168900	-3.02747900	1.50115900
C	-6.11772300	-4.72635400	2.99978300
H	-5.93179700	-6.65152900	3.95017000
H	-6.00489800	-2.82213300	1.99547500
H	-7.17823100	-4.63383100	3.22280000
C	-1.61906300	-6.02203100	0.39473000
C	-2.76579500	-6.57895600	-0.17383800
C	-0.38809700	-6.14776900	-0.26189800

C	-2.68147400	-7.25490300	-1.38960000
H	-3.72916400	-6.48105300	0.32451400
C	-0.30685700	-6.83159900	-1.46892300
H	0.50908500	-5.71098000	0.18029200
C	-1.45587400	-7.38322400	-2.03557500
H	-3.57843600	-7.68495600	-1.82937200
H	0.65364800	-6.93556700	-1.96923000
H	-1.39318300	-7.91404000	-2.98272500

Electronic Energy (0K) = -2709.340753

Electronic Energy (0K) + ZPE = -2708.536187

Enthalpy (298K) = -2708.482752

Free Energy (298K) = -2708.628982

TS_{A4}

Number of imaginary frequencies: 1

C	-2.66787900	0.39647500	1.27101000
H	-2.61726200	1.48195200	1.13346300
H	-3.48632400	0.02146900	0.64476800
H	-2.88996700	0.18629400	2.31996900
C	-1.37007600	-0.27022800	0.90839800
O	-0.78451500	-0.98012800	1.71310900
C	-0.79810100	-0.05557700	-0.45513600
C	-1.39320700	0.78388300	-1.34143500
H	-2.29466700	1.29929600	-1.01132500
C	-0.95205500	1.15295400	-2.67819800
C	-1.33890000	2.41357900	-3.16519700
C	-0.14406600	0.34039300	-3.49545100
C	-0.88432400	2.87500500	-4.39267700
H	-1.98971800	3.03727000	-2.55369700
C	0.30052600	0.80185200	-4.73049700

H	0.10111100	-0.67356600	-3.18517900
C	-0.05370400	2.07337800	-5.17463600
H	-1.18058800	3.86099900	-4.74402600
H	0.91621400	0.15811400	-5.35548100
H	0.30235900	2.43420800	-6.13732500
C	0.45499100	-0.74298200	-0.71059700
C	0.97333300	-1.90696200	-0.69722800
C	2.12906500	-2.76047200	-0.82279700
C	2.34536600	-3.48760800	-2.00209400
C	3.06528600	-2.82484100	0.22075500
C	3.50333700	-4.24070400	-2.14633400
H	1.60268000	-3.44541700	-2.79767000
C	4.21679600	-3.58620000	0.06973600
H	2.88337700	-2.25997300	1.13376700
C	4.43798000	-4.28987200	-1.11361500
H	3.67741400	-4.79504600	-3.06538600
H	4.94475300	-3.63195200	0.87587900
H	5.34154800	-4.88355800	-1.22890400
Au	2.16582900	0.43986100	-1.34383900
P	3.90887500	1.77301500	-2.14554800
C	-0.66266600	-3.44703400	-0.67214500
C	-0.30522700	-4.12940700	0.43103300
H	0.69896700	-4.54531300	0.51892900
N	-1.08507200	-4.27490000	1.54893300
C	-2.51034100	-4.10888300	1.51121100
C	-3.10463400	-3.02826900	2.15792900
C	-3.27689100	-5.05240700	0.82777900
C	-4.49042100	-2.89884800	2.12040000
H	-2.47693200	-2.29065600	2.65509000
C	-4.65766200	-4.90599200	0.78731800

H	-2.78122800	-5.89033500	0.34065700
C	-5.26441400	-3.83268500	1.43783400
H	-4.96572300	-2.05908300	2.62261100
H	-5.26253600	-5.63635500	0.25560300
H	-6.34613500	-3.72463800	1.41059500
O	1.01498700	-5.16731700	2.64536900
O	-1.23784900	-6.09903100	3.32985700
S	-0.39184600	-4.97345300	2.96790100
C	-0.56098500	-3.71112700	4.18142600
C	-1.51053100	-3.85360400	5.18870300
C	0.25413200	-2.58370100	4.09112200
C	-1.63684400	-2.83990800	6.12936200
H	-2.13541100	-4.74217500	5.22940600
C	0.10894900	-1.58406800	5.03846700
H	0.97395000	-2.48474300	3.28122400
C	-0.83437700	-1.69685600	6.06831000
H	-2.37012400	-2.93644900	6.92786700
H	0.73552800	-0.69507900	4.98617700
C	-0.98669000	-0.59818200	7.07165800
H	-1.59160800	-0.91376700	7.92729000
H	-1.47540900	0.27549500	6.62156100
H	-0.01228100	-0.25992200	7.44236100
C	-1.35110400	-3.27600800	-1.77956400
H	-1.33565200	-2.34000800	-2.33917000
H	-1.94870300	-4.08720200	-2.20092600
C	5.01660800	0.83510100	-3.24139600
C	6.30662800	1.29141600	-3.53297300
C	4.55550300	-0.35565500	-3.81101100
C	7.12204000	0.56085000	-4.38981200
H	6.67455300	2.21719500	-3.09112700

C	5.37564600	-1.08416200	-4.66661800
H	3.55115300	-0.71028600	-3.57335200
C	6.65797800	-0.62554000	-4.95428200
H	8.12508400	0.91555900	-4.61440900
H	5.01452900	-2.01356800	-5.10110200
H	7.30210800	-1.19780800	-5.61784500
C	4.96645200	2.48811800	-0.84988800
C	5.53348200	3.76002700	-0.96692200
C	5.24158600	1.70213000	0.27450600
C	6.37031200	4.23906300	0.03667300
H	5.32220300	4.37706000	-1.83925400
C	6.08205300	2.18424900	1.27117500
H	4.79445100	0.71060100	0.36513700
C	6.64410100	3.45336800	1.15280300
H	6.80907900	5.22982600	-0.05525300
H	6.29462700	1.57225600	2.14445800
H	7.29664700	3.83298800	1.93558400
C	3.24704800	3.16647600	-3.11079300
C	3.66986300	3.45343200	-4.40985400
C	2.25775400	3.95497900	-2.50961000
C	3.10454500	4.52250600	-5.10162700
H	4.43897400	2.84745300	-4.88552700
C	1.70014300	5.02098600	-3.20360400
H	1.92433500	3.72956000	-1.49537100
C	2.12312100	5.30448000	-4.50163800
H	3.43459400	4.74303300	-6.11408600
H	0.92837200	5.62686900	-2.73426900
H	1.68091000	6.13543600	-5.04644000

Electronic Energy (0K) = -3161.7814665

Electronic Energy (0K) + ZPE = -3160.968877

Enthalpy (298K) = -3160.913451

Free Energy (298K) = -3161.061633

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Number of imaginary frequencies: 0

C	-1.63163100	2.27386600	1.66765700
H	-1.28366300	3.30460000	1.54120300
H	-2.61614100	2.19755800	1.19023100
H	-1.73915100	2.05808600	2.73400600
C	-0.66776000	1.27876400	1.07606500
O	-0.23173500	0.38319000	1.79972600
C	-0.26093200	1.38291400	-0.35758900
C	-0.90711000	2.30244500	-1.12687400
H	-1.65119700	2.93658200	-0.64592200
C	-0.69598500	2.62173100	-2.53037200
C	-0.99235600	3.92941400	-2.95290100
C	-0.19359400	1.71363900	-3.47975100
C	-0.74533600	4.33387300	-4.25741000
H	-1.40108100	4.63635000	-2.23100700
C	0.02559900	2.11384700	-4.79405000
H	-0.00429300	0.68261900	-3.19209300
C	-0.23265700	3.42610800	-5.18288400
H	-0.96307900	5.35632100	-4.55830700
H	0.39745600	1.39412600	-5.52040700
H	-0.05055900	3.73700500	-6.20921000
C	0.89704700	0.57908700	-0.79370400
C	0.92067300	-0.77017700	-0.68627500
C	2.12209500	-1.60521200	-0.92179400
C	2.01864700	-2.84019500	-1.57758200
C	3.38986200	-1.19946500	-0.47468700

C	3.14788300	-3.61391900	-1.82954900
H	1.04272300	-3.18914200	-1.91333100
C	4.51729800	-1.97398500	-0.72262300
H	3.47897100	-0.27089900	0.08739300
C	4.40212000	-3.18195700	-1.40803700
H	3.04515000	-4.56080200	-2.35545800
H	5.48867000	-1.64138800	-0.36151200
H	5.28381700	-3.78910800	-1.60007800
Au	2.47067500	1.68649600	-1.63840200
P	4.08772000	3.02948800	-2.72944700
C	-0.30798100	-1.52775300	-0.29497200
C	-0.23767900	-2.05226900	1.05405000
H	0.75939300	-2.11179100	1.49900200
N	-1.19751700	-2.47736400	1.82932700
C	-2.60713300	-2.44546600	1.54682100
C	-3.28631400	-1.23764500	1.69094800
C	-3.25269400	-3.61914100	1.17074700
C	-4.64822700	-1.20476400	1.42017900
H	-2.74383700	-0.35055800	2.01355700
C	-4.61688700	-3.56841400	0.90538600
H	-2.68914800	-4.54357200	1.07360400
C	-5.30959400	-2.36589600	1.02514900
H	-5.19423000	-0.27046700	1.52200700
H	-5.13941700	-4.47216500	0.60328800
H	-6.37542400	-2.33463800	0.81333800
O	0.68052800	-2.77893000	3.58433900
O	-1.31766000	-4.34173900	3.63072100
S	-0.74908600	-3.01432100	3.51553600
C	-1.64768200	-1.86379900	4.47539200
C	-2.89447600	-2.23481000	4.97898000

C	-1.11984200	-0.58335600	4.64935300
C	-3.62279000	-1.29068900	5.68613400
H	-3.28148900	-3.23717400	4.81255400
C	-1.86990700	0.33926900	5.35955300
H	-0.15991600	-0.31193400	4.21818500
C	-3.12484300	0.00203000	5.88544300
H	-4.59738600	-1.55564700	6.09060700
H	-1.47899700	1.34331600	5.51489400
C	-3.90637900	1.00632000	6.66780600
H	-4.97121300	0.75555900	6.69585500
H	-3.79125500	2.01329500	6.25281300
H	-3.54887800	1.04371500	7.70499900
C	-1.35206100	-1.68375100	-1.12877000
H	-1.29188400	-1.27475500	-2.13594900
H	-2.25522700	-2.23103300	-0.87440000
C	3.33654200	4.57654000	-3.33883900
C	3.65155700	5.13180100	-4.58190000
C	2.41530200	5.22287300	-2.50628800
C	3.04961200	6.32054800	-4.98557700
H	4.36527500	4.63714400	-5.23897000
C	1.82862600	6.41776100	-2.90722000
H	2.15556600	4.78133000	-1.54272500
C	2.14255100	6.96511900	-4.14916500
H	3.29439800	6.74580000	-5.95620500
H	1.11234500	6.91343500	-2.25537900
H	1.67501500	7.89407500	-4.46795400
C	5.49546000	3.53566200	-1.68916600
C	6.08580900	4.79874300	-1.78136900
C	6.00099800	2.59702300	-0.78338400
C	7.17128800	5.11759900	-0.97014200

H	5.69957500	5.53359500	-2.48676400
C	7.08979100	2.91728300	0.01944900
H	5.53417900	1.61364200	-0.70960600
C	7.67211700	4.17952400	-0.07156700
H	7.62693500	6.10248800	-1.04239100
H	7.47924000	2.18486700	0.72276000
H	8.51881400	4.43397700	0.56189200
C	4.81833200	2.22462300	-4.19275200
C	6.12421700	2.48012100	-4.62090800
C	4.01034800	1.34562000	-4.92190300
C	6.61089200	1.86434800	-5.77028400
H	6.76234000	3.16089600	-4.05882300
C	4.49836900	0.73766800	-6.07299200
H	2.99616700	1.13791200	-4.57887700
C	5.79962900	0.99638700	-6.49646900
H	7.62835500	2.06373300	-6.09860600
H	3.86512600	0.05568300	-6.63574600
H	6.18488400	0.51643800	-7.39323200

Electronic Energy (0K) = -3161.8451835

Electronic Energy (0K) + ZPE = -3161.029672

Enthalpy (298K) = -3160.974564

Free Energy (298K) = -3161.123515

TS_{A4'}

Number of imaginary frequencies: 1

C	-1.27280900	0.73202300	1.43706900
H	-0.55037400	1.50392600	1.15106700
H	-2.20268800	0.94150300	0.88959300
H	-1.45897900	0.79830000	2.51152000
C	-0.79942400	-0.64796700	1.09756800

O	-0.73275600	-1.53433700	1.93274800
C	-0.41561000	-0.95888200	-0.31737700
C	0.22247200	-0.01994700	-1.06612900
H	0.39268600	0.94328600	-0.58120700
C	0.86660500	-0.14489900	-2.36539300
C	2.02219900	0.62555900	-2.57679400
C	0.41863600	-0.98969000	-3.39385500
C	2.73884700	0.52116900	-3.76218200
H	2.36108700	1.29516600	-1.78649600
C	1.12445700	-1.07401000	-4.58626900
H	-0.49705300	-1.56198100	-3.26372700
C	2.29025600	-0.32984800	-4.76967900
H	3.64318100	1.10855600	-3.90360900
H	0.76028900	-1.71979600	-5.38175800
H	2.83990900	-0.40397700	-5.70542000
C	-0.60105600	-2.31776100	-0.74172900
C	-0.09463200	-3.42340900	-1.15880200
C	-0.55750700	-4.64600200	-1.80182000
C	-1.64755900	-4.61800600	-2.68613700
C	0.09729400	-5.86616900	-1.57545500
C	-2.08041000	-5.78458700	-3.30518800
H	-2.15329400	-3.67355400	-2.88157900
C	-0.34924700	-7.03193400	-2.18521900
H	0.96241900	-5.88525900	-0.91169300
C	-1.43788500	-6.99416200	-3.05312000
H	-2.92616600	-5.74840300	-3.98805400
H	0.16130400	-7.97224100	-1.99052700
H	-1.78139800	-7.90521700	-3.53728900
Au	1.97108900	-3.14450600	-0.64050600
P	4.17350300	-2.68541700	0.00177500

C	-2.81443600	-2.17804100	-0.76794200
C	-3.05007400	-3.25481900	0.01978700
H	-2.78347500	-4.24606400	-0.35585100
N	-3.46923000	-3.22782000	1.31426700
C	-4.13185200	-2.08975100	1.88365800
C	-3.60299500	-1.43415100	2.99184200
C	-5.32367300	-1.66275300	1.29854900
C	-4.27947000	-0.33895800	3.51806200
H	-2.65340300	-1.75688900	3.41049100
C	-5.97974900	-0.55384400	1.82007700
H	-5.72990400	-2.20663100	0.44810900
C	-5.46156600	0.10567000	2.93188100
H	-3.87120700	0.17603200	4.38455800
H	-6.90624700	-0.21363900	1.36419900
H	-5.98179600	0.96689200	3.34424800
O	-3.36773000	-5.76926900	1.29912600
O	-4.18039700	-4.54158300	3.36688300
S	-3.25467100	-4.68219100	2.25945100
C	-1.59278000	-4.62123000	2.84427200
C	-1.33447500	-4.12213200	4.11760300
C	-0.56662500	-5.06664400	2.01059000
C	-0.01874400	-4.06717400	4.55746300
H	-2.15087800	-3.79707000	4.75813200
C	0.73994900	-5.00209200	2.47128600
H	-0.78611400	-5.46174100	1.01961300
C	1.03392500	-4.50103600	3.74621300
H	0.19760900	-3.68840300	5.55455900
H	1.55551100	-5.35286600	1.83693000
C	2.44702900	-4.46365900	4.23336900
H	2.54306200	-3.86247400	5.14274100

H	3.12316800	-4.05408200	3.47083100
H	2.80479900	-5.47611400	4.46200000
C	-3.22358700	-1.20017900	-1.54622700
H	-2.53655900	-0.45026500	-1.94207500
H	-4.27021200	-1.11307200	-1.84422900
C	4.85178000	-3.83666200	1.23345600
C	4.58064000	-5.20117900	1.07685500
C	5.64467300	-3.40066300	2.29816800
C	5.10749500	-6.12197000	1.97524600
H	3.95681600	-5.53923100	0.24769600
C	6.16293000	-4.32686200	3.19928100
H	5.85867800	-2.33986000	2.42312500
C	5.89650100	-5.68371000	3.03732600
H	4.89755400	-7.18168900	1.85062700
H	6.77789400	-3.98673100	4.02904200
H	6.30258800	-6.40386500	3.74390900
C	4.18418900	-1.02393400	0.75420500
C	5.17422500	-0.08001600	0.47396800
C	3.12618600	-0.68889600	1.60930800
C	5.09882900	1.19139300	1.03849200
H	6.00215000	-0.33068000	-0.18761500
C	3.05639500	0.58027000	2.17049900
H	2.35379200	-1.42738700	1.83292000
C	4.04103900	1.52341100	1.87942800
H	5.87009800	1.92512900	0.81677500
H	2.22979400	0.83344800	2.83124100
H	3.98231400	2.52016800	2.31042700
C	5.36626400	-2.62629800	-1.36748100
C	6.72019100	-2.91619200	-1.17655000
C	4.91246600	-2.20777000	-2.62263800

C	7.61173500	-2.78247900	-2.23648100
H	7.08024300	-3.24154800	-0.20123600
C	5.80962500	-2.06743100	-3.67531000
H	3.85444000	-1.98638400	-2.77477900
C	7.15847300	-2.35602100	-3.48213200
H	8.66452700	-3.01026000	-2.08737900
H	5.45149900	-1.73737400	-4.64820500
H	7.85994800	-2.25169200	-4.30662300

Electronic Energy (0K) = -3161.7878985

Electronic Energy (0K) + ZPE = -3160.975424

Enthalpy (298K) = -3160.920474

Free Energy (298K) = -3161.065116

A4'

Number of imaginary frequencies: 0

C	1.31293000	2.85940400	1.39995100
H	2.34500800	3.01944100	1.06514300
H	0.76381600	3.79144200	1.22648200
H	1.31668000	2.63306800	2.46862700
C	0.68967400	1.70807300	0.66479600
O	0.32510300	0.71258500	1.29295100
C	0.52620200	1.74499900	-0.81187300
C	0.95606900	2.82373200	-1.50821300
H	1.44349900	3.61532600	-0.93614800
C	0.91044100	3.10396800	-2.94174900
C	1.85431000	4.00759400	-3.45566700
C	-0.03441800	2.55474400	-3.82329400
C	1.87774200	4.32755400	-4.80809000
H	2.58947100	4.44629000	-2.77915000
C	-0.02475800	2.89238300	-5.16966400

H	-0.78482700	1.86356500	-3.44711300
C	0.93384600	3.77431400	-5.66915200
H	2.62758900	5.01863000	-5.18802300
H	-0.77322700	2.46913200	-5.83577100
H	0.93756700	4.03518700	-6.72509700
C	-0.03893100	0.48757700	-1.36817300
C	0.69600800	-0.37733300	-2.10609900
C	0.13668700	-1.67143800	-2.54365100
C	-1.09581100	-1.77167500	-3.20873900
C	0.85298700	-2.85616200	-2.30142300
C	-1.59284700	-3.00910400	-3.60943100
H	-1.65988100	-0.86629100	-3.42896800
C	0.34099600	-4.09270800	-2.67321800
H	1.82181500	-2.78869000	-1.80498400
C	-0.88439500	-4.17456300	-3.33375200
H	-2.54314000	-3.06137600	-4.13727800
H	0.90553100	-4.99741400	-2.45699100
H	-1.27819700	-5.14088800	-3.64049200
Au	2.63156400	0.11787700	-2.71037500
P	4.77851900	0.83873900	-3.41707600
C	-1.40336400	0.18673400	-0.82204500
C	-1.39380300	-0.92663800	0.10646400
H	-0.60152700	-1.66887700	-0.02589300
N	-2.20462600	-1.16792100	1.09885900
C	-3.24689600	-0.30216900	1.58631000
C	-2.88239900	0.81274300	2.33833900
C	-4.57587300	-0.61793000	1.32271000
C	-3.88605300	1.64628400	2.81605000
H	-1.82926600	1.01162900	2.53150000
C	-5.56660100	0.22800000	1.80890200

H	-4.82014000	-1.49893200	0.73478800
C	-5.22234500	1.35596000	2.54985400
H	-3.62261000	2.52385500	3.40073000
H	-6.61058800	0.00382200	1.60651500
H	-6.00247000	2.01309700	2.92615400
O	-0.76833700	-3.29502800	1.45085400
O	-3.16833600	-3.26943800	2.27305300
S	-1.87276200	-2.64038900	2.12610400
C	-1.37059300	-1.86537500	3.60856100
C	-2.29756600	-1.69884600	4.63616200
C	-0.07767600	-1.34302600	3.67492200
C	-1.90250000	-1.00043300	5.76717500
H	-3.30309100	-2.10210200	4.54559100
C	0.28775900	-0.64507100	4.81254300
H	0.61603500	-1.46600100	2.84737900
C	-0.61398600	-0.46553900	5.87133300
H	-2.60720300	-0.85998900	6.58405500
H	1.28965400	-0.22635500	4.88812900
C	-0.19125600	0.27358000	7.09886400
H	-1.05152500	0.57746900	7.70307000
H	0.39362100	1.16469000	6.84532700
H	0.44863100	-0.36065400	7.72590200
C	-2.48739800	0.93043700	-1.09889200
H	-2.40908800	1.75927000	-1.80041200
H	-3.47056900	0.73158300	-0.68273800
C	5.12539900	2.51105200	-2.76915900
C	5.54342800	3.56166300	-3.58751400
C	4.93789900	2.73272100	-1.39851900
C	5.77085100	4.82310000	-3.04096600
H	5.68633600	3.40003100	-4.65506700

C	5.17818900	3.98941900	-0.85541600
H	4.60240800	1.91473800	-0.75792700
C	5.59102200	5.03740800	-1.67804900
H	6.09307400	5.63889800	-3.68408200
H	5.04144300	4.15481700	0.21109700
H	5.77066500	6.02237700	-1.25314700
C	4.93183200	0.98248900	-5.22660700
C	6.15740600	0.86773200	-5.88922300
C	3.77489300	1.27828800	-5.95505200
C	6.22090500	1.05375100	-7.26657500
H	7.06246400	0.63442600	-5.32974900
C	3.84438600	1.47303100	-7.33000300
H	2.81723600	1.35523000	-5.43774400
C	5.06779900	1.35971400	-7.98543500
H	7.17518700	0.95995900	-7.77968500
H	2.94154700	1.70482000	-7.89087400
H	5.12301900	1.50508100	-9.06186400
C	6.17214400	-0.19691500	-2.86798200
C	7.43104600	0.33641200	-2.57420200
C	5.96380800	-1.57711300	-2.77540400
C	8.47069100	-0.50720000	-2.19611000
H	7.60029400	1.41047400	-2.64310000
C	7.00790200	-2.41678900	-2.40294100
H	4.97821200	-1.98981700	-2.99451900
C	8.26003600	-1.88135300	-2.11175000
H	9.44853000	-0.08946000	-1.96781500
H	6.84145700	-3.48909100	-2.33239400
H	9.07519800	-2.53700000	-1.81424200

Electronic Energy (0K) = -3161.8426306

Electronic Energy (0K) + ZPE = -3161.026229

Enthalpy (298K) = -3160.971225

Free Energy (298K) = -3161.119526

Pre'

Number of imaginary frequencies: 0

C	-2.77811500	2.10564700	0.17769400
H	-2.14507100	2.96552800	-0.06998900
H	-3.48459600	1.96599400	-0.64854900
H	-3.33375000	2.32244900	1.09253400
C	-1.95348700	0.87155800	0.40136400
O	-1.96651400	0.28830100	1.47405300
C	-1.10079500	0.35552400	-0.71357800
C	-1.02614700	1.00055600	-1.91062700
H	-1.66171000	1.88185000	-1.99970600
C	-0.25501300	0.72681000	-3.10809200
C	-0.53389800	1.52155000	-4.23543700
C	0.75032600	-0.25282400	-3.21448600
C	0.14578200	1.33475400	-5.42973300
H	-1.30010900	2.29195400	-4.16140600
C	1.43417700	-0.42998000	-4.40794600
H	1.00847300	-0.86980500	-2.35914000
C	1.13168100	0.35538600	-5.51925200
H	-0.09088700	1.95477600	-6.29086400
H	2.21102100	-1.18802700	-4.47315000
H	1.66843200	0.20620700	-6.45326800
C	-0.41171800	-0.86271000	-0.42714100
C	0.04473900	-2.00660900	-0.23995400
C	0.29205200	-3.40999600	-0.42250600
C	0.91827500	-4.18372200	0.56337000
C	-0.10413400	-4.00233900	-1.63178400

C	1.13973100	-5.53607400	0.34073600
H	1.22335400	-3.71314500	1.49650000
C	0.12402200	-5.35481400	-1.84349300
H	-0.58695900	-3.39224900	-2.39265100
C	0.74522500	-6.12223100	-0.85995100
H	1.62479900	-6.13486000	1.10755500
H	-0.18348900	-5.81222300	-2.78077100
H	0.92364600	-7.18128200	-1.03083700
Au	1.31159000	-0.74142200	1.02886700
Cl	2.97662500	0.05381400	2.46353800

Electronic Energy (0K) = -1364.9593263

Electronic Energy (0K) + ZPE = -1364.695543

Enthalpy (298K) = -1364.674008

Free Energy (298K) = -1364.748969

TS_A'

Number of imaginary frequencies: 1

C	-3.27596600	0.39058300	-2.57968900
C	-2.47739800	0.98941700	-1.76677700
C	-1.16341900	1.41309800	-2.22601800
C	-1.03449600	1.13266800	-3.67590300
O	-1.96862200	0.53791300	-4.22041200
C	-4.39904100	-0.32787500	-3.07460700
C	-4.95991400	-1.35285200	-2.29128300
C	-4.96497500	-0.01142700	-4.32075800
C	-6.08528200	-2.02727000	-2.74137600
H	-4.51036500	-1.59289600	-1.32987000
C	-6.07535000	-0.70953600	-4.76915000
H	-4.51815500	0.77352800	-4.92474100
C	-6.64021100	-1.71062700	-3.97971000

H	-6.52603400	-2.80926800	-2.12835900
H	-6.50981300	-0.46819900	-5.73598200
H	-7.51709400	-2.24821800	-4.33270600
H	0.36418000	2.59678500	-4.37152500
C	0.17344200	1.52146300	-4.45928800
H	0.02590500	1.26241800	-5.50920200
H	1.05786500	0.99763800	-4.07951200
C	-0.15777700	2.01449900	-1.54060600
C	-0.04594400	2.27694300	-0.11717700
C	0.60443900	3.45147300	0.29454700
C	-0.52629600	1.38902400	0.85857200
C	0.70505600	3.76645800	1.64233000
H	1.01002100	4.12507000	-0.45883800
C	-0.40491900	1.69833800	2.20805900
H	-0.95289700	0.43472100	0.55772300
C	0.19431700	2.89244800	2.60113600
H	1.19124400	4.68958200	1.94843400
H	-0.77926000	1.00098300	2.95426600
H	0.28074900	3.13418200	3.65791200
Au	-3.51788000	1.35677100	-0.00465200
H	0.68349200	2.37452800	-2.13596000
Cl	-4.68387700	1.78765200	2.00571800

Electronic Energy (0K) = -1364.9506824

Electronic Energy (0K) + ZPE = -1364.687421

Enthalpy (298K) = -1364.666686

Free Energy (298K) = -1364.739687

A'

Number of imaginary frequencies: 0

C	-0.19268800	-0.83160200	-2.05661600
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C	0.31739700	-0.26785500	-0.93082100
C	1.60710800	0.27796500	-1.35419300
C	1.73306700	0.02018300	-2.74683300
O	0.69843200	-0.65556400	-3.15893300
C	-1.41605300	-1.53084800	-2.42035100
C	-2.29432500	-2.00283200	-1.43203700
C	-1.73927400	-1.75716800	-3.76723400
C	-3.46461000	-2.66130700	-1.78289700
H	-2.04726200	-1.85349300	-0.38126800
C	-2.90921700	-2.42314200	-4.11090200
H	-1.07295400	-1.40546300	-4.55028900
C	-3.77912700	-2.87580900	-3.12319200
H	-4.13149300	-3.01886200	-1.00142200
H	-3.14201400	-2.58761500	-5.16074400
H	-4.69361500	-3.39817000	-3.39471800
H	3.37136000	1.18545200	-3.45624000
C	2.80107100	0.29026500	-3.71783600
H	2.37436100	0.40556300	-4.71819700
H	3.49991400	-0.55629600	-3.74780300
C	2.62346900	0.94646400	-0.69474900
C	2.85662200	1.11872800	0.70377000
C	3.63860300	2.22349500	1.10472500
C	2.37754300	0.22543100	1.68591500
C	3.86337400	2.47397200	2.44641200
H	4.03690400	2.89180000	0.34325000
C	2.63052600	0.46841200	3.02648200
H	1.85499500	-0.67811900	1.38468500
C	3.35425000	1.59808500	3.40723400
H	4.44353200	3.34124700	2.74994200
H	2.26626800	-0.22692000	3.77852700

H	3.54226100	1.78691400	4.46164600
Au	-0.65551500	0.02882100	0.84145900
H	3.36101600	1.43543200	-1.33596300
Cl	-1.80990900	0.42069400	2.88444100

Electronic Energy (0K) = -1364.9784212

Electronic Energy (0K) + ZPE = -1364.712080

Enthalpy (298K) = -1364.691848

Free Energy (298K) = -1364.762888

TS_{C'}

Number of imaginary frequencies: 1

C	-0.56449200	4.21452000	-3.44387600
C	-0.97588300	4.13268400	-2.19757700
C	-1.63183700	4.67114600	-1.14720700
H	-1.08996300	4.90499400	-0.22904400
N	-2.98471400	4.80676900	-1.05452900
C	-3.83913100	4.76877000	-2.20494900
C	-4.79562300	3.76201100	-2.31138600
C	-3.69916800	5.74051100	-3.19531200
C	-5.61919800	3.72624800	-3.43099900
H	-4.87123700	3.01649400	-1.52056500
C	-4.52733500	5.69432500	-4.31127200
H	-2.94585600	6.51929500	-3.08238300
C	-5.48577400	4.68986400	-4.42788100
H	-6.36397600	2.93913500	-3.52454200
H	-4.42466800	6.44647000	-5.08968200
H	-6.13179300	4.65862000	-5.30219300
O	-5.01198800	5.03641000	0.46872100
O	-2.65654500	5.10044500	1.44760800
S	-3.62697900	5.46056300	0.42781500

C	-3.57475600	7.20323600	0.15491100
C	-2.41945800	7.91069400	0.48837300
C	-4.67845900	7.82976800	-0.41796900
C	-2.38325200	9.27424500	0.24492200
H	-1.57437500	7.40418900	0.94896400
C	-4.61835400	9.19731100	-0.65318700
H	-5.56943900	7.25703900	-0.66457200
C	-3.47773200	9.93608500	-0.32701200
H	-1.49414900	9.84483500	0.50875600
H	-5.47397600	9.70429700	-1.09523300
C	-3.42118900	11.41153800	-0.56424600
H	-4.28176200	11.75987500	-1.14341800
H	-3.41151000	11.95836400	0.38705700
H	-2.50675300	11.69160700	-1.10026800
H	-0.62612400	5.15136100	-4.00100200
H	-0.11709500	3.37083000	-3.97058500
C	-2.94277400	0.17065500	-2.52038200
C	-2.45768900	0.94764600	-1.50679800
C	-1.10997100	1.29472400	-1.94369900
C	-0.90060700	0.68352500	-3.18272900
O	-1.97683500	-0.00689700	-3.52431800
C	-4.20614300	-0.49707100	-2.81298300
C	-4.29527900	-1.41113100	-3.87509800
C	-5.36342300	-0.24123400	-2.06020800
C	-5.49431000	-2.05095900	-4.16491300
H	-3.41375100	-1.62539500	-4.47361300
C	-6.55902800	-0.88310500	-2.35492300
H	-5.31936600	0.46989900	-1.23534600
C	-6.63343400	-1.79230000	-3.40776900
H	-5.53654400	-2.75824900	-4.99072300

H	-7.44175300	-0.66561600	-1.75707800
H	-7.57137500	-2.29363100	-3.63606000
H	-0.03043600	0.83384600	-5.11514300
C	0.25870500	0.57816800	-4.08902900
H	0.63081200	-0.45425600	-4.10443100
H	1.08126400	1.22701800	-3.77803900
C	-0.13784700	2.17433700	-1.40163300
C	0.18662200	2.41761600	-0.00338300
C	-0.29419200	1.60900600	1.03638200
C	1.08160600	3.45820500	0.30681000
C	0.06308000	1.87229500	2.35378600
H	-0.92655900	0.75539600	0.80895200
C	1.42526100	3.72662400	1.62130400
H	1.48010700	4.07050000	-0.50246600
C	0.90574100	2.93849600	2.65049900
H	-0.32195800	1.23822700	3.14893100
H	2.10329900	4.54524500	1.84981000
H	1.17346900	3.14876700	3.68336200
Au	-3.40572700	1.40378600	0.24873400
H	0.69458800	2.39306900	-2.07145900
Cl	-4.47150300	1.66042700	2.37423800

Electronic Energy (0K) = -2586.385671

Electronic Energy (0K) + ZPE = -2585.845393

Enthalpy (298K) = -2585.806062

Free Energy (298K) = -2585.919885

C'

Number of imaginary frequencies: 0

C	2.90116400	1.71014100	-1.62371100
C	2.30517700	0.81722500	-0.82337400

C	1.18182700	1.25492700	-0.00084400
H	1.20851100	1.09629500	1.08333800
N	0.14323000	1.89638300	-0.45662500
C	-0.23992400	2.00207700	-1.84591800
C	-0.82025700	0.88407500	-2.43565500
C	-0.07461300	3.20047600	-2.53458700
C	-1.21347200	0.95913000	-3.76658100
H	-0.95279900	-0.02543300	-1.85075600
C	-0.47899900	3.26096800	-3.86359000
H	0.36770300	4.06293900	-2.03844000
C	-1.04177800	2.14389800	-4.47819200
H	-1.65558800	0.08486400	-4.23962500
H	-0.34955200	4.18498000	-4.42093000
H	-1.35115100	2.19972500	-5.51898300
O	-2.28219900	1.59612200	0.43549100
O	-0.43590600	2.31444800	2.03348100
S	-1.12773900	2.40589800	0.76376100
C	-1.36507700	4.07083700	0.28821700
C	-0.41174200	5.01394300	0.68153300
C	-2.45035000	4.39911000	-0.52031100
C	-0.56429100	6.31802900	0.24569000
H	0.42718500	4.72880000	1.31243500
C	-2.58312300	5.71638500	-0.93659300
H	-3.16757200	3.63922600	-0.82013800
C	-1.64703700	6.68698400	-0.56732100
H	0.16173600	7.07319300	0.54098100
H	-3.42635600	5.99852200	-1.56341800
C	-1.78313100	8.10262600	-1.02501400
H	-2.67798000	8.24693900	-1.63706600
H	-1.83793700	8.78478600	-0.16810400

H	-0.90952800	8.40628400	-1.61477400
H	2.55377700	2.73599100	-1.71940800
H	3.80084200	1.43668300	-2.17228300
C	-0.36135000	-2.39447900	-1.54452400
C	0.41629300	-1.80732800	-0.57590700
C	1.64060500	-1.46706000	-1.25890200
C	1.51197900	-1.84088300	-2.56558200
O	0.30582800	-2.42687700	-2.75432700
C	-1.71720900	-2.92678000	-1.58517200
C	-2.15254100	-3.68356300	-2.68473200
C	-2.63045700	-2.67215200	-0.54939700
C	-3.44941100	-4.18066800	-2.73646400
H	-1.45979200	-3.88393800	-3.49874500
C	-3.92409500	-3.17441600	-0.60527700
H	-2.31573400	-2.06740300	0.30212900
C	-4.34232200	-3.93309000	-1.69712600
H	-3.76295200	-4.76933800	-3.59656500
H	-4.61414000	-2.96425800	0.20954700
H	-5.35665300	-4.32388400	-1.73861000
H	1.98191900	-0.84663300	-4.40081800
C	2.35533300	-1.66421300	-3.76712600
H	2.36876500	-2.57364200	-4.37916600
H	3.38698600	-1.42419700	-3.49077300
C	2.76587900	-0.62686700	-0.71512700
C	3.28062500	-1.03313100	0.65382900
C	3.33214600	-2.38587000	1.00495500
C	3.76914100	-0.09084800	1.56058900
C	3.83410400	-2.78250600	2.23877200
H	2.96054400	-3.13313300	0.30582200
C	4.26148600	-0.48478400	2.80315900

H	3.77291300	0.96719600	1.29927600
C	4.28911100	-1.83131600	3.14965700
H	3.85987100	-3.83969100	2.49421100
H	4.62801700	0.26637600	3.49966800
H	4.67039100	-2.14072800	4.12016800
Au	0.05271500	-1.49138700	1.40439100
H	3.61285300	-0.70139500	-1.41512700
Cl	-0.29494100	-1.23352300	3.75932100

Electronic Energy (0K) = -2586.441859

Electronic Energy (0K) + ZPE = -2585.898495

Enthalpy (298K) = -2585.859465

Free Energy (298K) = -2585.971797

TS_D'

Number of imaginary frequencies: 1

C	2.75771300	2.02329400	-0.97780500
C	2.19979300	0.86556000	-0.62219800
C	0.77941300	0.84841300	-0.17738100
H	0.56439600	0.81129700	0.88884600
N	-0.17365300	1.45827300	-0.89610500
C	-0.14706000	1.66688700	-2.32326900
C	-0.44104500	0.60322000	-3.17138100
C	0.12444900	2.93838000	-2.82522800
C	-0.42376200	0.80978500	-4.54618600
H	-0.70014100	-0.36655500	-2.75441000
C	0.13005900	3.13458200	-4.20172200
H	0.33290100	3.76059600	-2.14267400
C	-0.13640400	2.07142700	-5.06041600
H	-0.64828300	-0.01707900	-5.21525000
H	0.34731400	4.12118200	-4.60296000

H	-0.12701800	2.22900900	-6.13619000
O	-2.75330000	1.31995100	-0.95135100
O	-1.53211400	1.34157100	1.27018300
S	-1.70581700	1.83005700	-0.08831300
C	-1.67829800	3.58526500	-0.12710400
C	-0.77788100	4.25269100	0.70595000
C	-2.48681900	4.26221700	-1.03402300
C	-0.69868400	5.63203400	0.61972800
H	-0.15099300	3.70277000	1.40589000
C	-2.39378100	5.64688900	-1.09678200
H	-3.16518100	3.71287600	-1.68192400
C	-1.50332500	6.34807500	-0.27905800
H	-0.00319400	6.17262800	1.25922800
H	-3.01873900	6.19529900	-1.79884600
C	-1.41241400	7.83867400	-0.34096900
H	-1.88942100	8.23546700	-1.24227300
H	-1.90938900	8.29137300	0.52662800
H	-0.36934800	8.17378600	-0.32058300
H	2.20993000	2.96276900	-0.98008200
H	3.81178100	2.06202000	-1.24692000
C	-0.24434500	-2.13122500	-1.12069600
C	0.62374000	-1.42536400	-0.29295900
C	1.86856700	-1.42271300	-1.03109800
C	1.69220500	-2.09590800	-2.19143800
O	0.39739900	-2.55979300	-2.24207300
C	-1.65882900	-2.45328700	-1.04059800
C	-2.25661700	-3.29885900	-1.98788300
C	-2.46253200	-1.87553700	-0.04471700
C	-3.61745700	-3.56938100	-1.92825500
H	-1.64602400	-3.74547000	-2.76861400

C	-3.82250400	-2.14544000	0.00495300
H	-2.01260600	-1.20404000	0.68655500
C	-4.40525600	-2.99670100	-0.93247500
H	-4.06580500	-4.23317200	-2.66419500
H	-4.43164600	-1.68527800	0.77969100
H	-5.47066800	-3.21092400	-0.88785700
H	2.11784500	-1.97262700	-4.28341100
C	2.54069000	-2.39318400	-3.36180400
H	2.65020400	-3.47425400	-3.51339300
H	3.53918100	-1.96912800	-3.21588300
C	2.93514700	-0.45818000	-0.61142700
C	3.56883400	-0.82293800	0.72356000
C	4.07088200	-2.11742600	0.88969400
C	3.66470500	0.07496800	1.78651700
C	4.63121900	-2.51322100	2.09757200
H	4.00182900	-2.82445300	0.06232200
C	4.21918300	-0.32269700	3.00247500
H	3.29014600	1.09153000	1.67503100
C	4.69727000	-1.61762300	3.16448700
H	5.01201900	-3.52615200	2.21057900
H	4.27295700	0.38653000	3.82584100
H	5.12433400	-1.93003800	4.11477800
Au	0.55850400	-1.69711100	1.77148400
H	3.72843200	-0.40249600	-1.37211800
Cl	0.58527800	-2.16551000	4.10378600

Electronic Energy (0K) = -2586.4266361

Electronic Energy (0K) + ZPE = -2585.883773

Enthalpy (298K) = -2585.845474

Free Energy (298K) = -2585.956035

D'

Number of imaginary frequencies: 0

C	1.39216800	2.17989100	0.95801700
C	1.06853700	1.11284900	0.23461700
C	-0.37086500	0.61180200	0.07897700
H	-0.93198200	0.75514500	1.00697500
N	-1.14456800	1.28661900	-0.98116800
C	-0.63375000	1.33061300	-2.31908600
C	-1.10163300	0.41692400	-3.26444200
C	0.35446200	2.25657500	-2.66094800
C	-0.55677300	0.40997600	-4.54395500
H	-1.89539600	-0.27432600	-2.98673800
C	0.89519400	2.24424000	-3.94307700
H	0.69600700	2.96993200	-1.91242000
C	0.44475600	1.31806000	-4.88059600
H	-0.91788000	-0.30408000	-5.28027900
H	1.66836100	2.96074500	-4.21012100
H	0.87094700	1.30860500	-5.88124500
O	-3.43225100	2.01615200	-1.73426000
O	-2.89861200	1.82129200	0.73360400
S	-2.50461000	2.18977500	-0.62426300
C	-1.98952600	3.88443400	-0.61172000
C	-1.52805400	4.44770500	0.57756800
C	-2.00597700	4.61270100	-1.79770500
C	-1.07496400	5.75837000	0.56713900
H	-1.54577100	3.87079400	1.49994100
C	-1.54569800	5.92418700	-1.78756200
H	-2.38062500	4.16169600	-2.71358800
C	-1.07357400	6.51351300	-0.61220200
H	-0.71993100	6.21280800	1.49104600

H	-1.55601000	6.50495400	-2.70824400
C	-0.58993800	7.92927000	-0.59717200
H	-0.54533500	8.35134100	-1.60602400
H	-1.25333600	8.56318000	0.00459900
H	0.40835000	8.00212400	-0.14940200
H	0.63073300	2.76864600	1.46673600
H	2.42638000	2.50253000	1.06920500
C	-0.85515300	-1.94711400	-0.77833700
C	-0.13400800	-0.83930000	-0.29140100
C	1.20673700	-0.98790500	-0.80380800
C	1.24965200	-2.13136900	-1.52299300
O	0.00217900	-2.72109900	-1.49544100
C	-2.27806800	-2.25008800	-0.88197200
C	-2.72552800	-3.32651200	-1.65647400
C	-3.21205700	-1.42142600	-0.24459900
C	-4.08810000	-3.56806700	-1.78546400
H	-2.00636500	-3.96741500	-2.15975000
C	-4.57034500	-1.66221000	-0.38943600
H	-2.87621800	-0.58391000	0.36437600
C	-5.01303100	-2.73798900	-1.15760600
H	-4.42801800	-4.40796500	-2.38676000
H	-5.28486900	-1.00451400	0.10000800
H	-6.07819200	-2.92742800	-1.26753700
H	1.99050900	-3.04174900	-3.30108800
C	2.29875400	-2.85001000	-2.26660000
H	2.52543600	-3.81675200	-1.79997100
H	3.21573900	-2.25353800	-2.28095900
C	2.06526200	0.20211700	-0.49600400
C	3.33089300	-0.08884200	0.28011800
C	4.56695500	0.33116400	-0.20939800

C	3.28399500	-0.76843300	1.50120600
C	5.73768000	0.07506000	0.50271800
H	4.61135600	0.86333100	-1.15953300
C	4.44893000	-1.02664700	2.21235600
H	2.32057600	-1.09635700	1.89772400
C	5.68127400	-0.60442700	1.71457900
H	6.69436300	0.41002700	0.10735700
H	4.39516700	-1.55842200	3.16018600
H	6.59334300	-0.80715900	2.27173600
Au	-0.22834700	-2.08892600	1.56802400
H	2.35699900	0.68672000	-1.44241300
Cl	-0.05879000	-2.99006400	3.72566400

Electronic Energy (0K) = -2586.4822087

Electronic Energy (0K) + ZPE = -2585.938421

Enthalpy (298K) = -2585.899430

Free Energy (298K) = -2586.014005

1a' '

Number of imaginary frequencies: 0

C	-3.86147300	1.32156800	-0.52156400
H	-3.12655600	2.11904500	-0.36244900
H	-4.30141200	1.47230100	-1.51428200
H	-4.64689900	1.40291300	0.23321100
C	-3.22947700	-0.03829500	-0.40570900
O	-3.62138500	-0.84190000	0.42424100
C	-2.10547700	-0.40277300	-1.32498500
C	-1.65391800	0.48664500	-2.24919800
H	-2.16372800	1.45006800	-2.25909400
C	-0.59738400	0.39554600	-3.24216800
C	-0.36172800	1.54031100	-4.02527600

C	0.19495400	-0.74294000	-3.47297900
C	0.62696900	1.55454500	-4.99793400
H	-0.96977900	2.42792600	-3.85636600
C	1.18136400	-0.72622600	-4.44859900
H	0.03275900	-1.64130200	-2.88573600
C	1.40303800	0.41824300	-5.21289800
H	0.79324400	2.45166200	-5.58954100
H	1.78435400	-1.61573400	-4.61604600
H	2.17919000	0.42319800	-5.97487700
C	-1.58812700	-1.71679400	-1.12636400
C	-1.18525300	-2.83975400	-0.91669400
H	-0.82036100	-3.83037300	-0.74151800

Electronic Energy (0K) = -538.0595882

Electronic Energy (0K) + ZPE = -537.879477

Enthalpy (298K) = -537.866503

Free Energy (298K) = -537.919173

Pre'

Number of imaginary frequencies: 0

C	-1.93062300	2.40397300	0.12427000
H	-1.39884700	3.21260000	-0.39099000
H	-2.84216000	2.19187500	-0.44579800
H	-2.20033900	2.74009700	1.12744000
C	-1.06796700	1.18422800	0.24608300
O	-0.72937100	0.75632400	1.34026900
C	-0.61383200	0.48726300	-0.99677700
C	-0.86220800	1.01365600	-2.23129300
H	-1.42476900	1.94755400	-2.22124600
C	-0.52142300	0.57487500	-3.56638000
C	-0.92920000	1.41105600	-4.62370200

C	0.18006500	-0.60524700	-3.87740300
C	-0.64363900	1.08865300	-5.94125800
H	-1.47575700	2.32426000	-4.39340300
C	0.46648200	-0.92180700	-5.19560700
H	0.49635800	-1.28019200	-3.08885000
C	0.05776800	-0.07920300	-6.22940400
H	-0.96746300	1.74604400	-6.74401000
H	1.00939700	-1.83592800	-5.42285200
H	0.28440100	-0.33717000	-7.26121400
C	0.05900200	-0.74494200	-0.77407500
C	0.60210400	-1.82732300	-0.53930300
Au	1.96043200	-0.65085100	0.78885900
P	3.66347100	0.12534000	2.18544000
H	0.81283700	-2.88269300	-0.53914200
C	4.74186600	-1.22512800	2.74638500
C	5.28447900	-1.24900100	4.03378400
C	5.05422200	-2.24238800	1.83793200
C	6.13074100	-2.28919200	4.40692700
H	5.04927100	-0.45963700	4.74571600
C	5.90347600	-3.27552100	2.21528900
H	4.62838600	-2.22112600	0.83412600
C	6.43886500	-3.30012100	3.50134300
H	6.54897900	-2.30888300	5.41033800
H	6.14206600	-4.06588100	1.50781000
H	7.09630700	-4.11347700	3.79922900
C	3.01504300	0.94396300	3.67291700
C	3.66004700	2.04379800	4.24603500
C	1.86165100	0.42180900	4.26781900
C	3.15050100	2.61330100	5.40895900
H	4.55886400	2.45630800	3.78984600

C	1.36115700	0.99211200	5.43224500
H	1.35643700	-0.43090600	3.81322500
C	2.00443300	2.08905600	6.00050300
H	3.65073700	3.47003900	5.85409800
H	0.46313100	0.58463000	5.89023200
H	1.60752400	2.53897100	6.90759300
C	4.72678600	1.33668300	1.34533800
C	6.10897300	1.36740600	1.54603100
C	4.11977000	2.28552400	0.51467700
C	6.87640600	2.34398700	0.91772300
H	6.58696800	0.63302700	2.19244100
C	4.89087500	3.26176900	-0.10424800
H	3.04075500	2.25670400	0.35583700
C	6.26948000	3.28929700	0.09593800
H	7.95235100	2.36552300	1.07291300
H	4.41730500	3.99790400	-0.74932200
H	6.87295700	4.04972700	-0.39398300

Electronic Energy (0K) = -1709.4873372

Electronic Energy (0K) + ZPE = -1709.031523

Enthalpy (298K) = -1708.999086

Free Energy (298K) = -1709.099290

TS_{A'}

Number of imaginary frequencies: 1

C	-3.20447000	-0.16910500	-2.16874200
C	-2.50325200	0.70955500	-1.59058800
C	-1.36021000	1.36308600	-2.20077100
C	-1.19825800	0.85280800	-3.59367900
O	-1.95768400	-0.03295100	-3.97985500
H	-0.25552900	2.47493900	-4.61919300

C	-0.13006600	1.39460900	-4.48423800
H	-0.17876000	0.89996500	-5.45559800
H	0.85849300	1.23113400	-4.04083600
C	-0.55170400	2.31322500	-1.67522500
C	-0.52308300	2.81343900	-0.30893200
C	-0.26738700	4.17636800	-0.09229000
C	-0.69604200	1.96821400	0.80039400
C	-0.25227200	4.69443300	1.19657700
H	-0.09523600	4.82736000	-0.94778700
C	-0.64788000	2.48649700	2.08998900
H	-0.80918400	0.89567400	0.65233500
C	-0.44507900	3.85041100	2.28954700
H	-0.07355200	5.75577900	1.35099600
H	-0.76725800	1.81995200	2.94263700
H	-0.41702900	4.25195500	3.30030900
Au	-3.62427600	1.14059600	0.17536000
P	-4.71648300	1.81211800	2.14156700
H	0.16495600	2.77743600	-2.35520400
H	-3.93103800	-0.91630100	-2.43438900
C	-6.29413700	0.96852900	2.46246800
C	-7.09229400	0.61252100	1.37064300
C	-6.72654200	0.69185800	3.76286600
C	-8.31651500	-0.01272000	1.57888100
H	-6.74787500	0.82387900	0.35770800
C	-7.95030600	0.06172800	3.96455000
H	-6.10957600	0.96712300	4.61734800
C	-8.74266000	-0.29117500	2.87541100
H	-8.93375100	-0.29089500	0.72802300
H	-8.28343800	-0.15653900	4.97635400
H	-9.69595700	-0.78892900	3.03746900

C	-5.05039200	3.59841900	2.11250200
C	-6.13233100	4.16291700	2.79350500
C	-4.15464300	4.42178900	1.42167700
C	-6.31303500	5.54266100	2.77907600
H	-6.83356200	3.52840900	3.33408700
C	-4.33459400	5.79997500	1.41866000
H	-3.31498500	3.97556500	0.88487900
C	-5.41615200	6.35943700	2.09511200
H	-7.15821000	5.98156500	3.30386600
H	-3.63464700	6.43558200	0.88078800
H	-5.56368700	7.43677200	2.08588400
C	-3.67037200	1.50674300	3.59958100
C	-3.08514700	0.24119000	3.72631900
C	-3.43053700	2.48544500	4.56541200
C	-2.27000000	-0.04267100	4.81498300
H	-3.26982700	-0.52104800	2.96793300
C	-2.60631800	2.19775900	5.65102600
H	-3.87979800	3.47275500	4.46998700
C	-2.02764000	0.93860100	5.77606000
H	-1.81853500	-1.02704400	4.91282900
H	-2.41954500	2.96193400	6.40178600
H	-1.38516300	0.71829200	6.62531900

Electronic Energy (0K) = -1709.4767502

Electronic Energy (0K) + ZPE = -1709.021493

Enthalpy (298K) = -1708.989978

Free Energy (298K) = -1709.086040

A' '

Number of imaginary frequencies: 0

C	-0.44864800	0.08517800	-2.21760200
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C	0.08858700	0.18842000	-0.98875300
C	1.51902400	0.38457900	-1.25526400
C	1.68103700	0.40119300	-2.66865300
O	0.52505800	0.19522600	-3.24069900
H	3.59766200	1.22134400	-3.10327000
C	2.86493100	0.52842100	-3.52701500
H	2.57148100	0.87038300	-4.52287400
H	3.35630100	-0.44749100	-3.63613400
C	2.60529500	0.58359700	-0.42623800
C	2.70887400	0.41688100	0.99122400
C	3.67007500	1.19230900	1.67365800
C	1.93058000	-0.50796900	1.72092100
C	3.78873400	1.11109200	3.05029600
H	4.29908900	1.87335800	1.10293500
C	2.07952000	-0.60703700	3.09546900
H	1.26660600	-1.18724300	1.19314100
C	2.98949300	0.21461000	3.76181500
H	4.51247200	1.73090500	3.57271800
H	1.49492800	-1.33459800	3.65402100
H	3.09161600	0.13973500	4.84204600
Au	-0.94336300	0.37974400	0.80087600
P	-2.03705400	0.69558300	2.87291200
H	3.51591600	0.94738100	-0.91027000
H	-1.45303400	-0.02502100	-2.60359800
C	-3.43823500	1.85603500	2.79670400
C	-4.20636300	1.87655400	1.62796800
C	-3.78717700	2.67813700	3.87218600
C	-5.31879400	2.70639000	1.53956000
H	-3.92740000	1.24066100	0.78728300
C	-4.89931500	3.50923300	3.77747800

H	-3.19343100	2.66572400	4.78548000
C	-5.66471700	3.52166000	2.61418200
H	-5.91295600	2.72026700	0.62892700
H	-5.16886200	4.14715000	4.61586500
H	-6.53209100	4.17388600	2.54373700
C	-0.88078400	1.38108900	4.10615400
C	-0.86056500	0.95537200	5.43636100
C	0.01057000	2.37372700	3.68094500
C	0.03818400	1.52501800	6.33458100
H	-1.54712700	0.18060500	5.77483900
C	0.89736000	2.94783700	4.58392400
H	0.00884200	2.69064100	2.63681500
C	0.91194200	2.52284800	5.91122400
H	0.05113700	1.19078500	7.36931700
H	1.58793600	3.71825300	4.24806000
H	1.61122900	2.96661400	6.61628500
C	-2.69682600	-0.83919700	3.60063400
C	-3.82357200	-0.84971200	4.42793800
C	-2.02509300	-2.03681000	3.33127600
C	-4.27022800	-2.04704100	4.97847600
H	-4.35652200	0.07575200	4.64233600
C	-2.47189600	-3.23021500	3.88778500
H	-1.15504600	-2.03261900	2.67336700
C	-3.59534300	-3.23501500	4.71046200
H	-5.15004500	-2.05115100	5.61761500
H	-1.94766300	-4.15833200	3.67204900
H	-3.95131100	-4.16945000	5.13812500

Electronic Energy (0K) = -1709.5093144

Electronic Energy (0K) + ZPE = -1709.049058

Enthalpy (298K) = -1709.018318

Free Energy (298K) = -1709.112771

TS_{c'} ,

Number of imaginary frequencies: 1

C	-0.86850100	3.80443600	-3.68753500
C	-0.99590000	3.97996300	-2.39197100
C	-1.35541700	4.74876800	-1.33999600
H	-0.61146700	5.01784000	-0.58785000
N	-2.63889900	5.06515100	-1.01430600
C	-3.68922600	5.10627400	-1.99242300
C	-4.77009200	4.23457500	-1.88937000
C	-3.60938600	6.04282100	-3.02286200
C	-5.78972900	4.30964000	-2.83271100
H	-4.79387900	3.49994900	-1.08296800
C	-4.63078000	6.10422000	-3.96334100
H	-2.75455600	6.71725300	-3.06746200
C	-5.72018700	5.24078500	-3.86623800
H	-6.63776500	3.63200900	-2.76134900
H	-4.57826200	6.83091400	-4.77014900
H	-6.51918000	5.29432200	-4.60195100
O	-4.25818000	5.49205500	0.90640000
O	-1.74584900	5.53774300	1.31277300
S	-2.91295400	5.86531100	0.51052100
C	-2.89176700	7.57236300	0.07939500
C	-1.66745900	8.24071700	0.03333300
C	-4.08568200	8.20218500	-0.26258300
C	-1.65265800	9.57076700	-0.35354500
H	-0.74799700	7.73165600	0.31304500
C	-4.04492700	9.53598200	-0.64734500
H	-5.02712600	7.65967100	-0.22445600

C	-2.83677200	10.23641600	-0.69875100
H	-0.70874100	10.11248600	-0.38430900
H	-4.96886300	10.04750800	-0.91009000
C	-2.79434500	11.66941100	-1.12294800
H	-3.79932300	12.08284000	-1.25084800
H	-2.26053300	12.28264900	-0.38757000
H	-2.25922900	11.77916400	-2.07457200
H	-0.95800000	4.63729100	-4.38698700
H	-0.63776900	2.83134200	-4.12246100
C	-3.10125100	0.06075200	-2.03585600
C	-2.57097100	0.97540700	-1.18926300
C	-1.24534300	1.22549000	-1.75281900
C	-1.12313200	0.42773000	-2.89431900
O	-2.23077800	-0.28897600	-3.06084800
H	-0.38285800	0.19463500	-4.87238200
C	-0.02160500	0.15711200	-3.83848000
H	0.38238100	-0.84988700	-3.67201400
H	0.79834700	0.86992800	-3.72233600
C	-0.21358900	2.12638500	-1.38049700
C	0.20117400	2.52139500	-0.03921700
C	-0.35193300	1.98541400	1.13206100
C	1.26526400	3.43576100	0.07347000
C	0.12669300	2.38006700	2.37716100
H	-1.13846600	1.23750900	1.06687700
C	1.72431700	3.84326800	1.31506100
H	1.71219500	3.83626500	-0.83697900
C	1.15082200	3.31733000	2.47356300
H	-0.29952100	1.94416400	3.27855500
H	2.53763500	4.56128300	1.38519200
H	1.51462500	3.62845400	3.45006600

Au	-3.67252300	1.63827000	0.44683100
P	-5.10227200	2.07629000	2.29273300
H	0.60170300	2.20126500	-2.10175600
H	-4.05755900	-0.44459800	-2.08377200
C	-4.60311800	3.43333600	3.39876000
C	-3.23512700	3.64738300	3.57953900
C	-5.52662200	4.24957700	4.05742100
C	-2.78912700	4.66919800	4.40943100
H	-2.51812000	3.02320000	3.04548800
C	-5.07709700	5.27553100	4.88269600
H	-6.59556300	4.09038100	3.92158100
C	-3.71122800	5.48793700	5.05601400
H	-1.72087500	4.83979500	4.52924600
H	-5.79682300	5.91454400	5.38927000
H	-3.36582400	6.29758600	5.69501000
C	-6.81541800	2.45308900	1.78275100
C	-7.89800700	1.65082500	2.14904600
C	-7.02829500	3.57252200	0.96652300
C	-9.18036400	1.96586600	1.70440400
H	-7.74675500	0.77851200	2.78287700
C	-8.31067300	3.88496000	0.53266700
H	-6.18876800	4.20914000	0.68489300
C	-9.38852000	3.08040100	0.89892700
H	-10.01916100	1.33690200	1.99378100
H	-8.46834400	4.75898400	-0.09572500
H	-10.39144500	3.32406900	0.55591400
C	-5.23720900	0.59773200	3.35268100
C	-5.60284200	0.68500600	4.69961400
C	-5.02079800	-0.65741800	2.77459400
C	-5.74947600	-0.47289900	5.45616800

H	-5.77525000	1.65781800	5.15851900
C	-5.17515600	-1.81371100	3.53292200
H	-4.72667900	-0.72229400	1.72604200
C	-5.53775700	-1.72070000	4.87369800
H	-6.03112100	-0.40099600	6.50411600
H	-5.00654600	-2.78673100	3.07722200
H	-5.65321000	-2.62375300	5.46868500

Electronic Energy (0K) = -2930.9210529

Electronic Energy (0K) + ZPE = -2930.187134

Enthalpy (298K) = -2930.137644

Free Energy (298K) = -2930.270765

C'

Number of imaginary frequencies: 0

C	2.79127800	1.59720600	-2.04424200
C	2.21735300	0.85908700	-1.08647900
C	1.12984600	1.39802200	-0.28016800
H	1.17765100	1.29130100	0.81076700
N	0.07388200	1.99938100	-0.74073100
C	-0.31510600	2.06366400	-2.12905500
C	-0.82520400	0.90766700	-2.71299000
C	-0.20510900	3.26365400	-2.82487800
C	-1.20957700	0.95514500	-4.04777700
H	-0.92144000	-0.00100700	-2.11926600
C	-0.59764200	3.29275900	-4.15884500
H	0.19381000	4.14906700	-2.33260600
C	-1.09469300	2.14245600	-4.76732900
H	-1.60123200	0.05852800	-4.52226000
H	-0.51042600	4.21721700	-4.72334300
H	-1.39628100	2.17205700	-5.81136700

O	-2.35414800	1.66744600	0.11633700
O	-0.54277800	2.37853700	1.75133700
S	-1.21891600	2.49125900	0.47314200
C	-1.47782300	4.15776100	0.02479000
C	-0.53779800	5.11058400	0.42762400
C	-2.57412100	4.47906400	-0.77256000
C	-0.71715400	6.41829600	0.01446500
H	0.31073100	4.83099900	1.04834100
C	-2.73272700	5.80000100	-1.16586700
H	-3.28095300	3.71237200	-1.07912900
C	-1.81264500	6.78141100	-0.78472000
H	-0.00335500	7.18158600	0.31808800
H	-3.58489800	6.07681400	-1.78272100
C	-1.97744300	8.20023700	-1.22163300
H	-2.90382300	8.34539800	-1.78470300
H	-1.98787400	8.87729800	-0.35929700
H	-1.13817800	8.51086200	-1.85601700
H	2.46080000	2.60294100	-2.29097600
H	3.65569200	1.21144500	-2.58141700
C	-0.61635200	-2.27224600	-1.04581400
C	0.26174800	-1.61792600	-0.23355500
C	1.42348500	-1.41902800	-1.07623300
C	1.13963700	-1.93283400	-2.30870700
O	-0.10448100	-2.47737800	-2.30349200
H	1.45257300	-1.16975100	-4.28467400
C	1.85963200	-1.92856800	-3.60049500
H	1.78192900	-2.89933600	-4.10339000
H	2.92080500	-1.70349900	-3.45300400
C	2.62901400	-0.56970800	-0.76821900
C	3.23259100	-0.75598900	0.61227000

C	3.20742300	-2.00955800	1.23370800
C	3.89410000	0.29286000	1.25568900
C	3.80491400	-2.20004600	2.47568400
H	2.71124200	-2.84308200	0.73974900
C	4.48961900	0.10501700	2.50169800
H	3.95591700	1.27004800	0.77692000
C	4.44161800	-1.14042900	3.11942100
H	3.77388500	-3.18287000	2.94210700
H	5.00082000	0.93492200	2.98580600
H	4.90320000	-1.28725500	4.09359100
Au	0.00061500	-1.09480400	1.75152200
P	-0.30232700	-0.59344800	4.05249800
H	3.41540000	-0.80884900	-1.50212200
H	-1.61106900	-2.67353600	-0.89283700
C	-1.73360100	0.47942800	4.39950600
C	-2.82925200	0.40297900	3.53433400
C	-1.77451600	1.34816600	5.49390800
C	-3.95700100	1.18346500	3.76323900
H	-2.79022900	-0.26564700	2.67417400
C	-2.90463800	2.12860800	5.71936300
H	-0.92458000	1.41422800	6.17229000
C	-3.99304100	2.04810800	4.85438900
H	-4.80364800	1.12352700	3.08307800
H	-2.93312600	2.80314500	6.57205500
H	-4.87251500	2.66293700	5.03198300
C	-0.55371800	-2.11620800	5.02295800
C	-1.28155900	-2.13456300	6.21601600
C	0.05445000	-3.28936100	4.56308500
C	-1.40076600	-3.31823400	6.93741700
H	-1.75487100	-1.22445000	6.58248100

C	-0.06173100	-4.46883700	5.29084400
H	0.61958300	-3.27207300	3.62969500
C	-0.79267800	-4.48327800	6.47582300
H	-1.97185500	-3.33089900	7.86283800
H	0.41031800	-5.37863700	4.92736200
H	-0.89165100	-5.40713900	7.04117500
C	1.12442000	0.23829600	4.83333400
C	1.82197700	-0.31716300	5.90736100
C	1.53762900	1.46690500	4.30276300
C	2.91713900	0.35311100	6.44914100
H	1.51417400	-1.27270800	6.32789300
C	2.62341200	2.13638300	4.85367100
H	0.99748800	1.90232800	3.46162000
C	3.31639700	1.57880400	5.92723700
H	3.45397800	-0.08649900	7.28669800
H	2.93495500	3.09440100	4.44277800
H	4.16816700	2.10128500	6.35684600

Electronic Energy (0K) = -2930.9780686

Electronic Energy (0K) + ZPE = -2930.240871

Enthalpy (298K) = -2930.191368

Free Energy (298K) = -2930.326519

TS_{D'} ,

Number of imaginary frequencies: 1

C	3.27615800	1.30680500	-1.57834300
C	2.58883200	0.36413900	-0.93179600
C	1.38682500	0.69656200	-0.13240300
H	1.47039100	0.57949100	0.94660800
N	0.50640900	1.63678200	-0.51235600
C	0.21281500	1.98582800	-1.88391400

C	-0.36588400	1.05061400	-2.73682700
C	0.49321000	3.28131300	-2.31641800
C	-0.64852800	1.41624200	-4.04854300
H	-0.59514600	0.05249900	-2.37293700
C	0.19751800	3.63776100	-3.62677100
H	0.94008300	3.99681800	-1.62835300
C	-0.36859100	2.70553700	-4.49264500
H	-1.09398600	0.68991100	-4.72359900
H	0.41677400	4.64509900	-3.97141200
H	-0.59429400	2.98582400	-5.51872800
O	-1.95151900	1.31486100	0.22992200
O	-0.15376800	1.73760700	1.96482400
S	-0.76266600	2.02172600	0.67467000
C	-0.96516200	3.74917300	0.46199800
C	-0.04198900	4.60520000	1.06294300
C	-2.00130500	4.22221600	-0.34067000
C	-0.16912300	5.96783100	0.84585300
H	0.75839000	4.21203000	1.68569600
C	-2.10894300	5.59015900	-0.53959500
H	-2.69847600	3.52976200	-0.80589400
C	-1.19993000	6.47890400	0.04617400
H	0.53962800	6.65461300	1.30433800
H	-2.91040000	5.98004200	-1.16386200
C	-1.34486800	7.95242800	-0.15510800
H	-1.75332000	8.18329300	-1.14447700
H	-2.03712300	8.37276300	0.58602300
H	-0.38773300	8.47062500	-0.03849100
H	2.97606700	2.35092700	-1.59130800
H	4.19476400	1.04649300	-2.10071300
C	-0.53788300	-1.92657100	-1.02249300

C	0.53964600	-1.38359700	-0.35722700
C	1.66702700	-1.77055200	-1.17923800
C	1.20717200	-2.46766800	-2.24517500
O	-0.16176800	-2.59452100	-2.13660300
H	1.41611500	-2.61616900	-4.36570300
C	1.82636400	-3.05701900	-3.44875000
H	1.65823100	-4.13970000	-3.49853100
H	2.90618700	-2.88107900	-3.43640500
C	2.97706000	-1.10067500	-0.90996200
C	3.62662700	-1.53146000	0.39961800
C	3.43027700	-2.82258100	0.90022300
C	4.46369600	-0.66212700	1.10380700
C	4.05617700	-3.23453100	2.07418700
H	2.78299800	-3.51423100	0.36176200
C	5.08867500	-1.07195500	2.27853500
H	4.63322500	0.34508900	0.72496600
C	4.88770400	-2.35937300	2.76821800
H	3.89613500	-4.24527900	2.44553100
H	5.73637000	-0.38086400	2.81477200
H	5.37905000	-2.67888700	3.68471200
Au	0.36671400	-1.68388600	1.74117600
P	0.14598600	-2.11531400	4.03496600
H	3.69033300	-1.26788400	-1.73064400
H	-1.60201300	-1.94049200	-0.81384400
C	-1.13540800	-1.09627700	4.83020900
C	-2.22963000	-0.68366100	4.06320200
C	-1.05820000	-0.73922800	6.18007400
C	-3.24125800	0.07355400	4.64381200
H	-2.27952800	-0.95204200	3.00710600
C	-2.07167100	0.01983000	6.75571400

H	-0.20494800	-1.05266500	6.78093400
C	-3.16155600	0.42520100	5.98873400
H	-4.08881100	0.39485700	4.04294700
H	-2.00916400	0.29731300	7.80530900
H	-3.95014900	1.02219500	6.44108900
C	1.68252900	-1.75881900	4.94830600
C	2.21220700	-2.62437400	5.90767300
C	2.32729500	-0.54778700	4.67251300
C	3.37563200	-2.27509500	6.58942900
H	1.71796300	-3.56942500	6.12756900
C	3.48086500	-0.19875200	5.36375700
H	1.92026300	0.12296500	3.91328400
C	4.00645600	-1.06376000	6.32200000
H	3.78603600	-2.95287400	7.33431700
H	3.97716200	0.74509500	5.14873300
H	4.91233400	-0.79393900	6.86004900
C	-0.26990800	-3.85251900	4.38664600
C	-1.03032300	-4.22578500	5.49815500
C	0.22446800	-4.83501100	3.52135100
C	-1.29151800	-5.57104900	5.73968300
H	-1.42179900	-3.46836800	6.17573600
C	-0.03521100	-6.17816700	3.77007900
H	0.81039100	-4.54194900	2.64862200
C	-0.79516300	-6.54540300	4.87780700
H	-1.88713300	-5.85759000	6.60324700
H	0.34867400	-6.93767300	3.09307900
H	-1.00535500	-7.59542100	5.06807300

Electronic Energy (0K) = -2930.9618757

Electronic Energy (0K) + ZPE = -2930.225455

Enthalpy (298K) = -2930.176661

Free Energy (298K) = -2930.309809

D' '

Number of imaginary frequencies: 0

C	1.85057900	2.85321700	0.73406200
C	1.63150500	1.60002400	0.35424800
C	0.24236500	0.95829400	0.34321000
H	-0.14036400	0.91774100	1.37211700
N	-0.74503300	1.73569500	-0.41935700
C	-0.51391100	1.96169900	-1.82555400
C	-0.74261000	0.97299800	-2.78484900
C	-0.06621600	3.22509000	-2.21407700
C	-0.51129500	1.25177100	-4.12875600
H	-1.12455600	0.00062000	-2.48561100
C	0.16596100	3.49476600	-3.55766700
H	0.08937000	3.98555500	-1.45186300
C	-0.05442600	2.50784600	-4.51567600
H	-0.69265800	0.48261500	-4.87575100
H	0.51403100	4.48012100	-3.85824600
H	0.12458000	2.72141200	-5.56695400
O	-2.88190900	0.24144200	-0.57321300
O	-2.34283100	1.52190900	1.51342100
S	-2.34631900	1.45376700	0.05119000
C	-3.15154300	2.86731400	-0.62666800
C	-2.94314200	4.10608600	-0.01954100
C	-3.93650000	2.73338500	-1.76589000
C	-3.54032000	5.22589800	-0.57353300
H	-2.31987400	4.18531500	0.86911300
C	-4.52662800	3.87048800	-2.30543500
H	-4.07887900	1.75647600	-2.22174900

C	-4.33782400	5.12537400	-1.72247800
H	-3.39223000	6.20084200	-0.11166000
H	-5.14539600	3.78403700	-3.19644200
C	-4.96134500	6.35124000	-2.31054700
H	-5.62759000	6.10577700	-3.14320900
H	-5.53903100	6.90076400	-1.55790100
H	-4.19334600	7.04005800	-2.68424100
H	1.02914700	3.50175600	1.03712300
H	2.85539000	3.27177200	0.75752600
C	-0.11388100	-1.64775200	-0.41773400
C	0.53229300	-0.42880100	-0.16306600
C	1.89653200	-0.59973500	-0.42255400
C	2.05807400	-1.88017700	-0.89195300
O	0.87015500	-2.50549000	-0.92998100
H	3.06566900	-3.22275500	-2.19806500
C	3.24905600	-2.65167500	-1.28197000
H	3.51709600	-3.36585700	-0.49227300
H	4.09803900	-1.98047900	-1.43797800
C	2.71868200	0.60232000	-0.06508100
C	3.72349400	0.32006000	1.03438500
C	5.08718000	0.50019800	0.81261900
C	3.29576400	-0.14083200	2.28459100
C	6.01210800	0.22427300	1.81890600
H	5.42710500	0.86053100	-0.15807100
C	4.21640100	-0.42334100	3.28647200
H	2.22685200	-0.27314000	2.47665500
C	5.57992300	-0.24084400	3.05569700
H	7.07341100	0.37292800	1.63148600
H	3.86875400	-0.78750200	4.25238200
H	6.30032200	-0.45803100	3.84097000

Au	-0.31063600	-2.01084000	1.77758800
P	-0.30752600	-2.21991600	4.10623900
H	3.26087500	0.99038400	-0.93985200
H	-1.11506100	-1.83806900	-0.79872000
C	-1.90026700	-2.64267800	4.86374800
C	-2.68491200	-3.62326800	4.24764100
C	-2.33287700	-2.04048000	6.04832300
C	-3.89337400	-4.00298700	4.81889700
H	-2.34666800	-4.08545800	3.31989000
C	-3.54664300	-2.42202200	6.61188800
H	-1.72415500	-1.27632800	6.53002700
C	-4.32426400	-3.40083400	5.99917000
H	-4.50332800	-4.76403300	4.33844600
H	-3.88581200	-1.95233800	7.53201800
H	-5.27368000	-3.69397300	6.44103500
C	0.91549200	-3.41981600	4.70509700
C	0.78633600	-4.03030000	5.95620600
C	2.04516800	-3.67018900	3.91885200
C	1.78593800	-4.88221300	6.41487600
H	-0.09035300	-3.83737100	6.57314200
C	3.04517500	-4.51529900	4.38672600
H	2.13706200	-3.20058600	2.93722200
C	2.91357100	-5.12181300	5.63354600
H	1.68304700	-5.35969300	7.38634200
H	3.92309400	-4.70779900	3.77474500
H	3.69175000	-5.78895100	5.99685300
C	0.19913000	-0.59604800	4.75818300
C	-0.39528700	0.54136500	4.19579500
C	1.19435900	-0.45289200	5.72669300
C	0.01978000	1.80880000	4.58234200

H	-1.17640900	0.43487400	3.44095300
C	1.60269500	0.82195400	6.11460700
H	1.66265500	-1.33004400	6.17160300
C	1.02535100	1.94908300	5.53878300
H	-0.44106000	2.68532200	4.13083000
H	2.38215000	0.93120200	6.86502200
H	1.35813000	2.94082100	5.83594100

Electronic Energy (0K) = -2931.01743

Electronic Energy (0K) + ZPE = -2930.279776

Enthalpy (298K) = -2930.230631

Free Energy (298K) = -2930.366869

3a' '

Number of imaginary frequencies: 0

C	1.44997100	2.22360400	0.55898600
C	1.06027800	1.11656600	-0.06438300
C	-0.40767600	0.68992800	-0.20221600
H	-0.94508800	0.85346600	0.73839800
N	-1.15442800	1.44912000	-1.23160700
C	-0.62401800	1.56471700	-2.55642300
C	-1.03446800	0.66526100	-3.54086500
C	0.31938500	2.55098900	-2.85301800
C	-0.49241700	0.74549200	-4.81873200
H	-1.77743600	-0.08812900	-3.28869700
C	0.85917400	2.62575000	-4.13363600
H	0.62486500	3.24562600	-2.07279500
C	0.45553000	1.72289100	-5.11403300
H	-0.81158000	0.04414800	-5.58612800
H	1.59513600	3.39218600	-4.36534300
H	0.87873400	1.78374600	-6.11431000

O	-3.39872600	2.27323900	-2.01153200
O	-2.98170900	1.81919900	0.44576700
S	-2.52171200	2.31610400	-0.84774200
C	-2.00624700	3.99938900	-0.63576800
C	-1.53861900	4.41396300	0.61125000
C	-2.00978500	4.86337800	-1.72647100
C	-1.06193200	5.70790800	0.75592700
H	-1.56166500	3.73068700	1.45809100
C	-1.52752700	6.15706100	-1.56219900
H	-2.39068500	4.52716800	-2.68781200
C	-1.04322800	6.59555200	-0.32785800
H	-0.70049200	6.04516300	1.72653300
H	-1.52908000	6.84218200	-2.40830100
C	-0.51562400	7.98489500	-0.15197100
H	-0.59708600	8.56714600	-1.07507200
H	-1.06013100	8.51758900	0.63718000
H	0.53975900	7.96951500	0.14732500
H	0.72631100	2.91916200	0.98342000
H	2.50354200	2.48060400	0.66130600
C	-1.00506100	-1.88477100	-0.71906900
C	-0.27234200	-0.75683900	-0.55422800
C	1.08265900	-1.10292000	-0.82108500
C	1.10887000	-2.42688400	-1.12171500
O	-0.17173600	-2.90908000	-1.06173300
H	1.99888700	-3.86820900	-2.43104000
C	2.17602000	-3.39072500	-1.45939000
H	2.25411300	-4.18792000	-0.70925400
H	3.13795400	-2.87077600	-1.50389200
C	2.00414500	0.07261900	-0.68117900
C	3.25972500	-0.17092000	0.12032700

C	4.50025400	0.24579500	-0.36124100
C	3.19782500	-0.80130500	1.36764600
C	5.66047600	0.03557400	0.38260100
H	4.55621100	0.73697700	-1.33264200
C	4.35242400	-1.01400100	2.11021200
H	2.23176000	-1.12791100	1.75275200
C	5.58915400	-0.59554200	1.61961200
H	6.62058300	0.36561500	-0.00884800
H	4.28917400	-1.50828000	3.07759500
H	6.49301500	-0.76479500	2.20087800
H	2.30523300	0.43084700	-1.68090500
H	-2.05435600	-2.13405500	-0.63724200

Electronic Energy (0K) = -1759.5840982

Electronic Energy (0K) + ZPE = -1759.122589

Enthalpy (298K) = -1759.092514

Free Energy (298K) = -1759.185669

TS_E

Number of imaginary frequencies: 1

C	-6.59495200	-0.58826600	-5.87798900
C	-7.96502700	-0.76179900	-5.97315600
H	-8.39644200	-1.76584000	-5.89045200
N	-8.91019900	0.19741800	-6.13002600
C	-8.63938000	1.59137000	-6.34337700
C	-8.43435600	2.05433700	-7.64212700
C	-8.61442800	2.45752300	-5.25274400
C	-8.19490600	3.40931000	-7.84677000
H	-8.46664000	1.35427400	-8.47631000
C	-8.36581500	3.80930200	-5.46801100
H	-8.79007700	2.06261800	-4.25384300

C	-8.15822800	4.28292200	-6.76201100
H	-8.03354100	3.78361800	-8.85489300
H	-8.33594300	4.49502800	-4.62400400
H	-7.95893800	5.34042400	-6.92489900
O	-10.61795900	-1.68013900	-5.85543200
O	-11.27986500	0.70677400	-5.32688800
S	-10.59443600	-0.25972000	-6.16545800
C	-11.01656700	0.00890300	-7.85072300
C	-11.72709200	1.15105500	-8.20351800
C	-10.55534500	-0.89924100	-8.80557000
C	-11.98444100	1.38195000	-9.54923500
H	-12.06703500	1.84568800	-7.43941900
C	-10.81855200	-0.64468000	-10.14077900
H	-9.99793500	-1.78493700	-8.50638500
C	-11.53422600	0.49672900	-10.53151800
H	-12.54234300	2.26842800	-9.84472100
H	-10.46726000	-1.33982700	-10.90137400
C	-11.81173000	0.74614000	-11.97929700
H	-10.89320600	0.68100600	-12.57423600
H	-12.50240900	-0.00685500	-12.37909500
H	-12.25884600	1.73188000	-12.13991300
Au	-5.51976100	1.19675600	-5.74209000
P	-4.18695900	3.13264600	-5.43895900
C	-5.91981300	-1.81304100	-5.71520800
H	-4.83725300	-1.87744100	-5.82367100
H	-6.43666200	-2.76071000	-5.89811000
C	-4.65158400	-1.12142700	-3.14473000
C	-5.47697200	-2.04572700	-3.56909900
C	-6.29188000	-3.11443000	-3.47430300
H	-7.37068500	-2.96810800	-3.38971200

N	-5.88645900	-4.40445200	-3.68725100
C	-4.50165700	-4.77268600	-3.61134200
C	-3.87003000	-4.78092600	-2.36829600
C	-3.80750800	-5.08429800	-4.77779400
C	-2.52097200	-5.10842500	-2.29691600
H	-4.43847700	-4.52381200	-1.47577100
C	-2.45952100	-5.41550300	-4.69349400
H	-4.32492400	-5.06494700	-5.73403700
C	-1.81858700	-5.42701500	-3.45703400
H	-2.01796200	-5.11616700	-1.33324700
H	-1.90750000	-5.66146500	-5.59713400
H	-0.76393000	-5.68493900	-3.39706700
O	-8.30815600	-4.93299000	-4.17575500
O	-6.50661200	-6.62744300	-4.74580000
S	-7.08156000	-5.64319300	-3.84778000
C	-7.18890500	-6.32031000	-2.22670500
C	-6.35249800	-7.38034200	-1.88001500
C	-8.07569000	-5.75469100	-1.31227900
C	-6.41888200	-7.88191800	-0.58835800
H	-5.67221300	-7.80933600	-2.61171600
C	-8.12609900	-6.27616800	-0.02790500
H	-8.72773800	-4.93520400	-1.60597000
C	-7.30058500	-7.34051100	0.35343400
H	-5.78159600	-8.71714200	-0.30387900
H	-8.82484500	-5.85786200	0.69423200
C	-7.34561300	-7.87736100	1.74826100
H	-8.32621600	-7.71930800	2.20890400
H	-7.11708100	-8.94795300	1.77314200
H	-6.60303600	-7.37394400	2.38096800
H	-4.23977300	-0.36465100	-3.81845000

H	-4.35546400	-1.07059700	-2.09621400
C	-4.63307100	4.54729900	-6.49826000
C	-4.90886700	5.81921300	-5.99363700
C	-4.69372900	4.32093900	-7.87914600
C	-5.22987100	6.85822100	-6.86514000
H	-4.87477000	6.00563900	-4.92145600
C	-4.99993900	5.36315900	-8.74517600
H	-4.49717300	3.32328800	-8.27520600
C	-5.26959700	6.63379400	-8.23768800
H	-5.44317000	7.84751300	-6.46687200
H	-5.03574900	5.18277500	-9.81709000
H	-5.51399600	7.44891900	-8.91483800
C	-2.41074500	2.84922600	-5.75638300
C	-1.86137800	1.63206100	-5.33798500
C	-1.59110500	3.80442300	-6.36300700
C	-0.50729600	1.37584100	-5.51933600
H	-2.50291000	0.88449900	-4.86861800
C	-0.23710900	3.54049000	-6.55008400
H	-2.00771400	4.75545400	-6.69242800
C	0.30473100	2.32941100	-6.12930500
H	-0.08709400	0.42808100	-5.19074500
H	0.39624000	4.28551700	-7.02601600
H	1.36249100	2.12589400	-6.27958300
C	-4.26049000	3.71382500	-3.71252700
C	-3.29962100	4.58830200	-3.19285400
C	-5.29962400	3.26276800	-2.89186900
C	-3.38564500	5.01165300	-1.87177500
H	-2.48257500	4.93708200	-3.82405100
C	-5.38213900	3.68892700	-1.56930300
H	-6.04012100	2.56933600	-3.29448600

C	-4.42634000	4.56259000	-1.06027600
H	-2.63700000	5.69189200	-1.47250800
H	-6.19128400	3.33347800	-0.93548400
H	-4.48733800	4.89212000	-0.02565500

Electronic Energy (0K) = -3614.2531193

Electronic Energy (0K) + ZPE = -3613.430836

Enthalpy (298K) = -3613.373111

Free Energy (298K) = -3613.529573

E

Number of imaginary frequencies: 0

C	0.69427900	-0.16293000	-0.87600100
C	-0.43364100	0.39881600	-1.33131800
H	-0.71058500	0.39405500	-2.39471800
N	-1.31890300	1.11761300	-0.44789400
C	-1.15719400	2.54226000	-0.36211000
C	-0.75085400	3.27541200	-1.48045500
C	-1.38150600	3.19470300	0.85274200
C	-0.55332000	4.64818300	-1.37624300
H	-0.58556900	2.77032800	-2.42988000
C	-1.19477800	4.57029200	0.94302100
H	-1.70210500	2.61922100	1.71725200
C	-0.77603400	5.30033300	-0.16636300
H	-0.23373800	5.21128100	-2.25022400
H	-1.36587200	5.07040500	1.89390600
H	-0.62282800	6.37412900	-0.08786100
O	-2.77419600	-0.93730800	-0.35496100
O	-3.55874000	1.19703000	0.74555800
S	-2.89868000	0.51709800	-0.36257600
C	-3.68017800	1.00321800	-1.87366000

C	-4.25465200	2.26906000	-1.96975100
C	-3.63396200	0.14464800	-2.97290700
C	-4.78765900	2.67353000	-3.18735500
H	-4.29386100	2.92421900	-1.10252300
C	-4.17223000	0.56835400	-4.17891100
H	-3.19608400	-0.84567900	-2.87395200
C	-4.75353600	1.83550500	-4.30547700
H	-5.24218900	3.65887400	-3.27422100
H	-4.14975400	-0.09565500	-5.04190300
C	-5.32943500	2.27144700	-5.61558500
H	-4.59434800	2.17024100	-6.42302000
H	-6.19149600	1.65189000	-5.89262600
H	-5.66119400	3.31387200	-5.58373500
Au	1.13532900	-0.06266700	1.15920600
P	1.52904600	0.48093400	3.45282600
C	1.63467600	-0.76474200	-1.89180000
H	2.49875500	-0.10177200	-2.03469000
H	1.14456100	-0.86752100	-2.87553300
C	3.45856800	-2.44112100	-1.45921100
C	2.15811600	-2.10552300	-1.44934800
C	1.10933900	-3.03191500	-1.07861800
H	0.12710900	-2.86830500	-1.53839500
N	1.16280000	-4.03343300	-0.25151400
C	2.26363200	-4.36956300	0.61048100
C	2.49547300	-3.57313400	1.73037200
C	3.02756600	-5.49688900	0.32644600
C	3.54481700	-3.91366500	2.57514600
H	1.86631400	-2.69967700	1.92311700
C	4.07521000	-5.81924300	1.18142100
H	2.80869200	-6.09390500	-0.55519000

C	4.33199100	-5.02991600	2.29964800
H	3.74748200	-3.30513800	3.45365400
H	4.68956300	-6.69055000	0.97108300
H	5.15239200	-5.28811600	2.96466800
O	-1.27029300	-4.52707600	-1.01487900
O	0.06701700	-6.35246000	0.13780300
S	-0.38654900	-4.98258100	0.03964600
C	-0.83037500	-4.33174100	1.59526900
C	-0.33490900	-4.93701400	2.74987500
C	-1.58132900	-3.15470000	1.62549200
C	-0.62381700	-4.34483700	3.97120000
H	0.25966100	-5.84601800	2.69436000
C	-1.86809900	-2.59675600	2.85923200
H	-1.94177800	-2.68485700	0.71188600
C	-1.39598200	-3.17984000	4.04573500
H	-0.25118200	-4.79769400	4.88810600
H	-2.47225100	-1.69109000	2.90631300
C	-1.72869100	-2.56457600	5.36576800
H	-1.41937600	-1.51150000	5.39968100
H	-2.81275800	-2.57275100	5.53589700
H	-1.24925200	-3.09788800	6.19307900
H	4.19525300	-1.72730000	-1.82226600
H	3.82250400	-3.42057600	-1.16168100
C	-0.03809100	0.74144900	4.35594600
C	-0.06084200	1.03802700	5.72460900
C	-1.23584300	0.73162300	3.63619000
C	-1.26832100	1.30345500	6.35958400
H	0.86505300	1.05906400	6.29823100
C	-2.44438200	1.00841700	4.27225800
H	-1.22114200	0.51214000	2.56705000

C	-2.46000100	1.29003000	5.63437100
H	-1.28024500	1.52858500	7.42340100
H	-3.36721500	1.00228300	3.69466000
H	-3.40154500	1.50283100	6.13567200
C	2.35448200	2.11035200	3.55954000
C	3.08556000	2.51440500	4.68155900
C	2.15327700	3.01069000	2.50758200
C	3.61135000	3.80037900	4.74322300
H	3.25264500	1.82385000	5.50651800
C	2.66887700	4.30120600	2.57996000
H	1.58823400	2.69778400	1.62762400
C	3.40087300	4.69480000	3.69602800
H	4.18470700	4.10565600	5.61555900
H	2.50099800	4.99541500	1.75946900
H	3.81037700	5.70083100	3.75155200
C	2.53278100	-0.65126100	4.47148100
C	3.92760800	-0.63778300	4.35060400
C	1.92761200	-1.58700200	5.31568800
C	4.70235800	-1.51526700	5.10262900
H	4.41231800	0.07149000	3.68070400
C	2.70539900	-2.47414400	6.05404900
H	0.84370200	-1.61077800	5.41355600
C	4.09359000	-2.43040100	5.95962800
H	5.78595400	-1.48388700	5.01732400
H	2.22213300	-3.19159100	6.71393900
H	4.70217100	-3.11224500	6.54893400

Electronic Energy (0K) = -3614.3169115

Electronic Energy (0K) + ZPE = -3613.488783

Enthalpy (298K) = -3613.432476

Free Energy (298K) = -3613.580555

TS_{E1}

Number of imaginary frequencies: 1

C	-3.90876200	-1.33948500	-11.01243800
H	-4.79804600	-0.99258700	-11.54368700
H	-3.04121400	-0.78283600	-11.38412600
H	-3.74130200	-2.40231200	-11.22283200
C	-4.11061800	-1.09897200	-9.54711600
O	-5.11408700	-0.54685100	-9.12724800
C	-3.04549900	-1.55746700	-8.57933900
C	-1.81279200	-1.96504000	-9.02954200
H	-1.68489000	-1.95698800	-10.11244200
C	-0.63042400	-2.39143400	-8.32368500
C	0.48209100	-2.74381300	-9.11423200
C	-0.51540200	-2.48565900	-6.92199200
C	1.66273600	-3.17734900	-8.53278300
H	0.40185500	-2.67300400	-10.19753900
C	0.66627400	-2.92046100	-6.34609200
H	-1.35545100	-2.22163600	-6.28709300
C	1.75637700	-3.26666700	-7.14594100
H	2.51063200	-3.44612200	-9.15740100
H	0.74320300	-2.99184900	-5.26413100
H	2.68046800	-3.60702300	-6.68464200
C	-3.41925900	-1.47635900	-7.23437800
C	-3.82764100	-1.10827700	-6.11821800
C	-4.66063800	-1.31957200	-4.95472200
C	-4.14763300	-1.24637000	-3.65458100
C	-6.02041300	-1.59796000	-5.15232000
C	-4.98453800	-1.46822300	-2.56710400
H	-3.09044500	-1.03575400	-3.50072300

C	-6.85129500	-1.80856200	-4.05861200
H	-6.40900500	-1.64876100	-6.16828600
C	-6.33539900	-1.74600000	-2.76588600
H	-4.58016400	-1.42422300	-1.55837800
H	-7.90452200	-2.03034000	-4.21738600
H	-6.98470600	-1.92642100	-1.91278400
C	-4.02704600	1.58013900	-6.66318200
C	-3.78882300	1.86084900	-7.99103900
H	-2.88454500	1.47595000	-8.47202600
N	-4.57773500	2.54783300	-8.86043400
C	-5.82717300	3.16377800	-8.52083900
C	-5.83054800	4.43565600	-7.95029900
C	-7.01256100	2.48037000	-8.78039400
C	-7.04732600	5.03204000	-7.63530100
H	-4.88497500	4.94082300	-7.75694800
C	-8.22445100	3.08894600	-8.46844600
H	-6.96373100	1.48735400	-9.22302200
C	-8.24001600	4.36020500	-7.89729400
H	-7.06582800	6.02080900	-7.18161800
H	-9.15755100	2.56695200	-8.66859600
H	-9.18916200	4.83578400	-7.65906200
O	-2.93707500	1.79161200	-10.65880000
O	-5.25842700	2.55301400	-11.32442700
S	-4.06496800	2.70142400	-10.51139200
C	-3.50417000	4.36868400	-10.59028400
C	-4.35042600	5.35087700	-11.09608700
C	-2.24502900	4.67693300	-10.07400800
C	-3.91242900	6.66926000	-11.09531800
H	-5.33076500	5.08525500	-11.48310900
C	-1.83008500	5.99869500	-10.08307300

H	-1.59922700	3.89513300	-9.67944000
C	-2.65413400	7.01126800	-10.59317200
H	-4.55946800	7.45028200	-11.49023200
H	-0.84875100	6.25891800	-9.69016500
C	-2.17756000	8.42790700	-10.61840600
H	-1.64124500	8.68575800	-9.69845800
H	-1.47881500	8.58556000	-11.45013900
H	-3.00725400	9.12991100	-10.74672500
Au	-5.72802900	2.00130600	-5.53331500
P	-7.57286300	2.41454400	-4.09614500
C	-3.02894000	0.72402600	-6.12791400
H	-2.89157500	0.65289900	-5.04738700
H	-2.09450500	0.56574500	-6.67835300
C	-7.95479900	4.19999400	-3.94162800
C	-9.08041000	4.77705800	-4.53380600
C	-7.00770800	5.02604400	-3.32433000
C	-9.26445500	6.15742900	-4.49313400
H	-9.82093600	4.15262700	-5.02917000
C	-7.19488500	6.40253300	-3.28531800
H	-6.11689500	4.59258600	-2.86985100
C	-8.32464100	6.97168700	-3.87000300
H	-10.14827700	6.59455700	-4.95296400
H	-6.45517000	7.03303700	-2.79727200
H	-8.47019800	8.04895900	-3.83971700
C	-7.16301400	1.86989100	-2.39453600
C	-8.11924200	1.42495300	-1.47686000
C	-5.81901400	1.92774900	-2.00555500
C	-7.73788900	1.06306200	-0.18872800
H	-9.16562500	1.34857900	-1.76230200
C	-5.44355100	1.58468000	-0.71065000

H	-5.06216200	2.22752000	-2.73229100
C	-6.40325300	1.15092500	0.19931900
H	-8.48879800	0.71229800	0.51558500
H	-4.39666900	1.63836900	-0.41999000
H	-6.11111900	0.87267300	1.20940100
C	-9.11862100	1.58758600	-4.58549400
C	-10.34608300	1.81745800	-3.94807400
C	-9.05597600	0.66859300	-5.63850100
C	-11.48089700	1.12048200	-4.34610300
H	-10.42171800	2.55066600	-3.14614400
C	-10.19446700	-0.02783500	-6.03442200
H	-8.10580200	0.50819500	-6.15021000
C	-11.40456500	0.19481700	-5.38518000
H	-12.42898300	1.30282400	-3.84568700
H	-10.13451100	-0.74176800	-6.85268600
H	-12.29456300	-0.34991500	-5.69213400

Electronic Energy (0K) = -3161.7942987

Electronic Energy (0K) + ZPE = -3160.980121

Enthalpy (298K) = -3160.925041

Free Energy (298K) = -3161.073969

E1

Number of imaginary frequencies: 0

C	-0.59823900	-1.41599200	-3.56184400
H	-1.47215000	-0.79621900	-3.77889800
H	0.31842600	-0.82381100	-3.68128900
H	-0.56116200	-2.23546600	-4.29125600
C	-0.71456000	-1.96453000	-2.17655700
O	-1.72210900	-1.88863300	-1.50658800
C	0.51209200	-2.65771500	-1.59192400

C	1.37851500	-3.40413500	-2.40870800
H	1.33382800	-3.20932000	-3.48293700
C	2.29257100	-4.39904200	-1.99898000
C	3.28635700	-4.79700400	-2.92811300
C	2.26505000	-4.99626300	-0.71317100
C	4.26514700	-5.69628500	-2.55661400
H	3.28262300	-4.35751100	-3.92314400
C	3.24118600	-5.90387000	-0.35757600
H	1.44557300	-4.78210600	-0.03069200
C	4.24362600	-6.24424300	-1.27168500
H	5.04091400	-5.98470300	-3.25968200
H	3.21749300	-6.37388700	0.62123700
H	5.00340600	-6.96732200	-0.98512100
C	0.76024900	-2.43584700	-0.28282400
C	0.93238000	-1.88846000	0.88302800
C	0.46110000	-2.52173700	2.13212100
C	1.22734200	-2.45520400	3.30023500
C	-0.77477600	-3.18096400	2.14959800
C	0.75720300	-3.04203600	4.47017000
H	2.19481700	-1.95632400	3.29286100
C	-1.24650100	-3.74904700	3.32705800
H	-1.37189400	-3.21187200	1.23916300
C	-0.48125800	-3.68085000	4.48918600
H	1.35945800	-2.99556600	5.37468700
H	-2.21936400	-4.23625000	3.33704300
H	-0.85174500	-4.11987300	5.41260100
C	0.47081400	0.48301000	0.39606400
C	0.64748200	0.90362500	-0.86822500
H	1.54536200	0.63679900	-1.43270900
N	-0.26929700	1.61763700	-1.68275800

C	-1.46400900	2.20980500	-1.15335600
C	-1.39558500	3.37766500	-0.39178300
C	-2.69048800	1.60565000	-1.41754500
C	-2.56727700	3.94426100	0.09846700
H	-0.42617600	3.83138300	-0.18733600
C	-3.85938300	2.17391900	-0.91765400
H	-2.70920100	0.68791000	-2.00313200
C	-3.79693400	3.34205800	-0.16193100
H	-2.52172400	4.85472900	0.69256500
H	-4.81905200	1.70185800	-1.11753600
H	-4.71034900	3.78403300	0.23224800
O	1.41528400	1.44434800	-3.55555500
O	-0.87902600	2.40991800	-4.00052900
S	0.28631400	2.27217400	-3.13890500
C	0.88305800	3.88731100	-2.73811500
C	0.10017400	5.00024300	-3.02545000
C	2.08712400	4.00428400	-2.04157600
C	0.53729600	6.25276300	-2.60972500
H	-0.83845600	4.88199700	-3.56083400
C	2.50037100	5.26061200	-1.62806000
H	2.68859800	3.12352800	-1.82739700
C	1.73385100	6.40105800	-1.90521600
H	-0.06292600	7.13323900	-2.83211200
H	3.43715900	5.36925400	-1.08347200
C	2.20358100	7.74801300	-1.45455600
H	2.47161000	7.73840100	-0.39154600
H	3.10193100	8.05523000	-2.00467100
H	1.43785100	8.51473800	-1.60862700
Au	-1.19541300	0.60854100	1.64418800
P	-2.99528600	0.52434100	3.19904900

C	1.54303600	-0.47144100	0.87296600
H	1.86847600	-0.26088500	1.89922500
H	2.43411500	-0.46453600	0.22775700
C	-4.18577700	1.90983500	3.16833700
C	-5.55232300	1.71818100	2.95911700
C	-3.68985000	3.20461000	3.36170100
C	-6.41480300	2.81269300	2.94490600
H	-5.95021400	0.71526900	2.81200200
C	-4.55485200	4.29218900	3.35786700
H	-2.62042000	3.35854400	3.51490900
C	-5.91949100	4.09687600	3.14711200
H	-7.47882800	2.65702300	2.78171200
H	-4.16262100	5.29516600	3.51145900
H	-6.59588500	4.94852000	3.13981600
C	-4.01040700	-0.96975800	2.93988900
C	-4.59909900	-1.67372000	3.99295500
C	-4.21577800	-1.39596700	1.62278700
C	-5.38362900	-2.79325000	3.72877800
H	-4.44453800	-1.35230700	5.02190400
C	-5.00173000	-2.51316000	1.36221300
H	-3.74695100	-0.85014800	0.80262000
C	-5.58517300	-3.21282400	2.41632200
H	-5.83944700	-3.33854900	4.55205500
H	-5.15348600	-2.83992000	0.33588500
H	-6.19577300	-4.08979900	2.21331900
C	-2.44135600	0.45370300	4.93637800
C	-1.16818000	-0.05337500	5.21315100
C	-3.26359600	0.86618100	5.99109700
C	-0.72423700	-0.15069300	6.52833400
H	-0.52219100	-0.37015100	4.39218200

C	-2.81555300	0.76874100	7.30397500
H	-4.25677800	1.26523900	5.78746000
C	-1.54624800	0.26156600	7.57312000
H	0.26962900	-0.54164700	6.73568300
H	-3.45850400	1.09184700	8.11943900
H	-1.19649600	0.19206800	8.60061900

Electronic Energy (0K) = -3161.8132099

Electronic Energy (0K) + ZPE = -3160.997152

Enthalpy (298K) = -3160.942491

Free Energy (298K) = -3161.089023

TS_{E2}

Number of imaginary frequencies: 1

C	-3.45725600	-1.68339400	-11.07601200
H	-4.34265200	-1.42481900	-11.66223400
H	-2.61356500	-1.05454300	-11.38896900
H	-3.18698600	-2.72444500	-11.29004900
C	-3.77391300	-1.49349600	-9.61881800
O	-4.89338200	-1.16424300	-9.25733200
C	-2.68275000	-1.69612200	-8.61175200
C	-1.47026700	-2.18009800	-8.98199900
H	-1.35766000	-2.40794100	-10.04221600
C	-0.27244200	-2.45590000	-8.20747900
C	0.88508900	-2.80331900	-8.92666300
C	-0.19715600	-2.40344800	-6.80380300
C	2.07901400	-3.07156900	-8.27339100
H	0.83478700	-2.85529100	-10.01320300
C	0.99701200	-2.67676100	-6.15362700
H	-1.08114100	-2.16255900	-6.21870600
C	2.13778400	-3.00735600	-6.88368400

H	2.96408600	-3.33415200	-8.84765800
H	1.03901800	-2.63766200	-5.06781100
H	3.07064300	-3.22088200	-6.36694100
C	-3.02785600	-1.24510200	-7.28454300
C	-3.71271300	-1.29633200	-6.24932300
C	-4.42919600	-1.10604300	-5.05727900
C	-3.78586700	-1.21519900	-3.80798500
C	-5.79638700	-0.76486400	-5.12153200
C	-4.50070600	-0.96919500	-2.64755600
H	-2.73191700	-1.48362300	-3.77290300
C	-6.50214600	-0.53993600	-3.95023700
H	-6.28084300	-0.69845000	-6.09356400
C	-5.85518600	-0.63731600	-2.71813000
H	-4.00831600	-1.04296200	-1.68143300
H	-7.55767900	-0.28110300	-3.99203200
H	-6.41249600	-0.45313700	-1.80248000
C	-2.99932100	1.39954400	-7.92051100
C	-2.44500900	1.40659200	-9.17839000
H	-1.51047600	0.87233900	-9.37403300
N	-2.94859300	2.00345200	-10.30022100
C	-4.17231400	2.75371500	-10.33436400
C	-4.15281200	4.12013500	-10.05946100
C	-5.35798000	2.09310400	-10.64613100
C	-5.34500100	4.83682200	-10.10362300
H	-3.21115900	4.60567900	-9.80592100
C	-6.54435900	2.81848000	-10.68750000
H	-5.33805000	1.02050900	-10.83782600
C	-6.53553400	4.18680100	-10.42326700
H	-5.34462600	5.90214700	-9.88307800
H	-7.47634000	2.31424000	-10.93265300

H	-7.46355000	4.75278000	-10.46641900
O	-1.02061700	0.91782000	-11.54874900
O	-3.02590600	1.77408200	-12.83341700
S	-2.04614700	1.92884900	-11.77275200
C	-1.30667300	3.52275900	-11.87380300
C	-1.83220200	4.46757800	-12.74827600
C	-0.24835400	3.82231100	-11.01360800
C	-1.27148600	5.73963100	-12.76622700
H	-2.66167900	4.20944000	-13.40197800
C	0.28836300	5.09792500	-11.04373200
H	0.15021200	3.06827700	-10.33767200
C	-0.21341500	6.07338300	-11.91801600
H	-1.66429800	6.48946200	-13.45015900
H	1.11755400	5.35002400	-10.38470700
C	0.38472900	7.44369100	-11.93061600
H	0.27847000	7.92717100	-10.95151000
H	1.45899200	7.40154600	-12.14733000
H	-0.09005400	8.08459000	-12.67963400
Au	-4.79757900	2.22234500	-7.26322700
P	-6.74936800	3.12493300	-6.24987300
C	-2.27584600	0.56807100	-7.01962600
H	-2.40537700	0.70348400	-5.94576200
H	-1.26455500	0.22868100	-7.27665500
C	-7.01423700	4.89673500	-6.61413500
C	-7.94082600	5.32506100	-7.56776700
C	-6.16347400	5.83191700	-6.01392500
C	-8.03223400	6.67533100	-7.89683300
H	-8.59255200	4.60709000	-8.06238300
C	-6.25444200	7.17788300	-6.34910800
H	-5.42800200	5.50535900	-5.27857200

C	-7.19193100	7.60263900	-7.28900500
H	-8.76236700	7.00052000	-8.63485000
H	-5.59267100	7.89775900	-5.87294000
H	-7.26413000	8.65648900	-7.54771000
C	-6.56509400	3.05524900	-4.42618100
C	-7.63937800	3.24203200	-3.54931500
C	-5.28565600	2.84356400	-3.89966300
C	-7.43470000	3.21266700	-2.17419900
H	-8.64400800	3.40465500	-3.93339100
C	-5.08099300	2.82848900	-2.52338800
H	-4.44560100	2.68010200	-4.57698200
C	-6.15574500	3.01149500	-1.65913600
H	-8.27749100	3.35331800	-1.50151500
H	-4.08106800	2.66405000	-2.12766000
H	-5.99929800	2.99408100	-0.58299600
C	-8.29436100	2.26485300	-6.69369800
C	-9.56445500	2.72580200	-6.32128200
C	-8.18749500	1.08032500	-7.43164900
C	-10.69882000	1.99658900	-6.65879600
H	-9.67596900	3.66870200	-5.78832000
C	-9.32554400	0.35170300	-7.76602900
H	-7.20333500	0.73562800	-7.75390900
C	-10.58021200	0.80634500	-7.37330800
H	-11.68017600	2.36154300	-6.36504300
H	-9.22914400	-0.56825300	-8.33777700
H	-11.47070200	0.23875900	-7.63364000

Electronic Energy (0K) = -3161.7981319

Electronic Energy (0K) + ZPE = -3160.983261

Enthalpy (298K) = -3160.928784

Free Energy (298K) = -3161.073955

E2

Number of imaginary frequencies: 0

C	0.16269700	-3.92529300	-2.43764300
H	-0.88811100	-4.01108900	-2.72225000
H	0.63122600	-3.09298100	-2.98077000
H	0.68530500	-4.84317000	-2.72956400
C	0.25776300	-3.68733300	-0.96208600
O	-0.72980200	-3.68070300	-0.24121700
C	1.59262300	-3.40960700	-0.35971200
C	2.73583100	-3.83735700	-0.93561500
H	2.64394500	-4.29306000	-1.92315700
C	4.09666800	-3.78916400	-0.42185000
C	5.15261200	-3.85543100	-1.34435900
C	4.39797500	-3.70736700	0.94755500
C	6.47171800	-3.80238100	-0.91505200
H	4.92235400	-3.93677000	-2.40577000
C	5.71755600	-3.66800200	1.37405700
H	3.59223800	-3.70219300	1.67988400
C	6.75659000	-3.70921300	0.44522200
H	7.27947400	-3.84336400	-1.64175600
H	5.94012600	-3.61590800	2.43717200
H	7.78961300	-3.67998400	0.78371800
C	1.50759000	-2.56887500	0.85632500
C	0.63447100	-2.77816500	1.78151100
C	-0.22825800	-2.87669900	2.84711700
C	0.22829700	-3.38814900	4.09199100
C	-1.57607000	-2.44748600	2.70350200
C	-0.64114900	-3.44652100	5.16090600
H	1.26045800	-3.71804500	4.17964700

C	-2.43603100	-2.53235200	3.77809200
H	-1.90056300	-2.06128400	1.73938800
C	-1.96624200	-3.02531400	4.99988800
H	-0.30404700	-3.82495600	6.12135600
H	-3.47104000	-2.21342800	3.68044500
H	-2.64763700	-3.08126600	5.84584400
C	1.37575200	-0.39055200	-0.21490400
C	1.85186900	-0.44878500	-1.47431600
H	2.78900200	-0.96250800	-1.70275300
N	1.22487600	0.03008800	-2.64161400
C	0.11542800	0.93607500	-2.60076800
C	0.31631100	2.27802600	-2.27552300
C	-1.16108600	0.45375000	-2.87999600
C	-0.77270300	3.14389800	-2.24304400
H	1.32079100	2.62968700	-2.04165000
C	-2.24692400	1.32421000	-2.84330000
H	-1.28429700	-0.60054400	-3.12436600
C	-2.05015800	2.66799700	-2.53319700
H	-0.62409200	4.19287800	-1.99540300
H	-3.24579000	0.95287300	-3.06220000
H	-2.89676600	3.35063000	-2.51707400
O	2.92739700	-1.25923600	-3.98310500
O	1.04545700	-0.03765600	-5.15629800
S	2.05686900	-0.09606800	-4.11233800
C	3.05252900	1.36119800	-4.20300000
C	2.61209600	2.44734000	-4.95278000
C	4.22034300	1.42870300	-3.44142500
C	3.36260200	3.61749900	-4.94279600
H	1.69776100	2.37496100	-5.53631100
C	4.94969200	2.60701900	-3.44036800

H	4.55810800	0.56795400	-2.86832100
C	4.53396800	3.71661000	-4.18851900
H	3.03322300	4.47228500	-5.53085300
H	5.86508200	2.67276100	-2.85428900
C	5.34852700	4.97144200	-4.18292700
H	5.59115800	5.28105200	-3.15955900
H	6.30310000	4.81970000	-4.70260900
H	4.82583700	5.79561600	-4.67826400
Au	-0.45066600	0.34828700	0.45427400
P	-2.42601900	1.18373700	1.49752800
C	2.18364700	-1.16932800	0.79242700
H	2.18032000	-0.72267400	1.79165700
H	3.22950300	-1.32534400	0.49184300
C	-2.69265400	2.97171100	1.21756700
C	-3.66796900	3.46036200	0.34621900
C	-1.79095900	3.86471600	1.80976800
C	-3.75279300	4.82663500	0.08725500
H	-4.36433300	2.77866900	-0.13840700
C	-1.87661900	5.22602900	1.54544100
H	-1.01768600	3.49363900	2.48266400
C	-2.85964700	5.71006000	0.68400500
H	-4.51974800	5.19775500	-0.58916300
H	-1.17404400	5.91174100	2.01341300
H	-2.92675500	6.77575600	0.47794500
C	-2.25413100	1.02046000	3.31862500
C	-3.34430100	1.07489700	4.19293600
C	-0.96831800	0.84328400	3.84433500
C	-3.15122000	0.93633200	5.56348600
H	-4.35280400	1.21286600	3.80933300
C	-0.77523400	0.72062000	5.21697400

H	-0.11329200	0.79446100	3.16775500
C	-1.86857800	0.75868100	6.07697300
H	-4.00727200	0.97074600	6.23338000
H	0.22912800	0.58614300	5.61244500
H	-1.72259000	0.65275700	7.14957200
C	-3.96365200	0.32845500	1.01764000
C	-5.23984900	0.75735600	1.40722400
C	-3.84302800	-0.82679900	0.23585100
C	-6.36525400	0.02829700	1.03989500
H	-5.36173900	1.67312400	1.98353100
C	-4.97151600	-1.55634400	-0.12746400
H	-2.85410200	-1.15271600	-0.09225300
C	-6.23208300	-1.13094300	0.27848400
H	-7.35107000	0.36908400	1.34742500
H	-4.86304100	-2.45387700	-0.73161500
H	-7.11547100	-1.69875300	-0.00451900

Electronic Energy (0K) = -3161.8096249

Electronic Energy (0K) + ZPE = -3160.992472

Enthalpy (298K) = -3160.938141

Free Energy (298K) = -3161.082001

TS_{E3}

Number of imaginary frequencies: 1

C	-1.37379400	-1.69500900	-6.90347500
H	-1.07255800	-0.66397600	-7.12804200
H	-0.89081000	-1.97567000	-5.95976200
H	-1.02213500	-2.35568500	-7.69875600
C	-2.86371900	-1.81640600	-6.79449100
O	-3.50195500	-2.59587300	-7.48213700
C	-3.58091500	-0.96424800	-5.79598700

C	-2.92863500	0.04909200	-5.06250200
H	-1.83997900	0.05096000	-5.15885800
C	-3.37099900	0.56114800	-3.73925000
C	-2.74408200	1.69251900	-3.19804000
C	-4.30727700	-0.11919000	-2.95063300
C	-3.06708000	2.15287700	-1.92740600
H	-1.98123500	2.21720400	-3.77310000
C	-4.60976200	0.32585300	-1.66780300
H	-4.77839000	-1.02468600	-3.32485800
C	-4.00463000	1.47040100	-1.15605000
H	-2.57253600	3.03873200	-1.53341000
H	-5.32597400	-0.22884100	-1.06473800
H	-4.25612000	1.82235600	-0.15761800
C	-4.96470800	-0.98289000	-5.83522100
C	-6.15036200	-0.68752500	-5.95878600
C	-7.51526400	-0.33007600	-6.00278700
C	-8.02617200	0.53383000	-5.01345000
C	-8.35572400	-0.78137900	-7.03519500
C	-9.35434900	0.92556600	-5.05174200
H	-7.36366800	0.88356300	-4.22403500
C	-9.68448300	-0.37966400	-7.06557000
H	-7.95289000	-1.44424900	-7.79755900
C	-10.18433700	0.46811500	-6.07817800
H	-9.74735300	1.58559000	-4.27972900
H	-10.33354800	-0.72759200	-7.86502500
H	-11.22722700	0.77488100	-6.10730300
C	-4.54634300	1.92270200	-6.56248000
C	-5.10516200	1.34889600	-7.70331400
H	-4.60294300	0.50116100	-8.18200000
N	-6.24170800	1.73723700	-8.34034700

C	-6.79032600	3.05857500	-8.21594000
C	-5.96819300	4.15428400	-8.48581700
C	-8.13526000	3.22920600	-7.89643500
C	-6.49337900	5.43814800	-8.40468100
H	-4.92791100	3.99034600	-8.76225400
C	-8.65276400	4.51876600	-7.83354700
H	-8.76040100	2.35933800	-7.70902900
C	-7.83612300	5.61991500	-8.07983900
H	-5.85856900	6.29572900	-8.61335100
H	-9.70236400	4.66348900	-7.58845400
H	-8.25034000	6.62399300	-8.01856900
O	-6.04934100	-0.43738600	-9.66204400
O	-8.12916500	0.98873200	-9.90418300
S	-6.68832400	0.86173700	-9.79736000
C	-5.91573900	1.80064400	-11.06945100
C	-6.62858100	2.83098200	-11.67765500
C	-4.58178600	1.54039900	-11.38751300
C	-5.98663600	3.60797100	-12.63310700
H	-7.66491500	3.01931700	-11.40712600
C	-3.96348000	2.32953600	-12.34356600
H	-4.04521500	0.72500500	-10.90812900
C	-4.65326500	3.37136300	-12.97835100
H	-6.52882900	4.41444400	-13.12284900
H	-2.92619400	2.13583400	-12.61188800
C	-3.96551200	4.20083700	-14.01449300
H	-4.58128500	5.04965300	-14.32690200
H	-3.00931300	4.58563300	-13.64063900
H	-3.73875300	3.60123200	-14.90496200
Au	-5.56403900	3.14920400	-5.20169600
P	-6.53988500	4.56804600	-3.56111600

C	-3.19436500	1.53838100	-6.36480900
H	-2.56730200	2.19297200	-5.75857100
H	-2.64751800	1.10394300	-7.20821900
C	-7.58488100	5.91784200	-4.21064200
C	-8.84667200	5.59517200	-4.72452200
C	-7.15362100	7.24612800	-4.22476000
C	-9.67793500	6.59606800	-5.21284000
H	-9.18383400	4.55758700	-4.73089400
C	-7.98164200	8.24235900	-4.73665100
H	-6.17653800	7.51153400	-3.82465700
C	-9.24567100	7.92109600	-5.22095800
H	-10.66406700	6.34033600	-5.59483600
H	-7.64062500	9.27496200	-4.74115500
H	-9.89672200	8.70270600	-5.60582500
C	-5.20475000	5.38201800	-2.62019400
C	-5.32851800	5.67730500	-1.26038000
C	-4.02809000	5.72111500	-3.29887100
C	-4.28289300	6.30191700	-0.58698200
H	-6.23858800	5.41501500	-0.72247600
C	-2.99163100	6.35834400	-2.62523600
H	-3.92961700	5.48252600	-4.35937600
C	-3.11711200	6.64356500	-1.26717900
H	-4.38090700	6.52344000	0.47322600
H	-2.08194900	6.62428400	-3.15876900
H	-2.30274800	7.13284100	-0.73776000
C	-7.58105400	3.73323000	-2.32006300
C	-8.62243700	4.38036800	-1.64640200
C	-7.27895200	2.40575500	-2.00701500
C	-9.35554200	3.69639500	-0.68211000
H	-8.86249800	5.41814600	-1.87194600

C	-8.01174900	1.72489000	-1.04032900
H	-6.45662100	1.90653000	-2.52079100
C	-9.05455000	2.36982700	-0.38137500
H	-10.16578400	4.20286500	-0.16276700
H	-7.77154000	0.68899100	-0.80902500
H	-9.63440400	1.83922700	0.37034900

Electronic Energy (0K) = -3161.794815

Electronic Energy (0K) + ZPE = -3160.979986

Enthalpy (298K) = -3160.925426

Free Energy (298K) = -3161.069647

E3

Number of imaginary frequencies: 0

C	4.31755000	-3.87479200	0.38138400
H	4.61944200	-2.92031000	-0.06732200
H	4.74972300	-3.90901600	1.38932200
H	4.72191400	-4.69854200	-0.21071500
C	2.82777900	-4.00885000	0.44734300
O	2.23642800	-4.96053700	-0.03664700
C	2.04614000	-2.95380100	1.15840300
C	2.64672800	-1.72570800	1.70004900
H	3.73943700	-1.82472600	1.71169900
C	2.21808700	-1.22551700	3.06057600
C	2.67174300	0.02229300	3.50450800
C	1.48302800	-2.01694700	3.94705600
C	2.39029700	0.47097700	4.79064100
H	3.26631900	0.65411800	2.84442300
C	1.20011400	-1.56851900	5.23569800
H	1.14614700	-3.00598100	3.64367300
C	1.64602100	-0.32146200	5.66119700

H	2.75462500	1.44546500	5.11129000
H	0.63032500	-2.20469500	5.91023500
H	1.41654600	0.03288900	6.66430600
C	0.69413400	-2.96580500	1.02810100
C	-0.48673800	-2.64656200	0.82859400
C	-1.85022500	-2.34378900	0.71304100
C	-2.42955700	-1.42652100	1.61768400
C	-2.63829600	-2.92505400	-0.30104400
C	-3.77303100	-1.11418100	1.51731400
H	-1.80251300	-0.98334600	2.38923900
C	-3.98084600	-2.59394100	-0.39740300
H	-2.18197100	-3.62658800	-0.99564200
C	-4.54637200	-1.69654900	0.50847700
H	-4.22446500	-0.41975700	2.22318800
H	-4.59141700	-3.03542600	-1.18011300
H	-5.60224700	-1.44830000	0.42997400
C	0.99978700	-0.20042700	0.25070600
C	0.47567500	-0.66356200	-0.93882300
H	0.98996900	-1.45602700	-1.48939400
N	-0.68659200	-0.23805000	-1.55101700
C	-1.19889200	1.09281700	-1.39002700
C	-0.34484500	2.18101500	-1.58830400
C	-2.55084900	1.28816400	-1.11710100
C	-0.84205200	3.47335100	-1.47007500
H	0.70079900	2.00456900	-1.83576600
C	-3.04269600	2.58642500	-1.02451700
H	-3.20264800	0.42712300	-0.98877900
C	-2.19119100	3.67660100	-1.18557500
H	-0.17767700	4.32170100	-1.61582500
H	-4.09806100	2.74524500	-0.81552800

H	-2.58132100	4.68746500	-1.08257200
O	-0.44220600	-2.30209900	-3.02279900
O	-2.58267900	-0.95554000	-3.11188100
S	-1.13406800	-1.02191000	-3.03944800
C	-0.44108000	0.03240000	-4.26865200
C	-1.22081900	1.05260500	-4.80732200
C	0.90471300	-0.11832200	-4.60580900
C	-0.63603400	1.93187500	-5.70951100
H	-2.26564300	1.15519000	-4.52334700
C	1.46647400	0.77126600	-5.50766500
H	1.49565700	-0.92511000	-4.17830200
C	0.70799400	1.80625600	-6.07082100
H	-1.23193700	2.73262300	-6.14316400
H	2.51287400	0.66490500	-5.78895300
C	1.33068700	2.74449600	-7.05449600
H	1.53302800	2.23263700	-8.00394700
H	0.67841100	3.59704000	-7.26671100
H	2.29138100	3.12428100	-6.68775200
Au	0.01711700	1.05815500	1.60333400
P	-0.92724200	2.51467500	3.23814000
C	2.38714900	-0.64419300	0.50233800
H	3.00616800	0.20433000	0.82397400
H	2.86551900	-1.07480200	-0.38868400
C	-2.02130200	3.83553600	2.60635700
C	-3.28733900	3.47372000	2.13202300
C	-1.63293700	5.17682300	2.57922800
C	-4.16449000	4.44680400	1.66903200
H	-3.59035900	2.42552300	2.13585400
C	-2.50680300	6.14572400	2.09152200
H	-0.65401300	5.47425800	2.95066900

C	-3.77428200	5.78470400	1.64605300
H	-5.15316800	4.15931000	1.31758800
H	-2.19838300	7.18845300	2.07649500
H	-4.46071200	6.54472200	1.27983800
C	0.42606400	3.37346000	4.11135600
C	0.41264600	3.58363800	5.49164900
C	1.51537700	3.82058600	3.35321700
C	1.47772000	4.23689900	6.10620400
H	-0.42485400	3.23148500	6.09197200
C	2.57102900	4.48375300	3.96870900
H	1.53174400	3.64377100	2.27598700
C	2.55389500	4.68858300	5.34731000
H	1.46485600	4.39379400	7.18220600
H	3.41230900	4.83250000	3.37423000
H	3.38361300	5.19877000	5.83119500
C	-1.91684200	1.69319500	4.52958200
C	-2.88773900	2.37855400	5.26941000
C	-1.65728500	0.34941200	4.81210000
C	-3.59294400	1.71853300	6.26961500
H	-3.09240800	3.42858200	5.06526400
C	-2.36304600	-0.30743600	5.81571200
H	-0.88664500	-0.18150400	4.25131800
C	-3.33438300	0.37632900	6.54043700
H	-4.34858100	2.25407900	6.83954900
H	-2.15503600	-1.35436000	6.02690200
H	-3.89144300	-0.13617200	7.32142900

Electronic Energy (0K) = -3161.79976

Electronic Energy (0K) + ZPE = -3160.984182

Enthalpy (298K) = -3160.929535

Free Energy (298K) = -3161.074041

TS_{E4}

Number of imaginary frequencies: 1

C	-1.25013900	-1.52022400	-8.56731100
H	-1.14166100	-2.60036700	-8.69521000
H	-2.31909500	-1.30683900	-8.41866000
H	-0.92105700	-1.02924100	-9.48477200
C	-0.46833500	-1.02815900	-7.40006600
O	0.18707200	0.03739700	-7.45160400
C	-0.46516000	-1.73291200	-6.11412400
C	-1.20355200	-2.87539900	-5.95259700
H	-1.76073300	-3.22452400	-6.82097900
C	-1.41953200	-3.67107100	-4.76493500
C	-2.53444800	-4.53151900	-4.76671300
C	-0.61188200	-3.61893700	-3.61281100
C	-2.86414500	-5.27113000	-3.64114000
H	-3.15127600	-4.59323300	-5.66193500
C	-0.93415700	-4.37653000	-2.49718400
H	0.27474500	-2.99260900	-3.60121200
C	-2.06651100	-5.19091300	-2.50103400
H	-3.73921200	-5.91606900	-3.65249100
H	-0.29831400	-4.33230000	-1.61598700
H	-2.32023700	-5.77373700	-1.61852800
C	0.21966200	-1.07253600	-5.05685200
C	0.75518600	-0.46065100	-4.15315300
C	1.36516900	0.17615800	-3.03608900
C	0.95449400	-0.16666000	-1.73722800
C	2.38651600	1.12325900	-3.21272400
C	1.56035500	0.42620900	-0.63749900
H	0.15929900	-0.90039500	-1.61060800

C	2.99020800	1.70385800	-2.10585700
H	2.69682900	1.39180200	-4.22077900
C	2.58159300	1.35648500	-0.81925200
H	1.23767900	0.15775200	0.36590400
H	3.77996400	2.43860200	-2.24668300
H	3.05748300	1.81746500	0.04361900
C	-1.63620700	1.79479500	-8.10168500
C	-2.55030900	1.41139400	-9.04589900
H	-2.21675200	0.96784500	-9.98802500
N	-3.91569800	1.48599500	-8.96425300
C	-4.61916600	2.14427700	-7.90201500
C	-4.80268600	3.52420400	-7.96097600
C	-5.10150200	1.39463900	-6.83116200
C	-5.47754900	4.16274900	-6.92543200
H	-4.41279700	4.08109900	-8.81236900
C	-5.77624300	2.04161700	-5.80112400
H	-4.93837300	0.31803700	-6.81773000
C	-5.96399700	3.42191600	-5.85069300
H	-5.62600100	5.23952700	-6.95725400
H	-6.15342100	1.46835400	-4.95685200
H	-6.49025000	3.92466800	-5.04229300
O	-3.95871800	0.09347000	-11.08734600
O	-6.03493500	0.26492100	-9.64867000
S	-4.87129800	0.87645800	-10.26652800
C	-5.36543200	2.33042300	-11.12810600
C	-6.62930000	2.86486900	-10.88995000
C	-4.45054300	2.95665400	-11.97363300
C	-6.98256000	4.04591300	-11.52734700
H	-7.31828200	2.36251100	-10.21573400
C	-4.82444200	4.13754900	-12.59669400

H	-3.46653300	2.52545200	-12.14590400
C	-6.09122200	4.69626100	-12.38714900
H	-7.96775900	4.47609100	-11.35592800
H	-4.12474500	4.63833300	-13.26327500
C	-6.49359700	5.95257900	-13.09081700
H	-7.04750300	5.71856900	-14.00934100
H	-7.14992200	6.56914900	-12.46738800
H	-5.62168900	6.54907600	-13.37814400
Au	-1.95841300	2.38083000	-6.12025300
P	-2.14813100	2.91090000	-3.80140600
C	-0.30217600	1.47501100	-8.49437800
H	0.53020300	2.04384000	-8.08615500
H	-0.10457200	1.06758500	-9.49127400
C	-3.44660700	4.13744500	-3.38720000
C	-4.60979100	3.80222100	-2.69082800
C	-3.28678700	5.44427300	-3.86435300
C	-5.58673400	4.76683400	-2.45264500
H	-4.76346000	2.78782800	-2.32873800
C	-4.26829600	6.40100100	-3.63384100
H	-2.38985900	5.71772800	-4.42067200
C	-5.41883200	6.06489300	-2.92265600
H	-6.48323600	4.49688000	-1.89879600
H	-4.13289800	7.41302000	-4.00864000
H	-6.18364500	6.81586800	-2.73845200
C	-0.59857900	3.69390400	-3.21127300
C	-0.24312500	3.77771100	-1.86071600
C	0.22934300	4.28874400	-4.17047300
C	0.90779400	4.45860000	-1.48049100
H	-0.84606400	3.29720000	-1.09456500
C	1.37784400	4.97513100	-3.78599000

H	-0.03189900	4.21351200	-5.22686700
C	1.71459200	5.06630300	-2.43973000
H	1.17602400	4.51222500	-0.42750700
H	2.00922800	5.43630000	-4.54204800
H	2.61115600	5.60280900	-2.13688500
C	-2.50348900	1.43770500	-2.78274800
C	-2.71627200	1.48903100	-1.39723500
C	-2.58987000	0.20191600	-3.43399600
C	-2.97479000	0.32608700	-0.68104900
H	-2.70470400	2.44314500	-0.87337000
C	-2.86022600	-0.96004500	-2.71614700
H	-2.44524800	0.14920300	-4.51412800
C	-3.04243800	-0.90129400	-1.33894900
H	-3.13435400	0.38046200	0.39319000
H	-2.92963200	-1.91263100	-3.23813500
H	-3.24957400	-1.81116700	-0.77930100

Electronic Energy (0K) = -3161.7992553

Electronic Energy (0K) + ZPE = -3160.983194

Enthalpy (298K) = -3160.928688

Free Energy (298K) = -3161.075158

E4

Number of imaginary frequencies: 0

C	0.61644500	-2.96141300	-1.25273100
H	0.66241400	-4.04147200	-1.12005400
H	-0.41768200	-2.63031300	-1.07368700
H	0.85471600	-2.72734800	-2.29322200
C	1.50707700	-2.23065500	-0.32956000
O	1.95833000	-1.06551000	-0.63174900
C	1.90973700	-2.70425500	0.97075600

C	1.48039600	-3.94615000	1.39507900
H	0.84790400	-4.49642300	0.70190200
C	1.69068100	-4.63727100	2.63597800
C	0.88067100	-5.77014200	2.86726200
C	2.63223800	-4.26976500	3.61962900
C	0.97219600	-6.48104400	4.05196500
H	0.16861400	-6.07382000	2.10177300
C	2.73181300	-4.99613400	4.79445300
H	3.29729100	-3.43095000	3.44836000
C	1.89800000	-6.09209200	5.01984000
H	0.33305700	-7.34341600	4.22136000
H	3.46629900	-4.70804000	5.54286200
H	1.97875600	-6.65181700	5.94871100
C	2.65270700	-1.80920900	1.79265700
C	3.25977600	-1.06269400	2.53606200
C	3.99737200	-0.28449200	3.47401200
C	4.00067800	-0.65591600	4.82974500
C	4.73566900	0.83456900	3.06360400
C	4.72578800	0.08507800	5.75236900
H	3.42091900	-1.52319100	5.14234300
C	5.46086200	1.56695500	3.99432100
H	4.73156400	1.11967500	2.01351900
C	5.45570200	1.19755600	5.33721800
H	4.72252900	-0.20548500	6.80026000
H	6.02912300	2.43646900	3.67091700
H	6.02200600	1.77724600	6.06241400
C	-0.00708100	0.12674200	-1.45878600
C	-0.86031300	-0.12547800	-2.46712700
H	-0.51619500	-0.56564700	-3.40629300
N	-2.25590100	0.05069800	-2.46540300

C	-2.96765100	0.62178700	-1.36101500
C	-3.01979900	2.00579700	-1.19293000
C	-3.61299200	-0.22891100	-0.46594600
C	-3.73641000	2.53847100	-0.12529600
H	-2.49718000	2.65226200	-1.89704500
C	-4.31858100	0.30981200	0.60622900
H	-3.55887400	-1.30422400	-0.62809700
C	-4.38322900	1.69166300	0.77267300
H	-3.78513000	3.61674500	0.01065400
H	-4.82654200	-0.34874900	1.30731300
H	-4.93557600	2.11191400	1.61107800
O	-2.27230700	-0.86992200	-4.81724300
O	-4.45182700	-0.50053400	-3.58389200
S	-3.10566200	-0.07019300	-3.92809000
C	-3.18212800	1.58379800	-4.54528800
C	-4.35373400	2.31885600	-4.40160700
C	-2.02786900	2.15197000	-5.08744400
C	-4.36715700	3.64678300	-4.81433800
H	-5.24050600	1.85718600	-3.97444700
C	-2.06093400	3.47831900	-5.48708600
H	-1.12151500	1.56101500	-5.20276900
C	-3.22750000	4.24451200	-5.35579600
H	-5.27989900	4.23134000	-4.71399400
H	-1.17013500	3.93472100	-5.91642700
C	-3.23917000	5.67413300	-5.79577300
H	-2.47734300	6.25708500	-5.26404100
H	-3.01134600	5.75833300	-6.86546300
H	-4.21246800	6.14245700	-5.61943800
Au	-0.33696400	0.77883600	0.49660400
P	-0.38234800	1.26885200	2.81347300

C	1.41047400	-0.24131600	-1.74549600
H	2.09556800	0.61089900	-1.72077500
H	1.57303900	-0.79475600	-2.68168800
C	-1.87840700	2.08537100	3.47443800
C	-2.18315500	3.36016000	2.98189600
C	-2.71841500	1.49058100	4.41689300
C	-3.30829100	4.03567900	3.43682200
H	-1.53274500	3.82393700	2.23846900
C	-3.85197200	2.16769500	4.86291700
H	-2.48869600	0.50192800	4.81131000
C	-4.14621500	3.43805800	4.37805300
H	-3.53603000	5.02766200	3.05285200
H	-4.50246100	1.70074000	5.59893000
H	-5.02926400	3.96490400	4.73229500
C	0.96626900	2.38350200	3.32287400
C	1.05064100	2.88091100	4.62963800
C	1.88802400	2.81095200	2.36254100
C	2.05842000	3.77465400	4.97086700
H	0.31901500	2.57806000	5.37837100
C	2.87904600	3.72830200	2.70181700
H	1.81868800	2.42632800	1.34351600
C	2.96669300	4.20559000	4.00518700
H	2.12481400	4.15082200	5.98904800
H	3.58719000	4.06439300	1.94735300
H	3.74620600	4.91556600	4.27285500
C	-0.23338500	-0.29251900	3.74602200
C	0.57419400	-0.44389300	4.87416900
C	-0.99672000	-1.37794200	3.29326100
C	0.61763000	-1.66654800	5.54050100
H	1.18643800	0.38525400	5.22448900

C	-0.96317000	-2.59068600	3.97109400
H	-1.62146800	-1.26765100	2.40461600
C	-0.15339700	-2.73579400	5.09620800
H	1.26030600	-1.78210200	6.41146900
H	-1.56240000	-3.42704400	3.61717000
H	-0.11220600	-3.69052300	5.61719000

Electronic Energy (0K) = -3161.8123145

Electronic Energy (0K) + ZPE = -3160.994763

Enthalpy (298K) = -3160.940311

Free Energy (298K) = -3161.085609