

## *Supplementary Material*

### **Unveiling the mechanisms of gold/copper bimetallic catalysis in the synthesis of complex heterocyclic compounds**

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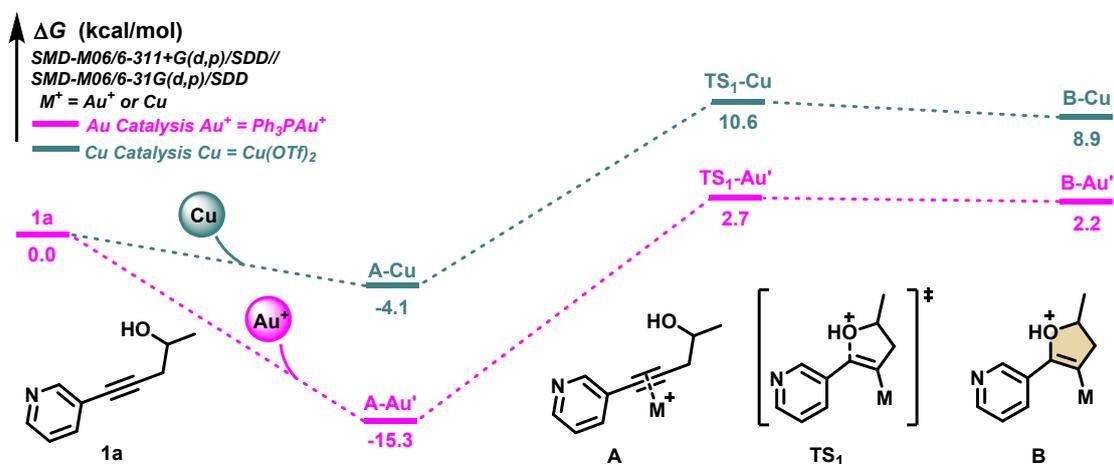
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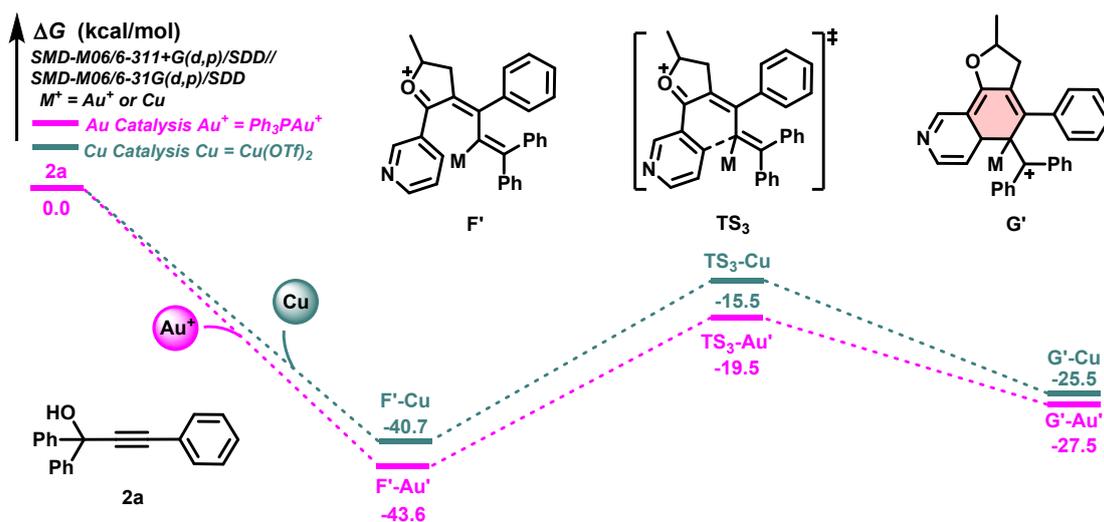
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To verify the validity of the simplified ligand model (CH<sub>3</sub>)<sub>3</sub>P, we conducted additional calculations for the key reaction steps—specifically, the *5-endo-dig* cyclization in the first cycle and the initial cyclization in the second cycle—using the PPh<sub>3</sub> ligand. As illustrated in the Figure S1-S2, the results demonstrate that the free energy profile for the gold-catalyzed pathway remains consistently lower than that of the copper-catalyzed pathway, indicating the gold-catalyzed pathway is energetically more favorable. This finding is fully consistent with the conclusions drawn from our initial calculations using the simplified (CH<sub>3</sub>)<sub>3</sub>P ligand, thereby validating the reliability of the mechanistic analysis based on the simplified (CH<sub>3</sub>)<sub>3</sub>P ligand model.



**Figure S1.** Reaction free energy profile for the PPh<sub>3</sub>Au<sup>+</sup>/Cu(OTf)<sub>2</sub>-catalyzed *5-endo-dig* cyclization.



**Figure S2.** Reaction free energy profile for the PPh<sub>3</sub>Au<sup>+</sup>/Cu(OTf)<sub>2</sub>-catalyzed cyclization from intermediate F' to G'.

## Cartesian Coordinates and Thermochemical Data (Energies in Hartree)

1a

Number of imaginary frequencies: 0

C	2.02969800	1.10555800	-0.03620500
C	2.48353600	-1.24566400	0.02471800
C	3.82934800	-0.92605200	0.11421900
C	4.19626800	0.41565700	0.12427100
N	3.31800400	1.41872200	0.05107000
H	2.14828700	-2.28028800	0.01350900
H	1.31950200	1.93168100	-0.09759900
H	4.58643800	-1.70325700	0.17563900
H	5.24760000	0.69691300	0.19428400
C	1.54373400	-0.21141500	-0.05383700
C	0.14639700	-0.46837100	-0.14915400
C	-1.04457500	-0.67438500	-0.23639100
C	-2.47479500	-0.92077600	-0.32372000
H	-2.71301600	-1.89701200	0.12115200
H	-2.78398700	-0.97060700	-1.37913900
O	-3.07857000	1.35308700	-0.35160400
H	-3.57450800	2.05634200	0.08089500
C	-3.31645900	0.15418900	0.35714300
C	-4.78589900	-0.21558400	0.33759200
H	-2.97303900	0.24844000	1.40372700
H	-5.39300200	0.57233000	0.80013200
H	-5.12958700	-0.34419600	-0.69650800
H	-4.97566800	-1.14503900	0.88742100

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

Electronic Energy (0 K) = -517.233093

Electronic Energy (0 K) + ZPE = -517.045679

Enthalpy (298 K) = -517.032999

Free Energy (298 K) = -517.085210

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

Electronic Energy (0 K) = -517.366899

### (CH<sub>3</sub>)<sub>3</sub>PAu<sup>+</sup>

Number of imaginary frequencies: 0

Au	0.95498000	-0.00004100	-0.00021000
P	-1.33529500	-0.00000800	-0.00042600
C	-2.00643200	1.46227800	-0.82813400
C	-2.00367700	-0.01294800	1.68121900
C	-2.00737800	-1.44921600	-0.85063200
H	-1.66808900	-1.46326600	-1.89096400
H	-1.67030200	-2.36391600	-0.35420100

H	-3.10346500	-1.40584200	-0.82716800
H	-1.66757000	0.87619800	2.22341200
H	-1.66056900	-0.90515000	2.21385600
H	-3.10001500	-0.01621600	1.63635800
H	-1.67293200	1.48687000	-1.87019000
H	-1.66359300	2.36992600	-0.32276000
H	-3.10253200	1.42406500	-0.80007900

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

Electronic Energy (0 K) = -596.575090

Electronic Energy (0 K) + ZPE = -596.459507

Enthalpy (298 K) = -596.450653

Free Energy (298 K) = -596.493132

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

Electronic Energy (0 K) = -596.624090

**A-Au**

Number of imaginary frequencies: 0

C	3.09419600	2.01568100	0.25157100
C	0.86959300	2.68857200	-0.36918400
C	1.31056700	4.00021300	-0.31107300
C	2.63968300	4.23921200	0.02756300
N	3.51681600	3.27129000	0.30412700
H	-0.16140700	2.44522200	-0.63049900
H	3.81347300	1.22852100	0.48247800
H	0.64070500	4.82699300	-0.52788400
H	3.01592500	5.26048900	0.07971100
C	1.77657400	1.66405100	-0.08357200
C	1.44268700	0.27141300	-0.11930500
C	1.44452100	-0.96446600	-0.10039300
C	1.73654300	-2.39595600	-0.09885400
H	1.17128200	-2.90740000	-0.88823300
H	1.43444100	-2.83428200	0.86345200
O	3.88326800	-1.90730500	0.72022100
H	4.83101800	-2.07074100	0.65363000
C	3.23534400	-2.63238100	-0.30216500
C	3.55067500	-4.11103100	-0.23753500
H	3.51149000	-2.23368600	-1.29500300
H	4.62409100	-4.28229600	-0.38037900
H	3.26854700	-4.51685600	0.74149100
H	3.02123100	-4.66959500	-1.01785600
Au	-0.77247300	-0.30739100	-0.03766500
P	-3.09300400	-0.11732600	0.09688000
C	-3.62491300	1.56620300	-0.33679400
C	-3.77679900	-0.42511400	1.75103900

C	-4.01250300	-1.21538600	-1.02068300
H	-3.71148800	-1.02955600	-2.05650200
H	-3.80168900	-2.26130500	-0.77595400
H	-5.08888600	-1.03175500	-0.91850800
H	-3.31992000	0.25758800	2.47441300
H	-3.56546600	-1.45417700	2.05814400
H	-4.86181100	-0.26602200	1.74026800
H	-3.29379400	1.81317900	-1.35093300
H	-3.18992100	2.28629100	0.36432000
H	-4.71828900	1.63652900	-0.28813900

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

Electronic Energy (0 K) = -1113.861092

Electronic Energy (0 K) + ZPE = -1113.557702

Enthalpy (298 K) = -1113.535100

Free Energy (298 K) = -1113.610601

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

Electronic Energy (0 K) = -1114.036556

**TS<sub>1</sub>-Au**

Number of imaginary frequencies: 1

C	3.38351500	1.52325100	0.92995400
C	2.01723900	2.04008100	-0.98193700
C	2.50191300	3.33541500	-0.90584700
C	3.42267000	3.64274100	0.09264100
N	3.86446300	2.75775400	0.99009200
H	1.30892200	1.74097300	-1.75211600
H	3.74763500	0.81145000	1.67267300
H	2.18528300	4.09460300	-1.61465700
H	3.82591100	4.65191500	0.17293800
C	2.45356600	1.10463400	-0.03427500
C	1.94153300	-0.23509500	-0.04779600
C	0.98017000	-1.10068200	-0.08147900
C	1.37822200	-2.54521000	-0.05876800
H	0.77289600	-3.16530600	-0.72818600
H	1.22430400	-2.93796300	0.95742600
O	3.41374500	-1.36783900	0.05786200
H	4.13645000	-1.06294800	-0.51425100
C	2.85375800	-2.61682200	-0.44759600
C	3.59463800	-3.78442400	0.14579200
H	2.94127100	-2.59217100	-1.54294100
H	4.64211200	-3.80511100	-0.17023200
H	3.55838000	-3.74420700	1.24023700
H	3.12628000	-4.71981400	-0.17993000
Au	-0.98482800	-0.36217200	-0.02028300

P	-3.20949800	0.38283700	0.09341800
C	-3.50687200	1.99613800	-0.69636400
C	-3.83919800	0.58844500	1.78924300
C	-4.40584300	-0.73682100	-0.70024400
H	-4.16313600	-0.84973300	-1.76187900
H	-4.36470300	-1.72310900	-0.22712000
H	-5.42144400	-0.33431900	-0.60365700
H	-3.22007300	1.31181700	2.32962300
H	-3.79852400	-0.36820600	2.32002900
H	-4.87588600	0.94539700	1.76789600
H	-3.24012500	1.94672100	-1.75705800
H	-2.89083100	2.76368800	-0.21678800
H	-4.56390000	2.27385900	-0.60437000

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

Electronic Energy (0 K) = -1113.844098

Electronic Energy (0 K) + ZPE = -1113.540803

Enthalpy (298 K) = -1113.519434

Free Energy (298 K) = -1113.592029

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

Electronic Energy (0 K) = -1114.013295

#### **B-Au**

Number of imaginary frequencies: 0

C	3.60775000	1.61564000	0.47754300
C	1.48941100	2.06782700	-0.54131700
C	1.79910000	3.41329600	-0.45987900
C	3.02736700	3.78536600	0.08441700
N	3.91736900	2.90737900	0.54278300
H	0.54862800	1.72965100	-0.97618400
H	4.34807000	0.92952100	0.89425200
H	1.10879100	4.16784500	-0.82642800
H	3.30420200	4.83730400	0.15033600
C	2.40877300	1.12690900	-0.05767400
C	2.10365600	-0.29152500	-0.10929900
C	1.03972900	-1.08288100	-0.12801400
C	1.45762000	-2.52928400	-0.11982300
H	0.90868100	-3.12742800	-0.85553500
H	1.24635400	-2.97033700	0.86567400
O	3.36740800	-1.14288500	-0.06867900
H	4.04884000	-0.80482900	-0.68262800
C	2.95039400	-2.56512900	-0.41453200
C	3.78058000	-3.49828300	0.40964000
H	3.14450800	-2.65118600	-1.48994300
H	4.84700600	-3.42923500	0.17560300

H	3.63130300	-3.30372800	1.47706800
H	3.45739100	-4.52438300	0.20222100
Au	-0.93198100	-0.43528600	-0.03048800
P	-3.16538200	0.30530100	0.10156600
C	-3.42665100	1.93972300	-0.66208300
C	-3.80321700	0.50165500	1.79640900
C	-4.38839000	-0.77032700	-0.71389200
H	-4.14423200	-0.87258500	-1.77632100
H	-4.37286900	-1.76507200	-0.25698500
H	-5.39474200	-0.34565800	-0.61481100
H	-3.17057000	1.20248900	2.35081000
H	-3.78710800	-0.46275400	2.31422200
H	-4.83151200	0.88235500	1.77488700
H	-3.16807500	1.89829600	-1.72546900
H	-2.78192600	2.67987300	-0.17577300
H	-4.47309100	2.25143400	-0.55894900

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

Electronic Energy (0 K) = -1113.849481

Electronic Energy (0 K) + ZPE = -1113.543638

Enthalpy (298 K) = -1113.522508

Free Energy (298 K) = -1113.594267

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

Electronic Energy (0 K) = -1114.017088

**C**

Number of imaginary frequencies: 0

C	1.43029300	-1.13046000	-0.20099000
C	0.87375300	0.14652000	-0.06679500
C	1.75269300	1.20821400	0.16631000
C	3.11013300	0.95323500	0.26111500
C	3.55255300	-0.35906600	0.11337000
N	2.73509000	-1.38653300	-0.11513600
H	1.37268800	2.22336600	0.26546500
H	0.77470200	-1.98049900	-0.38622800
H	3.81999000	1.75599200	0.44169800
H	4.61647200	-0.59006600	0.18019300
C	-0.56772600	0.34866300	-0.16768500
C	-1.30776400	1.44776000	0.03640800
C	-2.74148100	1.12455100	-0.25495400
C	-2.69455600	-0.40916700	-0.35930300
H	-3.43156300	1.44302500	0.53891500
H	-3.08733900	1.60030800	-1.18470100
H	-3.21426900	-0.78604000	-1.24788700
C	-3.19658900	-1.09766000	0.88771800

H	-4.26857500	-0.91263500	1.02435400
H	-3.03545800	-2.17922200	0.83304500
H	-2.66650600	-0.71207300	1.76821900
O	-1.29486400	-0.74674500	-0.53075600
H	-0.93471800	2.42200300	0.32777000

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

Electronic Energy (0 K) = -517.279454

Electronic Energy (0 K) + ZPE = -517.089454

Enthalpy (298 K) = -517.078416

Free Energy (298 K) = -517.125942

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

Electronic Energy (0 K) = -517.403251

**Cu(OTf)<sub>2</sub>**

Number of imaginary frequencies: 0

O	1.57241900	0.72284900	1.21039600
Cu	-0.00002800	0.78674800	0.00003400
S	2.53835000	0.68044800	0.04194800
C	3.06974900	-1.08490600	-0.03676900
F	3.82655200	-1.24951300	-1.09937600
F	1.99465900	-1.85042000	-0.12304500
F	3.74032800	-1.37224600	1.05732300
O	3.72383000	1.49369100	0.10340000
O	1.61446100	0.84151400	-1.15028400
O	-1.61445700	0.84151500	1.15030400
S	-2.53833500	0.68044100	-0.04197400
O	-3.72389400	1.49360200	-0.10345500
O	-1.57241800	0.72284900	-1.21040000
C	-3.06973200	-1.08491800	0.03679000
F	-1.99462700	-1.85046100	0.12260600
F	-3.82617600	-1.24961900	1.09960600
F	-3.74063200	-1.37209000	-1.05715600

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

Electronic Energy (0 K) = -2119.813572

Electronic Energy (0 K) + ZPE = -2119.753260

Enthalpy (298 K) = -2119.735540

Free Energy (298 K) = -2119.801349

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

Electronic Energy (0 K) = -2120.168644

**A-Cu**

Number of imaginary frequencies: 0

O	-1.64996400	-0.16810200	1.32401200
Cu	-0.37873900	-0.10157000	-0.24775700

S	-2.37621900	-1.38680400	0.78896400
C	-3.87218000	-0.65376100	0.00421900
F	-4.55240200	-1.59712600	-0.61105500
F	-3.48760600	0.26501100	-0.87517500
F	-4.61668200	-0.08646200	0.93266900
O	-2.83013100	-2.36411100	1.74789400
O	-1.53973400	-1.83624800	-0.37120200
O	2.71765000	0.42728300	-1.48288100
S	1.88016400	-0.53201100	-2.18959900
O	0.38341200	-0.27691100	-1.98232100
O	2.15714000	-0.85027000	-3.57539900
C	2.08322700	-2.10122400	-1.25132100
F	3.35065100	-2.46408400	-1.25197100
F	1.69585500	-1.90363400	0.02078300
F	1.34101000	-3.05776700	-1.77180700
C	2.88438100	0.41393200	1.83268400
C	0.95804500	0.64072100	3.27779600
C	1.70970900	0.04325900	4.27317500
C	3.01956200	-0.33262600	3.98062100
N	3.60187000	-0.15560600	2.79105500
H	-0.07057700	0.94978700	3.44489100
H	3.35015400	0.54669800	0.85506900
H	1.29492700	-0.13329000	5.26093100
H	3.63243500	-0.80567300	4.74808900
C	1.55407000	0.83608900	2.02250100
C	0.85115200	1.44308600	0.95233700
C	0.24409500	1.91721200	-0.00913900
C	-0.29198300	2.80138100	-1.04491000
H	-1.25374700	2.42867700	-1.42285500
H	0.41150100	2.80189600	-1.89059300
O	0.80059000	4.62588100	-0.05074200
H	0.73326200	5.53314800	0.26643700
C	-0.46608500	4.22750500	-0.52361500
C	-0.97158700	5.13577300	-1.62440600
H	-1.19943500	4.20141700	0.30351700
H	-1.09336100	6.16014400	-1.25223600
H	-0.25707700	5.15729700	-2.45599100
H	-1.94439600	4.80400100	-2.00508000

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

Electronic Energy (0 K) = -2637.074732

Electronic Energy (0 K) + ZPE = -2636.826052

Enthalpy (298 K) = -2636.794690

Free Energy (298 K) = -2636.891575

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

Electronic Energy (0 K) = -2637.565061

**TS<sub>1</sub>-Cu**

Number of imaginary frequencies: 1

O	-1.78383800	-1.38190300	-0.12267900
Cu	-0.64150500	0.21898000	0.52473000
S	-2.84882400	-0.47710400	-0.69650700
C	-4.19979700	-0.57654200	0.54755100
F	-5.16056700	0.26365700	0.21905800
F	-3.71962700	-0.25619900	1.74203600
F	-4.67077300	-1.80951500	0.58185900
O	-3.42631600	-0.85307900	-1.96636500
O	-2.30516700	0.90888700	-0.53432800
O	2.43772600	1.71862300	0.54078100
S	1.26200900	2.54368600	0.28855200
O	-0.00563600	1.99980000	0.93902600
O	1.35630200	3.98218900	0.44912300
C	0.89546200	2.26414400	-1.49282100
F	1.92387800	2.64222000	-2.22862300
F	0.68312300	0.95283600	-1.70451600
F	-0.18329300	2.92754200	-1.85998000
C	3.31580700	-1.68585900	-0.95735600
C	1.10928100	-2.52868700	-1.43648300
C	1.57908500	-2.86855700	-2.69562900
C	2.91131600	-2.60853900	-3.00012500
N	3.77145800	-2.03558400	-2.15201300
H	0.07722500	-2.71050700	-1.14281900
H	4.01847300	-1.20690700	-0.27332400
H	0.92709000	-3.33459300	-3.42841300
H	3.30881900	-2.87393900	-3.97977000
C	1.99424800	-1.91424000	-0.54219000
C	1.54076400	-1.46946500	0.74138300
C	0.73487000	-0.78628200	1.48212200
C	0.97982000	-0.74115500	2.95202700
H	0.23334800	-1.35315700	3.47585900
H	0.88260700	0.28108600	3.33920500
O	2.72121600	-2.11642900	2.00871000
H	2.41389500	-3.02131200	2.18442200
C	2.41573600	-1.25606700	3.15564100
C	3.44484000	-0.15952700	3.14974500
H	2.49531700	-1.88571200	4.04913400
H	4.45701500	-0.57261300	3.19501100
H	3.34445900	0.45805800	2.24864600
H	3.29667500	0.48803600	4.02040700

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

Electronic Energy (0 K) = -2637.059695

Electronic Energy (0 K) + ZPE = -2636.809935

Enthalpy (298 K) = -2636.780259

Free Energy (298 K) = -2636.872291

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

Electronic Energy (0 K) = -2637.545876

**B-Cu**

Number of imaginary frequencies: 0

O	-1.80709900	-1.55067400	0.23014700
Cu	-0.62183800	0.19363500	0.41343300
S	-2.86480300	-0.79913100	-0.53511600
C	-4.19328800	-0.54612900	0.71069000
F	-5.14656200	0.20091300	0.18993400
F	-3.68716400	0.06064600	1.77633900
F	-4.68509000	-1.71851500	1.06816300
O	-3.47651700	-1.46764100	-1.66151000
O	-2.29975700	0.57374700	-0.74395800
O	2.28891200	2.02505200	0.31219400
S	1.05445700	2.67613900	-0.11588800
O	-0.18727100	2.09484000	0.54133700
O	1.00398500	4.12575800	-0.16146600
C	0.82203500	2.11816300	-1.85224400
F	1.84801300	2.49865700	-2.59184100
F	0.74869300	0.77793700	-1.88645700
F	-0.29490500	2.61024700	-2.35357900
C	3.51033600	-2.30551600	-0.50716500
C	1.18866500	-2.41195800	-1.09154000
C	1.56885700	-3.06537800	-2.25101000
C	2.92190700	-3.31561400	-2.46436400
N	3.87797800	-2.95143900	-1.60963600
H	0.13749100	-2.23359800	-0.86971300
H	4.31505500	-1.99919000	0.16232900
H	0.82654200	-3.39244100	-2.97329600
H	3.24919300	-3.83793800	-3.36338300
C	2.17951700	-2.00441900	-0.18975600
C	1.81764600	-1.28248800	1.01558200
C	0.85359300	-0.49141300	1.45477000
C	1.08998700	-0.03698900	2.86414800
H	0.36371100	-0.49768500	3.54640200
H	0.96775900	1.05013300	2.94865500
O	2.87853400	-1.43064100	2.09932900
H	2.88893400	-2.34840900	2.43445900

C	2.52926100	-0.42367500	3.19644600
C	3.52950700	0.68376500	3.07501700
H	2.63472200	-0.99740000	4.12216700
H	4.55377500	0.31712400	3.18889300
H	3.41943900	1.19715600	2.11228500
H	3.33505700	1.41217100	3.87011600

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

Electronic Energy (0 K) = -2637.064226

Electronic Energy (0 K) + ZPE = -2636.813078

Enthalpy (298 K) = -2636.783164

Free Energy (298 K) = -2636.876091

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

Electronic Energy (0 K) = -2637.549435

**2a**

Number of imaginary frequencies: 0

C	1.66993400	-0.07890600	0.35972300
C	0.47912700	-0.08462500	0.58230600
C	-0.96784600	-0.04234000	0.82988200
C	3.07306700	-0.07405300	0.10230100
C	3.98702200	-0.25159700	1.15067800
C	3.55272200	0.10766200	-1.20259100
C	5.35117300	-0.24629100	0.89441300
H	3.61174800	-0.39115700	2.16188500
C	4.91850600	0.10955800	-1.44991400
H	2.84157100	0.24763800	-2.01360600
C	5.82048000	-0.06690900	-0.40411600
H	6.05323500	-0.38345900	1.71370500
H	5.28183300	0.25083200	-2.46530600
H	6.89008900	-0.06407600	-0.60111900
O	-1.13187100	-0.09191100	2.24336700
H	-2.05174100	-0.33514500	2.41057600
C	-1.49368900	1.27634300	0.25074700
C	-1.49616300	1.47173800	-1.13229200
C	-1.95172400	2.29056200	1.08458800
C	-1.96045500	2.66321800	-1.67163200
H	-1.13173200	0.67950500	-1.78608300
C	-2.42159100	3.48517400	0.54205500
H	-1.92801900	2.14282400	2.16106800
C	-2.42857700	3.67430500	-0.83407200
H	-1.95959700	2.80505300	-2.75024700
H	-2.77980500	4.27177600	1.20295000
H	-2.79473800	4.60736700	-1.25665900
C	-1.69230100	-1.24084600	0.21193900

C	-3.08391500	-1.19531700	0.08690600
C	-1.01961500	-2.41066200	-0.13397000
C	-3.78827500	-2.30123300	-0.37335500
H	-3.61897700	-0.27979400	0.34011700
C	-1.72410200	-3.51514700	-0.60293700
H	0.06331800	-2.45335400	-0.03677800
C	-3.10850700	-3.46453000	-0.72280900
H	-4.87069700	-2.25068000	-0.46854100
H	-1.18561600	-4.42032000	-0.87509800
H	-3.65753600	-4.32834200	-1.09091100

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

Electronic Energy (0 K) = -884.369729

Electronic Energy (0 K) + ZPE = -884.065830

Enthalpy (298 K) = -884.046500

Free Energy (298 K) = -884.115990

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

Electronic Energy (0 K) = -884.584804

**D-Au**

Number of imaginary frequencies: 0

C	-1.60391900	1.07768300	-0.66790800
C	-0.37757600	1.20600400	-0.74661600
C	0.97697100	1.80563100	-0.93783600
Au	-0.40277700	-0.83307000	0.19709100
P	0.38885500	-2.84282700	1.05073100
C	-0.56484100	-4.32573900	0.61565600
C	0.55297100	-2.87679700	2.85954100
C	2.06788300	-3.12698500	0.41132000
H	2.05223500	-3.14424700	-0.68455600
H	2.72423500	-2.30981000	0.73227600
H	2.46315800	-4.07824200	0.78815100
H	-0.42973800	-2.75534100	3.32595800
H	1.19850300	-2.05347800	3.18514300
H	0.99236600	-3.82873400	3.18051100
H	-0.63925300	-4.40946900	-0.47307300
H	-1.57499700	-4.25458800	1.03121100
H	-0.06975800	-5.21939700	1.01436100
C	-3.02475700	0.96164500	-0.60130900
C	-3.68236400	1.10580700	0.63068400
C	-3.76060300	0.72116100	-1.77091700
C	-5.06442500	1.01124700	0.68424300
H	-3.09846900	1.29956100	1.52829500
C	-5.14328200	0.63468600	-1.70392000
H	-3.23852400	0.61613300	-2.71892400

C	-5.79320300	0.77742800	-0.48032500
H	-5.57779200	1.12660500	1.63499800
H	-5.71706100	0.45570600	-2.60926100
H	-6.87716000	0.70886600	-0.43378100
O	0.78696700	2.78068700	-1.94676400
H	1.66336000	3.03746800	-2.26568100
C	1.35387500	2.43773200	0.40780600
C	1.67156600	1.64202700	1.51361200
C	1.32674000	3.82119400	0.55436100
C	1.96567400	2.22338300	2.73999400
H	1.70441100	0.55552400	1.41135100
C	1.62647300	4.40377700	1.78385200
H	1.06008300	4.44179100	-0.29646900
C	1.94515300	3.60962000	2.87776700
H	2.21918200	1.59381200	3.59019800
H	1.60487500	5.48625600	1.88299200
H	2.17802300	4.06595400	3.83674200
C	1.97972600	0.76274800	-1.43737000
C	3.31758100	0.78022800	-1.04366600
C	1.57012100	-0.16078200	-2.40587300
C	4.21976800	-0.13744900	-1.57853500
H	3.66319500	1.50818900	-0.31299200
C	2.46869100	-1.07879200	-2.93506700
H	0.53878700	-0.14849000	-2.75748600
C	3.79734800	-1.07399500	-2.51472700
H	5.25920100	-0.11413900	-1.26027300
H	2.13443600	-1.78964000	-3.68721800
H	4.50407500	-1.78964000	-2.92811500

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

Electronic Energy (0 K) = -1481.006306

Electronic Energy (0 K) + ZPE = -1480.585867

Enthalpy (298 K) = -1480.556977

Free Energy (298 K) = -1480.645962

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

Electronic Energy (0 K) = -1481.261196

**TS<sub>2</sub>-Au**

Number of imaginary frequencies: 1

C	0.99561100	-0.16141400	-0.21323600
C	-0.03119600	0.50136900	0.16799400
C	-0.35325600	1.90633500	0.64061800
Au	-1.70773600	-0.83116900	-0.10962400
P	-3.67151400	-2.06862500	-0.33299300
C	-3.47452400	-3.86094700	-0.57560000

C	-4.71980900	-1.52144900	-1.71673800
C	-4.74467600	-1.90240600	1.12695500
H	-4.21746300	-2.25345800	2.02030800
H	-4.99476200	-0.84446500	1.26677000
H	-5.66690500	-2.48147500	0.99539100
H	-4.19397300	-1.66392400	-2.66609300
H	-4.94540800	-0.45557800	-1.59973300
H	-5.65775400	-2.08982800	-1.73360900
H	-2.92230500	-4.28994600	0.26659400
H	-2.90905900	-4.05097700	-1.49353700
H	-4.45660100	-4.34367700	-0.64840300
C	1.50052300	-1.32332600	-0.89867200
C	1.21933400	-1.46347600	-2.26887900
C	2.22251400	-2.32683000	-0.23673000
C	1.64496200	-2.59249900	-2.95687800
H	0.65025800	-0.68384800	-2.77412100
C	2.65385600	-3.44573400	-0.93495800
H	2.42921000	-2.22735200	0.82671800
C	2.36661100	-3.58091300	-2.29190700
H	1.41766500	-2.69909900	-4.01477100
H	3.21120600	-4.22172900	-0.41662100
H	2.70410900	-4.46223600	-2.83172700
O	0.55635100	2.20949900	1.69494900
H	0.17095100	2.92238600	2.22191400
C	-0.15938800	2.85453700	-0.54436400
C	-0.61435500	2.50359100	-1.81946500
C	0.46292100	4.08909500	-0.37118800
C	-0.44902000	3.36779200	-2.89485600
H	-1.10179800	1.53958100	-1.97023900
C	0.63205400	4.95443200	-1.44943800
H	0.84128900	4.37664400	0.60666800
C	0.17813700	4.59762100	-2.71326000
H	-0.80921800	3.07804600	-3.87955400
H	1.12534000	5.91150800	-1.29645400
H	0.31186800	5.27387700	-3.55401300
C	-1.77665700	1.94897400	1.21185700
C	-2.84047700	2.58085000	0.57093200
C	-2.01303700	1.28227100	2.42169900
C	-4.12222400	2.52891900	1.11783500
H	-2.67690900	3.11895300	-0.35989300
C	-3.28870000	1.23576700	2.96812700
H	-1.18490800	0.78880300	2.92864200
C	-4.35093500	1.85785600	2.31369600
H	-4.94105200	3.03362300	0.61010900

H	-3.45440900	0.71708900	3.90989800
H	-5.34996300	1.82975000	2.74308300
C	4.97245900	-1.03745100	2.00045700
C	3.94310600	-0.13552500	1.70130700
C	3.07573200	0.23766200	2.73496700
C	3.28348500	-0.29022900	3.99743500
C	4.33982900	-1.17994900	4.18401400
N	5.17089600	-1.55421700	3.21001200
H	2.24969600	0.92115400	2.54199300
H	5.65906400	-1.34983600	1.21416600
H	2.63766900	-0.02416800	4.82942800
H	4.52122500	-1.61498300	5.16722900
C	3.77499900	0.36581800	0.34700300
C	2.82770600	1.21711400	-0.16573800
C	3.16490800	1.45860100	-1.61337100
C	4.49856200	0.71749700	-1.77914700
H	2.40016600	1.05516200	-2.29674200
H	3.25943200	2.52641900	-1.84174700
H	5.34128800	1.42234200	-1.74280900
C	4.61831500	-0.18378300	-2.97480400
H	4.54631700	0.40962400	-3.89309400
H	5.58005300	-0.70616400	-2.98233600
H	3.81427900	-0.92932100	-2.98000700
O	4.63327600	-0.09236800	-0.56420800
H	2.25773400	1.90026400	0.45174400

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

Electronic Energy (0 K) = -1998.290951

Electronic Energy (0 K) + ZPE = -1997.679698

Enthalpy (298 K) = -1997.639844

Free Energy (298 K) = -1997.754005

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

Electronic Energy (0 K) = -1998.663623

**E'-Au**

Number of imaginary frequencies: 0

C	1.23259900	-0.05099200	-0.28862900
C	0.03692600	0.45589100	0.06735700
C	-0.14355600	1.91484800	0.52133500
Au	-1.70850300	-0.71036100	-0.06618000
P	-3.73846500	-1.89725900	-0.13217700
C	-3.63238100	-3.68126600	-0.49512900
C	-4.93116300	-1.26432400	-1.35835600
C	-4.66335200	-1.82101000	1.43841600
H	-4.05912000	-2.25390400	2.24293400

H	-4.86594800	-0.77287700	1.68800900
H	-5.61116400	-2.36808600	1.36172800
H	-4.51006900	-1.35258500	-2.36537000
H	-5.12686400	-0.20490200	-1.15760600
H	-5.87446900	-1.82229700	-1.31162700
H	-3.01624500	-4.17353200	0.26466700
H	-3.15704700	-3.83042400	-1.47059600
H	-4.62974900	-4.13761000	-0.50320600
C	1.33746500	-1.41590200	-0.88527800
C	0.78951300	-1.65215600	-2.15393300
C	1.98684700	-2.47196900	-0.23792500
C	0.88719600	-2.90244200	-2.75525100
H	0.27737500	-0.83650000	-2.66453700
C	2.08222600	-3.72628300	-0.83679800
H	2.39266200	-2.32745000	0.76237100
C	1.53662000	-3.94438100	-2.09755200
H	0.45838900	-3.06168700	-3.74232200
H	2.57937700	-4.53783100	-0.31019400
H	1.61562200	-4.92284900	-2.56529900
O	0.81720500	2.18481700	1.55635500
H	0.51511200	2.96269900	2.04401600
C	0.10373100	2.82653000	-0.68168400
C	-0.49166800	2.54628800	-1.91873900
C	0.94064700	3.93808400	-0.58624800
C	-0.24918400	3.35171500	-3.02449800
H	-1.15221300	1.68449000	-2.01186900
C	1.18633500	4.74554900	-1.69559600
H	1.42454600	4.17156600	0.35937100
C	0.59546700	4.45447800	-2.91880600
H	-0.72296900	3.11708800	-3.97531100
H	1.84421600	5.60639100	-1.59794500
H	0.78794100	5.08313500	-3.78496100
C	-1.53315000	2.10300800	1.13600600
C	-2.55135400	2.84442700	0.54056300
C	-1.79927800	1.45055600	2.34790500
C	-3.81769500	2.90394600	1.12232500
H	-2.36843300	3.37766300	-0.38927700
C	-3.05734800	1.51387900	2.93115900
H	-1.00824600	0.87206500	2.82350200
C	-4.07736100	2.23644900	2.31287200
H	-4.59994500	3.48833600	0.64282700
H	-3.24449400	0.99800800	3.87085600
H	-5.06424800	2.28959300	2.76738800
C	5.08918900	-0.93168700	2.00901900

C	3.91448300	-0.26170800	1.61509000
C	2.95836700	0.05254300	2.59574400
C	3.22497400	-0.31102300	3.90282700
C	4.41810000	-0.97461000	4.18151700
N	5.33858600	-1.28316700	3.25976000
H	2.04199200	0.58001900	2.33199900
H	5.84472400	-1.18679400	1.26598500
H	2.52407400	-0.08729100	4.70096200
H	4.64819400	-1.27495400	5.20357500
C	3.71242600	0.09622400	0.23851000
C	2.53478900	0.76861300	-0.36011100
C	2.99959800	1.05603800	-1.80525200
C	4.33730700	0.33985200	-1.96860000
H	2.27251900	0.68271700	-2.53351800
H	3.10041900	2.13428100	-1.96191000
H	5.16129300	1.02483200	-2.19351500
C	4.36047400	-0.85342400	-2.88237400
H	4.16632600	-0.51514900	-3.90586200
H	5.33800100	-1.34445500	-2.86795600
H	3.58801500	-1.58189800	-2.60904200
O	4.66078100	-0.13855700	-0.59181300
H	2.37844500	1.69526400	0.20868300

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

Electronic Energy (0 K) = -1998.328672

Electronic Energy (0 K) + ZPE = -1997.713946

Enthalpy (298 K) = -1997.674679

Free Energy (298 K) = -1997.787337

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

Electronic Energy (0 K) = -1998.698430

#### **H<sub>2</sub>O**

Number of imaginary frequencies: 0

O	0.00000000	0.00000000	0.11835500
H	0.00000000	0.75707000	-0.47342100
H	0.00000000	-0.75707000	-0.47342100

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

Electronic Energy (0 K) = -76.388567

Electronic Energy (0 K) + ZPE = -76.366873

Enthalpy (298 K) = -76.363093

Free Energy (298 K) = -76.384516

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

Electronic Energy (0 K) = -76.422456

#### **F'-Au**

Number of imaginary frequencies: 0

C	-2.47503500	0.56965900	3.21321100
C	-1.19369300	0.04138400	3.34254900
C	-0.15167900	0.65171000	2.66309600
C	-0.42806400	1.79172300	1.90522100
C	-1.74997400	2.25926500	1.87049900
N	-2.76028800	1.65555000	2.48743300
H	0.86113800	0.26059500	2.73308500
H	-3.31414400	0.09716400	3.72403800
H	-1.02094600	-0.83312200	3.96256100
H	-1.98780000	3.15063100	1.28755400
C	0.57090700	2.51180900	1.12582400
C	1.51799600	2.08071600	0.20042200
C	1.38419300	4.45035400	0.24303700
C	2.29204100	3.31719600	-0.21237900
H	0.69701700	4.75643800	-0.55843600
H	2.49260300	3.35949900	-1.28758500
H	3.26012200	3.38551600	0.30674000
O	0.51830100	3.82477800	1.25632900
C	2.06424800	5.63593300	0.86161000
H	2.69915400	6.12492400	0.11503800
H	1.33866000	6.36909300	1.22610500
H	2.69788200	5.32213900	1.69910000
C	1.61726700	0.79241200	-0.37142000
C	0.70233000	-0.28341300	-0.13617300
C	1.01855100	-1.52851800	0.30702200
C	2.64768600	0.54586500	-1.40017500
C	2.32350500	-0.18199300	-2.55516100
C	3.97109700	0.97552900	-1.22298400
C	3.29060600	-0.45190500	-3.51298700
H	1.29631300	-0.50638900	-2.70869900
C	4.94205900	0.67291300	-2.16648700
C	4.60272400	-0.03105500	-3.31856100
H	3.01996600	-0.99762200	-4.41337600
H	5.96978900	0.98554200	-1.99998800
H	5.36254000	-0.25294800	-4.06376900
C	2.31964500	-1.88071700	0.91831600
C	3.12106100	-0.93702400	1.57774100
C	2.79956900	-3.19706800	0.82410900
C	4.36120300	-1.28535800	2.09865300
H	2.76876500	0.08617100	1.69526900
C	4.04227800	-3.54279500	1.33617600
H	2.19531200	-3.95223600	0.32567900
C	4.82881900	-2.58922500	1.97685400

H	4.95992700	-0.53538700	2.61105300
H	4.40004200	-4.56481500	1.23522700
H	5.79808500	-2.86390200	2.38577800
C	-0.01561100	-2.60043600	0.27246400
C	-0.64994800	-2.95465600	-0.92453700
C	-0.40519800	-3.24172000	1.45206500
C	-1.67021000	-3.90104200	-0.93448400
H	-0.32669300	-2.49071000	-1.85589000
C	-1.43581500	-4.17618000	1.44599300
H	0.10677600	-2.99711600	2.38259000
C	-2.07476400	-4.50469800	0.25345300
H	-2.13912200	-4.17947400	-1.87606600
H	-1.73448500	-4.65770100	2.37441700
H	-2.87142800	-5.24490500	0.24655100
Au	-1.33094600	0.09410400	-0.67252500
P	-3.62488800	0.33192700	-1.11679100
C	-4.26883600	2.02429700	-1.31287600
C	-4.64598700	-0.37186200	0.21691700
C	-4.17211700	-0.54594200	-2.61668200
H	-3.66667100	-0.13464800	-3.49665500
H	-3.90777800	-1.60585800	-2.52930500
H	-5.25733200	-0.45342300	-2.74557200
H	-4.52276000	0.24063800	1.11740100
H	-4.31627900	-1.39436900	0.43472000
H	-5.70387600	-0.38184700	-0.07290200
H	-3.75980700	2.52881400	-2.14044500
H	-4.09311400	2.58934100	-0.39097600
H	-5.34709200	1.99918600	-1.51333200
H	4.25374900	1.49965300	-0.31318600

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

Electronic Energy (0 K) = -1921.944379

Electronic Energy (0 K) + ZPE = -1921.357944

Enthalpy (298 K) = -1921.320040

Free Energy (298 K) = -1921.428669

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

Electronic Energy (0 K) = -1922.290578

#### **TS<sub>3</sub>-Au**

Number of imaginary frequencies: 1

C	2.37982700	-0.76922200	-2.75054700
C	1.05108700	-0.99821100	-2.55457800
C	0.17780100	0.08021500	-2.14328300
C	0.82659900	1.37947500	-2.12525300
C	2.22266000	1.46893000	-2.34666600

N	2.99813900	0.44589800	-2.62136400
H	-0.81887500	0.07415300	-2.59017600
H	3.02954800	-1.58955300	-3.05562600
H	0.64531900	-1.99209400	-2.72205700
H	2.69645700	2.44832100	-2.25176500
C	0.10995400	2.45710100	-1.59619100
C	-0.94249100	2.33082600	-0.65979900
C	-0.19873500	4.58087900	-0.81697200
C	-1.35543600	3.73053700	-0.28917600
H	0.52379500	4.79429900	-0.01664500
H	-1.50972500	3.86830500	0.78590200
H	-2.29354900	4.01278400	-0.79090100
O	0.51451000	3.71088700	-1.75858400
C	-0.59217500	5.83919500	-1.53614500
H	-1.10671500	6.51528600	-0.84475500
H	0.28303700	6.36051200	-1.93555500
H	-1.27284900	5.61050700	-2.36447400
C	-1.22007400	1.13797300	-0.00639100
C	-0.63682500	-0.14153000	-0.38519800
C	-1.37928800	-1.31696500	-0.40870500
C	-2.08708000	1.14941600	1.19804200
C	-1.72790900	0.48107900	2.37699300
C	-3.34067500	1.76925200	1.13646800
C	-2.59811600	0.43749300	3.45759400
H	-0.75177700	0.00013000	2.45097900
C	-4.21934800	1.70302100	2.21145000
C	-3.85084900	1.03950200	3.37585000
H	-2.29730000	-0.07435500	4.36872400
H	-5.19852400	2.16918200	2.13307900
H	-4.53651200	0.99170800	4.21825100
C	-2.84758600	-1.30713500	-0.53124400
C	-3.51064700	-0.37641200	-1.34466800
C	-3.61451100	-2.25278200	0.16671800
C	-4.89358100	-0.39760300	-1.46430500
H	-2.94169100	0.37263900	-1.89417400
C	-4.99934800	-2.24587400	0.07728100
H	-3.11326400	-2.98288600	0.79956600
C	-5.64257000	-1.32404200	-0.74449200
H	-5.38987300	0.31647500	-2.11733100
H	-5.57997400	-2.96885800	0.64495400
H	-6.72690100	-1.32836600	-0.82372300
C	-0.73531200	-2.63583300	-0.48969800
C	0.31572300	-3.02643100	0.35282900
C	-1.15389500	-3.53568200	-1.48685400

C	0.96998100	-4.23935600	0.16706300
H	0.58453100	-2.39327500	1.19899100
C	-0.48966400	-4.73787400	-1.68302700
H	-1.98168300	-3.26067300	-2.13817500
C	0.58108000	-5.08949100	-0.86275600
H	1.77300400	-4.52835400	0.84179100
H	-0.80800300	-5.40600900	-2.47938300
H	1.09527800	-6.03556400	-1.01310600
Au	1.33432200	-0.09830700	0.61979400
P	3.54637300	-0.06801300	1.36715000
C	4.28990300	1.57737000	1.58966900
C	4.62444300	-0.90256300	0.16187200
C	3.84002600	-0.93727700	2.93909200
H	3.29407900	-0.44166000	3.74827700
H	3.48019700	-1.96927000	2.85834400
H	4.91058700	-0.94605500	3.17711900
H	4.58575700	-0.36649000	-0.79478800
H	4.26951800	-1.92745800	0.00172100
H	5.65767100	-0.92823900	0.52946200
H	3.74654600	2.13392800	2.36005100
H	4.23351100	2.13338900	0.64738100
H	5.34150100	1.48148800	1.88650800
H	-3.65100900	2.26625000	0.21891300

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

Electronic Energy (0 K) = -1921.910436

Electronic Energy (0 K) + ZPE = -1921.323826

Enthalpy (298 K) = -1921.287226

Free Energy (298 K) = -1921.390905

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

Electronic Energy (0 K) = -1922.256721

**G'-Au**

Number of imaginary frequencies: 0

C	2.03069800	-1.99929800	-2.57312000
C	0.73775500	-1.72993400	-2.30530700
C	0.25382000	-0.33944900	-2.04629600
C	1.40140500	0.62579100	-2.16034000
C	2.71815600	0.17261000	-2.46555200
N	3.06420000	-1.06988800	-2.63079100
H	-0.49266900	-0.08309500	-2.82600400
H	2.32995500	-3.02428700	-2.78927200
H	0.01625300	-2.53939100	-2.35687600
H	3.50660500	0.92808500	-2.52685300
C	1.14003500	1.92375700	-1.81507100

C	-0.01451800	2.30305400	-1.06218000
C	1.57063800	4.05356600	-1.12548900
C	0.09477400	3.78096400	-0.83016900
H	2.15772000	3.98269300	-0.19614300
H	-0.19299000	4.09096500	0.17966600
H	-0.54283000	4.33439600	-1.53680500
O	2.00502400	2.93741400	-1.95836200
C	1.86447900	5.33628000	-1.84893300
H	1.56438600	6.19102100	-1.23291000
H	2.93201400	5.43198700	-2.06966200
H	1.30789600	5.37760800	-2.79253500
C	-0.81175400	1.36890100	-0.44692700
C	-0.63649100	-0.07072500	-0.74072400
C	-1.66740700	-0.98750700	-0.43876200
C	-1.71498000	1.83292900	0.64102300
C	-1.59104700	1.36687900	1.95530600
C	-2.70653100	2.77948600	0.36319900
C	-2.44805800	1.81391600	2.95384100
H	-0.80515100	0.64965900	2.20360300
C	-3.56991600	3.21979500	1.35920300
C	-3.44771800	2.73447000	2.65701400
H	-2.33257500	1.43994300	3.96862100
H	-4.34622900	3.94162100	1.11647700
H	-4.12424400	3.07806000	3.43572400
C	-3.06742700	-0.54728300	-0.33323100
C	-3.59985000	0.28110500	-1.33106300
C	-3.91347500	-1.03130300	0.67371700
C	-4.94745900	0.61203500	-1.32559200
H	-2.95152100	0.64947600	-2.12581900
C	-5.24724900	-0.65200400	0.70871500
H	-3.50751300	-1.69017300	1.44013100
C	-5.76860500	0.16093600	-0.29600800
H	-5.35692000	1.23069800	-2.12040000
H	-5.88949700	-1.00413100	1.51207600
H	-6.81976400	0.43834200	-0.27843500
C	-1.49933000	-2.44676100	-0.40970700
C	-0.50597400	-3.10816100	0.32798300
C	-2.37951400	-3.23056800	-1.18221000
C	-0.35045200	-4.48643700	0.24763600
H	0.12461600	-2.53887800	1.01265200
C	-2.20663500	-4.60178100	-1.28214900
H	-3.17114800	-2.74202900	-1.74646700
C	-1.18734000	-5.23457700	-0.57182600
H	0.42012600	-4.97746800	0.83704900

H	-2.87243200	-5.18332900	-1.91469800
H	-1.06193500	-6.31215100	-0.64198000
Au	1.10690600	-0.40259800	0.76145300
P	3.26232900	-0.50974700	1.62213900
C	4.14284600	1.07634000	1.49953000
C	4.25923500	-1.67963000	0.65212800
C	3.44663500	-1.03009800	3.35319700
H	2.93268800	-0.32531500	4.01426800
H	3.00672300	-2.02328100	3.48966300
H	4.50990300	-1.06783600	3.62012000
H	4.25804100	-1.38965900	-0.40688300
H	3.82803800	-2.68383200	0.73259200
H	5.28950800	-1.69778400	1.02862400
H	3.64350800	1.83016100	2.11722600
H	4.13798300	1.41630900	0.45739100
H	5.18053100	0.96088000	1.83596800
H	-2.82167400	3.14831400	-0.65559400

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

Electronic Energy (0 K) = -1921.916437

Electronic Energy (0 K) + ZPE = -1921.328318

Enthalpy (298 K) = -1921.291667

Free Energy (298 K) = -1921.395275

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

Electronic Energy (0 K) = -1922.263441

#### **TS<sub>4</sub>-Au**

Number of imaginary frequencies: 1

C	-1.80782200	-0.24823400	3.15921700
C	-0.77299100	-0.58089200	2.36164300
C	0.12477500	0.47705100	1.76348500
C	-0.62414400	1.81125600	1.79489800
C	-1.65114700	1.99932800	2.76787200
N	-2.22103900	1.04669100	3.44774900
H	1.01758500	0.56852600	2.42174600
H	-2.40870100	-1.03071300	3.62319200
H	-0.52213200	-1.63005600	2.21843900
H	-2.02203800	3.01569900	2.92547700
C	-0.23680300	2.80683900	0.93639300
C	0.63530400	2.60416700	-0.17715400
C	-0.32767200	4.75307400	-0.24842000
C	0.82353100	3.93206200	-0.84468200
H	-1.20731400	4.69496400	-0.90779300
H	0.77791000	3.89786300	-1.93918600
H	1.78961700	4.38458200	-0.56826000

O	-0.69480200	4.07048500	0.98260400
C	0.00068700	6.18307600	0.07553500
H	0.26004400	6.72708800	-0.83940900
H	-0.84977300	6.68802800	0.54391700
H	0.85391100	6.23238200	0.76215100
C	0.96603800	1.32157400	-0.50193900
C	0.53859000	0.16392800	0.31268800
C	1.60962600	-0.91408800	0.13999900
C	1.80321500	0.86101700	-1.59385900
C	1.69559100	-0.54604500	-1.86148200
C	2.89421700	1.56435300	-2.09799000
C	2.69127400	-1.19611300	-2.63473100
H	0.69111300	-0.95566000	-1.93138200
C	3.87691500	0.88512700	-2.80676400
C	3.79170200	-0.49625300	-3.06802000
H	2.56616500	-2.24941900	-2.88024700
H	4.75277900	1.43231800	-3.14849100
H	4.57875900	-0.98562300	-3.63449400
C	3.02102700	-0.63362500	0.54943600
C	3.40600800	0.55002600	1.19745400
C	4.02068400	-1.57832800	0.26141600
C	4.73007000	0.76492000	1.56010400
H	2.67203400	1.31501000	1.42985100
C	5.34252900	-1.36006500	0.61684800
H	3.75384100	-2.49364200	-0.26519400
C	5.70235100	-0.18643800	1.27378500
H	4.99884800	1.68270200	2.07712000
H	6.09511400	-2.10722600	0.37768900
H	6.73742300	-0.01394500	1.55832200
C	1.18455400	-2.32468100	0.36618900
C	0.24823800	-2.99788100	-0.43353900
C	1.62779100	-2.96287900	1.53723200
C	-0.24221900	-4.24321100	-0.06758100
H	-0.09069800	-2.56660600	-1.37369200
C	1.11569100	-4.19862100	1.91592600
H	2.33954100	-2.46077100	2.18764700
C	0.17959200	-4.84345000	1.11668600
H	-0.94820600	-4.75375900	-0.71826600
H	1.45538800	-4.65628200	2.84140000
H	-0.21004800	-5.81642300	1.40505300
Au	-1.49761600	-0.33147700	-0.45560700
P	-3.75754700	-0.70869400	-0.99261300
C	-4.59564600	0.51956100	-2.04613600
C	-4.73217700	-0.71976500	0.54693700

C	-4.14352200	-2.30836900	-1.77794600
H	-3.68134700	-2.35802200	-2.76956800
H	-3.74015500	-3.12115100	-1.16379300
H	-5.22787300	-2.43856700	-1.87980400
H	-4.59397200	0.22956400	1.07666300
H	-4.37269500	-1.52557600	1.19659100
H	-5.79823400	-0.87039900	0.33669000
H	-4.13857500	0.53308600	-3.04089100
H	-4.49111500	1.51501900	-1.60203800
H	-5.66137400	0.27790400	-2.14147500
H	3.02957500	2.61498800	-1.85191600

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

Electronic Energy (0 K) = -1921.867933

Electronic Energy (0 K) + ZPE = -1921.281325

Enthalpy (298 K) = -1921.245199

Free Energy (298 K) = -1921.346905

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

Electronic Energy (0 K) = -1922.212667

**H'-Au**

Number of imaginary frequencies: 0

C	-1.43591000	0.72993000	3.37144300
C	-0.73535100	0.00674200	2.47378300
C	0.42384600	0.60825900	1.72513800
C	0.30539600	2.12115800	1.77205700
C	-0.39162500	2.71475100	2.87099400
N	-1.21150700	2.07016700	3.64730500
H	1.33210600	0.35165700	2.32211800
H	-2.24326800	0.27378100	3.94211000
H	-0.94633900	-1.05193200	2.34850100
H	-0.27737800	3.78800700	3.03854500
C	0.88464800	2.89474300	0.79290700
C	1.39272700	2.36426600	-0.41561500
C	1.38358100	4.72368900	-0.46623700
C	1.95516400	3.50158500	-1.20255800
H	0.46213100	5.06057800	-0.96362800
H	1.67066200	3.49249500	-2.26090100
H	3.05699500	3.49841500	-1.15961500
O	0.98441700	4.23532800	0.84489200
C	2.34057500	5.86767000	-0.28625100
H	2.64111000	6.26371200	-1.26241300
H	1.88055400	6.67992000	0.28437700
H	3.23958000	5.53436300	0.24521700
C	1.24833200	1.01211400	-0.65484000

C	0.55234500	0.10123800	0.28333500
C	1.21485400	-1.29644600	-0.00751100
C	1.78916500	0.26728200	-1.72878200
C	1.37951300	-1.14928800	-1.55335400
C	2.65438900	0.63678600	-2.76021100
C	2.12495700	-2.14504900	-2.34198200
H	0.34156700	-1.15719500	-1.96754100
C	3.22206900	-0.35508100	-3.53510800
C	2.97613600	-1.74421100	-3.31841700
H	1.91638600	-3.20084200	-2.17645300
H	3.91371100	-0.07204300	-4.32559800
H	3.48884700	-2.47125100	-3.94176100
C	2.64725500	-1.45923800	0.55305400
C	3.43003500	-0.39201300	1.00735800
C	3.24666200	-2.72711900	0.52143700
C	4.74522100	-0.58692000	1.42526900
H	3.03137400	0.61719600	1.04109500
C	4.55835400	-2.92339400	0.93164500
H	2.66942400	-3.58592600	0.18262800
C	5.31637500	-1.85093000	1.39153900
H	5.32091800	0.26413900	1.78215300
H	4.98733800	-3.92226000	0.89620500
H	6.34127900	-2.00196900	1.72153500
C	0.33526100	-2.47113700	0.40872500
C	-0.59699400	-3.06312100	-0.44970400
C	0.39848000	-2.94695900	1.72364000
C	-1.45774900	-4.06356400	-0.00322100
H	-0.67520600	-2.75419600	-1.49119500
C	-0.46204400	-3.94108400	2.17560000
H	1.12887600	-2.52526800	2.41272900
C	-1.40133500	-4.50083500	1.31490700
H	-2.16590500	-4.50914800	-0.69896100
H	-0.39267100	-4.28280500	3.20571800
H	-2.07014300	-5.28376400	1.66413700
Au	-1.54421600	0.12550100	-0.38987400
P	-3.85394700	0.07406300	-0.87432000
C	-4.52012300	1.13368700	-2.20006000
C	-4.84353100	0.51483100	0.59142500
C	-4.42943700	-1.60138100	-1.30889700
H	-3.91602200	-1.94722600	-2.21316400
H	-4.18751200	-2.28808500	-0.49001500
H	-5.51255800	-1.61136600	-1.48246000
H	-4.62373200	1.54614200	0.88797900
H	-4.56901500	-0.14311700	1.42363300

H	-5.91664200	0.41558900	0.38707000
H	-4.05990800	0.86800900	-3.15728700
H	-4.29253000	2.18287100	-1.98496700
H	-5.60732300	1.01111700	-2.27678400
H	2.93333200	1.67532700	-2.91753100

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

Electronic Energy (0 K) = -1921.887412

Electronic Energy (0 K) + ZPE = -1921.300558

Enthalpy (298 K) = -1921.263772

Free Energy (298 K) = -1921.371127

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

Electronic Energy (0 K) = -1922.232363

**D-Cu**

Number of imaginary frequencies: 0

C	-0.22294300	-1.03505400	-1.84577100
C	-1.12178900	-0.23223900	-1.59088000
C	-2.37495200	0.58070000	-1.64787400
C	0.85935000	-1.91249200	-2.09674200
C	0.89524300	-3.17024700	-1.47114600
C	1.90058000	-1.51259000	-2.95383900
C	1.96726800	-4.01517800	-1.70250600
H	0.08632700	-3.45916900	-0.80426600
C	2.96740500	-2.36781300	-3.17302700
H	1.85681900	-0.53365600	-3.42422900
C	3.00050900	-3.61360200	-2.54756300
H	2.00417000	-4.98671500	-1.21768900
H	3.77774600	-2.06540800	-3.83094600
H	3.84248600	-4.27976400	-2.72081100
O	-2.51054700	0.94806900	-3.01147700
H	-2.79430600	1.87025600	-3.04243300
C	-3.57259600	-0.24888200	-1.19670200
C	-3.45060300	-1.30821900	-0.29998200
C	-4.83939100	0.12125500	-1.64960000
C	-4.58193500	-1.98960500	0.13834900
H	-2.47468500	-1.60217700	0.07813300
C	-5.96763600	-0.56172400	-1.21325400
H	-4.94198500	0.94239900	-2.35567400
C	-5.84202400	-1.61970400	-0.31684400
H	-4.46736800	-2.81166200	0.84136500
H	-6.94948700	-0.26768600	-1.57746300
H	-6.72567300	-2.15443200	0.02394900
C	-2.16013400	1.83073800	-0.78220100
C	-2.79584700	2.01631300	0.44496800

C	-1.23806500	2.78890600	-1.23078100
C	-2.50443500	3.13702000	1.21655900
H	-3.50286500	1.27471800	0.80886900
C	-0.95407100	3.90889100	-0.45714800
H	-0.73147100	2.64744900	-2.18459900
C	-1.58387600	4.08034300	0.77239200
H	-2.99968600	3.26863100	2.17538900
H	-0.23434700	4.64205500	-0.81341000
H	-1.35594500	4.94978200	1.38399700
O	1.63792100	1.61170500	1.01264100
Cu	0.26545100	0.48802600	-0.09231800
S	2.42806100	1.91052000	-0.22589700
C	3.89782100	0.80460500	-0.13646500
F	4.55780400	0.89024500	-1.27860900
F	3.50428900	-0.43860500	0.05734300
F	4.66990000	1.19307400	0.85985000
O	2.92485600	3.25244500	-0.42495200
O	1.61141500	1.30234900	-1.34785200
O	-0.79476500	-0.20043500	1.36304100
S	-0.14977900	-1.47325100	1.90961300
O	-1.08787500	-2.57968900	2.01400100
O	1.14495500	-1.69785300	1.26280300
C	0.22317500	-0.96199700	3.63410500
F	1.03564300	0.07972800	3.62853000
F	-0.89958400	-0.64174400	4.25606200
F	0.80369200	-1.97080500	4.26433900

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

Electronic Energy (0 K) = -3004.222440

Electronic Energy (0 K) + ZPE = -3003.857523

Enthalpy (298 K) = -3003.820154

Free Energy (298 K) = -3003.929837

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

Electronic Energy (0 K) = -3004.793218

#### **TS<sub>2</sub>-Cu**

Number of imaginary frequencies: 1

C	1.19557300	0.42404600	-0.27327900
C	0.36367200	0.91588800	0.55098600
C	0.14446200	2.07766700	1.49007900
C	1.43318500	-0.49153500	-1.35249400
C	0.81431000	-0.22920100	-2.58583700
C	2.20693400	-1.65338700	-1.19317600
C	0.97328100	-1.11460400	-3.64404200
H	0.19153700	0.65814200	-2.69211300

C	2.36795200	-2.52333100	-2.25927600
H	2.64781800	-1.87696400	-0.22415900
C	1.75683800	-2.25341100	-3.48399100
H	0.47283100	-0.91885200	-4.58862900
H	2.96028500	-3.42604100	-2.13258600
H	1.87937000	-2.94648000	-4.31298300
O	1.23802100	2.06039800	2.40784300
H	0.93013800	2.45077800	3.23663900
C	0.14549400	3.36146000	0.66068000
C	-0.61608900	3.44120200	-0.50963300
C	0.90345300	4.46148700	1.05537600
C	-0.61177600	4.60263600	-1.27119800
H	-1.22739400	2.59595400	-0.82224700
C	0.90755500	5.62487200	0.28796600
H	1.50919300	4.40647500	1.95666100
C	0.15341000	5.69819600	-0.87702500
H	-1.21333900	4.64580700	-2.17655200
H	1.50684600	6.47536100	0.60592000
H	0.15863100	6.60613200	-1.47590200
C	-1.15114800	1.84658100	2.26840000
C	-2.24492600	2.70366400	2.21190200
C	-1.23733800	0.67494300	3.03616000
C	-3.42127300	2.37793600	2.88245400
H	-2.19610700	3.61498900	1.62129500
C	-2.41814100	0.34479000	3.69087800
H	-0.36915400	0.02065000	3.12164900
C	-3.51792800	1.19519100	3.60549800
H	-4.27423900	3.04959600	2.82160500
H	-2.47766300	-0.57904900	4.26199100
H	-4.44689900	0.93619600	4.10751200
C	5.46069600	-0.99329000	0.69940700
C	4.38732600	-0.11041900	0.88390200
C	3.68420100	-0.17220700	2.09444600
C	4.08497500	-1.09599200	3.04403000
C	5.16521400	-1.92696900	2.75496500
N	5.84789300	-1.88195700	1.60869200
H	2.83134100	0.48055900	2.27747900
H	6.02281800	-0.96865800	-0.23376700
H	3.56299800	-1.18468300	3.99236500
H	5.49417500	-2.66895800	3.48286400
C	3.99766100	0.79901600	-0.17696200
C	3.02162200	1.77258200	-0.18935200
C	3.05605500	2.44295100	-1.53368900
C	4.26251600	1.78271500	-2.21481700

H	2.13185600	2.27163000	-2.10830400
H	3.17504200	3.52909700	-1.44769000
H	5.13856100	2.44576800	-2.18468300
C	4.04086600	1.26391500	-3.60701900
H	3.79330200	2.09660000	-4.27468200
H	4.93833000	0.77087900	-3.99361500
H	3.21057500	0.54797100	-3.62579600
O	4.61577800	0.65436500	-1.34636100
H	2.64462400	2.23403200	0.71521400
O	-2.27066100	-2.29197900	0.91670600
Cu	-1.11534100	-0.48161200	0.55719900
S	-1.02207600	-3.00627100	1.30403000
C	-0.54432500	-3.96419400	-0.19375500
F	0.67715800	-4.45091400	-0.02575300
F	-0.55818000	-3.17639000	-1.25391700
F	-1.39509900	-4.95988100	-0.37036800
O	-1.07520900	-3.95622400	2.39623700
O	0.05868900	-1.95382000	1.37772300
O	-2.48264900	0.64708900	-0.22934900
S	-2.89086300	0.31839300	-1.65765700
O	-2.87166900	1.49632500	-2.51678300
O	-2.27302500	-0.91153000	-2.14481400
C	-4.66342400	-0.08589300	-1.40470100
F	-4.77997400	-1.10374100	-0.56847800
F	-5.30307600	0.96265900	-0.90599600
F	-5.20731000	-0.41187200	-2.56882200

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

Electronic Energy (0 K) = -3521.513518

Electronic Energy (0 K) + ZPE = -3520.956769

Enthalpy (298 K) = -3520.908159

Free Energy (298 K) = -3521.041280

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

Electronic Energy (0 K) = -3522.205348

**E'-Cu**

Number of imaginary frequencies: 0

C	1.52659900	0.51387600	-0.34755500
C	0.49846700	0.78721500	0.46064000
C	0.43492200	1.92928600	1.47328300
C	1.41006800	-0.50304800	-1.43191700
C	0.55290700	-0.23966700	-2.50593800
C	2.13312400	-1.70342400	-1.42963800
C	0.43759400	-1.13764800	-3.56307900
H	-0.03290100	0.67984600	-2.50604300

C	2.01492900	-2.60184100	-2.48432000
H	2.75362300	-1.96230900	-0.57347800
C	1.17678400	-2.31496100	-3.55949500
H	-0.24798400	-0.91874900	-4.37787400
H	2.56765200	-3.53845200	-2.45751200
H	1.08322000	-3.02116000	-4.38130900
O	1.58609800	1.80855200	2.32762400
H	1.37425300	2.24483100	3.16358800
C	0.46912600	3.25047900	0.70721400
C	-0.38440800	3.44010400	-0.38666900
C	1.35076300	4.27164200	1.05813000
C	-0.34573700	4.62263700	-1.11385400
H	-1.09222400	2.66026100	-0.66424500
C	1.38977200	5.45769600	0.32525100
H	2.02485300	4.13701100	1.90124300
C	0.54529700	5.63558800	-0.76402800
H	-1.02058300	4.74834900	-1.95800100
H	2.08395400	6.24473500	0.61322000
H	0.57542100	6.56062900	-1.33558200
C	-0.81193900	1.76719800	2.34102200
C	-1.83402600	2.70966600	2.40995000
C	-0.93554200	0.57874000	3.07605500
C	-2.97410600	2.45578100	3.16847900
H	-1.75952100	3.63840300	1.84962700
C	-2.07811300	0.32199000	3.82413700
H	-0.12836600	-0.15389500	3.05199400
C	-3.10637500	1.26025000	3.86405200
H	-3.77034300	3.19590100	3.20123900
H	-2.16743100	-0.61664400	4.36699800
H	-4.00741500	1.05790800	4.43813800
C	5.69429900	-1.06461400	0.56325300
C	4.48004500	-0.36371100	0.69938500
C	3.70609300	-0.57758700	1.85374300
C	4.17865100	-1.47359700	2.79487200
C	5.39043400	-2.11730700	2.55500900
N	6.14499800	-1.91915800	1.46646900
H	2.76287200	-0.05291200	2.00246500
H	6.31115900	-0.91293400	-0.32244600
H	3.61540500	-1.68233400	3.69897000
H	5.77740300	-2.83469200	3.27853700
C	4.04573600	0.53048200	-0.33634800
C	2.81522900	1.35409600	-0.36228500
C	2.99127900	2.21027600	-1.63299200
C	4.21925700	1.65113600	-2.34557900

H	2.10719800	2.14277000	-2.27580700
H	3.12538100	3.26248500	-1.36445900
H	5.01876400	2.38952500	-2.46635600
C	3.96823100	0.90314000	-3.62449900
H	3.60913700	1.61080000	-4.37951500
H	4.88471400	0.43854000	-4.00055600
H	3.20077300	0.13200500	-3.48831600
O	4.79611100	0.68215900	-1.36542600
H	2.82097000	1.96658500	0.55022100
O	-2.34514500	-2.05715500	0.93727700
Cu	-1.03288000	-0.42397800	0.44701300
S	-1.19899500	-2.94603600	1.28329700
C	-1.03029700	-4.04413200	-0.18082600
F	0.10746700	-4.72130100	-0.09668400
F	-1.02377100	-3.31963600	-1.28617400
F	-2.04294500	-4.89442100	-0.21994100
O	-1.33668700	-3.82300600	2.43118300
O	0.04317700	-2.10523500	1.22032200
O	-2.44556600	0.80024500	-0.19742800
S	-3.01539600	0.59768600	-1.58499700
O	-2.93586300	1.80787800	-2.39830200
O	-2.61564000	-0.66760800	-2.19434200
C	-4.79240300	0.39464100	-1.17747100
F	-4.95994700	-0.65288800	-0.38618700
F	-5.25006600	1.47841500	-0.56361200
F	-5.48551900	0.20912600	-2.29422000

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

Electronic Energy (0 K) = -3521.547464

Electronic Energy (0 K) + ZPE = -3520.988080

Enthalpy (298 K) = -3520.939608

Free Energy (298 K) = -3521.073396

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

Electronic Energy (0 K) = -3522.239556

**F'-Cu**

Number of imaginary frequencies: 0

C	3.24140500	-3.82710500	1.52711500
C	3.76127400	-2.54232400	1.38462700
C	2.96262000	-1.47089900	1.74168500
C	1.66794300	-1.72239400	2.20813300
C	1.24387100	-3.05866500	2.31466500
N	2.01321300	-4.08750000	1.98267600
H	3.34883700	-0.45524600	1.68640700
H	3.85112800	-4.69340900	1.26978800

H	4.77206600	-2.38599800	1.01683200
H	0.22810700	-3.27254800	2.64471500
C	0.77661600	-0.65077300	2.59841300
C	0.64147900	0.66510500	2.08767400
C	-0.96093100	0.25249500	3.75605800
C	-0.25160300	1.39806600	3.04882000
H	-1.83815600	-0.07674100	3.18306100
H	-0.94660600	2.07349200	2.53843600
H	0.32918000	1.98733200	3.77551500
O	-0.00396800	-0.86554800	3.62300100
C	-1.26568900	0.44804500	5.21005700
H	-1.98451400	1.26688000	5.32014100
H	-1.70790500	-0.45245100	5.64615900
H	-0.35942300	0.70597200	5.77022800
C	1.19077300	1.19992300	0.86265900
C	1.49243800	0.36195800	-0.19859000
C	2.25164000	-0.07620600	-1.19584400
C	1.37819100	2.66898400	0.71895300
C	1.18470300	3.31418900	-0.50756800
C	1.87234800	3.39804300	1.80732300
C	1.44345300	4.67277600	-0.62627000
H	0.79650000	2.75568800	-1.35666300
C	2.14585900	4.75342600	1.67672500
C	1.92140800	5.39544700	0.46286600
H	1.26533700	5.16956500	-1.57642800
H	2.53765600	5.30814300	2.52582800
H	2.12345500	6.45926200	0.36436700
C	3.72939600	0.00321700	-1.14336200
C	4.38745300	0.95489600	-0.35137600
C	4.49434600	-0.91291300	-1.87578500
C	5.77361400	0.97851500	-0.28588300
H	3.81037300	1.69446200	0.20271500
C	5.88228400	-0.88676000	-1.80586800
H	3.99339200	-1.65525500	-2.49348700
C	6.52555700	0.05509600	-1.00924300
H	6.27099800	1.72845400	0.32472200
H	6.46273600	-1.60717000	-2.37736400
H	7.61156900	0.07630900	-0.95740400
C	1.61645200	-0.74907600	-2.36105100
C	1.64824500	-0.13682300	-3.61702700
C	1.01467900	-1.99742900	-2.20949400
C	1.06077200	-0.76593100	-4.70704400
H	2.12849400	0.83462600	-3.72967100
C	0.43660000	-2.62796400	-3.30563400

H	0.98853400	-2.46983200	-1.22841400
C	0.45635700	-2.01204400	-4.55170500
H	1.07271000	-0.28216900	-5.68093400
H	-0.04429600	-3.59412200	-3.17374800
H	-0.00458000	-2.50137100	-5.40667900
H	2.07961400	2.89610800	2.75062200
O	-1.58060400	-1.87951100	1.56832300
Cu	-0.51302800	0.33699600	-0.04064500
S	-1.85828400	-2.28871800	0.18293700
C	-3.69125200	-2.26295400	0.07435100
F	-4.08030900	-2.47959000	-1.17200300
F	-4.15961800	-1.09063800	0.47950200
F	-4.18838600	-3.21373700	0.85593800
O	-1.45806900	-3.63378700	-0.20912600
O	-1.47634100	-1.22692200	-0.80956900
O	-2.17690900	1.43577900	0.59251100
S	-2.38363600	2.23638200	-0.66585700
O	-2.62905800	3.65435600	-0.45914300
O	-1.35397500	1.84820800	-1.65886600
C	-3.95757400	1.56778000	-1.34773000
F	-3.80037100	0.32633700	-1.76901400
F	-4.89426800	1.59859200	-0.41133100
F	-4.33772900	2.32350300	-2.36898200

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

Electronic Energy (0 K) = -3445.162254

Electronic Energy (0 K) + ZPE = -3444.630528

Enthalpy (298 K) = -3444.583643

Free Energy (298 K) = -3444.713276

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

Electronic Energy (0 K) = -3445.832635

#### TS<sub>3</sub>-Cu

Number of imaginary frequencies: 1

C	-1.12116500	3.65893800	-2.52075600
C	-1.94052900	2.73300500	-1.93379900
C	-1.76773100	2.41169200	-0.55336900
C	-0.69321800	3.09294400	0.10729800
C	0.08446400	4.02885900	-0.61918000
N	-0.12202700	4.32175200	-1.88117900
H	-2.69528300	2.25708700	0.01609100
H	-1.27091300	3.93025300	-3.56512600
H	-2.74865700	2.27484100	-2.50032800
H	0.92332800	4.50869600	-0.11607600
C	-0.29032300	2.65453000	1.38853900

C	-0.58238400	1.39295100	1.92493500
C	1.11842300	2.46993000	3.14670600
C	0.13723800	1.29932500	3.23611100
H	2.06162800	2.13923800	2.69264400
H	0.64169800	0.33348400	3.35807600
H	-0.54205800	1.43274900	4.09251900
O	0.52089600	3.36708300	2.14733100
C	1.33918000	3.24138600	4.41366100
H	1.80473400	2.59155400	5.16240700
H	2.00300500	4.09466100	4.24493300
H	0.38815700	3.60867400	4.81751500
C	-1.28663800	0.34470900	1.23034900
C	-1.57957000	0.47590100	-0.14384300
C	-2.49022200	-0.19854500	-0.97161200
C	-1.83733100	-0.79711400	2.02172500
C	-1.90915200	-2.09762400	1.51388100
C	-2.41213000	-0.52696100	3.27020300
C	-2.51299500	-3.10613600	2.25361200
H	-1.44728700	-2.33932600	0.55914900
C	-3.03167900	-1.53553300	3.99822900
C	-3.07598100	-2.83088600	3.49556200
H	-2.53055000	-4.11807700	1.85685700
H	-3.48122200	-1.30415000	4.96100000
H	-3.54783800	-3.62436200	4.06997800
C	-3.92189400	0.02024500	-0.84244100
C	-4.49061100	0.48085400	0.36304300
C	-4.76863700	-0.13989700	-1.96051500
C	-5.84973000	0.73810400	0.45198400
H	-3.87085800	0.59125800	1.24942800
C	-6.12400600	0.12545700	-1.86572200
H	-4.34439200	-0.44584000	-2.91351800
C	-6.66968000	0.56014900	-0.65906200
H	-6.27321400	1.07436500	1.39473900
H	-6.75884900	0.00584100	-2.73980400
H	-7.73468600	0.76720800	-0.58741200
C	-1.94510400	-0.98507300	-2.06983000
C	-2.51592500	-2.22669900	-2.41115300
C	-0.78590800	-0.55684000	-2.74058800
C	-1.92169100	-3.02092400	-3.37716400
H	-3.39149100	-2.58201300	-1.87075400
C	-0.20917200	-1.35141200	-3.71955700
H	-0.35032600	0.41254900	-2.51127000
C	-0.76888000	-2.58595700	-4.03275200
H	-2.34817300	-3.99263100	-3.61296600

H	0.68794900	-1.00591900	-4.22651100
H	-0.30463100	-3.21743200	-4.78631400
H	-2.41160900	0.48818700	3.66251300
O	2.32492500	2.18435000	0.29529900
Cu	0.37343300	-0.10247900	0.01387400
S	2.62416700	1.62286300	-1.02813900
C	4.26031100	0.82347300	-0.79762800
F	4.61077400	0.15845200	-1.88907000
F	4.23423200	-0.00764400	0.23337800
F	5.16883700	1.76342100	-0.55897700
O	2.81809300	2.55432600	-2.13068100
O	1.72872600	0.46350200	-1.37843600
O	1.66639300	-1.11445800	1.30918900
S	1.51250300	-2.53284100	0.83853400
O	1.32434100	-3.51339500	1.89891000
O	0.59758900	-2.58840400	-0.32165600
C	3.15080900	-2.94245900	0.11302800
F	3.38362500	-2.21738600	-0.96943700
F	4.11277900	-2.72966200	0.99918100
F	3.15673800	-4.22584900	-0.22920800

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

Electronic Energy (0 K) = -3445.126813

Electronic Energy (0 K) + ZPE = -3444.596193

Enthalpy (298 K) = -3444.550266

Free Energy (298 K) = -3444.676112

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

Electronic Energy (0 K) = -3445.794286

#### **G'-Cu**

Number of imaginary frequencies: 0

C	-0.82075300	3.80160900	-2.25015800
C	-1.37341500	2.60755700	-1.93063400
C	-1.37349800	2.15715900	-0.52336600
C	-0.51058700	2.96713200	0.35448800
C	-0.01279700	4.20887800	-0.13082200
N	-0.16857300	4.61866200	-1.35739200
H	-2.42156900	2.46468400	-0.21823800
H	-0.85778800	4.16745000	-3.27352100
H	-1.91172400	2.01972100	-2.67026400
H	0.56738200	4.83284400	0.54920400
C	-0.16757200	2.43822700	1.59238100
C	-0.52033000	1.13632700	1.96490700
C	1.12921500	2.01704100	3.37952100
C	0.10279200	0.88235700	3.29564100

H	2.07294600	1.69986100	2.91281800
H	0.55234300	-0.11567000	3.35516800
H	-0.64219900	0.96559800	4.10262600
O	0.59082000	3.05630000	2.49455400
C	1.34522700	2.60259200	4.74291700
H	1.76248700	1.84090600	5.41015400
H	2.04690500	3.44103300	4.70317200
H	0.39833800	2.95586200	5.16832100
C	-1.31441000	0.26990300	1.14850600
C	-1.57631400	0.69566300	-0.18443400
C	-2.53842100	-0.03883800	-1.04300200
C	-1.97686100	-0.91187200	1.76941400
C	-1.97241100	-2.18316800	1.19047500
C	-2.69496200	-0.70663100	2.95456200
C	-2.66145000	-3.22801400	1.79571200
H	-1.39752300	-2.37311100	0.28805400
C	-3.38949300	-1.75128600	3.54995600
C	-3.37033200	-3.01706300	2.97290700
H	-2.63027100	-4.21608600	1.34343800
H	-3.94836600	-1.57366500	4.46559500
H	-3.90626500	-3.83837300	3.44253100
C	-3.93912800	0.25811800	-0.87516700
C	-4.42005700	0.96819100	0.25331200
C	-4.88151300	-0.05979900	-1.88480700
C	-5.75754100	1.31192400	0.37259100
H	-3.74483100	1.21784000	1.07016700
C	-6.21341800	0.29009100	-1.75749300
H	-4.54412200	-0.55559900	-2.79092700
C	-6.66489700	0.97321500	-0.62756900
H	-6.09619000	1.84400400	1.25849100
H	-6.90839000	0.04125000	-2.55608700
H	-7.71316400	1.24499600	-0.53267200
C	-2.02303700	-0.96198200	-2.04570700
C	-2.66820200	-2.18985500	-2.29609200
C	-0.81842400	-0.69485600	-2.72201700
C	-2.12745500	-3.10249500	-3.18820900
H	-3.57015400	-2.44197100	-1.74109500
C	-0.28590900	-1.61014700	-3.61838900
H	-0.29202900	0.24347100	-2.55960000
C	-0.93667000	-2.81723200	-3.85505400
H	-2.62882900	-4.05352100	-3.35225100
H	0.64906100	-1.37817000	-4.12257900
H	-0.51222300	-3.54079200	-4.54669000
H	-2.73900800	0.28676000	3.40017100

O	2.32545700	2.25395000	0.29435800
Cu	0.40179600	-0.16214600	0.05689900
S	2.51055300	1.72716300	-1.06247000
C	4.19669200	1.00320700	-1.02388200
F	4.43559800	0.32066500	-2.13322100
F	4.32597700	0.20016200	0.02168500
F	5.08615500	1.98311400	-0.92066800
O	2.51776300	2.68201900	-2.16290900
O	1.65542700	0.51689900	-1.34621200
O	1.68967700	-1.13862300	1.34556200
S	1.63581100	-2.55999000	0.84905400
O	1.51014200	-3.55975300	1.89940500
O	0.73683600	-2.65838600	-0.31728100
C	3.30775300	-2.82129800	0.13093700
F	3.45810500	-2.09879400	-0.96791100
F	4.24272300	-2.48718900	1.00798900
F	3.44715100	-4.10347600	-0.18210000

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

Electronic Energy (0 K) = -3445.142902

Electronic Energy (0 K) + ZPE = -3444.612096

Enthalpy (298 K) = -3444.566142

Free Energy (298 K) = -3444.691350

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

Electronic Energy (0 K) = -3445.810979

**TS<sub>4</sub>-Cu**

Number of imaginary frequencies: 1

C	-0.94559000	2.94890700	-3.13586300
C	-1.55155700	1.96431100	-2.43047000
C	-1.51748500	1.96976600	-0.94303300
C	-0.56115400	2.99875700	-0.41990300
C	-0.02121400	3.95810800	-1.29240900
N	-0.20567900	3.97260200	-2.59628200
H	-2.54300000	2.31460200	-0.63628600
H	-1.02337200	2.95968700	-4.22217400
H	-2.15055800	1.21469200	-2.94229200
H	0.62838800	4.72636200	-0.87066700
C	-0.20593000	2.92382200	0.94069100
C	-0.49594600	1.83418800	1.74506200
C	1.08820300	3.23561400	2.75838600
C	0.15122500	2.06017300	3.07663800
H	2.07266500	2.85201700	2.45628400
H	0.70134200	1.18410700	3.44158700
H	-0.58079200	2.34305800	3.85214400

O	0.52986500	3.85288100	1.55549900
C	1.20431800	4.28126700	3.82906500
H	1.64369500	3.84295700	4.73190700
H	1.84559800	5.10667700	3.50508600
H	0.21703200	4.68502100	4.08430800
C	-1.13083300	0.67676300	1.18658700
C	-1.46895900	0.64120600	-0.18349300
C	-2.42596500	-0.45486400	-0.58820700
C	-1.75372800	-0.42104400	1.93220600
C	-2.07817200	-1.55830600	1.13072500
C	-2.28316800	-0.28755600	3.20793000
C	-3.02766000	-2.48990300	1.62288600
H	-1.26818400	-2.00961600	0.54505500
C	-3.20580600	-1.22877500	3.66062800
C	-3.60688500	-2.30838000	2.86004100
H	-3.24251700	-3.38143900	1.03745800
H	-3.64585600	-1.10497200	4.64750600
H	-4.32919800	-3.02389900	3.24267300
C	-3.86511000	-0.05987600	-0.51903900
C	-4.38199700	0.68177900	0.55831300
C	-4.71170600	-0.28946000	-1.61713900
C	-5.68971900	1.13819700	0.55333700
H	-3.76034000	0.89775000	1.42343700
C	-6.02076900	0.17787300	-1.62243200
H	-4.33616100	-0.80755700	-2.49405500
C	-6.51996000	0.88366800	-0.53642000
H	-6.06337700	1.69969500	1.40592400
H	-6.64693500	-0.00754700	-2.49153800
H	-7.54529700	1.24474500	-0.53973200
C	-2.01475500	-1.37679000	-1.66907100
C	-2.72837700	-2.56860300	-1.89129300
C	-0.85156200	-1.14556100	-2.41500400
C	-2.29559600	-3.48620600	-2.83354200
H	-3.61312000	-2.78568800	-1.29444800
C	-0.43197600	-2.05768300	-3.37459300
H	-0.25647900	-0.24936500	-2.26007100
C	-1.14574400	-3.23152600	-3.58119000
H	-2.84695400	-4.41181300	-2.97835300
H	0.47326300	-1.85239600	-3.93997000
H	-0.80100900	-3.95813500	-4.31275800
H	-2.04611600	0.58061700	3.81810100
O	2.48922000	2.17574800	0.00051500
Cu	0.53400700	0.02191600	0.15921500
S	2.71274300	1.43118000	-1.24273100

C	4.31361500	0.57655800	-0.95875500
F	4.55617700	-0.29665600	-1.92531300
F	4.30152600	-0.05504800	0.20698500
F	5.28811100	1.47861100	-0.94034600
O	2.89716400	2.18184300	-2.47588500
O	1.75575100	0.26976400	-1.39483800
O	1.56435800	-1.07533100	1.52966000
S	1.45476900	-2.56070400	1.32216900
O	1.33443100	-3.31290500	2.56424300
O	0.53424500	-2.91294200	0.22519500
C	3.10379800	-2.99390500	0.64304100
F	3.27820200	-2.42031300	-0.53808900
F	4.06106200	-2.59765500	1.46798500
F	3.18240800	-4.31099900	0.49315900

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

Electronic Energy (0 K) = -3445.110925

Electronic Energy (0 K) + ZPE = -3444.580395

Enthalpy (298 K) = -3444.535244

Free Energy (298 K) = -3444.658885

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

Electronic Energy (0 K) = -3445.778181

**H'-Cu**

Number of imaginary frequencies: 0

C	-0.96527300	3.22935800	-2.77291700
C	-1.49802000	2.13535400	-2.18084200
C	-1.54002300	2.02862200	-0.68954900
C	-0.59922800	3.02618700	-0.06234400
C	-0.15167200	4.11952200	-0.82078200
N	-0.34942600	4.26780700	-2.11589000
H	-2.57385100	2.36175800	-0.40509400
H	-0.99148300	3.32212200	-3.85790600
H	-1.96883200	1.36304700	-2.78310100
H	0.43887600	4.88658900	-0.31717400
C	-0.17803900	2.81102400	1.26490600
C	-0.37105000	1.62533200	1.94815900
C	1.16957000	3.00049300	3.06689800
C	0.35289300	1.70819100	3.25481900
H	2.18236400	2.75013300	2.72329000
H	1.01133800	0.84810700	3.43412900
H	-0.33704700	1.79094300	4.11150300
O	0.54594700	3.70249100	1.94859300
C	1.20067900	3.91847100	4.25531700
H	1.69387400	3.42240900	5.09872500

H	1.75300800	4.83601600	4.02983800
H	0.18247700	4.18991600	4.55967600
C	-1.02356800	0.54114400	1.27758600
C	-1.47823200	0.65654700	-0.05861000
C	-2.44689900	-0.49693300	-0.39047700
C	-1.45163700	-0.73297300	1.81102800
C	-2.09260000	-1.49467100	0.74301300
C	-1.33302400	-1.26716200	3.08473600
C	-2.88416400	-2.65203200	1.12631300
H	-1.19220800	-2.10264200	0.37933300
C	-1.96397100	-2.47919200	3.34383200
C	-2.75719700	-3.15780900	2.39054200
H	-3.45259900	-3.17377800	0.35778300
H	-1.86525300	-2.91367900	4.33677900
H	-3.25663700	-4.07995700	2.67136700
C	-3.86428600	0.06353600	-0.17783100
C	-4.47421100	0.05587400	1.07773800
C	-4.53932800	0.67758000	-1.23866000
C	-5.72846800	0.62856000	1.26836000
H	-3.97722000	-0.39428100	1.93732700
C	-5.78918000	1.25428300	-1.04835500
H	-4.08997600	0.69220800	-2.22965800
C	-6.39067500	1.23048400	0.20582800
H	-6.18509100	0.60241400	2.25501800
H	-6.29604600	1.72099600	-1.88970600
H	-7.37005500	1.67908600	0.35328300
C	-2.28274900	-1.19716700	-1.73573300
C	-3.30074000	-2.03973700	-2.19685700
C	-1.09093300	-1.13451200	-2.45991400
C	-3.13158600	-2.79554400	-3.35121200
H	-4.24660300	-2.09274700	-1.65912600
C	-0.92363500	-1.88890200	-3.61768800
H	-0.27819500	-0.48232200	-2.14357800
C	-1.94036800	-2.72320800	-4.06596900
H	-3.93743500	-3.44097200	-3.69357900
H	0.01231000	-1.81684000	-4.16629600
H	-1.80703300	-3.31249700	-4.97010300
H	-0.78920200	-0.74921100	3.86996100
O	2.50809400	2.11697000	0.16762700
Cu	0.59462400	0.02188600	0.12676100
S	2.61730900	1.61261100	-1.20477600
C	4.21987300	0.71551300	-1.23204900
F	4.34949500	0.03275800	-2.36026900
F	4.29311100	-0.12327600	-0.20790800

F	5.21380500	1.58962900	-1.13905800
O	2.68896900	2.56865100	-2.29763400
O	1.64256800	0.48147300	-1.46922600
O	1.70413900	-1.14204300	1.39567000
S	1.55522400	-2.62774200	1.25379600
O	1.76039100	-3.36162400	2.49358200
O	0.37486500	-3.00559600	0.44475900
C	2.95786100	-3.07918300	0.16259200
F	2.85228900	-2.44069100	-0.99392500
F	4.10352800	-2.75943200	0.74027700
F	2.93458900	-4.38553700	-0.06245800

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

Electronic Energy (0 K) = -3445.135532

Electronic Energy (0 K) + ZPE = -3444.604386

Enthalpy (298 K) = -3444.559241

Free Energy (298 K) = -3444.682690

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

Electronic Energy (0 K) = -3445.804405

**G''-Cu**

Number of imaginary frequencies: 0

C	2.05409000	-4.24247900	0.39024000
C	2.19671300	-2.89339700	0.68294300
C	1.58078200	-1.95731300	-0.13942900
C	0.84986700	-2.46252500	-1.22952000
C	0.75459500	-3.85147400	-1.42787300
N	1.35065900	-4.72875300	-0.64407300
H	1.00227600	-0.41706500	1.09040000
H	2.53579300	-4.98355100	1.02757300
H	2.78432300	-2.57651600	1.54195300
H	0.16856000	-4.23656600	-2.26281000
C	0.23090400	-1.51730900	-2.09238700
C	0.32636300	-0.10005400	-1.93037900
C	-1.01197600	-0.65641500	-3.80286500
C	-0.20505200	0.49917300	-3.20998700
H	-0.80664200	-0.81255600	-4.86575000
H	0.63212900	0.75988500	-3.87122700
H	-0.81515800	1.39325200	-3.04372400
O	-0.44391300	-1.86891600	-3.14081300
C	-2.48931400	-0.62809300	-3.52428500
H	-2.93884200	0.21285000	-4.06311200
H	-2.96695600	-1.55426500	-3.85748600
H	-2.70043900	-0.49446200	-2.45702700
C	0.97525900	0.44826700	-0.82021300

C	1.63775900	-0.48834400	0.18990300
C	3.02588000	-0.02826100	0.61335300
C	1.19450700	1.89396200	-0.66010700
C	1.56464100	2.68649900	-1.75387000
C	1.03171200	2.49602200	0.59702900
C	1.76739000	4.05004700	-1.59489900
H	1.73158600	2.22985800	-2.72645700
C	1.21459800	3.86203100	0.74441300
C	1.58285300	4.64108700	-0.34902400
H	2.06710900	4.65315200	-2.44825400
H	1.05862300	4.31975100	1.71770700
H	1.72352800	5.71263900	-0.22968600
C	3.17170000	0.51855400	1.95487800
C	2.40017800	0.04538200	3.03632000
C	4.03739300	1.60511900	2.19705500
C	2.50356700	0.61909300	4.29501400
H	1.71800400	-0.79486700	2.90127800
C	4.12868600	2.18161300	3.45449300
H	4.60082200	2.02843300	1.36780400
C	3.36683100	1.69011500	4.51221300
H	1.90223500	0.22693900	5.11178700
H	4.78790900	3.03330800	3.60702800
H	3.43711000	2.14541600	5.49714500
C	4.13553600	-0.15523000	-0.30012800
C	3.94694700	-0.30541900	-1.69326400
C	5.47012900	-0.19773600	0.17019200
C	5.01777000	-0.45628300	-2.55882700
H	2.94327100	-0.27871700	-2.11115200
C	6.53666500	-0.35271400	-0.69911800
H	5.65863300	-0.13902100	1.23923800
C	6.32236900	-0.47702100	-2.07088600
H	4.83410800	-0.55632200	-3.62642800
H	7.54817800	-0.39057500	-0.30080800
H	7.16199900	-0.59811200	-2.75090500
H	0.71367500	1.90328500	1.45188300
O	-0.84339000	-1.49364500	1.68066400
Cu	-1.13834100	0.01484200	-0.42882200
S	-1.84505300	-2.33300500	0.99405100
C	-3.37713300	-2.10818700	1.97847400
F	-4.37615600	-2.76733400	1.41121300
F	-3.68908900	-0.82391000	2.05161100
F	-3.18507600	-2.57774700	3.20298500
O	-1.60158300	-3.76743800	0.95184600
O	-2.22729100	-1.73097300	-0.33413600

O	-1.88955900	1.47116600	0.70752700
S	-2.57932700	2.47841800	-0.17811800
O	-2.58346900	3.83107300	0.35363300
O	-2.22861200	2.28487000	-1.59472200
C	-4.32288400	1.90901600	-0.09425400
F	-4.41119800	0.66066200	-0.54842700
F	-4.76620400	1.94637300	1.15143500
F	-5.08426400	2.68890900	-0.85023900

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

Electronic Energy (0 K) = -3445.204571

Electronic Energy (0 K) + ZPE = -3444.671068

Enthalpy (298 K) = -3444.625184

Free Energy (298 K) = -3444.752223

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

Electronic Energy (0 K) = -3445.872921

**TS<sub>4</sub>-Cu**

Number of imaginary frequencies: 1

C	2.28350900	-3.86965700	-1.05469800
C	2.27866900	-2.69412400	-0.31469900
C	1.56883000	-1.59533600	-0.78761100
C	0.88339400	-1.77341800	-2.00494400
C	0.94704200	-3.00778200	-2.67032500
N	1.63882200	-4.03794900	-2.21627400
H	0.77955100	-0.56717900	0.83270300
H	2.83888000	-4.73181000	-0.68657800
H	2.81857700	-2.65054600	0.62702900
H	0.40854300	-3.13902800	-3.60887000
C	0.14162600	-0.67143000	-2.52477100
C	0.10677800	0.61287500	-1.93697800
C	-1.22422400	0.53592800	-3.88200500
C	-0.50741700	1.52917300	-2.96576500
H	-1.06879100	0.74485100	-4.94406700
H	0.28615900	2.06774900	-3.50281500
H	-1.20591800	2.25471200	-2.53703400
O	-0.52096100	-0.75014000	-3.64715200
C	-2.68292600	0.34167400	-3.56320300
H	-3.23363100	1.25159600	-3.82556000
H	-3.10220400	-0.49764000	-4.12560300
H	-2.84079700	0.15351900	-2.49248500
C	0.77372700	0.84470200	-0.72716500
C	1.45778700	-0.31141800	-0.00370600
C	2.77534000	0.17099300	0.63513800
C	1.07960500	2.10419700	-0.12480700

C	1.02360100	3.34638700	-0.77890500
C	1.76011400	1.99530800	1.13651500
C	1.72004900	4.42562100	-0.26739100
H	0.48155500	3.45213700	-1.71323500
C	2.48522300	3.11333700	1.61705200
C	2.48834200	4.29309400	0.90678700
H	1.69074000	5.37930300	-0.78738200
H	2.99026500	3.04261400	2.57797000
H	3.04061800	5.15149200	1.28165600
C	3.11748300	-0.31260200	1.98479600
C	2.28502700	-1.16354900	2.73429400
C	4.27685500	0.18804200	2.61004300
C	2.61449600	-1.51365300	4.03862400
H	1.37572700	-1.58611600	2.30863100
C	4.59713200	-0.16025400	3.91231500
H	4.92131700	0.87379500	2.06303300
C	3.76890700	-1.01814100	4.63376300
H	1.95774500	-2.18248000	4.58937900
H	5.49657700	0.24440800	4.37064100
H	4.02092700	-1.29388200	5.65483400
C	3.91208600	0.37439800	-0.31572200
C	3.95863400	1.40025100	-1.27001800
C	4.96410200	-0.55779000	-0.31188100
C	5.00726500	1.48598800	-2.17867300
H	3.18712600	2.16357900	-1.29328100
C	6.00532700	-0.47669100	-1.22680100
H	4.95807200	-1.36746500	0.41432500
C	6.03286800	0.54756200	-2.16661400
H	5.02368200	2.30318500	-2.89637300
H	6.79834600	-1.22049600	-1.20241200
H	6.85023500	0.61740000	-2.88033500
H	1.32402800	1.34076600	1.89180900
O	-0.83816100	-2.06124700	1.22365900
Cu	-1.35568700	0.10905800	-0.45462500
S	-1.84088500	-2.64458300	0.31765000
C	-3.38793100	-2.63371100	1.30252600
F	-4.39675800	-3.08113000	0.56912800
F	-3.66015000	-1.40061700	1.70581600
F	-3.24471800	-3.41344900	2.36510500
O	-1.65187100	-4.02239600	-0.10908300
O	-2.19028700	-1.70353200	-0.80962300
O	-1.85375600	1.22117300	1.11986700
S	-2.55768100	2.48561400	0.69627100
O	-2.45209300	3.56472700	1.66494200

O	-2.32837400	2.80242100	-0.72139700
C	-4.31679300	1.96062500	0.73392200
F	-4.50922600	0.95661400	-0.12088800
F	-4.65788900	1.56131100	1.94762600
F	-5.09351000	2.97398100	0.37488400

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

Electronic Energy (0 K) = -3445.174552

Electronic Energy (0 K) + ZPE = -3444.641092

Enthalpy (298 K) = -3444.596065

Free Energy (298 K) = -3444.719988

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

Electronic Energy (0 K) = -3445.840866

**H''-Cu**

Number of imaginary frequencies: 0

C	2.30433000	3.89751400	0.90471500
C	2.30883400	2.71102900	0.18182900
C	1.63459700	1.60280500	0.68467200
C	0.94901600	1.79165200	1.90342100
C	1.00139100	3.03741100	2.54716700
N	1.67420300	4.07184400	2.07250500
H	0.88223000	0.56185500	-0.94134800
H	2.83828100	4.76388400	0.51472700
H	2.82922300	2.66462600	-0.77083400
H	0.46165000	3.17823200	3.48374800
C	0.19385800	0.70254300	2.44369600
C	0.07984900	-0.56360300	1.83824400
C	-1.13961500	-0.48618000	3.85023100
C	-0.52180000	-1.48501100	2.86659100
H	-0.92478700	-0.72606200	4.89557000
H	0.27004400	-2.08970000	3.33216500
H	-1.28236500	-2.15812500	2.45712500
O	-0.40787700	0.78232200	3.60053400
C	-2.60674600	-0.22856000	3.62963200
H	-3.17354900	-1.13562600	3.86699600
H	-2.96399500	0.58413200	4.26909400
H	-2.81569300	0.03854900	2.58529600
C	0.78093700	-0.80638000	0.64570100
C	1.51732500	0.31014400	-0.07005700
C	2.78712300	-0.41955900	-0.65240400
C	1.09378800	-2.02795700	0.01813900
C	0.66990100	-3.33219900	0.28981900
C	2.07420200	-1.75084200	-1.07216700
C	1.30163000	-4.38369100	-0.34819100

H	-0.14024100	-3.52049600	0.99058300
C	2.84168600	-2.92941700	-1.53654400
C	2.41888600	-4.17859100	-1.21854100
H	0.97019600	-5.40012300	-0.15001500
H	3.67488400	-2.76973700	-2.21910200
H	2.93061300	-5.04819400	-1.62326100
C	3.39190200	0.20931700	-1.90336800
C	2.66283300	1.04289700	-2.75865400
C	4.68372300	-0.16359100	-2.29349100
C	3.21491400	1.50054700	-3.95161500
H	1.65111000	1.36153900	-2.50961200
C	5.23238600	0.28725600	-3.48868300
H	5.27340400	-0.81215500	-1.64763600
C	4.50053300	1.12516100	-4.32259000
H	2.62846800	2.15521500	-4.59195100
H	6.23912200	-0.01793100	-3.76537500
H	4.92922900	1.48392600	-5.25529800
C	3.81139800	-0.60253000	0.46870700
C	3.90368000	-1.76942800	1.23212400
C	4.66712100	0.45807400	0.79762900
C	4.80397200	-1.86975600	2.29046800
H	3.27671700	-2.62893600	1.00998000
C	5.56342400	0.36183000	1.85369400
H	4.64499600	1.37085400	0.20649900
C	5.63434800	-0.80427100	2.60966200
H	4.85465300	-2.79429600	2.86139500
H	6.21401600	1.20299000	2.08214000
H	6.33820700	-0.88276800	3.43493400
H	1.46224800	-1.44739600	-1.95569000
O	-0.86598300	1.94519500	-1.24436600
Cu	-1.36513600	-0.10637200	0.35023200
S	-1.86122700	2.58790800	-0.36623500
C	-3.40890300	2.56102700	-1.35172000
F	-4.40746800	3.06132600	-0.63956800
F	-3.70560700	1.31534600	-1.69640800
F	-3.25069900	3.28699600	-2.44908800
O	-1.64718400	3.97812700	0.00229800
O	-2.21981700	1.68970300	0.79239100
O	-1.92006800	-1.31663800	-1.12826500
S	-2.76201700	-2.47882600	-0.66697900
O	-2.81964200	-3.56827200	-1.62830800
O	-2.52661100	-2.82107000	0.74432600
C	-4.44199300	-1.73775000	-0.65398200
F	-4.47191500	-0.69872400	0.17984200

F	-4.77545000	-1.32484800	-1.86490100
F	-5.32452300	-2.63698000	-0.24172700

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

Electronic Energy (0 K) = -3445.204168

Electronic Energy (0 K) + ZPE = -3444.669638

Enthalpy (298 K) = -3444.624298

Free Energy (298 K) = -3444.750091

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

Electronic Energy (0 K) = -3445.870280

**TS<sub>5</sub>-Cu**

Number of imaginary frequencies: 1

C	2.71289600	3.84263700	0.67590000
C	2.66664800	2.55535200	0.15977600
C	1.88825200	1.58605800	0.79942400
C	1.16448000	2.02242200	1.94063400
C	1.27245500	3.35839000	2.36009900
N	2.03865200	4.25123100	1.75994500
H	0.78871700	0.11338200	-0.73640500
H	3.32877800	4.59435800	0.18303500
H	3.23066100	2.31906500	-0.73739000
H	0.70483000	3.68979900	3.22994700
C	0.34084600	1.08348800	2.62052600
C	0.26556300	-0.27476400	2.27445600
C	-1.27673300	0.24728800	3.98111100
C	-0.64562400	-0.94603200	3.24856400
H	-1.21439700	0.16221200	5.07023900
H	-0.08305700	-1.60044600	3.92844800
H	-1.41420800	-1.55298200	2.75103200
O	-0.42200200	1.40568900	3.64017000
C	-2.67620500	0.56672700	3.52406100
H	-3.34493000	-0.26153400	3.78297800
H	-3.04757900	1.47996800	3.99870300
H	-2.70436200	0.70427500	2.43487000
C	0.98733100	-0.72637800	1.19083400
C	1.72494200	0.20680700	0.33923700
C	2.71487200	-0.66486900	-0.47991200
C	0.98645600	-1.99952900	0.53688100
C	0.28929400	-3.17867900	0.79111000
C	1.75076900	-1.84623600	-0.66573400
C	0.37440400	-4.20747400	-0.13753600
H	-0.32978700	-3.29102000	1.67816800
C	1.86325000	-2.92871300	-1.56584800
C	1.14425500	-4.07907600	-1.30779700

H	-0.18139800	-5.12537500	0.03397800
H	2.48908700	-2.83881800	-2.45185700
H	1.17929800	-4.90743200	-2.01080100
C	3.20184800	-0.14881500	-1.83117100
C	2.50532600	0.80119900	-2.58601700
C	4.33951600	-0.73778000	-2.39427400
C	2.94673200	1.15722600	-3.85739800
H	1.61323200	1.28818800	-2.19644300
C	4.77292000	-0.38771800	-3.66809300
H	4.89615400	-1.48241500	-1.82739100
C	4.07902400	0.56544500	-4.40471100
H	2.39293800	1.90605100	-4.41893400
H	5.66048800	-0.86146800	-4.08158900
H	4.41928000	0.84688700	-5.39858700
C	3.89099300	-1.04549400	0.43265200
C	4.11240700	-2.35137000	0.87772500
C	4.80292600	-0.05482900	0.81543000
C	5.19752100	-2.65117000	1.69791600
H	3.44449900	-3.15699300	0.57970300
C	5.88296300	-0.35257800	1.63493100
H	4.67440800	0.96532900	0.46008400
C	6.08372700	-1.65471500	2.08426500
H	5.34859400	-3.67648400	2.02823200
H	6.57405000	0.43763700	1.91949300
H	6.93152600	-1.89050800	2.72323400
H	0.75121300	-0.75700300	-1.19851000
O	-0.38119200	2.41018500	-1.65044300
Cu	-1.76721900	-0.01876300	-0.29631800
S	-1.26307800	2.84546100	-0.56870300
C	-2.89305600	3.12434800	-1.37214200
F	-3.79498700	3.46258300	-0.46482400
F	-3.29666400	2.01255600	-1.98261000
F	-2.78721800	4.09211500	-2.26740300
O	-0.95660500	4.07838800	0.13567600
O	-1.60489200	1.71971200	0.39995500
O	-2.01463300	-1.76122400	-0.95103300
S	-2.94056500	-2.65747000	-0.14633800
O	-2.91062000	-4.03240900	-0.61598600
O	-2.86326300	-2.40981800	1.29543800
C	-4.59318500	-2.01176000	-0.63098300
F	-4.70493000	-0.72956900	-0.28546500
F	-4.75827700	-2.11569600	-1.93887400
F	-5.53705700	-2.70284000	-0.01234500

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

Electronic Energy (0 K) = -3445.138887  
 Electronic Energy (0 K) + ZPE = -3444.612213  
 Enthalpy (298 K) = -3444.567258  
 Free Energy (298 K) = -3444.692355  
**SMD-M06/6-311+G(d,p)/SDD**  
 Electronic Energy (0 K) = -3445.805715

## H<sub>2</sub>

Number of imaginary frequencies: 0  

H	0.00000000	0.00000000	0.37115800
H	0.00000000	0.00000000	-0.37115800

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

Electronic Energy (0 K) = -1.168727  
 Electronic Energy (0 K) + ZPE = -1.158600  
 Enthalpy (298 K) = -1.155296  
 Free Energy (298 K) = -1.170086

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

Electronic Energy (0 K) = -1.169720

## TS<sub>5</sub>

Number of imaginary frequencies: 1

C	0.75541100	-4.02227500	0.09004400
C	0.09619400	-2.83027700	-0.13619100
C	0.81893500	-1.62556000	-0.18855100
C	2.22136500	-1.73777400	0.01544100
C	2.78307500	-3.01015900	0.22556500
N	2.08538200	-4.13037000	0.26382600
H	-0.05110800	-0.07189700	-1.84654500
H	0.18937500	-4.95305800	0.13092800
H	-0.98025400	-2.83939500	-0.28106400
H	3.86149400	-3.08896100	0.37104100
C	3.01122500	-0.55095300	0.03202500
C	2.48819000	0.69895800	-0.11653300
C	4.84315000	0.77439400	0.02281900
C	3.60267300	1.69224000	0.01635100
H	5.50687300	0.98172500	0.86975700
H	3.51223800	2.28397500	0.93795700
H	3.64751300	2.40265200	-0.82176300
O	4.34669800	-0.58162400	0.22220000
C	5.60460500	0.80268700	-1.27933500
H	6.04637300	1.79243900	-1.44323700
H	6.40815800	0.05935700	-1.28256200
H	4.92720800	0.58565000	-2.11541300
C	1.09859300	0.85215900	-0.30314300

C	0.24508500	-0.31301600	-0.47051000
C	-1.20292600	0.18293600	-0.18344900
C	0.32838900	1.99286400	-0.57381500
C	0.66291700	3.35646200	-0.70356700
C	-1.00452400	1.53458400	-0.90927500
C	-0.31147300	4.25327600	-1.07071600
H	1.67447000	3.69777900	-0.48953400
C	-2.01140200	2.51243700	-1.18338700
C	-1.64738000	3.82694300	-1.30340400
H	-0.06891900	5.30914600	-1.16632500
H	-3.04422600	2.19877600	-1.32786700
H	-2.39748800	4.57207100	-1.56158400
C	-2.37719300	-0.57886800	-0.79395600
C	-2.25923000	-1.43945400	-1.89134900
C	-3.66381100	-0.32806000	-0.30128100
C	-3.38033100	-2.03480500	-2.46160900
H	-1.28221400	-1.66438800	-2.31216500
C	-4.78612800	-0.91508700	-0.87496700
H	-3.78863500	0.33741900	0.55123000
C	-4.64968900	-1.77605400	-1.95782200
H	-3.25416500	-2.70769800	-3.30705100
H	-5.77113400	-0.69992600	-0.46632100
H	-5.52450300	-2.24380500	-2.40382100
C	-1.39895900	0.35604900	1.32853100
C	-1.54334200	1.60131400	1.94533400
C	-1.47034500	-0.78501500	2.13636300
C	-1.73446000	1.70109200	3.32191000
H	-1.51239700	2.51272200	1.35362100
C	-1.65659400	-0.68760300	3.50871800
H	-1.38208800	-1.77092600	1.68505100
C	-1.78826200	0.56018100	4.11117600
H	-1.84433500	2.68475100	3.77385600
H	-1.70159000	-1.59359700	4.10934000
H	-1.93694400	0.63961300	5.18577800
H	-0.64750500	0.75945800	-2.07620300

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

Electronic Energy (0 K) = -1325.263810

Electronic Energy (0 K) + ZPE = -1324.797757

Enthalpy (298 K) = -1324.771938

Free Energy (298 K) = -1324.851626

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

Electronic Energy (0 K) = -1325.566201

Number of imaginary frequencies: 0

C	1.05890600	1.76037100	0.05538700
C	-0.27988800	2.13328500	-0.12351400
C	-1.08544800	0.92120300	-0.21073100
C	-0.25136200	-0.19215800	-0.12148700
C	-2.47476600	0.77665800	-0.34646600
C	-0.79284800	-1.49764500	-0.18791400
C	-2.20822200	-1.65428000	-0.32895400
C	-3.00484800	-0.48979100	-0.40090400
C	-2.74911100	-2.95655500	-0.39700400
H	-3.83063700	-3.06746400	-0.49722800
C	-0.68841700	-3.90784700	-0.23238300
C	-0.04428100	-2.69979700	-0.15108000
H	-0.11209400	-4.83258400	-0.20419200
H	1.03719300	-2.67034700	-0.06213700
C	-0.64560400	3.47672100	-0.17329200
H	-1.68369800	3.76878300	-0.32015300
C	2.03973100	2.72734600	0.20658200
H	3.08081500	2.44843500	0.35913700
C	0.34431500	4.44384100	-0.03037400
H	0.07899700	5.49806800	-0.06644200
C	1.67422200	4.07213400	0.16323600
H	2.43603700	4.83961000	0.28079300
C	-3.59808700	1.75917000	-0.49500400
C	-4.83393500	0.84243200	-0.38383800
H	-3.55448800	2.28482400	-1.45910500
H	-3.61141500	2.52552800	0.29241100
H	-5.54608800	1.00553900	-1.20037700
C	1.20757400	0.23681800	0.05825300
O	-4.34446400	-0.52145500	-0.54348400
N	-2.03183300	-4.05676600	-0.35059800
C	1.72003500	-0.26165800	1.41915800
C	2.58868300	-1.34672400	1.55265900
C	1.24097700	0.34201600	2.58695000
C	2.97380500	-1.80726800	2.80929500
H	2.98540300	-1.83858500	0.66686500
C	1.62249300	-0.11557700	3.84130200
H	0.55639400	1.18553600	2.51255000
C	2.49493200	-1.19365100	3.95947200
H	3.65461400	-2.65273100	2.88269400
H	1.23586100	0.37523300	4.73198300
H	2.79739000	-1.55158100	4.94101000
C	2.10505600	-0.13023600	-1.12792600
C	1.56271600	-0.52280500	-2.35301900

C	3.49404400	0.02996100	-1.04579400
C	2.37858400	-0.76207200	-3.45512800
H	0.48618100	-0.64159600	-2.45220700
C	4.31022500	-0.20933200	-2.14441100
H	3.94845300	0.33498100	-0.10479300
C	3.75576300	-0.60909100	-3.35660900
H	1.92852000	-1.07122300	-4.39611200
H	5.38670300	-0.08199700	-2.05072400
H	4.39387700	-0.79964000	-4.21657500
C	-5.51896400	0.93742400	0.95717800
H	-5.95659800	1.93311300	1.09365100
H	-6.31658700	0.19300900	1.04561600
H	-4.79397400	0.76672900	1.76356700

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

Electronic Energy (0 K) = -1324.179806

Electronic Energy (0 K) + ZPE = -1323.727854

Enthalpy (298 K) = -1323.702027

Free Energy (298 K) = -1323.782278

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

Electronic Energy (0 K) = -1324.481255

**PPh<sub>3</sub>Au<sup>+</sup>**

Number of imaginary frequencies: 0

Au	0.33283400	1.29406900	-1.65323600
P	-0.03076200	-0.10563500	0.13710100
C	1.29571200	0.06762500	1.35095300
C	1.01096500	0.06431000	2.71945100
C	2.62051700	0.12912400	0.90369300
C	2.05671800	0.12380700	3.63487700
H	-0.01797200	0.01336100	3.07143200
C	3.65677200	0.18402500	1.82532900
H	2.83702200	0.12763000	-0.16507300
C	3.37313900	0.18443400	3.18979900
H	1.83968800	0.12377600	4.69986200
H	4.68631000	0.23220300	1.48043300
H	4.18561700	0.23497400	3.91020700
C	-1.59856000	0.28967200	0.94289900
C	-1.88662000	1.62770800	1.23729100
C	-2.47995700	-0.72403400	1.32766900
C	-3.05238900	1.94696200	1.91845100
H	-1.19503000	2.41587300	0.93804900
C	-3.64808200	-0.39268800	2.00673900
H	-2.25735800	-1.76548400	1.10310300
C	-3.93313900	0.93636700	2.29993200

H	-3.27848000	2.98466400	2.14883600
H	-4.33653400	-1.17838800	2.30669900
H	-4.84900700	1.18956300	2.82797100
C	-0.08467100	-1.82692700	-0.40879700
C	0.60091600	-2.81960400	0.29642100
C	-0.87297800	-2.16182300	-1.51616300
C	0.49274200	-4.14544700	-0.11058600
H	1.21316900	-2.56317800	1.15897100
C	-0.97796200	-3.48765600	-1.91080300
H	-1.40875000	-1.38448100	-2.06190200
C	-0.29237100	-4.47774700	-1.20897000
H	1.02527500	-4.92029500	0.43449000
H	-1.59042700	-3.75052000	-2.76921200
H	-0.37050700	-5.51524100	-1.52382100

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

Electronic Energy (0 K) = -1171.340186

Electronic Energy (0 K) + ZPE = -1171.065627

Enthalpy (298 K) = -1171.046653

Free Energy (298 K) = -1171.115977

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

Electronic Energy (0 K) = -1171.518516

**A-Au'**

Number of imaginary frequencies: 0

C	4.45632900	1.85148700	0.40949200
C	2.38209700	2.56358100	-0.58425100
C	2.84011800	3.86546500	-0.46628200
C	4.09945700	4.08013300	0.08781000
N	4.89657800	3.09762300	0.51526200
H	1.40719600	2.34766400	-1.02089100
H	5.10671500	1.04898600	0.76180800
H	2.23483900	4.70327800	-0.80010200
H	4.48613100	5.09357300	0.19170300
C	3.20349300	1.52517600	-0.13452700
C	2.84377300	0.14110000	-0.19804600
C	2.80286700	-1.09400900	-0.17390100
C	3.06269300	-2.53141200	-0.18008100
H	2.49907900	-3.02276500	-0.98329500
H	2.73087000	-2.97114700	0.77164500
O	5.20755800	-2.08704800	0.67305400
H	6.14946700	-2.28860200	0.63392900
C	4.55928200	-2.80082500	-0.35749100
C	4.84128900	-4.28577100	-0.28482000
H	4.86129100	-2.41153300	-1.34650800

H	5.91359200	-4.48071000	-0.40407500
H	4.52765700	-4.68595800	0.68700300
H	4.31808200	-4.83324300	-1.07719600
Au	0.61512000	-0.36974200	-0.08936400
P	-1.70106600	-0.08914100	0.04902500
C	-2.09321500	1.65361000	-0.28632100
C	-3.07163000	2.02554200	-1.20993400
C	-1.38452900	2.63541400	0.41778700
C	-3.33331700	3.37518100	-1.43037600
H	-3.62937900	1.26773300	-1.75788400
C	-1.65433500	3.97890900	0.19528500
H	-0.62596400	2.34532900	1.14703400
C	-2.62694400	4.34807200	-0.73239800
H	-4.09421200	3.66487100	-2.15048300
H	-1.10686100	4.74050300	0.74535900
H	-2.83406800	5.40047600	-0.91038700
C	-2.60922700	-1.07943800	-1.16693100
C	-2.06040700	-1.23228900	-2.44468800
C	-3.86361400	-1.62021400	-0.87395000
C	-2.76726100	-1.91571100	-3.42525600
H	-1.08123900	-0.80771500	-2.67045800
C	-4.56200400	-2.31037000	-1.85919900
H	-4.29616200	-1.50381100	0.11859700
C	-4.01687500	-2.45604000	-3.13068300
H	-2.34125200	-2.03252300	-4.41853000
H	-5.53629100	-2.73515500	-1.63144300
H	-4.56660400	-2.99585100	-3.89769400
C	-2.36709100	-0.47611100	1.68881300
C	-3.42856100	0.25515900	2.22948300
C	-1.83150900	-1.55973700	2.39168300
C	-3.94641500	-0.10018100	3.47006600
H	-3.84961100	1.09907300	1.68464700
C	-2.35691600	-1.91151100	3.62850500
H	-1.00217300	-2.12593400	1.96741100
C	-3.41123000	-1.17925400	4.16741800
H	-4.76919400	0.46933300	3.89451900
H	-1.93817900	-2.75189700	4.17603000
H	-3.81659100	-1.44995700	5.13917300

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

Electronic Energy (0 K) = -1688.626436

Electronic Energy (0 K) + ZPE = -1688.163601

Enthalpy (298 K) = -1688.131241

Free Energy (298 K) = -1688.232103

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

Electronic Energy (0 K) = -1688.931641

**TS<sub>1</sub>-Au'**

Number of imaginary frequencies: 1

C	4.67384600	1.64968800	0.73993600
C	2.87563300	1.98375700	-0.82230600
C	3.15914200	3.33780700	-0.77094300
C	4.21298100	3.76791400	0.03157400
N	4.96200600	2.94440100	0.76784800
H	2.07451300	1.59504400	-1.44941600
H	5.28774700	0.99498000	1.35998400
H	2.58389000	4.05027900	-1.35502900
H	4.46671900	4.82639300	0.08216800
C	3.64101100	1.10673100	-0.03954700
C	3.33110300	-0.29215400	-0.02893100
C	2.51353100	-1.29194400	-0.03426400
C	3.10222700	-2.66645900	-0.01163900
H	2.57036900	-3.36969100	-0.66087400
H	3.02860400	-3.06490000	1.01111000
O	4.97363300	-1.22835100	0.03892000
H	5.63158700	-0.84188800	-0.56070700
C	4.56447500	-2.54102800	-0.44071600
C	5.46313200	-3.60179100	0.13676100
H	4.61677300	-2.51955900	-1.53819600
H	6.49412200	-3.50073100	-0.21616500
H	5.46019000	-3.55135100	1.23114700
H	5.10205400	-4.59177900	-0.16362700
Au	0.49056600	-0.73060800	0.00515900
P	-1.75693700	-0.02993800	0.02678800
C	-1.87007100	1.72493700	-0.44294600
C	-2.86090600	2.20390200	-1.30225900
C	-0.94181400	2.61327100	0.11289000
C	-2.91913700	3.56182800	-1.60247300
H	-3.58754900	1.51996800	-1.73801500
C	-1.01089800	3.96829700	-0.18333200
H	-0.16853400	2.24027100	0.78690300
C	-1.99823500	4.44201300	-1.04449900
H	-3.68920600	3.93217200	-2.27461000
H	-0.29406200	4.65708900	0.25748000
H	-2.04848800	5.50202600	-1.28120200
C	-2.81682100	-0.94082400	-1.13365900
C	-2.27479100	-1.32187300	-2.36555800
C	-4.15573200	-1.21725100	-0.84576000
C	-3.06860200	-1.96715100	-3.30517500

H	-1.22786800	-1.10974300	-2.58603000
C	-4.94393000	-1.86870600	-1.78877500
H	-4.58264600	-0.92625800	0.11295800
C	-4.40247000	-2.24168800	-3.01502000
H	-2.64551600	-2.26286100	-4.26200500
H	-5.98492400	-2.08663900	-1.56319100
H	-5.02248900	-2.75199800	-3.74802300
C	-2.54155300	-0.16634300	1.65934800
C	-3.42168200	0.80947900	2.13363400
C	-2.28194600	-1.30590100	2.42757500
C	-4.03441600	0.64348600	3.37132900
H	-3.63000100	1.69721900	1.53776400
C	-2.90190700	-1.46836200	3.66002900
H	-1.59214500	-2.06520600	2.05728300
C	-3.77524700	-0.49214300	4.13234000
H	-4.71717200	1.40396400	3.74208500
H	-2.69710100	-2.35405800	4.25624000
H	-4.25415800	-0.61661900	5.10059700

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

Electronic Energy (0 K) = -1688.608800

Electronic Energy (0 K) + ZPE = -1688.145184

Enthalpy (298 K) = -1688.115078

Free Energy (298 K) = -1688.209442

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

Electronic Energy (0 K) = -1688.907940

**B-Au'**

Number of imaginary frequencies: 0

C	4.80632400	1.65984500	0.51584100
C	2.71487100	1.92623500	-0.61820100
C	2.89001900	3.29389600	-0.50616600
C	4.04664300	3.77100500	0.10857000
N	4.98981300	2.97376800	0.60765400
H	1.83781600	1.50878100	-1.11287600
H	5.58318400	1.03860000	0.96628500
H	2.15025900	3.98360800	-0.90385300
H	4.21983300	4.84307400	0.19908600
C	3.68834900	1.06931700	-0.08704100
C	3.51424700	-0.37048500	-0.15323200
C	2.52425800	-1.25204100	-0.18966900
C	3.06542700	-2.65568000	-0.17690200
H	2.58294600	-3.29835600	-0.92126000
H	2.87698900	-3.11512000	0.80469000
O	4.84669200	-1.10634900	-0.08891400

H	5.50686900	-0.70753700	-0.68945500
C	4.56179900	-2.55888300	-0.44437600
C	5.45460700	-3.42031100	0.39210700
H	4.78269200	-2.62350700	-1.51595700
H	6.51545700	-3.25271800	0.18330100
H	5.26578300	-3.25046900	1.45752000
H	5.23196500	-4.46989700	0.17038900
Au	0.51783800	-0.72738800	-0.10478700
P	-1.74093800	-0.04093700	0.02876100
C	-1.87556200	1.76514800	-0.17142800
C	-2.87975500	2.36049400	-0.93798800
C	-0.94508800	2.56789000	0.49878800
C	-2.94772900	3.74750800	-1.03379300
H	-3.61018700	1.74428400	-1.46042100
C	-1.02272200	3.95178400	0.40581200
H	-0.16042400	2.10542600	1.10019000
C	-2.02297300	4.54145500	-0.36403000
H	-3.72923600	4.20832200	-1.63294700
H	-0.30147500	4.57093500	0.93443200
H	-2.08114100	5.62441400	-0.44135300
C	-2.81567100	-0.76643600	-1.24658300
C	-2.29270100	-0.93505100	-2.53286000
C	-4.14518000	-1.10562200	-0.98593500
C	-3.09596400	-1.43400300	-3.55068800
H	-1.25294400	-0.67265900	-2.73288600
C	-4.94258900	-1.61207100	-2.00726300
H	-4.55939100	-0.97529200	0.01265500
C	-4.42000100	-1.77466800	-3.28611800
H	-2.68713600	-1.56305600	-4.54986100
H	-5.97635300	-1.87886800	-1.80177600
H	-5.04675200	-2.17149600	-4.08108500
C	-2.51471500	-0.41959400	1.62996900
C	-3.48033300	0.41637500	2.19796700
C	-2.15261400	-1.60461200	2.27773000
C	-4.07701600	0.06379600	3.40345900
H	-3.76679200	1.34124900	1.69890200
C	-2.75497300	-1.95375200	3.48025800
H	-1.39639500	-2.25356200	1.83514100
C	-3.71506600	-1.11797800	4.04342800
H	-4.82568200	0.71664100	3.84530100
H	-2.47040900	-2.87484400	3.98278600
H	-4.18223400	-1.38718600	4.98761300

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

Electronic Energy (0 K) = -1688.614594

Electronic Energy (0 K) + ZPE = -1688.148797

Enthalpy (298 K) = -1688.118944

Free Energy (298 K) = -1688.211922

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

Electronic Energy (0 K) = -1688.912101

**F'-Au'**

Number of imaginary frequencies: 0

C	1.08693800	0.91019400	-3.56155200
C	-0.14792600	0.26560200	-3.52986300
C	-1.15090700	0.78486800	-2.72722700
C	-0.89009400	1.95431100	-2.00492100
C	0.37797500	2.53948000	-2.13770300
N	1.35470300	2.02547800	-2.87705100
H	-2.12469800	0.30263900	-2.67677800
H	1.90059200	0.50834700	-4.16642200
H	-0.30942900	-0.63359100	-4.11795500
H	0.60961500	3.44828800	-1.57956000
C	-1.83296300	2.60098400	-1.10146100
C	-2.64089200	2.11827400	-0.07088800
C	-2.61488800	4.49383700	-0.09066900
C	-3.40275000	3.31590900	0.46102000
H	-1.84652400	4.82785200	0.62110100
H	-3.45899400	3.33664400	1.55397400
H	-4.43384000	3.34552400	0.07830500
O	-1.85832900	3.91702100	-1.21233700
C	-3.42311100	5.65020200	-0.60244600
H	-3.98184600	6.10105100	0.22490400
H	-2.78419600	6.42154100	-1.04305800
H	-4.14135200	5.31324200	-1.35883900
C	-2.63921200	0.82185000	0.48430000
C	-1.77305700	-0.24878100	0.09140800
C	-2.17219900	-1.47539900	-0.33470200
C	-3.50186200	0.54247800	1.65156600
C	-2.98607000	-0.16841100	2.74585900
C	-4.85336100	0.91581100	1.66517000
C	-3.79462500	-0.47491300	3.83105000
H	-1.93487900	-0.45120300	2.74868200
C	-5.66622800	0.57637500	2.73737600
C	-5.13731800	-0.10902100	3.82720800
H	-3.37602400	-1.00629300	4.68228500
H	-6.71957800	0.84509000	2.71964800
H	-5.77323500	-0.36059400	4.67257800
C	-3.56330800	-1.78793800	-0.73846400

C	-4.41536700	-0.83000400	-1.30544500
C	-4.07034300	-3.08118900	-0.53596700
C	-5.72886500	-1.14299700	-1.63519900
H	-4.04606400	0.17423000	-1.50631100
C	-5.38519300	-3.39061400	-0.85434800
H	-3.42605500	-3.84605600	-0.10665700
C	-6.22058400	-2.42334900	-1.40696200
H	-6.36731000	-0.38479500	-2.08368800
H	-5.76018000	-4.39518200	-0.67227500
H	-7.24752300	-2.66991500	-1.66606200
C	-1.17934700	-2.57205800	-0.50088600
C	-0.35414700	-2.97358700	0.55699100
C	-1.03507200	-3.20627400	-1.73961900
C	0.61228000	-3.95793400	0.37315800
H	-0.48513300	-2.51498100	1.53690600
C	-0.06422300	-4.18536900	-1.92725100
H	-1.69311400	-2.92479900	-2.56161500
C	0.76608300	-4.55943900	-0.87339200
H	1.24666700	-4.25312800	1.20710800
H	0.03986700	-4.66342700	-2.89926900
H	1.52367400	-5.32590000	-1.02016400
Au	0.31206700	0.09806100	0.35818700
P	2.67578700	0.12379700	0.44405800
H	-5.28575600	1.42106800	0.80439400
C	3.27141700	-1.06178900	1.69167800
C	2.47417400	-1.33779100	2.80600100
C	4.51562800	-1.68389800	1.55648400
C	2.91675900	-2.23077700	3.77624200
H	1.50271600	-0.85073100	2.90639800
C	4.95157500	-2.57967600	2.52534100
H	5.14058300	-1.47226200	0.68920500
C	4.15268800	-2.85419600	3.63236900
H	2.29421900	-2.44449100	4.64197400
H	5.91753400	-3.06680300	2.41562300
H	4.49557700	-3.55868000	4.38661900
C	3.52041100	1.69725100	0.79602200
C	3.46171500	2.72889200	-0.15018300
C	4.15703800	1.91297700	2.02022100
C	4.04366300	3.95866400	0.13108000
H	2.98518800	2.56025100	-1.11763400
C	4.73015700	3.15074100	2.29615400
H	4.21046600	1.11560200	2.75979800
C	4.67387000	4.17225900	1.35498800
H	4.00854400	4.75311200	-0.61095000

H	5.22699800	3.31275900	3.24981600
H	5.12631500	5.13705900	1.57231700
C	3.31848600	-0.49414900	-1.14745700
C	4.48432800	-0.01321200	-1.74647200
C	2.60417200	-1.53245200	-1.75608100
C	4.92161800	-0.56035800	-2.94982800
H	5.05172200	0.79059100	-1.28029700
C	3.05153300	-2.08326900	-2.95008900
H	1.69318100	-1.91511600	-1.29246100
C	4.20839900	-1.59297100	-3.55146500
H	5.82685100	-0.17873400	-3.41616700
H	2.49009000	-2.89350800	-3.41184900
H	4.55697900	-2.01783800	-4.49008200

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

Electronic Energy (0 K) = -2496.709794

Electronic Energy (0 K) + ZPE = -2495.962642

Enthalpy (298 K) = -2495.915232

Free Energy (298 K) = -2496.046752

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

Electronic Energy (0 K) = -2497.189582

### TS<sub>3</sub>-Au'

Number of imaginary frequencies: 1

C	-0.11762200	2.18513600	3.42000500
C	-1.31072300	1.83834300	2.85370700
C	-1.54569700	0.47687800	2.45985200
C	-0.48981600	-0.44386700	2.81926700
C	0.70911400	0.05993800	3.38418900
N	0.91268800	1.32468700	3.66926700
H	-2.56198300	0.10365900	2.59597000
H	0.05010800	3.21513700	3.73356600
H	-2.09044400	2.58584000	2.73477700
H	1.52837600	-0.63810700	3.57440900
C	-0.58804200	-1.75598500	2.34697500
C	-1.36365500	-2.15182900	1.23046400
C	0.18059300	-3.83546700	1.83437800
C	-1.11509300	-3.62812500	1.05309700
H	1.05242500	-3.69129400	1.17495300
H	-1.01950900	-3.93469100	0.00577600
H	-1.92514200	-4.22782800	1.49581700
O	0.22499200	-2.71494700	2.77723700
C	0.28948800	-5.11791100	2.60549600
H	0.27103900	-5.96849800	1.91576800
H	1.22150500	-5.16231000	3.17685200

H	-0.55162400	-5.21960300	3.30066000
C	-1.86991900	-1.24236000	0.30621900
C	-1.82834600	0.20258800	0.49888600
C	-2.83778000	1.06139400	0.09665700
C	-2.36808500	-1.74902500	-0.99758500
C	-1.96576300	-1.19555700	-2.22079900
C	-3.33324800	-2.76293300	-1.00474600
C	-2.51100800	-1.65132700	-3.41357600
H	-1.21447400	-0.40490600	-2.23978700
C	-3.89651500	-3.19761600	-2.19871700
C	-3.48393500	-2.64719700	-3.40672600
H	-2.17603200	-1.22226900	-4.35493600
H	-4.66231500	-3.96938000	-2.18167200
H	-3.91780900	-2.99305800	-4.34167200
C	-4.20690000	0.56375000	-0.15156500
C	-4.80676000	-0.37464600	0.69776300
C	-4.92563100	1.01489000	-1.26772200
C	-6.09175800	-0.83902300	0.44768400
H	-4.26467700	-0.74760300	1.56597700
C	-6.19306100	0.51803500	-1.53950000
H	-4.46967200	1.74514700	-1.93432400
C	-6.78326700	-0.40368000	-0.67833300
H	-6.55052300	-1.55124700	1.12965200
H	-6.72711800	0.85674900	-2.42398400
H	-7.78163700	-0.78147100	-0.88501100
C	-2.64923600	2.51644100	0.06405200
C	-1.46033500	3.13083800	-0.35986100
C	-3.67364100	3.34779500	0.55885800
C	-1.27974900	4.50415300	-0.25286800
H	-0.67613500	2.53028600	-0.82308300
C	-3.48852800	4.71717100	0.67759500
H	-4.60790000	2.90150400	0.89290400
C	-2.28814100	5.30119200	0.27788800
H	-0.35152100	4.95250600	-0.60003000
H	-4.28499800	5.33393100	1.08667400
H	-2.14673800	6.37558100	0.36582500
Au	0.28897500	0.46042900	-0.07983200
P	2.55781800	0.21189200	-0.61053400
H	-3.67798500	-3.18293000	-0.06123600
C	2.79281900	-1.27624700	-1.62816800
C	1.83830600	-2.29632600	-1.56770000
C	3.94581100	-1.44801900	-2.39930100
C	2.03558700	-3.48041000	-2.26915700
H	0.93682500	-2.15491800	-0.96692100

C	4.13716100	-2.63249500	-3.10142900
H	4.69450100	-0.65816000	-2.44927700
C	3.18506700	-3.64647200	-3.03616800
H	1.28719500	-4.26863200	-2.22465000
H	5.03337100	-2.76515000	-3.70212700
H	3.33946900	-4.57000000	-3.58890100
C	3.53353000	-0.06213500	0.89963700
C	3.60007200	0.97073700	1.84183600
C	4.12173800	-1.29868100	1.18027600
C	4.26651500	0.77441400	3.04405900
H	3.12203500	1.92976600	1.63991500
C	4.78139400	-1.49042700	2.39084800
H	4.07087200	-2.11085800	0.45646400
C	4.85568900	-0.45733300	3.31947400
H	4.30260100	1.57740500	3.77560300
H	5.24246700	-2.45158800	2.60528700
H	5.36980900	-0.61305900	4.26487400
C	3.31945600	1.59158400	-1.51084800
C	4.64069700	1.98483800	-1.28310200
C	2.55879000	2.23657400	-2.49185500
C	5.19196700	3.01885100	-2.03225400
H	5.23673900	1.48711200	-0.51975700
C	3.11747500	3.26398700	-3.24132500
H	1.52806300	1.92621100	-2.67007000
C	4.43310600	3.65673100	-3.00851700
H	6.21904900	3.32614900	-1.85168500
H	2.52544700	3.76239900	-4.00480400
H	4.86855900	4.46571700	-3.58987600

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

Electronic Energy (0 K) = -2496.676062

Electronic Energy (0 K) + ZPE = -2495.930455

Enthalpy (298 K) = -2495.883862

Free Energy (298 K) = -2496.011772

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

Electronic Energy (0 K) = -2497.152412

**G'-Au'**

Number of imaginary frequencies: 0

C	-0.79586100	2.42039400	3.88910000
C	-1.70997500	1.85302800	3.08317200
C	-1.59682000	0.42921000	2.63663700
C	-0.32550700	-0.17473500	3.18435900
C	0.53925800	0.57712900	4.04340400
N	0.36946400	1.81835100	4.36674600

H	-2.44650700	-0.10792500	3.12228400
H	-0.95108700	3.44203300	4.23363200
H	-2.60951900	2.41090800	2.84369500
H	1.43084800	0.06597500	4.41769500
C	-0.08084800	-1.45882000	2.81761800
C	-0.89244800	-2.12325600	1.83783300
C	0.96362200	-3.44352600	2.44461500
C	-0.42761000	-3.54789100	1.81171800
H	1.72001400	-3.25869800	1.66276100
H	-0.40655900	-3.99296100	0.81056400
H	-1.08305600	-4.17870100	2.43251100
O	0.91826600	-2.23686700	3.25942000
C	1.36691400	-4.59828500	3.31504400
H	1.41601900	-5.51755400	2.72097100
H	2.34964100	-4.43073100	3.76630400
H	0.63557200	-4.74502500	4.11817900
C	-1.75288000	-1.46269500	1.00560700
C	-1.88526900	0.02122800	1.17831400
C	-2.38728300	0.90040000	0.19814700
C	-2.33731400	-2.30421600	-0.07945800
C	-1.79770500	-2.34113900	-1.36832400
C	-3.35212700	-3.20652900	0.25076800
C	-2.28443300	-3.23535400	-2.31471100
H	-0.99277000	-1.65587700	-1.63558800
C	-3.84303800	-4.09819600	-0.69707200
C	-3.31237600	-4.11353500	-1.98276500
H	-1.85324400	-3.24612600	-3.31360500
H	-4.63925800	-4.78764500	-0.42632700
H	-3.69372200	-4.81322600	-2.72256600
C	-3.18724400	0.44500300	-0.97907800
C	-4.37719400	-0.26180800	-0.78999800
C	-2.82701400	0.83583400	-2.27261100
C	-5.17211600	-0.60588800	-1.87730800
H	-4.67989200	-0.54057700	0.21881800
C	-3.60805500	0.46984900	-3.36137000
H	-1.92053700	1.42450300	-2.42272200
C	-4.78080000	-0.25474400	-3.16535900
H	-6.09417500	-1.15941300	-1.71618300
H	-3.30826500	0.76149500	-4.36514400
H	-5.39693900	-0.53261200	-4.01706100
C	-2.50825000	2.38676800	0.37581700
C	-1.42737700	3.27006300	0.47689500
C	-3.80516600	2.91713100	0.43873500
C	-1.63395300	4.63143500	0.67702500

H	-0.40485700	2.89236600	0.41863200
C	-4.01091000	4.27057200	0.66462000
H	-4.66145200	2.25329700	0.33531800
C	-2.92444600	5.13357600	0.78728300
H	-0.77808000	5.29719500	0.75576700
H	-5.02511500	4.65524900	0.73887500
H	-3.08574300	6.19543500	0.95587200
Au	-0.04284100	0.48735700	-0.22600200
P	2.19036300	0.29979000	-0.88433400
H	-3.76086300	-3.20307600	1.26093800
C	2.46816900	-1.17078500	-1.90895700
C	1.79060800	-2.34301500	-1.55498400
C	3.34052700	-1.17352400	-2.99827200
C	1.97829600	-3.50791200	-2.28559500
H	1.10920500	-2.33582600	-0.70216900
C	3.52519700	-2.34467400	-3.72819200
H	3.87260900	-0.26698700	-3.28222500
C	2.84564500	-3.50620800	-3.37613300
H	1.43882200	-4.41195500	-2.01048100
H	4.20177600	-2.34645100	-4.57903000
H	2.99082900	-4.41525100	-3.95446300
C	3.20428300	0.09251000	0.60907600
C	3.03801500	1.01570800	1.64824200
C	4.11024000	-0.96116900	0.74737300
C	3.77393500	0.88371100	2.81817100
H	2.32409300	1.83565100	1.54630200
C	4.83722000	-1.09249200	1.92732900
H	4.24799500	-1.68002900	-0.05929400
C	4.66907300	-0.17490500	2.95895200
H	3.63477700	1.60092500	3.62394800
H	5.54193500	-1.91307000	2.03716400
H	5.23651400	-0.28413700	3.87985500
C	2.82001500	1.74895900	-1.76766600
C	4.18034100	2.07199800	-1.72980700
C	1.93373800	2.53316700	-2.51224100
C	4.64671400	3.17203100	-2.43931900
H	4.87065100	1.46638600	-1.14337100
C	2.40767300	3.63065000	-3.22124600
H	0.87079000	2.28597200	-2.53005400
C	3.76195400	3.94889400	-3.18291100
H	5.70308000	3.42628800	-2.40881800
H	1.71864500	4.24264900	-3.79753800
H	4.12992700	4.81229500	-3.73170200

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

Electronic Energy (0 K) = -2496.691791

Electronic Energy (0 K) + ZPE = -2495.943449

Enthalpy (298 K) = -2495.897253

Free Energy (298 K) = -2496.023212

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

Electronic Energy (0 K) = -2497.169449