Supporting Information for

Mechanistic Insights into Synergistic Catalysis by Au(I), Ga(III), and Counterions in Nakamura Reaction.

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Table S1: NBO charges on C1 and C2 of the Au/Ga stabilized reactant complex for the terminal alkynes **1a** – **1f**.

Entry	NBO charge (C_1)	NBO charge (C_2)
1a (**R** = C_6H_5)	-0.06	-0.24
1b (**R** = 4-FC_6H_4)	-0.06	-0.24
1c (**R** = 4-OMe C_6H_4)	-0.04	-0.26
1d (**R** = CH_3)	-0.03	-0.27
1e (**R** = C_2H_5)	-0.01	-0.28
1f (**R** = $CH(CH_3)_2$	-0.003	-0.280

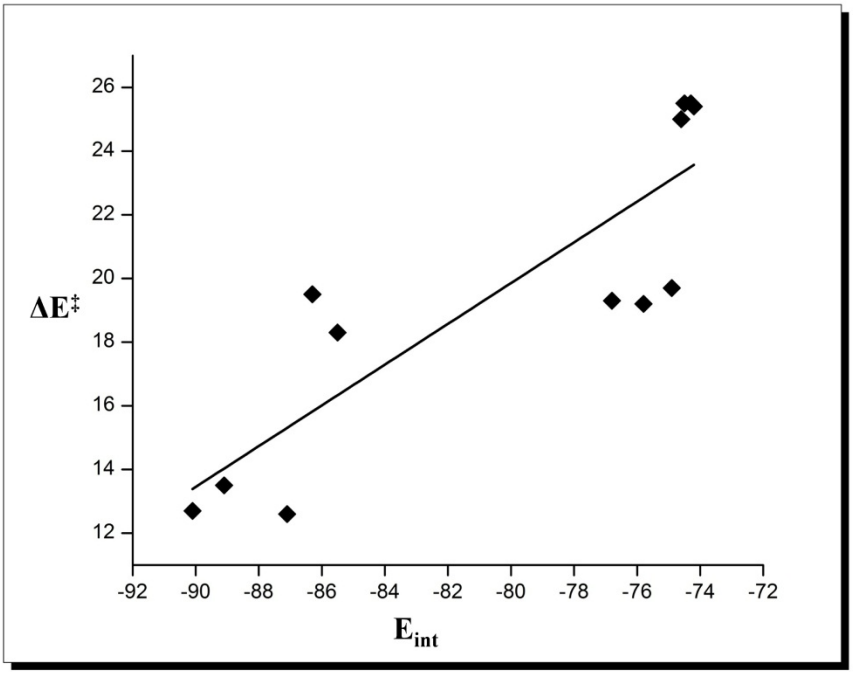

*Figure S1. Linear fitting of the activation energy ($\Delta E^{\ddagger}$) with respect to interaction energy (E_{int}), (R^2= 0.71) for both transition state (TS (C1) and TS (C2)) of each alkyne (**1a - 1f**). Energies are in kcal/mol.*

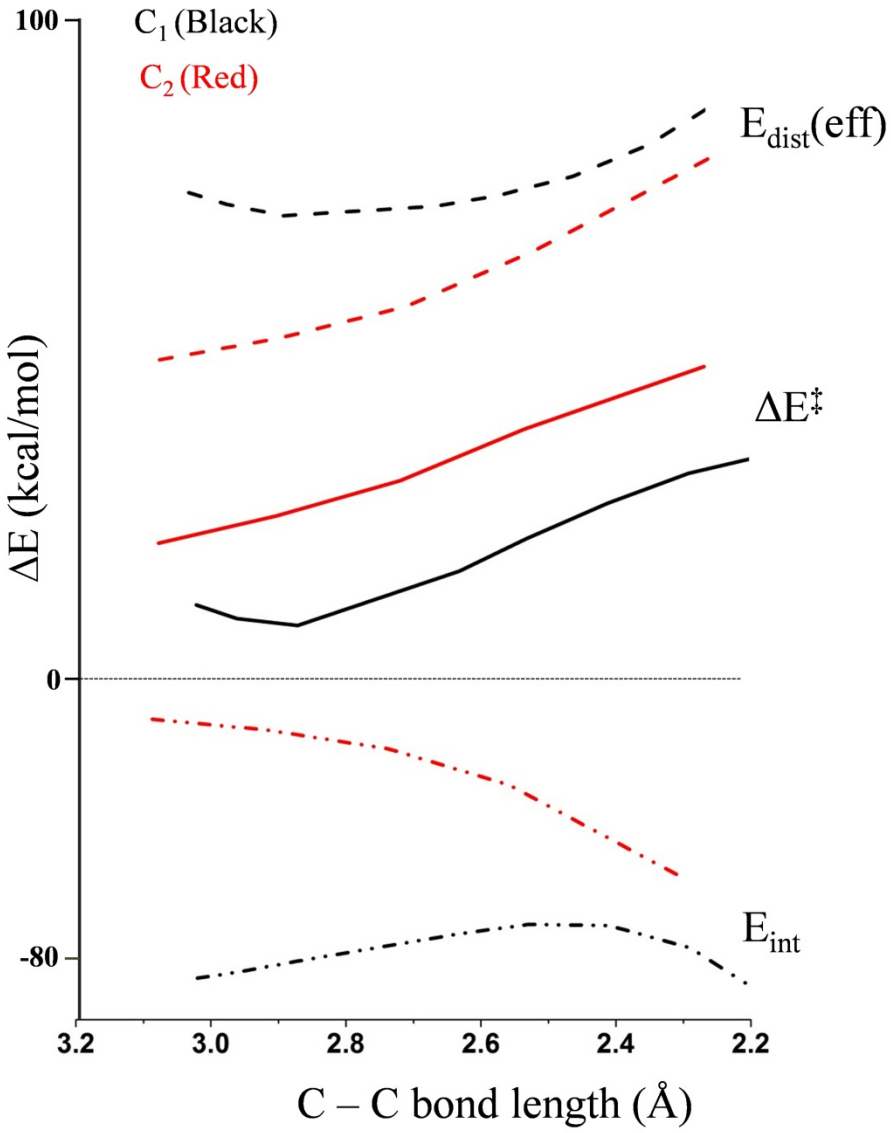

Figure S2. Interaction energy (E_{int}), effective distortion energy (E_{dist} (eff)) and activation energy ($\Delta E^{\ddagger}$) for two TS (C1 attack and C2 attack) are plotted along the reaction coordinate defined between the anionic carbon of the dianion and C1/C2. Black lines are shown for the TS (C_1) and red for TS (C_2).

Distortion and interaction energies calculated along the reaction coordinate

Fig S2 depicts the changes of distortion energy, interaction energy, and the activation energy for the isomeric transition states calculated along the reaction coordinate. These results are in good agreement with those obtained from single point calculations at the TS geometry.

Coordinates, electronic energies (E), zero–point energy correction to electronic energy (E_{ZPE}), zero–point energy correction to Gibb's free energies (G_{ZPE}), and zero–point energy corrected enthalpies (H_{ZPE}) at 298.15 K, and low energy vibrational frequencies for all systems optimized at MO62X/6-31+G(d), LANL2dZ (for Au and Ga) (BS1) level of theory and single point at M062x/TZVP, LANL2TZ (f) (for Au) level of theory

4a)

E_{elec}(BS1) = -3231.4268522 Hartree E_{ZPE} = 0.870193 Hartree H_{ZPE} = 0.915910 Hartree G_{ZPE} = 0.789011 Hartree

E_{elec}(BS2)= -2158.6973459 Hartree

Low frequencies (cm^{-1}) 5.3159 14.5583 15.6891 25.0093 33.3453 36.4507 43.9586 52.8353 62.4188

Au	2.39451400	-0.28090900	0.24991700
P	0.09772300	-0.33073200	-0.04694200
N	4.53573400	-0.23187500	0.52815900
N	5.14787400	-1.14514900	1.20756500
N	6.43458400	-0.84471800	1.21480400
H	7.06653800	-1.46207200	1.70890500
C	5.43531600	0.70164600	0.07067000
C	5.26329800	1.86427000	-0.69732100
H	4.28044100	2.16805700	-1.04362200
C	6.40190400	2.58477700	-0.98002000
H	6.32858900	3.49163800	-1.56970300
C	7.68034200	2.17374000	-0.51946000
H	8.54326900	2.77986400	-0.77193000

C	7.86096300	1.03466300	0.23536700
H	8.83882100	0.72523600	0.58475000
C	6.69808400	0.30352200	0.52104200
C	-0.68490100	-1.17036400	1.38832900
C	0.17663500	-1.97890900	2.14862400
H	1.23552700	-2.01411000	1.90866600
C	-0.28856700	-2.75375600	3.20397300
H	0.40388300	-3.36800500	3.76932900
C	-1.64000000	-2.72651900	3.52510900
H	-2.02357200	-3.32067100	4.34807700
C	-2.50230800	-1.92482600	2.78589100
H	-3.55811800	-1.89154000	3.03804700
C	-2.05869200	-1.14101000	1.71324600
C	-3.09619100	-0.30902300	1.02062000
C	-3.87825100	-0.86644400	-0.01310400
C	-4.89766500	-0.09476100	-0.57305300
H	-5.50953200	-0.52123700	-1.36347300
C	-5.16525800	1.20454200	-0.14262400
C	-4.38830900	1.72557600	0.89025100
H	-4.60421800	2.73061300	1.24430800
C	-3.36561100	0.99159100	1.49458500
C	-0.54893900	1.39893000	-0.33663300
C	0.62174600	2.36220500	-0.62411500
C	-1.62952800	1.51309900	-1.42780400
H	-0.99591800	1.68556600	0.62315900
C	0.13576100	3.80277600	-0.80747600
H	1.14591700	2.03328200	-1.53481800
H	1.34898600	2.32155500	0.19621400
C	-2.09743000	2.96408700	-1.58148600
H	-1.22017300	1.17994300	-2.38974800
H	-2.48429200	0.87285100	-1.19998400
C	-0.93257100	3.90084200	-1.89476000
H	0.98986700	4.44673000	-1.04181000
H	-0.27852400	4.16298600	0.14371100
H	-2.85188300	3.01109600	-2.37335900
H	-2.59291900	3.28199100	-0.65442700
H	-1.28443600	4.93283700	-1.98812600
H	-0.49289400	3.62481300	-2.86325800
C	-0.25212800	-1.37523600	-1.53003900
C	0.58298600	-0.91366400	-2.73816900
C	0.03673400	-2.85799400	-1.24195200
H	-1.32144200	-1.25071700	-1.75332500

C	0.25290700	-1.75773300	-3.97283600
H	1.64836000	-1.03994100	-2.49234000
H	0.43467800	0.14990300	-2.95043200
C	-0.26301700	-3.71690300	-2.47474300
H	1.09891600	-2.96362000	-0.97008000
H	-0.54417000	-3.21203900	-0.38427100
C	0.51500300	-3.23970400	-3.70183100
H	0.84601700	-1.41108600	-4.82492100
H	-0.80302700	-1.61157100	-4.23827200
H	-0.03045500	-4.76360400	-2.25514500
H	-1.33877900	-3.66742000	-2.68695700
H	0.24713300	-3.83988500	-4.57659400
H	1.58987000	-3.38860200	-3.53065000
C	-3.68548000	-2.30093100	-0.48680700
C	-3.88688600	-2.47000000	-1.99730500
C	-4.63943100	-3.24278100	0.26268400
H	-2.65936300	-2.60482200	-0.24528800
H	-3.29951200	-1.75072100	-2.57961700
H	-3.59802900	-3.48087600	-2.30047100
H	-4.93706200	-2.34339300	-2.27788700
H	-4.46662500	-3.21796400	1.34143900
H	-5.67864400	-2.94947500	0.07916500
H	-4.50952800	-4.27400200	-0.08053000
C	-6.29775100	2.00884900	-0.75094200
C	-7.65423400	1.36497500	-0.43755300
C	-6.11927200	2.18853600	-2.26255600
H	-6.27906000	3.00288200	-0.28626500
H	-7.79770400	1.24669200	0.64042200
H	-8.46955600	1.98044800	-0.82954800
H	-7.73048300	0.37423700	-0.89959900
H	-5.16572900	2.67236200	-2.49480000
H	-6.14421100	1.22236100	-2.77882200
H	-6.92527300	2.80493900	-2.67191300
C	-2.63017000	1.57602500	2.69545200
C	-3.40053700	1.26207900	3.98722100
C	-2.39999000	3.08868600	2.60103200
H	-1.64904000	1.08997300	2.76787500
H	-3.50829000	0.18589300	4.14266400
H	-2.88143200	1.68231300	4.85435400
H	-4.40288300	1.70107900	3.94232600
H	-1.95730200	3.38424000	1.64393100
H	-3.33502500	3.64474900	2.72057200

H	-1.72887500	3.41207800	3.40206100

4b)

Eelec(BS1) = -1414.4964726 Hartree EZPE = 0.362987 Hartree HZPE = 0.387414 Hartree GZPE = 0.304945 Hartree

Eelec(BS2)= -1414.8440791 Hartree
Low frequencies (cm-1) 7.3306 15.0823 21.1691 38.4228 57.3150 57.9177 76.2393 86.5125 94.2254

Au	-0.95889400	-0.59662500	-0.31442200
P	1.33700700	-0.66737300	-0.33338600
N	-3.10874300	-0.57128300	-0.26985200
N	-3.78529500	-1.38462100	-1.01415800
N	-5.06651500	-1.15778300	-0.79129200
H	-5.74487000	-1.71391300	-1.29701700
C	-3.95975000	0.21791000	0.46802200
C	-3.71651900	1.23483000	1.40508700
H	-2.70560500	1.52929500	1.66739100
C	-4.82537500	1.82883800	1.96524400
H	-4.69640400	2.61999900	2.69529300
C	-6.14338400	1.43457800	1.61460700
H	-6.97974100	1.93721700	2.08785100
C	-6.39426900	0.43778200	0.69645700
H	-7.40175400	0.13964400	0.43160200
C	-5.26166600	-0.16475800	0.12806100
C	1.90985800	-1.80340500	-1.64507800
H	2.98470600	-1.97447800	-1.55659800
C	1.93526300	-1.40643100	1.22841600
H	2.98302200	-1.70606100	1.15689200
C	2.04559500	0.98999200	-0.62544500
C	1.20765000	1.92795200	-1.24581100
H	0.19981900	1.64395700	-1.53733200
C	1.64267100	3.22448000	-1.49386400
H	0.98100000	3.93252000	-1.98090700
C	2.92087100	3.60689300	-1.09996100

H	3.26680000	4.62027200	-1.27502600
C	3.76119900	2.68499900	-0.48424100
H	4.76430000	2.97335200	-0.18519400
C	3.35162100	1.36920800	-0.25392100
C	4.31445000	0.42231200	0.37492800
C	4.94610800	-0.55892400	-0.39490500
C	5.80964600	-1.47461500	0.20275100
H	6.29861600	-2.23158200	-0.40200400
C	6.05809600	-1.40587400	1.57234100
C	5.46247100	-0.40446800	2.33740100
H	5.67084500	-0.33590900	3.40012300
C	4.59916000	0.51018900	1.74043100
H	4.77584300	-0.58620200	-1.46800400
H	4.12569000	1.28683300	2.33497600
H	6.72926800	-2.11931100	2.03892000
H	1.81436000	-0.69247000	2.04635100
H	1.31332300	-2.28300800	1.43037900
H	1.37972400	-2.75395000	-1.54005300
H	1.68031000	-1.37539200	-2.62355400

4c)

Eelec(BS1) = -1018.7155527 Hartree EZPE = 0.252765 Hartree HZPE = 0.269632 Hartree GZPE = 0.207273 Hartree

Eelec(BS2)= -1018.9320104 Hartree

Low frequencies (cm-1) 32.6975 54.9085 60.0658 80.2058 93.0533 120.9003 161.5588 171.4837 205.3845

Au	2.45129500	-0.36593400	-0.20007900
P	0.24153000	-0.49821500	0.36421600
C	0.13924800	-1.12327900	2.07149300
H	-0.90497500	-1.33383500	2.31635600
C	-0.51489800	-1.76362100	-0.70804800
H	-1.49531400	-2.05789500	-0.32455100
C	-0.50467900	1.15136400	0.21827900
C	0.34482400	2.26286100	0.32104100

H	1.40817200	2.12550400	0.49933300
C	-0.15648100	3.55146700	0.19133100
H	0.51143600	4.40135800	0.27668600
C	-1.51180900	3.73938100	-0.06589300
H	-1.90921200	4.74178300	-0.18526800
C	-2.36152500	2.64238000	-0.16382800
H	-3.42192600	2.78476400	-0.34766700
C	-1.88424700	1.33920700	-0.00670000
C	-2.84050100	0.20044700	-0.07024000
C	-3.19626200	-0.48388000	1.09674700
C	-4.04347200	-1.58835100	1.03263800
H	-4.32201100	-2.11096800	1.94203900
C	-4.54854300	-2.00691100	-0.19738500
C	-4.22868000	-1.30310100	-1.35782500
H	-4.63922500	-1.61461900	-2.31263300
C	-3.38302300	-0.19889200	-1.29489700
H	-2.83167600	-0.12758600	2.05709400
H	-3.12420200	0.34680300	-2.19826000
H	-5.20730900	-2.86734700	-0.24876000
H	-0.61834900	-1.37462200	-1.72323600
H	0.15381700	-2.62850300	-0.71877100
H	0.72637600	-2.04188900	2.15092300
H	0.53942500	-0.37538700	2.75944600

Ga Cycle:

5)

E_{elec}(BS1) = -3231.4268522 Hartree E_{ZPE} = 0.218196 Hartree H_{ZPE} = 0.253417 Hartree G_{ZPE} = 0.149976 Hartree

E_{elec}(BS2)= -5155.0883481 Hartree

Low frequencies (cm^{-1}) 26.0535 28.4277 30.3884 41.0241 45.9543 49.4194 55.3734 62.9580 69.1997

C	2.21043900	-2.64800600	0.75943800

C	1.91532300	-1.64392100	1.85506900
C	2.74935600	-1.71672800	3.09096400
H	2.96103000	-2.18387400	0.10185900
H	2.56549700	-0.84116500	3.71255500
H	2.49418800	-2.62863100	3.64318300
O	1.03650400	-0.79611700	1.75918600
C	1.05034300	-3.01744700	-0.13221800
O	0.18928400	-2.20594000	-0.43384900
Ga	-0.06247200	-0.21658500	0.15662000
O	-1.67653500	-1.20327400	1.18577800
O	1.49941200	-0.01884200	-0.85131000
S	2.50123600	1.17147200	-0.90073000
O	2.66812500	1.67920100	-2.23513100
O	2.36772600	2.01900800	0.26231800
S	-2.62983100	-0.85542000	0.08043600
O	-3.80977700	-0.09670300	0.38456200
O	-1.68326000	-0.32035900	-0.98551900
C	-3.24014700	-2.45202300	-0.60033500
C	4.02420600	0.20026700	-0.56463800
F	-3.91723500	-2.21097900	-1.70763700
F	-4.03070800	-3.01000600	0.30233900
F	-2.23401700	-3.27425300	-0.86572700
F	5.09492800	0.94639800	-0.74238800
F	4.01401800	-0.24030300	0.70871100
F	4.10073000	-0.87567500	-1.35345800
H	3.80688400	-1.77955100	2.81645900
H	2.67775300	-3.54030200	1.18456700
C	0.99726000	-4.41040500	-0.67237500
H	1.95205900	-4.66352200	-1.14519300
H	0.84746100	-5.11257100	0.15556100
H	0.18106800	-4.49919800	-1.38826300
O	-0.50076600	1.36538100	0.99622300
S	-0.54611000	2.73154700	0.24782300
O	-0.01914100	3.79342100	1.06465200
O	-0.12790000	2.52318700	-1.12927800
C	-2.36492800	3.00953400	0.18459800
F	-2.58248700	4.28921700	-0.08720700
F	-2.91283100	2.70745100	1.35180000
F	-2.90511900	2.26392800	-0.76648800

6)

E_{elec}(BS1) = -4192.7751424 Hartree E_{ZPE} = 0.248022 Hartree H_{ZPE} = 0.291979 Hartree
G_{ZPE} = 0.165732 Hartree

E_{elec}(BS2)= -6116.7002027 Hartree

Low frequencies (cm^{-1}) 11.9806 17.0156 19.5014 22.1621 31.5364 35.0642 37.0984 42.1584 46.9403

C	1.89655700	1.04441100	0.40095900
C	0.92167100	1.34058400	1.49254600
C	1.42569800	2.10410100	2.66914100
H	2.77807600	1.68927300	0.44294200
H	0.70826100	2.05760800	3.48734900
H	2.40851900	1.72494500	2.96323500
O	-0.25804900	0.98163600	1.46940000
C	1.33848100	0.99258000	-0.98829200
O	0.19472500	0.58277300	-1.20911300
Ga	-1.18585000	-0.07415400	0.08500600
O	0.30371200	-1.55937000	0.57978200
O	-2.31388500	1.18069400	-0.70801500
S	-2.60407700	2.63688400	-0.31341300
O	-3.77682900	3.12638600	-0.99513200
O	-2.37542900	2.89640400	1.09135300
S	-0.26030000	-2.52989900	-0.41630500
O	-0.65239900	-3.84259500	0.02094700
O	-1.29510900	-1.68588700	-1.13500200
C	1.08859800	-2.78832200	-1.63994100
C	-1.18609700	3.47194300	-1.14606000
F	0.62571300	-3.53622600	-2.63215200
F	2.08573600	-3.40741000	-1.03822000
F	1.50414900	-1.62837500	-2.12303200
F	-1.40961700	4.77772700	-1.20554800
F	-0.05388700	3.28109100	-0.43894100
F	-0.98524000	3.00739400	-2.37119600
H	1.55771900	3.14609900	2.35218200
H	2.30207600	0.02737000	0.57378800
C	2.20918600	1.38647900	-2.12202400
H	2.75160200	2.30724800	-1.89717900
H	2.97276200	0.60074900	-2.20083400
H	1.61800300	1.45802100	-3.03470200
O	-2.28951100	-0.86018600	1.36606700
S	-3.81408400	-0.78117300	1.58767300
O	-4.17514200	-1.51459300	2.77920800
O	-4.33882100	0.54700800	1.35193900
C	-4.37457200	-1.79713400	0.16786400
F	-5.69244300	-1.96150600	0.23076500
F	-3.78687300	-2.98583300	0.18919000
F	-4.06937500	-1.18096500	-0.96900500
O	3.99093200	-0.76246000	-0.60445900
S	5.13522800	0.11654100	-0.28301300
O	6.42294800	-0.27775100	-0.83659700
O	4.80465100	1.55246800	-0.35112300
C	5.32498500	-0.14797800	1.52260600

F	6.28427700	0.62248200	2.03128000
F	4.17527900	0.16629800	2.16128700
F	5.60613000	-1.41538500	1.80825600

TS1)

E_{elec}(BS1) = -4192.769360242 Hartree E_{ZPE} = 0.248022 Hartree H_{ZPE} = 0.291979 Hartree G_{ZPE} = 0.165732 Hartree

E_{elec}(BS2)= -6116.6943159 Hartree

Low frequencies (cm^{-1}) -829.5346 17.5750 28.1130 30.5750 35.2131 37.9151 46.5830 49.3364 53.8710

C	-1.23904200	0.66859400	-2.00282300
C	-0.58479600	-0.53585000	-2.21320700
C	-0.84886900	-1.35274600	-3.44401200
H	-1.93292600	1.02126100	-2.75334500
H	-1.21387700	-2.33789200	-3.13843200
H	-1.57677100	-0.87957800	-4.10435000
O	0.27645800	-1.06503300	-1.41719600
C	-1.02499900	1.45824600	-0.86231000
O	-0.25637700	1.13201200	0.09582500
Ga	0.97900700	-0.33746500	0.14240400
O	-1.89395800	-1.35288300	0.69838600
O	2.40230300	0.87190500	0.42493200
S	2.79423000	1.92260800	-0.62374800
O	4.21889500	1.96346700	-0.85463900
O	1.85510300	1.92871100	-1.73481400
S	-1.21492300	-1.32809300	2.01153600
O	-1.36555600	-2.47426000	2.87473000
O	0.21385800	-0.86938600	1.83990000
C	-2.00459500	0.06214700	2.91830300
C	2.43605200	3.44911000	0.32675200
F	-1.54903000	0.08904200	4.16419700
F	-3.31676300	-0.16951400	2.93983900
F	-1.77353500	1.22561700	2.34380200
F	2.78484900	4.50769800	-0.40367100
F	1.14136600	3.54309700	0.61391600
F	3.12877700	3.46574200	1.45953700
H	0.09795100	-1.50196300	-3.97089300
H	-3.45221400	-1.48420700	0.60338800
C	-1.67972400	2.80067400	-0.73483400
H	-0.93106500	3.55614000	-0.99752000
H	-2.54539900	2.89309700	-1.39184400
H	-1.98159400	2.95460600	0.30227900
O	2.16370300	-1.84971800	0.29679800

S	3.20713900	-2.07034100	-0.80175400
O	3.23764900	-3.43930200	-1.27330600
O	3.19395100	-0.97208300	-1.75725500
C	4.74403000	-1.86358100	0.17322900
F	5.79506200	-2.03363900	-0.62717000
F	4.79752300	-2.77497100	1.14190800
F	4.80188000	-0.65674000	0.71213400
O	-4.46112900	-1.40966000	0.48100900
S	-4.81634500	0.01128100	-0.07505600
O	-6.20329500	0.28936900	0.19825000
O	-3.77064100	0.96361400	0.22323200
C	-4.69901900	-0.32940800	-1.88053300
F	-4.55067200	0.82111800	-2.53011200
F	-3.65848500	-1.11232700	-2.13168500
F	-5.80284600	-0.92784200	-2.30377300

TS2)

E_{elec}(BS1) =-3231.3889801 Hartree E_{ZPE} = 0.213515 Hartree H_{ZPE} = 0.248182 Hartree G_{ZPE} = 0.145421 Hartree

E_{elec}(BS2)= -5155.0533072 Hartree

Low frequencies (cm^{-1}) -1129.1506 16.6450 27.1796 32.8754 42.5706 47.1594 50.9275 61.6106 67.2142

C	2.27111500	-2.31994000	0.77630300
C	1.93258900	-1.57652600	1.97399000
C	2.83540500	-1.63786000	3.16393600
H	2.22668800	-1.15408600	-0.05431900
H	2.57096200	-0.85266000	3.87141600
H	2.72988000	-2.61797100	3.64169400
O	0.91239600	-0.85225000	2.03703400
C	1.17816500	-2.88249900	0.01606800
O	0.11183200	-2.24854100	-0.13813700
Ga	-0.17330300	-0.38492200	0.48158500
O	-1.91873500	-1.07931300	1.32409200
O	1.67316900	-0.18817300	-0.53797300
S	2.65714000	1.04362300	-0.89185300
O	2.63224900	1.30368000	-2.30189200
O	2.57598600	2.04591700	0.13652700
S	-2.73826300	-0.79511800	0.08751500
O	-3.91762600	0.01288900	0.21183500
O	-1.65803800	-0.36167500	-0.88663500

C	-3.32201500	-2.42963000	-0.52666600
C	4.24007000	0.15313900	-0.57264400
F	-3.83193300	-2.26231900	-1.73396600
F	-4.25356400	-2.87168600	0.30118800
F	-2.32790900	-3.29964500	-0.57866700
F	5.24688300	0.92460200	-0.92238000
F	4.33350800	-0.14146600	0.72704200
F	4.27902500	-0.98295500	-1.26391900
H	3.87619100	-1.53410500	2.84586300
H	3.18669800	-2.90048300	0.81537700
C	1.33056000	-4.20448700	-0.66661800
H	2.20685800	-4.17345900	-1.32258200
H	1.50335500	-4.98913700	0.07598900
H	0.43578100	-4.42348600	-1.24869200
O	-0.37490800	1.36046000	1.02033600
S	-0.39147200	2.61040400	0.09204100
O	0.15602200	3.75512200	0.77135200
O	0.04672100	2.21056200	-1.23566700
C	-2.20695400	2.93709800	-0.03709500
F	-2.37860800	4.22761700	-0.28252600
F	-2.80354300	2.62126400	1.10278900
F	-2.73138400	2.23155100	-1.02440900

7)

E_{elec}(BS1) = -3231.4399584 Hartree E_{ZPE} = 0.217989 Hartree H_{ZPE} = 0.253590Hartree G_{ZPE} = 0.145581 Hartree

E_{elec}(BS2)= -5155.0533072 Hartree

Low frequencies (cm^{-1}) 12.0045 21.0496 23.1071 29.3276 33.6773 38.7208 41.1525 43.9271 49.5567

C	1.77363800	1.49965400	0.26339500
C	0.89759800	1.53501500	1.42384500
C	1.42376100	2.16537300	2.67644100
H	2.60242800	2.20688000	0.31525200
H	0.79923800	1.88327600	3.52347000
H	2.46414300	1.86995800	2.83589700
O	-0.26004700	1.07645700	1.45000000
C	1.16437200	1.40062200	-1.05557500
O	0.08007200	0.82439200	-1.25201800
Ga	-1.11022200	-0.02797600	0.08576300
O	0.55563600	-1.33070000	0.52624900
O	-2.47101000	1.02400400	-0.65844200
S	-3.00262000	2.38041000	-0.17977400
O	-4.26733000	2.69137800	-0.80205500

O	-2.77539100	2.60767500	1.23116100
S	0.13550000	-2.32877700	-0.50466200
O	-0.03803500	-3.70771400	-0.12984300
O	-1.02699900	-1.63161500	-1.18078900
C	1.48375400	-2.33689500	-1.75798800
C	-1.78459600	3.48640000	-1.00882100
F	1.04872600	-2.96818400	-2.84226500
F	2.52790300	-2.97157000	-1.26381600
F	1.83360900	-1.09929700	-2.09329700
F	-2.22127700	4.74101200	-0.97899000
F	-0.60449300	3.44699000	-0.36461500
F	-1.57385900	3.13170400	-2.26967400
H	1.39679800	3.25403500	2.55252500
H	2.46072900	0.38635300	0.34448400
C	1.87488600	1.99352200	-2.22704300
H	1.80717700	3.08490300	-2.14655100
H	2.93300100	1.71499200	-2.19463300
H	1.39774600	1.66405800	-3.14993900
O	-2.07995100	-0.99285100	1.36439800
S	-3.58418300	-1.21876200	1.59398200
O	-3.78560700	-2.01152300	2.78695400
O	-4.37386600	-0.02644100	1.36683200
C	-3.94883400	-2.33003400	0.18146200
F	-5.19544700	-2.78558000	0.28777000
F	-3.11180200	-3.35936000	0.17258000
F	-3.83250100	-1.66299100	-0.96090100
O	3.31739500	-0.63513200	0.36571000
S	4.68420900	-0.24052900	-0.14941700
O	5.47109500	-1.36018200	-0.62105900
O	4.62977900	0.97798500	-0.95641700
C	5.47672700	0.31318600	1.40464700
F	6.70430400	0.76621400	1.17215900
F	4.75357100	1.31180800	1.93533900
F	5.54408100	-0.67092100	2.29139500

8)

E_{elec}(BS1) = -4192.8003031 Hartree E_{ZPE} = 0.248237 Hartree H_{ZPE} = 0.292047 Hartree G_{ZPE} = 0.165963 Hartree

E_{elec}(BS2)= -6116.7256982Hartree

Low frequencies (cm^{-1}) 11.1854 15.2210 25.1188 30.2609 31.0638 32.0535 35.5057 42.9918 44.9853

C	-1.23904200	0.66859400	-2.00282300
C	-0.58479600	-0.53585000	-2.21320700

C	-0.84886900	-1.35274600	-3.44401200
H	-1.93292600	1.02126100	-2.75334500
H	-1.21387700	-2.33789200	-3.13843200
H	-1.57677100	-0.87957800	-4.10435000
O	0.27645800	-1.06503300	-1.41719600
C	-1.02499900	1.45824600	-0.86231000
O	-0.25637700	1.13201200	0.09582500
Ga	0.97900700	-0.33746500	0.14240400
O	-1.89395800	-1.35288300	0.69838600
O	2.40230300	0.87190500	0.42493200
S	2.79423000	1.92260800	-0.62374800
O	4.21889500	1.96346700	-0.85463900
O	1.85510300	1.92871100	-1.73481400
S	-1.21492300	-1.32809300	2.01153600
O	-1.36555600	-2.47426000	2.87473000
O	0.21385800	-0.86938600	1.83990000
C	-2.00459500	0.06214700	2.91830300
C	2.43605200	3.44911000	0.32675200
F	-1.54903000	0.08904200	4.16419700
F	-3.31676300	-0.16951400	2.93983900
F	-1.77353500	1.22561700	2.34380200
F	2.78484900	4.50769800	-0.40367100
F	1.14136600	3.54309700	0.61391600
F	3.12877700	3.46574200	1.45953700
H	0.09795100	-1.50196300	-3.97089300
H	-3.45221400	-1.48420700	0.60338800
C	-1.67972400	2.80067400	-0.73483400
H	-0.93106500	3.55614000	-0.99752000
H	-2.54539900	2.89309700	-1.39184400
H	-1.98159400	2.95460600	0.30227900
O	2.16370300	-1.84971800	0.29679800
S	3.20713900	-2.07034100	-0.80175400
O	3.23764900	-3.43930200	-1.27330600
O	3.19395100	-0.97208300	-1.75725500
C	4.74403000	-1.86358100	0.17322900
F	5.79506200	-2.03363900	-0.62717000
F	4.79752300	-2.77497100	1.14190800
F	4.80188000	-0.65674000	0.71213400
O	-4.46112900	-1.40966000	0.48100900
S	-4.81634500	0.01128100	-0.07505600
O	-6.20329500	0.28936900	0.19825000
O	-3.77064100	0.96361400	0.22323200
C	-4.69901900	-0.32940800	-1.88053300
F	-4.55067200	0.82111800	-2.53011200
F	-3.65848500	-1.11232700	-2.13168500
F	-5.80284600	-0.92784200	-2.30377300

Au Cycle:

10)

E_{elec}(BS1) = -4953.864825 Hartree E_{ZPE} = 0.684931Hartree H_{ZPE} = 0.752087 Hartree G_{ZPE} = 0.574773 Hartree

E_{elec}(BS2)= -6877. 9772159 Hartree

Low frequencies (cm^{-1}) 9.1776 13.2655 14.7081 21.0139 25.8699 27.0243 29.8801 34.3776 35.2472

C	2.09377000	-1.67792000	2.41768500
C	3.25541000	-0.90250600	2.53046000
C	3.86589900	-0.65373000	3.87809200
H	1.69680100	-2.15283500	3.30464300
H	4.95145100	-0.75265000	3.80821900
H	3.64898500	0.38061500	4.16525000
O	3.84907700	-0.34962500	1.54800500
C	1.43914900	-1.87766100	1.20997200
O	1.78647200	-1.35166600	0.08657400
Ga	3.36535400	-0.42087700	-0.30850400
O	0.93288800	1.17510000	-1.21629500
O	4.77183100	-1.49221800	-0.89649700
S	4.93811800	-2.96157900	-0.46585200
O	6.32090500	-3.36943700	-0.49485500
O	4.09956900	-3.25652600	0.68594100
S	1.34704500	0.40673900	-2.38717900
O	1.28806600	1.03455700	-3.69732300
O	2.63644100	-0.33384600	-2.15186400
C	0.08325100	-0.94905500	-2.48507900
C	4.11146700	-3.78437500	-1.87902800
F	-0.82235900	-0.62279800	-3.41871500
F	-0.56958300	-1.07650500	-1.32995300
F	0.62332300	-2.10955200	-2.80720800
F	4.11628700	-5.09910500	-1.68547000
F	2.85118300	-3.36364100	-1.95382400
F	4.73352200	-3.50660800	-3.01330000
H	3.47039200	-1.33295200	4.63474900
C	0.22118900	-2.74848900	1.13242900
H	0.39705100	-3.51521500	0.37110000
H	-0.01075900	-3.21559300	2.09073500
H	-0.63065600	-2.14623400	0.79943200
Au	-2.22533100	0.90882600	0.67314500
P	-4.46805600	0.65161600	0.03996400
N	-1.91068400	2.80503900	-1.15320900
N	-2.00414400	2.17732100	-2.28165800

N	-1.01431700	2.58262100	-3.07807200
H	-0.81463900	2.06114500	-3.92331500
C	-0.80273600	3.61477400	-1.18834600
C	-0.19890000	4.38930700	-0.18170300
H	-0.65665800	4.48765800	0.79769300
C	1.01198800	4.96652500	-0.48810600
H	1.54880600	5.53076800	0.26617300
C	1.61268900	4.80743600	-1.76588300
H	2.58853200	5.24900900	-1.93149600
C	1.02478400	4.06861500	-2.76758200
H	1.50424900	3.90270600	-3.72465400
C	-0.20024900	3.46805900	-2.44180900
C	-5.08604500	2.14050100	-0.82145900
H	-6.16706500	2.07802600	-0.97000300
C	-5.51429700	0.50396500	1.53955400
H	-6.57695400	0.64025600	1.32972500
C	-4.71557600	-0.76806900	-1.08994800
C	-3.61441400	-1.06226800	-1.90402400
H	-2.73906300	-0.42260400	-1.86699900
C	-3.62835700	-2.15429400	-2.76368800
H	-2.76156200	-2.35679000	-3.38406400
C	-4.74496500	-2.98373800	-2.80008500
H	-4.76043700	-3.85367400	-3.44891900
C	-5.85241200	-2.68925400	-2.01122700
H	-6.73855500	-3.31593000	-2.05490000
C	-5.86676600	-1.57385500	-1.16824700
C	-7.11428500	-1.27090200	-0.41328700
C	-7.91635600	-0.19043800	-0.79321800
C	-9.06397000	0.12549600	-0.07023000
H	-9.67874400	0.96762700	-0.37215500
C	-9.42502600	-0.64337600	1.03461200
C	-8.64895700	-1.74217400	1.39790300
H	-8.93499100	-2.35163900	2.24932600
C	-7.50334700	-2.05880800	0.67277600
H	-7.64004300	0.39339300	-1.66707900
H	-6.89012800	-2.90928200	0.95861100
H	-10.31561200	-0.39463000	1.60261800
H	-5.35814100	-0.47323100	2.00332600
H	-5.17208600	1.27573600	2.23537400
H	-4.83621800	3.01979000	-0.22195300
H	-4.56855900	2.22332400	-1.78021700
C	-0.62295200	0.40384200	2.33489200
C	-0.07274800	1.13676600	1.51489800
H	0.59340900	1.71773700	0.89310300
S	3.73345700	2.51225700	0.53744700
O	3.85344600	1.38732400	-0.49360100
O	3.90214300	3.80280700	-0.09276100
O	2.60984600	2.29720000	1.44211300
C	5.27463900	2.27166900	1.56248800

F	4.95220400	1.91107100	2.80010600
F	5.93154700	3.42236700	1.61853600
F	6.05823400	1.35149000	1.02559100
C	-0.98457800	-0.43282400	3.45282300
C	-0.18876800	-0.36301200	4.60536300
C	-2.05762400	-1.32904400	3.40003600
C	-0.46665300	-1.18826800	5.68798500
H	0.64638300	0.33003300	4.63054500
C	-2.32816200	-2.15032900	4.48866600
H	-2.66182200	-1.38339000	2.49862700
C	-1.53473000	-2.08261000	5.63161400
H	0.15238900	-1.13438600	6.57761900
H	-3.15807600	-2.84793500	4.44258900
H	-1.74840900	-2.72631700	6.47880100

TS3)

E_{elec}(BS1) = -4953.8479615 Hartree E_{ZPE} = 0.683765 Hartree H_{ZPE} = 0.749626 Hartree G_{ZPE} = 0.578932 Hartree

E_{elec}(BS2)= -6877.9557793 Hartree

Low frequencies (cm^{-1}) -388.1651 20.2362 20.9865 26.6550 29.6444 31.7870 33.6386 37.3759 38.9082

C	-1.85914300	-1.18588100	-2.50387500
C	-2.69892800	-0.03464300	-2.56114400
C	-2.99653700	0.64884200	-3.85401000
H	-1.65503200	-1.68056600	-3.44659600
H	-4.07892600	0.61947500	-4.01520800
H	-2.70933400	1.70071000	-3.74919000
O	-3.17652800	0.50394900	-1.53051600
C	-1.86009600	-2.01794200	-1.33834600
O	-2.12806400	-1.59048900	-0.18101300
Ga	-3.05553600	0.01162000	0.33353400
O	-0.09428800	-0.10697500	1.27826700
O	-4.76165700	-0.65786500	0.60987900
S	-5.51302300	-1.64782500	-0.30308300
O	-6.91624400	-1.33151600	-0.37846600
O	-4.75498800	-1.92745500	-1.51689400
S	-0.92621200	-0.51982600	2.40425000
O	-0.56528700	-0.05355800	3.73377800
O	-2.39941000	-0.31084900	2.11040800
C	-0.79991400	-2.37937000	2.49605700
C	-5.35158100	-3.16663100	0.70996900
F	-0.21678700	-2.71733200	3.63819800
F	-0.04893700	-2.82577700	1.49044900
F	-1.99281900	-2.93920500	2.43122600

F	-6.04600100	-4.14377000	0.14189300
F	-4.06896700	-3.52093900	0.76342600
F	-5.79979200	-2.95884900	1.93525300
H	-2.48038700	0.19049500	-4.69749200
C	-1.52339200	-3.46790400	-1.44989000
H	-2.48167700	-3.99505500	-1.54774700
H	-0.90718900	-3.68313100	-2.32500400
H	-1.03433400	-3.80527000	-0.53494900
Au	1.99700200	1.32404200	-1.02275900
P	4.23173600	0.87184500	-0.45831700
N	3.42440700	2.70551000	2.80127200
N	2.77064900	1.92633500	3.59042900
N	1.46689600	1.97675900	3.28161200
H	0.80773600	1.36485000	3.75879600
C	2.52933600	3.29402500	1.93500000
C	2.72654900	4.22358100	0.89848800
H	3.71464200	4.62003700	0.68859900
C	1.61179200	4.62102500	0.19002900
H	1.71448100	5.34333600	-0.61346800
C	0.31632300	4.13376900	0.50551700
H	-0.53252800	4.49409300	-0.06529200
C	0.10198500	3.23061900	1.52777100
H	-0.89382600	2.88335100	1.78472600
C	1.24506100	2.81617200	2.23334900
C	5.38514800	2.16341100	0.13467000
H	6.41504300	1.80338600	0.07158600
C	5.01351900	0.23333200	-1.99286300
H	6.08571700	0.05862600	-1.88176500
C	4.16600000	-0.47137900	0.79479900
C	3.03379200	-0.45399800	1.61801500
H	2.30080000	0.34144600	1.51264600
C	2.79639200	-1.46215600	2.54549200
H	1.92167200	-1.40760200	3.18686300
C	3.68644100	-2.52669800	2.64251500
H	3.50760600	-3.32778100	3.35295800
C	4.82088200	-2.55425000	1.83504500
H	5.53395000	-3.36936300	1.92113400
C	5.08848000	-1.52764400	0.92439800
C	6.34743300	-1.59452700	0.13391500
C	7.39373800	-0.70568500	0.39571800
C	8.55543900	-0.73845800	-0.37211600
H	9.36148200	-0.04199100	-0.16274600
C	8.68569200	-1.66972800	-1.40052600
C	7.65998600	-2.58087400	-1.64469700
H	7.76318100	-3.31532200	-2.43735500
C	6.49923400	-2.54683600	-0.87729600
H	7.29297000	0.00514300	1.21148300
H	5.68512000	-3.23898900	-1.07787700
H	9.58856300	-1.69256800	-2.00233600

H	4.51398500	-0.69577000	-2.28514400
H	4.84064200	0.97997700	-2.77355100
H	5.27005800	3.04627700	-0.50071000
H	5.13582900	2.42174300	1.16831800
C	-0.00433000	-0.26594800	-2.09633200
C	-0.02444800	0.94438000	-1.67907000
H	-0.81071800	1.67845900	-1.52513400
S	-3.10541800	3.12036400	-0.18767800
O	-2.93383500	1.85256300	0.67482000
O	-3.12744800	4.27820200	0.67409400
O	-2.22702300	3.12845600	-1.34903400
C	-4.82891000	2.92310900	-0.87665600
F	-4.77023500	2.80099800	-2.19562500
F	-5.53552900	3.99666700	-0.56985400
F	-5.41422700	1.84858400	-0.36485200
C	0.88542300	-1.42125200	-2.24720400
C	1.19788100	-1.97109800	-3.49363700
C	1.45074900	-1.95881000	-1.08250300
C	2.08162500	-3.04366100	-3.57335800
H	0.76033600	-1.54844700	-4.39390100
C	2.34399800	-3.02243300	-1.16979800
H	1.19220400	-1.52310100	-0.12112100
C	2.65683400	-3.56772000	-2.41457300
H	2.32833500	-3.46683600	-4.54193800
H	2.79025300	-3.41572200	-0.25975500
H	3.34559200	-4.40425800	-2.48547800

TS4)

E_{elec}(BS1) = -4953.835929 Hartree E_{ZPE} = 0.684180 Hartree H_{ZPE} = 0.750425 Hartree G_{ZPE} = 0.575540 Hartree

E_{elec}(BS2)= -6877.9466428 Hartree

Low frequencies (cm^{-1}) -380.6515 10.1945 15.7812 19.1048 20.9423 23.6886 25.9610 28.3680 32.2301

C	2.15504600	-1.73869200	1.59290100
C	3.06708800	-0.74596400	2.03516000
C	3.29407200	-0.53521000	3.49890100
H	1.82357700	-2.47053200	2.31914900
H	4.35557400	-0.35431000	3.67791600
H	2.75256600	0.37420400	3.78583700
O	3.69887400	0.02082400	1.25517900
C	2.03016600	-2.07480700	0.22194700
O	2.39816800	-1.31324700	-0.71959200

Ga	3.55215900	0.21900600	-0.66141500
O	1.04302900	1.17982800	-0.97812000
O	5.19618300	-0.47161200	-1.17814200
S	5.72543400	-1.87141800	-0.80353800
O	7.16035700	-1.86982700	-0.66911800
O	4.88972300	-2.49742200	0.21222400
S	1.40274900	0.99292200	-2.38838300
O	1.06410100	2.02270100	-3.35165600
O	2.84681700	0.54262100	-2.46808100
C	0.44028800	-0.51368900	-2.91645200
C	5.34150900	-2.77321700	-2.35207000
F	-0.42703400	-0.16998100	-3.86109100
F	-0.24107600	-0.99334700	-1.87423000
F	1.23829100	-1.45923600	-3.38067100
F	5.72312200	-4.03818700	-2.21591100
F	4.03008800	-2.74076200	-2.57385700
F	5.97420700	-2.23004500	-3.37789500
H	2.94230700	-1.37923900	4.09393500
C	1.41112800	-3.37188000	-0.18682200
H	2.23801200	-4.06418900	-0.38833800
H	0.77786200	-3.78998800	0.59866600
H	0.85088200	-3.23199900	-1.11283500
Au	-2.49137400	-0.44778300	1.12989400
P	-4.64409300	0.13746800	0.42701800
N	-1.99013000	2.01694900	-0.44630700
N	-1.58772700	2.25883300	-1.64578300
N	-0.76410500	3.30911600	-1.62600600
H	-0.21093500	3.47698600	-2.46027700
C	-1.38109200	2.90662000	0.40924600
C	-1.46115300	3.04675200	1.80491300
H	-2.09473000	2.39255400	2.39826400
C	-0.69186000	4.03658000	2.37791000
H	-0.70985900	4.17632000	3.45375900
C	0.14204900	4.87289300	1.59552500
H	0.75610900	5.61602300	2.09329900
C	0.22445400	4.75454900	0.22450100
H	0.89597500	5.37138900	-0.35981100
C	-0.56043500	3.74748300	-0.35297000
C	-5.01638200	1.88479400	0.82323400
H	-6.07042400	2.10512900	0.64339200
C	-5.90899100	-0.80373400	1.36673000
H	-6.90663400	-0.36967600	1.27349400
C	-4.87604000	-0.11436200	-1.37330600
C	-3.70219900	-0.18791200	-2.13606600
H	-2.73701500	-0.06028600	-1.65656500
C	-3.75108300	-0.40539700	-3.50899200
H	-2.82671100	-0.44407400	-4.07358800
C	-4.97951400	-0.57674900	-4.13595200
H	-5.02924000	-0.75792700	-5.20510300

C	-6.15168200	-0.51112400	-3.38949800
H	-7.11676600	-0.63743000	-3.87160500
C	-6.12250600	-0.26648700	-2.01439900
C	-7.42598600	-0.19381900	-1.29448000
C	-7.95696300	1.03490600	-0.89289500
C	-9.16174900	1.08911400	-0.19519600
H	-9.56349500	2.04862900	0.11548200
C	-9.85490100	-0.08467500	0.09246900
C	-9.35128200	-1.31019600	-0.33950100
H	-9.89622000	-2.22583700	-0.13208100
C	-8.14676100	-1.36300800	-1.03470000
H	-7.42706300	1.94962000	-1.14429300
H	-7.74468400	-2.31684300	-1.36570400
H	-10.79165300	-0.04323600	0.63902100
H	-5.92805200	-1.84066600	1.02196600
H	-5.59932000	-0.79214200	2.41578000
H	-4.78452900	2.05466600	1.87894100
H	-4.37536300	2.52332200	0.21253100
C	-0.69987700	-1.32462600	1.98979500
C	0.21316500	-0.65826000	1.41965300
H	0.55888600	0.18046400	0.82408200
S	3.26492500	2.90244800	0.80671100
O	3.70306000	2.07152900	-0.41119800
O	3.20583200	4.30219800	0.44719400
O	2.16250600	2.29370700	1.53415700
C	4.76208900	2.74154400	1.91114900
F	4.40837000	2.18562200	3.06764100
F	5.25184500	3.94780100	2.15712000
F	5.70244800	2.00041300	1.34549000
C	-0.82162500	-2.47469100	2.88096500
C	-1.60495400	-3.58462600	2.54076600
C	-0.12421200	-2.47108100	4.09629700
C	-1.66181700	-4.68393300	3.39092200
H	-2.15752600	-3.57908600	1.60495000
C	-0.19704300	-3.56855500	4.94790900
H	0.46017000	-1.59626500	4.36621300
C	-0.96049100	-4.67909900	4.59523100
H	-2.26048100	-5.54580300	3.11401900
H	0.34434000	-3.55516000	5.88856000
H	-1.01283600	-5.53603100	5.25880300

11)

E_{elec}(BS1) = -4953.8680307 Hartree E_{ZPE} = 0.686437 Hartree H_{ZPE} = 0.752835 Hartree
G_{ZPE} = 0.57698 Hartree

E_{elec}(BS2)= -6877.9793358 Hartree

Low frequencies (cm^{-1}) 9.5085 12.3115 15.7118 22.5857 27.3736 30.7232 31.1081 35.0505 36.4082

C	-1.53794300	-2.19387300	-1.44737000
C	-2.24441000	-1.06586500	-2.13414400
C	-2.15679800	-1.00469700	-3.62240600
H	-1.70591100	-3.10095200	-2.03512200
H	-2.88087700	-1.72935500	-4.01697900
H	-2.42362100	-0.00480300	-3.96468200
O	-2.88294500	-0.18689900	-1.54880200
C	-1.91332100	-2.47436000	-0.02866300
O	-2.45949500	-1.64836400	0.71209800
Ga	-3.52390700	0.00187400	0.30056400
O	-1.83428000	0.98922900	0.94022900
O	-5.10816800	-0.99303400	0.10968000
S	-5.41981400	-2.31394600	-0.59442600
O	-6.69111000	-2.28554700	-1.27056200
O	-4.24574800	-2.83471800	-1.29868500
S	-2.20486700	0.89767800	2.40236600
O	-2.13261200	2.08296200	3.21510600
O	-3.53149600	0.17791900	2.33001600
C	-0.98822900	-0.33364600	3.10353100
C	-5.61389300	-3.41118300	0.85990300
F	-0.32223700	0.23139700	4.08819200
F	-0.15227200	-0.71880200	2.15283500
F	-1.65076800	-1.38760500	3.55682900
F	-5.84512600	-4.64825900	0.43939900
F	-4.48828400	-3.40421900	1.57317700
F	-6.61524100	-3.00212700	1.61599400
H	-1.15824000	-1.28294500	-3.96730000
C	-1.55990700	-3.81054500	0.53292400
H	-2.38768400	-4.48184400	0.27041100
H	-0.63970300	-4.20501500	0.09514800
H	-1.49195200	-3.74337900	1.61964700
Au	2.31063800	-0.07272800	-0.47501700
P	4.54311900	0.56805500	0.06158200
N	1.48534200	2.44964700	0.99700800
N	0.48161300	2.52759200	1.80075900
N	-0.38194600	3.43932200	1.34375600
H	-1.29487200	3.53016600	1.78218000
C	1.26783300	3.31873600	-0.04898800
C	2.03086100	3.59988500	-1.19610000
H	2.97392100	3.09232400	-1.37849900
C	1.52498700	4.52990800	-2.07897700
H	2.08023600	4.77488200	-2.97857200

C	0.28272700	5.17292700	-1.84591100
H	-0.08021400	5.88812300	-2.57697400
C	-0.48317800	4.90585000	-0.73166000
H	-1.44628700	5.37365100	-0.56309600
C	0.04058100	3.96114300	0.16461400
C	4.65700200	2.02964500	1.16024800
H	5.69692100	2.31004400	1.33910600
C	5.51490800	1.04648600	-1.42194500
H	6.43237600	1.58505100	-1.17576100
C	5.41004700	-0.81030400	0.92488900
C	4.57027500	-1.72489900	1.57704100
H	3.49709500	-1.54858800	1.57957100
C	5.07702200	-2.85246800	2.21390800
H	4.40219900	-3.53810100	2.71658700
C	6.44546400	-3.09940400	2.18658100
H	6.85466400	-3.98500200	2.66255700
C	7.29326500	-2.19706100	1.55421700
H	8.36590600	-2.36853500	1.54639900
C	6.79956900	-1.04166200	0.94017800
C	7.78820600	-0.09348400	0.35271100
C	8.07730500	1.10814200	1.00518900
C	8.98395600	2.01094600	0.45547700
H	9.19755100	2.94282600	0.96964800
C	9.62237200	1.71236200	-0.74608200
C	9.36632500	0.50014600	-1.38387800
H	9.87247300	0.25738300	-2.31296800
C	8.45893700	-0.40117600	-0.83360800
H	7.59608700	1.32410900	1.95499200
H	8.24798800	-1.34243800	-1.33425400
H	10.32694000	2.41638000	-1.17717200
H	5.75853800	0.15251000	-2.00154500
H	4.86947900	1.68263000	-2.03517000
H	4.12247700	2.85825700	0.68910900
H	4.14439100	1.80873500	2.09880000
C	-0.01046200	-1.89063700	-1.36787300
C	0.40163500	-0.71711200	-0.85596900
H	-0.38950100	-0.02964700	-0.54451500
S	-3.57433700	2.94259800	-0.43533800
O	-4.33508900	1.65383800	-0.07948600
O	-3.18600500	3.69412700	0.74999900
O	-2.60251200	2.73834000	-1.49064500
C	-4.96601700	3.88079300	-1.16365100
F	-4.51378200	5.08294600	-1.50975400
F	-5.94416500	4.01695900	-0.28404600
F	-5.41942000	3.25786900	-2.24094300
C	0.87235200	-3.00953000	-1.80165300
C	0.61557500	-3.73086400	-2.97414400
C	1.98191200	-3.38177100	-1.03008300
C	1.45440300	-4.76329700	-3.38235000

H	-0.23992400	-3.47378900	-3.59489200
C	2.82037500	-4.41596200	-1.43304500
H	2.17469700	-2.85499900	-0.10061600
C	2.56256900	-5.10904800	-2.61352300
H	1.24091300	-5.29711000	-4.30309700
H	3.67279800	-4.68365300	-0.81565900
H	3.21379800	-5.91852200	-2.92749200

12)

E_{elec}(BS1) = -4953.8675579 Hartree E_{ZPE} = 0.685582 Hartree H_{ZPE} = 0.752245 Hartree G_{ZPE} = 0.574158 Hartree

E_{elec}(BS2)= -6877.9779709 Hartree

Low frequencies (cm^{-1}) 8.5452 10.0737 14.7677 18.6610 19.6112 25.2932 27.4983 29.9197 30.6703

C	1.80872900	1.86595900	-0.98136200
C	2.72007300	0.93736700	-1.70944200
C	2.87160300	1.06369000	-3.18714100
H	1.80570000	2.84696300	-1.46017100
H	3.90573900	0.84167100	-3.45723900
H	2.23947400	0.28671700	-3.63572000
O	3.28871400	-0.00675600	-1.15366800
C	2.03908400	2.00579900	0.49079500
O	2.40488800	1.06313300	1.20304100
Ga	3.33814700	-0.63391000	0.70651400
O	1.33674400	-1.40147700	0.86297100
O	5.01795900	0.13216800	1.05714200
S	5.59099000	1.49744400	0.65941400
O	6.95535100	1.39831300	0.20802400
O	4.63483000	2.28815100	-0.11748200
S	1.47721600	-1.59253400	2.34177400
O	1.07427800	-2.84072300	2.94353300
O	2.90335900	-1.15319900	2.59545200
C	0.39580300	-0.26325900	3.08789700
C	5.62170800	2.31024900	2.30075500
F	-0.49638500	-0.82926800	3.88188700
F	-0.22357500	0.39591300	2.12036100
F	1.14003100	0.57830700	3.78605500
F	6.14087200	3.52437800	2.17122700
F	4.37643700	2.42126500	2.75987100
F	6.34356700	1.60747000	3.15466300
H	2.56768100	2.04412900	-3.55302000
C	1.72570100	3.31417100	1.12763800

H	2.63216800	3.92462700	1.02133200
H	0.90378200	3.82032500	0.61515800
H	1.51622900	3.16964100	2.18804200
Au	-2.56576500	1.08116000	-0.99763000
P	-4.66511700	0.05597700	-0.57650600
N	-1.63676000	-1.71422800	0.04510500
N	-1.35321800	-2.31804300	1.14545400
N	-0.73832000	-3.47452500	0.86322000
H	-0.31430800	-3.98011200	1.63126700
C	-1.17016600	-2.47231300	-1.00328000
C	-1.21744000	-2.25175200	-2.39059400
H	-1.67167600	-1.34983400	-2.79197400
C	-0.65366100	-3.21804000	-3.19484000
H	-0.65928000	-3.09117300	-4.27245900
C	-0.04658000	-4.37759800	-2.64926100
H	0.40559500	-5.09718900	-3.32386000
C	0.01232500	-4.60821300	-1.29214800
H	0.51075500	-5.47838000	-0.88145300
C	-0.56863400	-3.62398900	-0.47817300
C	-4.78481200	-1.58392000	-1.38789600
H	-5.79758200	-1.98757900	-1.32326600
C	-6.05502900	1.00482800	-1.31069800
H	-6.97998800	0.42815800	-1.37418800
C	-4.95975600	-0.20650300	1.21727200
C	-3.80532100	-0.22575300	2.01360400
H	-2.82968500	-0.13116300	1.54566700
C	-3.88643300	-0.38122400	3.39357300
H	-2.97587200	-0.41009400	3.98126600
C	-5.13072400	-0.49058400	4.00349000
H	-5.20698800	-0.59744000	5.08104200
C	-6.28410600	-0.47265800	3.22592000
H	-7.26042200	-0.57189300	3.69154900
C	-6.21817800	-0.35209000	1.83520000
C	-7.49691300	-0.39195300	1.07070400
C	-7.85712500	-1.53560900	0.35235000
C	-9.03516500	-1.56210500	-0.39036500
H	-9.30315900	-2.45458800	-0.94722100
C	-9.87243500	-0.44845500	-0.40939800
C	-9.53866800	0.68158000	0.33453600
H	-10.19516000	1.54605000	0.33439400
C	-8.36070800	0.70674400	1.07582300
H	-7.21185500	-2.40890200	0.38942100
H	-8.08970200	1.59049500	1.64703100
H	-10.78836700	-0.46618600	-0.99126200
H	-6.22927100	1.91173000	-0.72626500
H	-5.73500400	1.30009600	-2.31427100
H	-4.50550800	-1.46841800	-2.43946000
H	-4.07216000	-2.26167200	-0.91223700
C	-0.72593300	1.96011900	-1.33791200

C	0.37818200	1.26050200	-1.02873000
H	0.33404300	0.23389300	-0.66363000
S	3.34090700	-2.96841800	-1.22179600
O	3.81929100	-2.34168000	0.10552700
O	3.41966100	-4.40950300	-1.15285900
O	2.13915000	-2.33198700	-1.72931900
C	4.71320100	-2.41532900	-2.36026300
F	4.18070800	-1.80403200	-3.41799500
F	5.40166600	-3.46654500	-2.77416900
F	5.53331600	-1.56931700	-1.75262000
C	-0.64945900	3.35465600	-1.82810300
C	-1.19783300	4.40787000	-1.08121000
C	-0.04405300	3.65706600	-3.05618900
C	-1.10230900	5.72205900	-1.52717200
H	-1.70304200	4.18001200	-0.14531900
C	0.03323900	4.97111600	-3.51175300
H	0.33989200	2.84259400	-3.66560700
C	-0.48607400	6.01003600	-2.74427900
H	-1.52148700	6.52460800	-0.92788800
H	0.49801100	5.18224300	-4.47013000
H	-0.42298700	7.03447100	-3.09635000

13)

E_{elec}(BS1) = -5915.6642169 Hartree E_{ZPE} = 0.726453 Hartree H_{ZPE} = 0.802345 Hartree G_{ZPE} = 0.602807 Hartree

E_{elec}(BS2)= -7840.0280379 Hartree

Low frequencies (cm^{-1}) 7.3219 8.8278 11.7671 17.0153 18.2848 19.6710 22.7942 27.1478 28.6688

C	1.76673700	1.13838800	2.26873100
C	2.53308100	1.70755000	1.10915900
C	2.75741200	3.17721100	1.06931900
H	2.00710400	1.73936100	3.15052400
H	3.68158200	3.34898200	1.63913200
H	2.90330500	3.49776200	0.03757700
O	3.01849000	1.01625100	0.20718500
C	2.01555000	-0.30597300	2.58757300
O	2.38387300	-1.13612100	1.74773300
Ga	3.41586300	-0.88958800	0.04219400
O	1.62665900	-1.26627400	-0.94306000
O	5.03451300	-0.93766200	1.00763000
S	5.50843700	-0.21288800	2.26593900
O	6.84872800	0.29664200	2.13913700
O	4.46020800	0.65964700	2.80405600

S	1.81719100	-2.76317900	-0.91677300
O	1.67595300	-3.51059600	-2.13788400
O	3.11563800	-2.89058700	-0.15553600
C	0.50588300	-3.38113200	0.25080400
C	5.57523600	-1.62157200	3.43527900
F	-0.39440900	-4.06293100	-0.43388800
F	-0.07674300	-2.35570000	0.85461900
F	1.06603600	-4.16536000	1.15554300
F	5.88721400	-1.16618900	4.64187900
F	4.37777200	-2.20323000	3.49294300
F	6.47411200	-2.50535000	3.04520100
H	1.94647400	3.73716500	1.53756500
C	1.73233800	-0.75823400	3.98053700
H	2.60488500	-0.47140200	4.58104600
H	0.85367700	-0.25397500	4.39144100
H	1.62079000	-1.84218000	4.00620200
Au	-2.21880000	0.21083700	0.36382700
P	-4.44406600	-0.37970200	-0.24709500
N	-1.60363900	-0.81030700	-2.33995100
N	-0.78557300	-1.77818800	-2.58423200
N	0.15199300	-1.35646900	-3.43569000
H	0.96986000	-1.93587100	-3.60778600
C	-1.17217000	0.30546600	-3.02040200
C	-1.67137600	1.61953500	-3.05228600
H	-2.54538900	1.89812800	-2.47229700
C	-0.98864900	2.53053600	-3.82825100
H	-1.32670800	3.56052100	-3.87118200
C	0.16271900	2.15840700	-4.56755900
H	0.66969100	2.91414900	-5.15827200
C	0.67103500	0.87830000	-4.54123700
H	1.56704100	0.59860200	-5.08144400
C	-0.01919800	-0.04170300	-3.73655100
C	-4.89920300	0.22959400	-1.91292600
H	-5.92832700	-0.03619700	-2.16331100
C	-5.66921100	0.41681900	0.86406400
H	-6.68869300	0.38465800	0.47497100
C	-4.68394400	-2.19976300	-0.27679200
C	-3.51815800	-2.95153700	-0.48853300
H	-2.57252400	-2.44266300	-0.65818800
C	-3.55643000	-4.34223500	-0.50668200
H	-2.64484400	-4.90111000	-0.68354200
C	-4.75989500	-5.00334400	-0.28877100
H	-4.79728100	-6.08816100	-0.28774700
C	-5.92258700	-4.26972200	-0.08002500
H	-6.87021100	-4.77675800	0.07708600
C	-5.90814300	-2.87229600	-0.08922300
C	-7.20631100	-2.16266700	0.09409300
C	-7.86191300	-1.59021200	-0.99960600
C	-9.05842600	-0.89899200	-0.82371800

H	-9.55681700	-0.45505100	-1.67978100
C	-9.61855700	-0.78696100	0.44710300
C	-8.99038400	-1.38793400	1.53621700
H	-9.43145400	-1.31686100	2.52547400
C	-7.79431000	-2.07766300	1.35898100
H	-7.43370100	-1.70150700	-1.99189700
H	-7.29481100	-2.53818900	2.20707900
H	-10.54858600	-0.24516100	0.58591900
H	-5.63785800	-0.06008700	1.84699200
H	-5.35005000	1.45728000	0.97896000
H	-4.79810300	1.31917300	-1.92285000
H	-4.20371900	-0.20024800	-2.63841100
C	0.22537600	1.16848200	2.02935200
C	-0.28176900	0.65979700	0.89380200
H	0.44262200	0.32268200	0.14970900
S	3.70740800	-0.13611500	-2.91210300
O	4.29018800	-0.69102300	-1.60355500
O	3.00425900	-1.15972400	-3.67339900
O	3.08928700	1.16139300	-2.73776100
C	5.28454500	0.13470600	-3.80069100
F	5.00007800	0.61366500	-5.00796500
F	5.94469200	-1.00469700	-3.92565700
F	6.02920200	1.01170000	-3.14570800
C	-0.57812600	1.67439200	3.17710900
C	-0.29596200	2.91612800	3.75910500
C	-1.64656200	0.92366200	3.68351100
C	-1.07435500	3.40643000	4.80206500
H	0.51472300	3.52714900	3.36834600
C	-2.41981000	1.40981500	4.73445800
H	-1.85703200	-0.05031300	3.24991800
C	-2.13822700	2.65342700	5.29413300
H	-0.85322800	4.38093300	5.22505800
H	-3.23836900	0.81055100	5.12121100
H	-2.74173800	3.03321100	6.11226700
O	-1.77857000	3.46481900	0.82616700
S	-0.60296600	4.21520100	0.07479800
O	0.00870000	5.16718000	0.97131600
O	0.18844700	3.28486300	-0.69555500
C	-1.63380600	5.17806400	-1.10312100
F	-0.83567700	5.74017000	-1.99602300
F	-2.48495400	4.36825200	-1.72137100
F	-2.30803700	6.10839400	-0.45079800
H	-1.64762000	2.48092300	0.75066700

TS5)

E_{elec}(BS1) = -5915.6539833 Hartree E_{ZPE} = 0.722429 Hartree H_{ZPE} = 0.797473 Hartree G_{ZPE} = 0.602078 Hartree

E_{elec}(BS2)= -7840.0144129 Hartree

Low frequencies (cm^{-1}) -990.8461 10.4486 13.8306 15.4089 18.6621 21.9414 25.2386 26.5850 28.0934

C	1.79189200	-1.19429500	2.35889000
C	2.84562400	-0.14948100	2.09038600
C	3.54643700	0.46695100	3.24507600
H	1.96659600	-1.61092700	3.35436200
H	4.38542700	-0.20887300	3.46346000
H	3.92587000	1.44918600	2.96530400
O	3.17696200	0.16597500	0.94185600
C	1.74488600	-2.32657300	1.36748800
O	2.05861300	-2.19737100	0.18256200
Ga	3.18499100	-0.81435000	-0.75580200
O	1.32677300	-0.21382600	-1.46423200
O	4.74394100	-1.80459400	-0.40199400
S	5.23771000	-2.57414300	0.82335300
O	6.65191500	-2.41327100	1.03563300
O	4.32296100	-2.41502400	1.95958700
S	1.32366900	-1.20511900	-2.60272800
O	0.94173500	-0.73435800	-3.90645400
O	2.66576300	-1.87082900	-2.43218000
C	0.07715500	-2.50315500	-2.09881600
C	4.96621400	-4.29653100	0.25862800
F	-0.81611600	-2.63537200	-3.06127500
F	-0.52900200	-2.12832100	-0.97881300
F	0.68924400	-3.65659200	-1.89720900
F	5.35197600	-5.12847700	1.21625600
F	3.66783100	-4.48267700	0.02363200
F	5.65078200	-4.53353400	-0.84373500
H	2.90116400	0.54534600	4.11846600
C	1.23769600	-3.64369800	1.84494000
H	2.08437000	-4.13610100	2.34073000
H	0.43672100	-3.52007100	2.57891900
H	0.91911100	-4.24779600	0.99509600
Au	-2.13125200	0.10289400	0.54147400
P	-4.35334400	-0.05676700	-0.11030500
N	-1.99912500	1.87296600	-1.86375100
N	-1.13255100	1.19374600	-2.54352100
N	-0.08855200	1.96873600	-2.82484100
H	0.72601400	1.58431800	-3.29846900
C	-1.49780600	3.13896300	-1.67161400
C	-2.02752200	4.25128800	-0.99394900
H	-2.99125500	4.19827600	-0.49856300
C	-1.26243700	5.39579300	-0.97837300

H	-1.62346900	6.27481700	-0.45536400
C	0.00718000	5.45138500	-1.61037200
H	0.57444200	6.37501800	-1.55769400
C	0.54486100	4.37137900	-2.27537400
H	1.52014100	4.40438600	-2.74670300
C	-0.24271700	3.20882500	-2.29211900
C	-5.03338300	1.62473000	-0.33945600
H	-6.11425300	1.59592700	-0.49231600
C	-5.33670200	-0.76872200	1.26550700
H	-6.40699000	-0.57945100	1.16133900
C	-4.64462100	-0.97335600	-1.66837300
C	-3.54606800	-1.05230000	-2.53417900
H	-2.60251400	-0.59099900	-2.25820600
C	-3.64848500	-1.69689000	-3.76319800
H	-2.78816700	-1.72494200	-4.42305700
C	-4.84566700	-2.30148100	-4.12766200
H	-4.93302800	-2.81737000	-5.07868900
C	-5.93977000	-2.24071700	-3.26985400
H	-6.88115900	-2.70523000	-3.54852900
C	-5.86548000	-1.56710200	-2.04834200
C	-7.09264900	-1.51292100	-1.20331200
C	-7.87769100	-0.35732100	-1.16094100
C	-9.00263400	-0.29744100	-0.34137100
H	-9.60262300	0.60665200	-0.31260000
C	-9.36182400	-1.39972600	0.43138900
C	-8.60600400	-2.56865100	0.36444800
H	-8.89201600	-3.43538600	0.95196700
C	-7.48103100	-2.62638600	-0.45324700
H	-7.60700000	0.49089800	-1.78358700
H	-6.88182000	-3.53166100	-0.50047800
H	-10.23590400	-1.35266800	1.07285200
H	-5.16160900	-1.84629100	1.32361200
H	-4.96590900	-0.30630600	2.18537100
H	-4.80292800	2.21083200	0.55542000
H	-4.52903700	2.07182500	-1.19932200
C	0.35037500	-0.60946100	2.31396000
C	-0.06003500	0.20724200	1.32500600
H	0.64783600	0.49844000	0.55073100
S	3.34017300	1.93811000	-1.93789000
O	4.02531800	0.58795300	-1.66017500
O	2.72206200	1.96227500	-3.25747400
O	2.57911800	2.40917500	-0.79868200
C	4.83338300	2.98822000	-2.07452000
F	4.43734100	4.22778400	-2.34359800
F	5.61189000	2.55239900	-3.04949100
F	5.49779100	2.97582500	-0.93070400
C	-0.50773300	-1.00039400	3.46445300
C	-0.17120600	-0.57667400	4.75615300
C	-1.66006800	-1.77086700	3.27566600

C	-0.99010900	-0.89738300	5.83235200
H	0.69792100	0.05932800	4.90053600
C	-2.46879400	-2.10536000	4.36023400
H	-1.91187800	-2.11845100	2.27638500
C	-2.13763800	-1.66528200	5.63774300
H	-0.73806600	-0.53630700	6.82390900
H	-3.35660600	-2.71010300	4.20311600
H	-2.77147000	-1.91772000	6.48167700
O	-1.14296500	2.13550400	2.74115400
S	0.02064200	2.90177300	3.34905200
O	-0.36081000	3.69073300	4.50029900
O	1.22400300	2.06894100	3.44056900
C	0.38671000	4.08044300	1.99394300
F	1.53288400	4.70758200	2.22682600
F	0.47627400	3.41625700	0.84573700
F	-0.58783700	4.97920100	1.90523300
H	-0.74378100	1.16578200	1.92792400

14)

E_{elec}(BS1) = -3539.7669073 Hartree E_{ZPE} = 0.334692 Hartree H_{ZPE} = 0.376262 Hartree G_{ZPE} = 0.258361 Hartree

E_{elec}(BS2)= -5463.5328875 Hartree

Low frequencies (cm^{-1}) 17.0457 25.3607 30.7475 34.6101 39.2050 40.0309 42.4444 47.7010 52.2153

C	-1.61502000	-0.08871700	-1.64644800
C	-0.21256400	-0.33884600	-2.12790500
C	0.00586200	-0.51426600	-3.58964500
H	-2.17371000	0.39386300	-2.45409300
H	0.00118500	0.49155400	-4.02944900
H	0.97440000	-0.98303700	-3.76330400
O	0.74151400	-0.43895400	-1.36005600
C	-1.72072900	0.78120100	-0.41477000
O	-0.86280800	0.78246000	0.46422400
Ga	1.05492000	0.11872700	0.51227200
O	0.09623300	-1.46746200	1.52186400
O	1.61612900	1.83833400	-0.03504300
S	1.10518500	2.82753400	-1.08216600
O	2.17682500	3.45051000	-1.81397900
O	-0.04289000	2.29454900	-1.82809300
S	0.15501800	-0.74512600	2.84188600
O	0.57323300	-1.45497400	4.01606600
O	0.89801000	0.52150100	2.46423300
C	-1.60522900	-0.19058800	3.15754800

C	0.37466200	4.10555100	0.00939300
F	-1.99277700	-0.65034500	4.33104900
F	-2.40296200	-0.67940600	2.21111900
F	-1.67768900	1.12896700	3.14830500
F	-0.10937800	5.08531300	-0.74174800
F	-0.62230600	3.56740000	0.71069600
F	1.28608200	4.58250600	0.83482000
H	-0.80481100	-1.09439400	-4.03875600
C	-2.93536800	1.62721600	-0.25028900
H	-2.77489800	2.51732700	-0.87292400
H	-3.83170300	1.11398200	-0.60842000
H	-3.03369100	1.93041600	0.79209700
C	-2.28971200	-1.43064000	-1.29213500
C	-1.58515200	-2.47042000	-0.83465100
H	-0.50774700	-2.47237000	-0.68986100
S	2.96830600	-2.19664200	0.05744700
O	2.68920600	-0.75459100	0.54262700
O	3.78944400	-2.91541600	0.99746600
O	1.77100300	-2.80670700	-0.49793500
C	4.03638300	-1.81007200	-1.38211800
F	4.37335600	-2.94326200	-1.98431900
F	5.12729400	-1.17657600	-0.98833000
F	3.37244700	-1.04415500	-2.24630600
C	-3.77181600	-1.46159600	-1.41105200
C	-4.42356000	-1.01395700	-2.56633700
C	-4.53929600	-1.94168500	-0.34360800
C	-5.81074300	-1.05971600	-2.65814200
H	-3.84518800	-0.65266400	-3.41361800
C	-5.92726400	-1.98549500	-0.43620300
H	-4.03838400	-2.25926400	0.56613900
C	-6.56599400	-1.54466300	-1.59230100
H	-6.30184000	-0.72173800	-3.56487300
H	-6.51004300	-2.35608900	0.40084500
H	-7.64831700	-1.57505700	-1.66243100
H	-2.10445000	-3.39313700	-0.59302000

15)

E_{elec}(BS1) = -653.9589975 Hartree E_{ZPE} = 0.240243 Hartree H_{ZPE} = 0.255908 Hartree G_{ZPE} = 0.198169 Hartree

E_{elec}(BS2)= -654.183495 Hartree

Low frequencies (cm^{-1}) 37.1892 62.3301 74.2337 75.7087 99.4939 141.2190 163.4685 200.0141 234.5421

C	-1.23069700	0.08691500	-0.00316200
C	-2.67785600	0.48232400	0.05494400

C	-3.72080100	-0.60352500	-0.11112300
H	-3.69057200	-1.28598200	0.74219700
H	-4.69966500	-0.13037300	-0.18645100
O	-3.01590000	1.63913000	0.21668000
C	-0.94558500	-1.38878300	-0.15618500
O	-1.37659000	-2.18575200	0.65156000
H	-3.52554000	-1.20601100	-1.00498500
C	-0.22862000	-1.85187300	-1.40721300
H	0.53248000	-1.14622700	-1.74363400
H	0.20796200	-2.83695500	-1.23509700
H	-0.98078800	-1.93917100	-2.20197800
C	-0.22930900	0.99476700	0.09982300
C	-0.44370800	2.48421000	0.21292700
H	-1.05669600	2.86619200	-0.60679100
C	1.18578700	0.53601600	0.13519400
C	2.13925400	1.13529400	-0.69874400
C	1.58938000	-0.49743400	0.98881000
C	3.45339900	0.68343200	-0.70872000
H	1.83943200	1.94327000	-1.36103000
C	2.91052500	-0.93670100	0.99005800
H	0.86670800	-0.94522900	1.66440000
C	3.84281200	-0.35399900	0.13704600
H	4.17642700	1.14251500	-1.37586700
H	3.21033000	-1.73424800	1.66268300
H	4.87149600	-0.70065900	0.13471300
H	-0.99530500	2.71869500	1.12740800
H	0.51616300	3.00331700	0.23658000

16)

E_{elec}(BS1) = -653.9603445 Hartree E_{ZPE} = 0.240716 Hartree H_{ZPE} = 0.255949 Hartree G_{ZPE} = 0.198910 Hartree

E_{elec}(BS2)= -654.1903767 Hartree

Low frequencies (cm^{-1}) 33.8930 55.1575 71.5199 99.3946 113.1044 139.7202 150.0703 171.5533 210.8677

C	-1.29531400	-0.00745800	0.25814200
C	-2.29167600	0.79529800	-0.43983800
C	-2.08070700	2.28397500	-0.59551300
H	-1.05472600	2.50858300	-0.90072400
H	-2.79155000	2.65778500	-1.33274500
O	-3.31029400	0.28696500	-0.93506800
C	-1.46405800	-1.37362300	0.30045100
O	-2.50924200	-1.98393200	-0.22360500
H	-2.24961400	2.79332500	0.35817900

C	-0.48252300	-2.31789200	0.92294300
H	0.18991200	-2.70652000	0.14982200
H	0.12199600	-1.82526100	1.68512900
H	-1.02400700	-3.16068100	1.35789800
C	-0.08403800	0.62010700	0.86383400
C	-0.19476200	1.44334200	1.91401800
H	-1.15764600	1.62201100	2.38338100
C	1.23921000	0.33013500	0.24292100
C	1.33828700	0.05721000	-1.12651100
C	2.41087300	0.31926900	1.01062700
C	2.57462300	-0.18621200	-1.71697500
H	0.43597600	0.04227200	-1.73171300
C	3.64574700	0.07168200	0.42279000
H	2.34549800	0.48221900	2.08274700
C	3.73344000	-0.17741800	-0.94523500
H	2.63133700	-0.38571400	-2.78280700
H	4.54162400	0.06173300	1.03621100
H	4.69748400	-0.37363100	-1.40422100
H	0.66108800	1.97327400	2.32182600
H	-3.08569800	-1.26415100	-0.62353200

17)

E_{elec}(BS1) = -2068.0383989 Hartree E_{ZPE} = 0.591660 Hartree H_{ZPE} = 0.631227 Hartree G_{ZPE} = 0.516963 Hartree

E_{elec}(BS2)= -654.1903767 Hartree

Low frequencies (cm^{-1}) -38.7254 19.0183 21.9154 29.2764 35.2541 38.6382 40.9769 46.1402 50.0894

C	4.36453900	1.01612300	-0.84142100
C	4.89184300	-0.16209700	-1.66115500
C	4.68940900	-0.08321000	-3.15535800
H	4.72184900	1.93199900	-1.33619700
H	5.41307200	0.62697200	-3.57297100
H	4.85560200	-1.06450700	-3.60093700
O	5.45226800	-1.09778600	-1.13088500
C	5.00696800	0.97029600	0.54911500
O	4.39127600	0.63355700	1.53788200
H	3.68564100	0.28146600	-3.38687000
C	6.46008500	1.36689800	0.62950600
H	7.04878900	0.74752200	-0.05415500
H	6.57454100	2.41210700	0.32176300
H	6.82274000	1.24127000	1.64971900
Au	0.08577500	-0.31508900	-0.75386200
P	-2.23601700	-0.69589400	-0.38430800

N	0.13656000	-1.86465200	2.32257000
N	0.82244300	-0.79264700	2.53752100
N	2.06110800	-0.95233100	2.06216600
H	2.71877300	-0.17358200	2.02192300
C	0.94573300	-2.76401400	1.66578000
C	0.69001000	-4.05618400	1.17445200
H	-0.27613800	-4.52704100	1.32413300
C	1.71575800	-4.68730900	0.50289700
H	1.56241300	-5.68472300	0.10349700
C	2.97686400	-4.06403600	0.31360400
H	3.74775500	-4.59850000	-0.23241400
C	3.25171500	-2.80159100	0.79614900
H	4.20647300	-2.31193600	0.63308900
C	2.20182400	-2.16965300	1.48099600
C	-2.56711700	-2.36461300	0.29886800
H	-3.64026200	-2.56028300	0.36897400
C	-3.17015100	-0.66297600	-1.96560400
H	-4.17760600	-1.07600300	-1.88860100
C	-2.96791700	0.47326900	0.83157800
C	-2.07092900	0.94232700	1.80224600
H	-1.04574400	0.58135200	1.80702300
C	-2.47404100	1.85110300	2.77477300
H	-1.76266900	2.18334000	3.52444200
C	-3.77885800	2.33219700	2.77265600
H	-4.10062700	3.05622800	3.51496600
C	-4.68016700	1.86935500	1.82025200
H	-5.70789500	2.22144500	1.82185600
C	-4.30032300	0.92612500	0.86093100
C	-5.34815500	0.42839400	-0.07506200
C	-5.92361000	-0.83104300	0.11710100
C	-6.88714600	-1.30945100	-0.76754200
H	-7.32573700	-2.29024100	-0.61134600
C	-7.29134700	-0.52754100	-1.84773400
C	-6.74454400	0.74134200	-2.02737100
H	-7.06403700	1.35818700	-2.86159600
C	-5.78346700	1.21937600	-1.14088900
H	-5.61491500	-1.42985700	0.96974200
H	-5.34527100	2.20362300	-1.28301100
H	-8.03760500	-0.90195300	-2.54127600
H	-3.22196600	0.36248800	-2.33961300
H	-2.58261600	-1.25535700	-2.67394100
H	-2.09692100	-3.10444600	-0.35633600
H	-2.09822400	-2.41931800	1.28580100
C	2.84012500	1.02202900	-0.76620500
C	2.10309300	-0.07605000	-1.00319900
H	2.66358300	-0.97351100	-1.28140800
C	2.25556900	2.32481800	-0.33253700
C	2.58772900	3.51916800	-0.98284300
C	1.35391100	2.38532400	0.73717200

C	2.01808800	4.72948000	-0.59872400
H	3.27429800	3.49954500	-1.82636500
C	0.78184300	3.59354600	1.12337700
H	1.10777900	1.47300800	1.27364900
C	1.11026900	4.77106900	0.45644900
H	2.27807700	5.64004500	-1.13038300
H	0.08039000	3.61324400	1.95239500
H	0.66574600	5.71430800	0.75881900

18)

E_{elec}(BS1) = -3029.8346532 Hartree E_{ZPE} = 0.632589Hartree H_{ZPE} = 0.681477 Hartree G_{ZPE} = 0.544118 Hartree

E_{elec}(BS2)= -3030.6694571 Hartree

Low frequencies (cm^{-1}) -24.2743 10.4728 18.2775 20.1438 26.2867 26.9001 30.5329 38.8085 40.6068

C	-3.99869700	-1.51514000	-0.90432700
C	-4.79704600	-0.30529600	-0.40974300
C	-4.92939000	0.85654400	-1.36246400
H	-4.35342000	-1.74705000	-1.91996600
H	-5.68449800	0.60667900	-2.11768700
H	-5.25378700	1.74276100	-0.81629100
O	-5.30443700	-0.30331800	0.69143800
C	-4.33873600	-2.70945600	-0.00527200
O	-3.59369000	-3.09395200	0.86963400
H	-3.98868300	1.05272700	-1.88337200
C	-5.66334000	-3.38099400	-0.26272500
H	-6.46505900	-2.63606100	-0.27024700
H	-5.64139700	-3.86137800	-1.24749800
H	-5.85505800	-4.12924900	0.50623700
Au	0.10565300	0.04824400	0.02948300
P	2.42717500	0.39782700	0.39652400
N	0.40535100	-1.18228800	3.13949600
N	-0.17868100	-2.16553400	2.54169100
N	-1.48755200	-1.91212800	2.43701800
H	-2.08855100	-2.50954400	1.86883000
C	-0.54765200	-0.23050200	3.42524100
C	-0.44213000	1.03809000	4.02241700
H	0.50942900	1.39992400	4.39763700
C	-1.59398200	1.79144800	4.10669800
H	-1.55704900	2.77865500	4.55587300
C	-2.83637400	1.30889500	3.61912400
H	-3.71272700	1.94415000	3.70066200
C	-2.96454300	0.06140600	3.04450100

H	-3.90817200	-0.30552500	2.65399500
C	-1.78528700	-0.69547300	2.95957800
C	2.73129700	1.16594800	2.03304000
H	3.76945600	1.49010200	2.13647000
C	3.11389100	1.59233000	-0.81220700
H	4.08053700	1.99799300	-0.50708100
C	3.39681300	-1.16507700	0.36351500
C	2.66864400	-2.32315000	0.67001100
H	1.62384300	-2.24331300	0.95643300
C	3.26420900	-3.57953400	0.63673800
H	2.67904400	-4.45584100	0.89753900
C	4.59850200	-3.70124600	0.26471000
H	5.07004500	-4.67801300	0.21591200
C	5.33558700	-2.56000400	-0.03251700
H	6.38498600	-2.64049400	-0.30190000
C	4.76087300	-1.28733500	0.03336600
C	5.63755500	-0.11187000	-0.23063700
C	6.06233100	0.70001400	0.82478200
C	6.85323600	1.81992100	0.58057700
H	7.17322400	2.44611900	1.40773500
C	7.23770600	2.13110000	-0.72192700
C	6.84812400	1.30558300	-1.77462800
H	7.15430800	1.53792200	-2.78989200
C	6.05874400	0.18585500	-1.52897100
H	5.77489000	0.44116300	1.84019900
H	5.74001000	-0.45200900	-2.34904000
H	7.84758500	3.00784300	-0.91556600
H	3.21360200	1.10435800	-1.78540200
H	2.37807400	2.39560000	-0.90607200
H	2.06470300	2.02929300	2.12816500
H	2.47794900	0.43149700	2.80346500
C	-2.49950900	-1.24102600	-0.93749100
C	-1.92369800	-0.25581600	-0.22591200
H	-2.60006600	0.36097700	0.37202600
C	-1.71302100	-2.21018400	-1.75344700
C	-1.99427400	-2.41578800	-3.10832400
C	-0.66437700	-2.93097300	-1.16972300
C	-1.22554700	-3.29212600	-3.86911100
H	-2.79936700	-1.85907200	-3.58328200
C	0.10448100	-3.80828800	-1.92855800
H	-0.46412300	-2.80443300	-0.10850100
C	-0.17168600	-3.98841300	-3.28177900
H	-1.44428100	-3.42455500	-4.92436400
H	0.92032100	-4.34950300	-1.45862100
H	0.42910200	-4.66939200	-3.87652500
S	-1.09655500	3.26811400	-1.81295100
O	-1.67336200	1.86096300	-2.24762800
O	0.16988000	3.12685700	-1.13092400
O	-1.28516400	4.17240600	-2.91465200

C	-2.31999000	3.72704800	-0.52270200
F	-3.53247600	3.77816700	-1.05588100
F	-1.99895500	4.91385600	-0.03415900
F	-2.30474800	2.82596400	0.45060800
H	-1.41450400	1.12434900	-1.61616200

TS6)

E_{elec}(BS1) = -3029.8239803 Hartree E_{ZPE} = 0.628063 Hartree H_{ZPE} = 0.677060 Hartree G_{ZPE} = 0.539883 Hartree

E_{elec}(BS2)= -3030.654666 Hartree

Low frequencies (cm^{-1}) -943.2915 8.6446 13.8184 19.2430 24.6798 31.0766 34.6672 43.7441 45.0932

C	-3.16826100	2.70504600	-0.41067500
C	-4.14340900	1.72721700	-1.07895500
C	-5.26548600	1.17606600	-0.24389600
H	-3.75060700	3.45991300	0.13245900
H	-5.59004000	1.87806000	0.52715600
H	-6.09874200	0.90120200	-0.89308900
O	-3.95978400	1.37362900	-2.22829100
C	-2.37065000	3.38752700	-1.53682800
O	-1.31614100	2.94257700	-1.92504400
H	-4.90160000	0.26399700	0.24975000
C	-3.02384400	4.59487900	-2.16454700
H	-3.20034300	5.37123400	-1.41222400
H	-2.39374100	4.98368100	-2.96434300
H	-3.99873600	4.30254200	-2.57070400
Au	0.11359600	0.08199700	0.32507300
P	2.34139400	-0.52527800	0.09022500
N	0.50391100	-0.98985900	-3.08179800
N	-0.00248400	0.19483500	-3.10656700
N	-1.31643300	0.12184600	-2.86746600
H	-1.85656700	0.97839200	-2.78424600
C	-0.50698400	-1.88455600	-2.80612800
C	-0.49194200	-3.28417700	-2.67387800
H	0.42699800	-3.84460900	-2.81192300
C	-1.68614000	-3.89975600	-2.36512800
H	-1.71987800	-4.97701800	-2.23872200
C	-2.87980400	-3.15594600	-2.18490700
H	-3.78812300	-3.68052300	-1.90738500
C	-2.91959500	-1.78524100	-2.33223100
H	-3.83104000	-1.21445700	-2.19320400
C	-1.70177000	-1.16539700	-2.65501500
C	2.50228900	-2.13762100	-0.76325400

H	3.48344200	-2.58139700	-0.58133100
C	3.08711500	-0.81402100	1.74184800
H	4.03919000	-1.34536300	1.68165600
C	3.31111900	0.74099200	-0.81466200
C	2.56291300	1.64255800	-1.58429900
H	1.48543300	1.53008500	-1.66370100
C	3.18121500	2.68412100	-2.26895000
H	2.57793100	3.35932300	-2.86627200
C	4.55678200	2.85593100	-2.17044900
H	5.04715000	3.67467700	-2.68776300
C	5.31053700	1.96724500	-1.41012700
H	6.38815200	2.08360000	-1.33903400
C	4.71064800	0.89618900	-0.74336700
C	5.59017900	-0.03896000	0.01164600
C	5.82534400	-1.33133100	-0.46592400
C	6.61844300	-2.21861600	0.25799000
H	6.79168800	-3.22115000	-0.12074200
C	7.19635900	-1.81591100	1.46013600
C	6.99670200	-0.51687600	1.92376700
H	7.45570200	-0.19474900	2.85317400
C	6.20320300	0.36859400	1.19995500
H	5.38973100	-1.63171200	-1.41482300
H	6.03199800	1.37766300	1.56489100
H	7.81044300	-2.50790200	2.02745900
H	3.23019400	0.14216100	2.25161600
H	2.36932600	-1.40826000	2.31473900
H	1.71772800	-2.79712300	-0.37938500
H	2.33283000	-1.97841200	-1.83133000
C	-2.24339000	1.95761700	0.54312300
C	-1.95976900	0.65051500	0.34256900
H	-2.51362800	0.15696100	-0.45590100
C	-1.63957900	2.77135100	1.63061200
C	-1.26547100	2.17251800	2.84354200
C	-1.43417800	4.14811900	1.47973100
C	-0.68912000	2.92702100	3.85810600
H	-1.45189100	1.11532100	3.00304700
C	-0.84668300	4.90137800	2.49179300
H	-1.71046300	4.64518900	0.55375100
C	-0.47137600	4.29309300	3.68541200
H	-0.41957300	2.44615800	4.79317000
H	-0.68367400	5.96442100	2.34522400
H	-0.02088600	4.88004600	4.47946100
S	-3.17505100	-2.15102400	1.88491700
O	-3.95414600	-1.75821700	0.71933100
O	-2.23700000	-1.01840500	2.33978900
O	-3.81789600	-2.79105700	3.00824700
C	-1.93976300	-3.34944100	1.25154800
F	-2.55493300	-4.36100500	0.65135700
F	-1.20026100	-3.81958400	2.24833900

F	-1.13619900	-2.74714100	0.37442700
H	-1.96906100	-0.26131500	1.46584300

1b
(**R** = 4-F-C_6H_4)

Au/Ga stabilized Reactant complex:

E_{elec}(BS1) = -5053.0696434 Hartree E_{ZPE} = 0.676318 Hartree H_{ZPE} = 0.744216 Hartree G_{ZPE} = 0.565446 Hartree

E_{elec}(BS2)= -6977.2248508 Hartree

Low frequencies (cm^{-1}) 9.8089 12.0989 16.2404 19.1153 22.1418 24.7567 27.3605 32.8862 36.3731

C	2.15613700	2.77974300	-0.75429000
C	3.31349700	2.24291500	-1.33426800
C	3.92913600	2.90033000	-2.53346800
H	1.77130800	3.71726300	-1.13238800
H	5.01560100	2.91361500	-2.42322800
H	3.69572200	2.28970400	-3.41216400
O	3.89737700	1.18635200	-0.92693300
C	1.50171400	2.17355500	0.30979600
O	1.84128200	1.05191900	0.84185900
Ga	3.40080000	0.05387000	0.53975700
O	0.93782800	-1.72296800	0.19905400
O	4.80739100	0.47545900	1.68772700
S	4.98351200	1.87810700	2.29984400
O	6.36416800	2.14998500	2.61402400
O	4.17499500	2.85411600	1.58483500
S	1.35674600	-1.90104700	1.58729900
O	1.29694100	-3.22896500	2.17642100
O	2.64737600	-1.18724600	1.88808900
C	0.09995600	-0.93910600	2.55060100
C	4.11639600	1.62368300	3.89391700
F	-0.83808300	-1.79263700	2.98972400
F	-0.51253700	-0.03824500	1.78248900
F	0.63708400	-0.32920500	3.59085200
F	4.09188700	2.76985100	4.56576600
F	2.86591000	1.23489700	3.65716900
F	4.73063300	0.70380300	4.61959100
H	3.54953000	3.91245300	-2.68161500
C	0.28985400	2.80404600	0.92812100
H	0.44571000	2.86026000	2.00975400
H	0.09131700	3.79741400	0.52291100
H	-0.57609300	2.15594900	0.75379000

Au	-2.20537600	-0.31639200	-1.03921200
P	-4.44637300	-0.55170400	-0.39476400
N	-1.90005900	-2.96028600	-0.91934900
N	-1.98223600	-3.21347600	0.34795100
N	-0.98075300	-4.02659700	0.68624400
H	-0.77207400	-4.17450600	1.66648000
C	-0.78824400	-3.58791100	-1.42358500
C	-0.19501200	-3.52202100	-2.69711800
H	-0.66637900	-2.97034900	-3.50456500
C	1.02072200	-4.14921300	-2.84618300
H	1.54995800	-4.08840400	-3.79061200
C	1.63637600	-4.84831700	-1.77326700
H	2.61488600	-5.28366200	-1.93914700
C	1.05935500	-4.93762800	-0.52692900
H	1.55015600	-5.42705100	0.30553100
C	-0.17110900	-4.28051900	-0.37716900
C	-5.05348200	-2.23209600	-0.77864800
H	-6.13556100	-2.29028700	-0.63841100
C	-5.49668600	0.56853400	-1.39847000
H	-6.55468300	0.30049500	-1.36001300
C	-4.70353400	-0.27255400	1.39594700
C	-3.59393400	-0.56021400	2.20071300
H	-2.69537300	-0.96647000	1.74883500
C	-3.62783200	-0.34494700	3.57354100
H	-2.75475100	-0.58255100	4.17179900
C	-4.77348400	0.18645300	4.15681400
H	-4.80634400	0.37858600	5.22457800
C	-5.88746000	0.46077900	3.36968200
H	-6.79437400	0.85274500	3.82102600
C	-5.88035600	0.21797000	1.99329300
C	-7.12993300	0.46639200	1.22139900
C	-7.90145500	-0.60970600	0.77237200
C	-9.04832800	-0.38848600	0.01407600
H	-9.63977300	-1.23136900	-0.32980200
C	-9.44033500	0.91311300	-0.29264700
C	-8.69535100	1.99102600	0.18137600
H	-9.00560800	3.00676100	-0.04315400
C	-7.55013300	1.76883300	0.94097900
H	-7.60151700	-1.62132600	1.03254000
H	-6.96027000	2.60682400	1.30314000
H	-10.33149100	1.08790900	-0.88703800
H	-5.37226300	1.59813000	-1.05380500
H	-5.13512400	0.50018500	-2.42866800
H	-4.79315500	-2.46892000	-1.81362500
H	-4.53915800	-2.94182400	-0.12660600
C	-0.59440500	1.13385400	-1.99487900
C	-0.05425100	0.03825200	-1.85821400
H	0.59667900	-0.81929300	-1.76889500
S	3.75514600	-1.62191600	-2.01100300

O	3.84632600	-1.45846400	-0.49080100
O	3.90145100	-3.01145200	-2.38492600
O	2.65866800	-0.84065600	-2.57174600
C	5.33030200	-0.80355300	-2.58942300
F	5.04583600	0.25106100	-3.34641800
F	6.01474100	-1.67269700	-3.32016800
F	6.07332600	-0.42239400	-1.56368200
C	-0.95291500	2.49568800	-2.30090100
C	-0.17312000	3.18343500	-3.24304700
C	-2.00890800	3.15518400	-1.66088900
C	-0.44368100	4.51177900	-3.54001700
H	0.65000200	2.66834600	-3.72763600
C	-2.28516000	4.48463200	-1.95213100
H	-2.60284400	2.62145300	-0.92435700
C	-1.49718000	5.14000200	-2.88769700
H	0.14287700	5.06629500	-4.26363400
H	-3.09303500	5.01982000	-1.46669400
F	-1.76067100	6.41827500	-3.17053600

TS(C1)

E_{elec}(BS1) = -5053.0548246 Hartree E_{ZPE} = 0.676045 Hartree H_{ZPE} = 0.742576 Hartree G_{ZPE} = 0.571378 Hartree

E_{elec}(BS2)= -6977.2046509 Hartree

Low frequencies (cm^{-1}) -388.5810 21.2772 24.7142 27.8362 30.8686 34.0190 34.3543 36.4067 39.5220

C	-1.82458400	-1.31526900	-2.42229400
C	-2.69873200	-0.19743700	-2.56129600
C	-2.98712000	0.40639300	-3.89512300
H	-1.58481800	-1.85639300	-3.33061900
H	-4.06622100	0.35255400	-4.07064300
H	-2.71675100	1.46689000	-3.84365900
O	-3.21699900	0.37984500	-1.57229100
C	-1.82442400	-2.07879600	-1.21111700
O	-2.11678900	-1.59244700	-0.08291400
Ga	-3.10313300	0.00765800	0.32040300
O	-0.15082200	0.01704700	1.33171400
O	-4.78867700	-0.70499800	0.61543300
S	-5.49590100	-1.75622300	-0.26409900
O	-6.90338800	-1.47656600	-0.39005200
O	-4.70102600	-2.08022400	-1.44257800
S	-1.00087900	-0.34517100	2.46189900
O	-0.67790300	0.20270100	3.76942900

O	-2.47016400	-0.18178600	2.12492600
C	-0.84253800	-2.19385000	2.66221100
C	-5.32791400	-3.21974800	0.82584300
F	-0.27062500	-2.45683500	3.82903900
F	-0.06739400	-2.68189400	1.69406500
F	-2.02362000	-2.77893300	2.61026500
F	-5.98883000	-4.23690400	0.28949300
F	-4.03986300	-3.54430500	0.92505800
F	-5.80924200	-2.96273500	2.02883500
H	-2.45096300	-0.08913600	-4.70435000
C	-1.45666000	-3.52515700	-1.23763900
H	-2.40248500	-4.07552400	-1.32961400
H	-0.81814000	-3.77266500	-2.08786100
H	-0.98315100	-3.80662200	-0.29614800
Au	1.92645100	1.39452900	-1.02228500
P	4.16408400	1.01528900	-0.41912000
N	3.24671500	3.00018700	2.71093600
N	2.60520100	2.25165200	3.53873900
N	1.30217600	2.25977100	3.22333800
H	0.65406600	1.66203200	3.73210600
C	2.34432200	3.52388100	1.81199200
C	2.52991800	4.39797800	0.72649100
H	3.51187900	4.79895600	0.49740300
C	1.41111700	4.73665900	-0.00601800
H	1.50366200	5.41472500	-0.84838600
C	0.12327600	4.24413100	0.33187700
H	-0.72939600	4.56046800	-0.25889700
C	-0.07939400	3.39237700	1.39972000
H	-1.07032400	3.04022900	1.66891800
C	1.06812200	3.03758400	2.13092700
C	5.27827300	2.35503300	0.13915800
H	6.31475800	2.00884100	0.12761900
C	4.97804500	0.34670800	-1.92350700
H	6.05173600	0.19511400	-1.79477700
C	4.11450000	-0.28343300	0.88121800
C	2.97975900	-0.25357900	1.70128300
H	2.23195600	0.52266900	1.56229300
C	2.75690600	-1.23032500	2.66567400
H	1.87941500	-1.16680600	3.30256600
C	3.66448600	-2.27586900	2.80427500
H	3.49793800	-3.05222500	3.54450900
C	4.79932600	-2.31668500	1.99809000
H	5.52378800	-3.11793800	2.11306200
C	5.05169500	-1.32151900	1.04862900
C	6.31047600	-1.40327500	0.25936400
C	7.34401300	-0.49144000	0.49179800
C	8.50726100	-0.53421700	-0.27273900
H	9.30331200	0.18004500	-0.08649800
C	8.65106000	-1.49871600	-1.26830500

C	7.63798800	-2.43169300	-1.48143000
H	7.75216200	-3.19187100	-2.24781200
C	6.47452800	-2.38926300	-0.71780700
H	7.23179200	0.24500300	1.28300400
H	5.67560200	-3.10440400	-0.89850200
H	9.55503900	-1.53028500	-1.86811200
H	4.50027000	-0.59957500	-2.19587400
H	4.80059100	1.06761900	-2.72715000
H	5.17036600	3.19901000	-0.54828400
H	4.99178900	2.66565300	1.14860200
C	-0.00682800	-0.31221000	-2.03029400
C	-0.07689600	0.91856500	-1.68469700
H	-0.88937200	1.63351400	-1.58650400
S	-3.23670100	3.07493300	-0.39886300
O	-3.02751300	1.87018200	0.54262300
O	-3.30824700	4.28235600	0.38949600
O	-2.34891600	3.04130700	-1.55281700
C	-4.94542800	2.77180900	-1.08590500
F	-4.87017100	2.57704700	-2.39523400
F	-5.69511800	3.83238000	-0.84589900
F	-5.49311700	1.70622000	-0.51621800
C	0.92804800	-1.43793500	-2.08448500
C	1.34961500	-2.01563000	-3.28560200
C	1.44946500	-1.89818700	-0.86625200
C	2.30481500	-3.02736700	-3.27504700
H	0.94784400	-1.65640200	-4.22850900
C	2.41209900	-2.89945600	-0.84491200
H	1.10904000	-1.44048300	0.05823600
C	2.82299600	-3.44288700	-2.05422500
H	2.66326400	-3.48580500	-4.18975900
H	2.84460300	-3.24631200	0.08899100
F	3.76398200	-4.39800400	-2.04690300

TS(C2)

E_{elec}(BS1) = -5053.0404442 Hartree E_{ZPE} = 0.675288 Hartree H_{ZPE} = 0.742621 Hartree G_{ZPE} = 0.563849 Hartree

E_{elec}(BS2)= -6977.2046509 Hartree

Low frequencies (cm^{-1}) -387.3459 6.2706 12.4262 14.3177 19.6588 22.9158 25.5885 26.4568 30.2896

C	2.14372600	2.14623900	-0.88911700
C	3.08049500	1.39094300	-1.64175600
C	3.30191100	1.69077900	-3.09009800
H	1.79700700	3.07981200	-1.31438700
H	4.37121200	1.65296800	-3.30821400

H	2.82235500	0.88754500	-3.66210400
O	3.73851700	0.42395100	-1.16649200
C	2.01183300	1.97450300	0.51232100
O	2.39043800	0.93313100	1.12319400
Ga	3.58897300	-0.45092100	0.55203200
O	1.09089600	-1.55753300	0.45602300
O	5.21040200	0.04146100	1.30237900
S	5.69173700	1.49415900	1.50067400
O	7.12653200	1.58728600	1.40391200
O	4.84142700	2.43393100	0.78200000
S	1.43796500	-1.84424800	1.85148400
O	1.13364700	-3.14732300	2.41004800
O	2.86476300	-1.40349900	2.10696800
C	0.41547000	-0.63388400	2.83249100
C	5.26216600	1.71868500	3.26884600
F	-0.48303000	-1.30085800	3.54751700
F	-0.23370700	0.18166400	1.99887000
F	1.16897500	0.08892600	3.64266200
F	5.60305200	2.94703000	3.64134700
F	3.95063900	1.56663900	3.43002400
F	5.90197500	0.83738600	4.01832500
H	2.88498900	2.65616600	-3.38037100
C	1.36955000	3.02924000	1.35311000
H	2.18568300	3.58720800	1.82854600
H	0.76145000	3.71588000	0.76097400
H	0.77748900	2.55634100	2.13903300
Au	-2.45828200	0.61113800	-0.85509600
P	-4.61261700	-0.18380400	-0.41103600
N	-1.98385100	-2.26779300	-0.29795400
N	-1.55325300	-2.90307200	0.73681000
N	-0.66702200	-3.82245700	0.34633300
H	-0.09411500	-4.24693200	1.06869000
C	-1.32945900	-2.74577900	-1.41057200
C	-1.40895400	-2.36837300	-2.76164100
H	-2.09084300	-1.58617200	-3.08520600
C	-0.57509700	-3.02298200	-3.64296200
H	-0.58933600	-2.75694500	-4.69482400
C	0.32185800	-4.02842900	-3.20576200
H	0.98878300	-4.48788300	-3.92766000
C	0.40327600	-4.41865800	-1.88605000
H	1.12268200	-5.15762800	-1.55560900
C	-0.44911900	-3.75263700	-0.99561100
C	-5.01322200	-1.65974400	-1.41543900
H	-6.07369700	-1.90655600	-1.33353800
C	-5.85180700	1.05835800	-0.95326400
H	-6.85799700	0.64100800	-1.02836900
C	-4.86039300	-0.59537500	1.35761800
C	-3.69499800	-0.81813900	2.10436600
H	-2.72380600	-0.76716500	1.62159900

C	-3.75990200	-1.11655200	3.46159500
H	-2.84283200	-1.29563300	4.01062000
C	-4.99454600	-1.17297200	4.09674800
H	-5.05581100	-1.39545000	5.15748200
C	-6.15773600	-0.94558600	3.36862000
H	-7.12744700	-0.99204300	3.85588300
C	-6.11334700	-0.67067800	1.99978700
C	-7.40848800	-0.44559200	1.29640200
C	-7.96146800	-1.42691900	0.46959000
C	-9.15690300	-1.18929900	-0.20585700
H	-9.57594400	-1.95711400	-0.84883500
C	-9.81911700	0.02587500	-0.04620600
C	-9.29442000	0.99346900	0.80852700
H	-9.81506900	1.93536500	0.95018200
C	-8.09922300	0.75555100	1.48061000
H	-7.45720100	-2.38427700	0.37050200
H	-7.68066600	1.51033800	2.14100400
H	-10.74894200	0.21251200	-0.57392600
H	-5.85719400	1.90198100	-0.25837900
H	-5.52983500	1.41978100	-1.93418800
H	-4.77273600	-1.43899700	-2.45979900
H	-4.39279300	-2.49116000	-1.07668000
C	-0.71688800	1.81862900	-1.33350700
C	0.24099600	1.02130700	-1.10924000
H	0.62597000	0.02809500	-0.90261100
S	3.40449900	-2.43102800	-1.78917700
O	3.79404700	-2.08855100	-0.34114600
O	3.37375000	-3.86670100	-1.96402700
O	2.29919500	-1.62098400	-2.27785100
C	4.92198100	-1.85150800	-2.71110000
F	4.56399300	-0.98103100	-3.65270600
F	5.50084700	-2.89128200	-3.29303700
F	5.79171000	-1.27290400	-1.89742100
C	-0.91866400	3.22567500	-1.66591800
C	-1.73312300	4.04817300	-0.87554100
C	-0.27967100	3.77166600	-2.78753100
C	-1.88178100	5.39578800	-1.17736100
H	-2.24071200	3.62336600	-0.01381100
C	-0.43529000	5.11571600	-3.10714100
H	0.32976400	3.12797800	-3.41486100
C	-1.23080300	5.90724200	-2.29160700
H	-2.49641100	6.05141300	-0.57109300
H	0.04528800	5.55641700	-3.97326400
F	-1.38158700	7.20185500	-2.59222900

1c
(**R** = 4-OMe-C_6H_4)

Au/Ga stabilized Reactant complex:

E_{elec}(BS1) = -5068.3435551 Hartree E_{ZPE} = 0.716856 Hartree H_{ZPE} = 0.786041 Hartree G_{ZPE} = 0.604867 Hartree

E_{elec}(BS2)= -6992.4977817Hartree

Low frequencies (cm^{-1}) -2.4791 12.8609 12.8973 17.2342 21.4368 23.9567 26.2015 29.5391 33.5132

C	2.14233400	2.68401000	0.65658600
C	3.33634700	2.50471900	-0.05503300
C	3.97321300	3.66750100	-0.75745300
H	1.73746600	3.68274300	0.75050300
H	5.05640300	3.62143100	-0.62645900
H	3.76678500	3.57254000	-1.82867900
O	3.94200100	1.39084300	-0.17836300
C	1.46906800	1.63677000	1.27039200
O	1.82054700	0.39884100	1.21238400
Ga	3.41542800	-0.31207200	0.53765100
O	0.99591500	-1.75720500	-0.65579900
O	4.78187600	-0.47830700	1.79256400
S	4.92649100	0.45845900	3.00619900
O	6.30153100	0.57016600	3.42750000
O	4.09970200	1.64469300	2.84335000
S	1.40201900	-2.56438700	0.49112700
O	1.35105400	-4.01297800	0.37957200
O	2.67800000	-2.06545400	1.11486400
C	0.12538300	-2.17472800	1.77867300
C	4.06633000	-0.55553600	4.26715500
F	-0.78789700	-3.15777300	1.78482100
F	-0.51427000	-1.04076500	1.49405800
F	0.65398100	-2.08430100	2.98494600
F	4.09766100	0.07325800	5.43725100
F	2.79807600	-0.72292700	3.90080500
F	4.64642000	-1.73815500	4.39017600
H	3.58583300	4.62154900	-0.39655000
C	0.22566100	1.88849200	2.07010200
H	0.35405500	1.43182100	3.05633100
H	0.01356000	2.95372600	2.17272700
H	-0.62114200	1.39094100	1.58488200
Au	-2.22282600	0.15006700	-1.02796800
P	-4.44945000	-0.39328700	-0.56433400

N	-1.86638700	-2.25026600	-2.19501200
N	-1.95514500	-3.06958700	-1.19760100
N	-0.97010400	-3.96503900	-1.28996600
H	-0.76942500	-4.56540800	-0.49896100
C	-0.76664600	-2.58668300	-2.94536500
C	-0.17159300	-1.94211600	-4.04467300
H	-0.62745200	-1.06353400	-4.48996900
C	1.02821200	-2.45116900	-4.48628100
H	1.55651100	-1.96350200	-5.29777100
C	1.62862600	-3.58364500	-3.87449900
H	2.59631100	-3.91097500	-4.23666200
C	1.05097500	-4.23520100	-2.80812400
H	1.53234800	-5.06534600	-2.30555500
C	-0.16462600	-3.70213300	-2.35448100
C	-5.05191000	-1.65605700	-1.74017300
H	-6.13255600	-1.78672300	-1.64533900
C	-5.50974900	1.07290600	-0.86946900
H	-6.56930400	0.81969300	-0.94212000
C	-4.69291300	-1.04974100	1.12702200
C	-3.57263100	-1.68411700	1.67776700
H	-2.67907600	-1.80708000	1.07540700
C	-3.59055800	-2.16934600	2.98033200
H	-2.70838600	-2.65802900	3.37995000
C	-4.73154400	-2.00381500	3.75832600
H	-4.75207700	-2.35877400	4.78388100
C	-5.85755200	-1.39352700	3.21505100
H	-6.76221800	-1.28679000	3.80689700
C	-5.86617700	-0.93050100	1.89634300
C	-7.12858100	-0.35660700	1.35361800
C	-7.87892400	-1.07555800	0.41836900
C	-9.03947300	-0.53080900	-0.12537800
H	-9.61359000	-1.09694600	-0.85229900
C	-9.46720200	0.73453500	0.27186900
C	-8.74375500	1.44155100	1.23020200
H	-9.08255900	2.42066100	1.55384700
C	-7.58393300	0.89575400	1.77358500
H	-7.55228900	-2.07091500	0.12932500
H	-7.01079500	1.44867800	2.51311300
H	-10.36952800	1.16203800	-0.15338900
H	-5.36376600	1.80693300	-0.07302400
H	-5.16951300	1.51174500	-1.81215100
H	-4.79771700	-1.33505300	-2.75386900
H	-4.52809800	-2.59328100	-1.53851700
C	-0.56206500	1.84754000	-1.27583600
C	-0.05655200	0.77629600	-1.60304200
H	0.56564600	-0.06717600	-1.86072700
S	3.76170200	-0.57634000	-2.49318400
O	3.91164100	-1.14061800	-1.07748400
O	3.87800900	-1.62763400	-3.47938700

O	2.65671300	0.37084900	-2.57807100
C	5.32059800	0.43395000	-2.67623400
F	5.01401800	1.72049800	-2.81173000
F	5.96282600	0.03853800	-3.76691800
F	6.11245000	0.27897800	-1.62858700
C	-0.87815800	3.21929700	-0.98086400
C	-0.04538000	4.21137600	-1.50914200
C	-1.94375200	3.59453000	-0.14878600
C	-0.26132600	5.55353400	-1.21796100
H	0.78666100	3.92028500	-2.14282000
C	-2.16556000	4.92686900	0.14378000
H	-2.58817600	2.82749500	0.27214600
C	-1.32717500	5.91653400	-0.38815100
H	0.40095200	6.29973200	-1.63958700
H	-2.98243600	5.23737700	0.78579800
O	-1.62889900	7.18629400	-0.04358600
C	-0.81260700	8.22194600	-0.55332900
H	-0.84022600	8.24489900	-1.64891700
H	-1.22436200	9.15030400	-0.15970200
H	0.22439500	8.11073700	-0.21582000

TS(C1)

E_{elec}(BS1) = -5068.3281259 Hartree E_{ZPE} = 0.717516 Hartree H_{ZPE} = 0.785984 Hartree G_{ZPE} = 0.608868 Hartree

E_{elec}(BS2)= -6992.4977817Hartree

Low frequencies (cm^{-1}) -388.2630 17.6566 20.5281 22.3203 24.9526 28.2943 30.7482 34.6728 35.1380

C	-1.76025300	-1.54289900	-2.27990900
C	-2.68037300	-0.48709700	-2.55138300
C	-2.96696400	-0.04333800	-3.94727700
H	-1.47242900	-2.15977600	-3.12351800
H	-4.02747800	-0.22250300	-4.15268700
H	-2.79999300	1.03782900	-3.99452700
O	-3.24860600	0.16384700	-1.63832500
C	-1.76078900	-2.18211900	-0.99855500
O	-2.10565100	-1.60074000	0.06799200
Ga	-3.15997700	-0.01366200	0.28788300
O	-0.22742300	0.17101900	1.37871500
O	-4.83196000	-0.74673200	0.60500600
S	-5.49366600	-1.87904200	-0.20655700
O	-6.86889300	-1.57863900	-0.51365700
O	-4.60247500	-2.37312600	-1.25028000

S	-1.10806400	-0.10358400	2.50927400
O	-0.83847000	0.56825000	3.77026200
O	-2.56941600	-0.00169300	2.11659300
C	-0.91953400	-1.92180300	2.88323900
C	-5.49391500	-3.18763700	1.07469600
F	-0.38593900	-2.06138600	4.08918700
F	-0.09904200	-2.47830900	1.99239500
F	-2.08523500	-2.53855200	2.84432900
F	-6.06405000	-4.27704200	0.57600400
F	-4.23851600	-3.47004400	1.41235700
F	-6.15919300	-2.78902200	2.14427200
H	-2.35381600	-0.56188100	-4.68442700
C	-1.32595200	-3.60414000	-0.87055300
H	-2.24583900	-4.20333600	-0.89680200
H	-0.67487100	-3.91128800	-1.69106900
H	-0.83909600	-3.75844300	0.09327000
Au	1.82211700	1.41732400	-1.03227300
P	4.06386600	1.16661400	-0.38496300
N	3.04169000	3.36948900	2.52924900
N	2.41931000	2.66133800	3.40603900
N	1.12030400	2.59847600	3.08126600
H	0.48675900	2.02112800	3.62997400
C	2.13002000	3.79242700	1.58753400
C	2.29378200	4.58964900	0.44091100
H	3.26324900	5.00619400	0.18735900
C	1.16998200	4.83303000	-0.32076600
H	1.24484100	5.44883100	-1.21134200
C	-0.10234600	4.31980500	0.04392400
H	-0.96014300	4.56347500	-0.57315600
C	-0.28309200	3.53922800	1.16836600
H	-1.26214700	3.16742500	1.45423900
C	0.86931400	3.28401700	1.93251200
C	5.12758700	2.58952100	0.04999300
H	6.17695100	2.28563400	0.06672700
C	4.90039900	0.38979800	-1.82434000
H	5.98202400	0.30936200	-1.69683900
C	4.06024100	-0.02055200	1.01852200
C	2.90887600	0.00649000	1.81545700
H	2.12204100	0.72599000	1.60494600
C	2.72125000	-0.90536200	2.84868900
H	1.82664900	-0.84744800	3.46218800
C	3.68286700	-1.88314000	3.08290200
H	3.54365700	-2.61146900	3.87568200
C	4.83391400	-1.92098400	2.30028200
H	5.59684700	-2.67201200	2.48446800
C	5.04862300	-0.98934200	1.28009900
C	6.32071400	-1.06940800	0.51178300
C	7.30695700	-0.09332700	0.67839300
C	8.47931600	-0.14013000	-0.07221800

H	9.23899200	0.62341900	0.06326300
C	8.68002500	-1.17197300	-0.98668100
C	7.71608200	-2.16873900	-1.12903500
H	7.87791000	-2.98224800	-1.83023400
C	6.54355700	-2.12327000	-0.37930600
H	7.15328900	0.69455500	1.41074300
H	5.78040800	-2.88963700	-0.49935200
H	9.59081900	-1.20657100	-1.57603500
H	4.46949600	-0.60390500	-1.98605000
H	4.67600100	1.01007400	-2.69719400
H	4.98567500	3.36406100	-0.70907300
H	4.82575900	2.97638700	1.02808000
C	-0.00543800	-0.44653900	-1.94638000
C	-0.13903400	0.80351100	-1.69029200
H	-0.99515400	1.47158500	-1.66222700
S	-3.38326200	2.96816500	-0.71787600
O	-3.15211300	1.86059300	0.33077700
O	-3.50825800	4.23804500	-0.04162300
O	-2.47438400	2.86087600	-1.85038500
C	-5.06995700	2.54848400	-1.39956900
F	-4.96726200	2.24737300	-2.68663500
F	-5.85929000	3.59816700	-1.25907700
F	-5.58917000	1.51564500	-0.74914100
C	0.99198100	-1.51594400	-1.90900500
C	1.50540100	-2.11557100	-3.05710100
C	1.50190200	-1.88769100	-0.65225600
C	2.53293800	-3.05452800	-2.97011100
H	1.12049100	-1.82964700	-4.03210800
C	2.52694100	-2.81056100	-0.55550400
H	1.10104200	-1.41304800	0.23958400
C	3.05108300	-3.39635600	-1.71640500
H	2.92689900	-3.49606900	-3.87759000
H	2.94906200	-3.07787500	0.40931800
O	4.06118500	-4.27952800	-1.52403000
C	4.71936300	-4.79027000	-2.66526600
H	5.14413800	-3.97916800	-3.26985500
H	5.52072700	-5.42681300	-2.29055200
H	4.04023600	-5.38912700	-3.28283900

TS(C2)

E_{elec}(BS1) = -5068.3139218 Hartree E_{ZPE} = 0.717688 Hartree H_{ZPE} = 0.786355 Hartree G_{ZPE} = 0.606323 Hartree

E_{elec}(BS2)= -6992.4663654 Hartree

Low frequencies (cm^{-1}) -387.4975 8.7126 14.5750 18.8408 21.1291 22.3820 27.0954 28.7397 30.3455

C	2.16701100	2.15993300	-0.26344200
C	3.07046900	1.61644100	-1.21181000
C	3.28590900	2.30360800	-2.52311400
H	1.83571700	3.17969100	-0.41574100
H	4.34830000	2.27926400	-2.77367200
H	2.75448400	1.72398000	-3.28706900
O	3.70597600	0.53859200	-1.03593600
C	2.06275800	1.62782800	1.04684200
O	2.43209600	0.45748800	1.35268700
Ga	3.57870900	-0.74954400	0.39755900
O	1.05546700	-1.73599400	0.13411300
O	5.23402100	-0.48495300	1.19702700
S	5.74813200	0.86710100	1.73311800
O	7.18205300	0.96343600	1.62420800
O	4.90122100	1.96698500	1.29055800
S	1.44174000	-2.38613300	1.39094400
O	1.10898600	-3.78134700	1.60444200
O	2.89336200	-2.06364500	1.68403500
C	0.50932800	-1.44929200	2.70465800
C	5.36271900	0.65817900	3.51358200
F	-0.37845800	-2.25849000	3.27089500
F	-0.14668900	-0.42871400	2.14961400
F	1.32672500	-0.98253900	3.63287600
F	5.69283000	1.77237000	4.15736300
F	4.05909300	0.44262000	3.66492200
F	6.03813100	-0.35977500	4.01875500
H	2.91798700	3.33052400	-2.51289000
C	1.47033600	2.44464400	2.14855900
H	2.30825400	2.93387300	2.66072500
H	0.79046600	3.21028300	1.76776500
H	0.96737300	1.78961500	2.86129400
Au	-2.47228500	0.81264500	-0.61627500
P	-4.60785800	-0.12142700	-0.39307500
N	-2.00205200	-2.14818100	-0.72571900
N	-1.58467800	-3.03418700	0.11042000
N	-0.75154000	-3.86839600	-0.51725600
H	-0.18672900	-4.47903800	0.06371300
C	-1.39383400	-2.36972900	-1.94066900
C	-1.48768100	-1.67695700	-3.15918400
H	-2.13342500	-0.80863800	-3.26127300
C	-0.71499000	-2.14033500	-4.20246600
H	-0.74353200	-1.63030900	-5.15979000
C	0.13735400	-3.26105300	-4.05132800
H	0.75746000	-3.56602200	-4.88760600
C	0.23362500	-3.95761700	-2.86512600
H	0.92154500	-4.78588400	-2.74844600
C	-0.55708800	-3.48480100	-1.80934800
C	-4.96363200	-1.31447200	-1.73547700

H	-6.02029900	-1.58885900	-1.74242800
C	-5.90242400	1.16277900	-0.60211200
H	-6.89119000	0.73166400	-0.77254700
C	-4.81888500	-0.93957000	1.23503500
C	-3.63726900	-1.25346000	1.92097900
H	-2.67506500	-1.07400200	1.45159300
C	-3.67308400	-1.81176500	3.19427200
H	-2.74292500	-2.05547900	3.69429800
C	-4.89677900	-2.04230800	3.81158400
H	-4.93693700	-2.46569400	4.81038300
C	-6.07717800	-1.73733200	3.14161300
H	-7.03867800	-1.92718500	3.61008100
C	-6.06001700	-1.20384000	1.85076900
C	-7.36794900	-0.94706200	1.18471200
C	-7.80743800	-1.77400000	0.14726000
C	-9.01137500	-1.51368100	-0.50313300
H	-9.34081800	-2.16110800	-1.30993000
C	-9.79623100	-0.43204400	-0.10954900
C	-9.38488200	0.37218000	0.95167200
H	-10.00109300	1.20645800	1.27196900
C	-8.18101300	0.11140100	1.60003100
H	-7.20443200	-2.63191000	-0.13703700
H	-7.85039400	0.74406700	2.41945400
H	-10.73264000	-0.22568800	-0.61793500
H	-5.93153200	1.80223000	0.28383500
H	-5.61450700	1.77395000	-1.46217500
H	-4.70723000	-0.83906700	-2.68719400
H	-4.33159700	-2.19393100	-1.59832300
C	-0.69457900	2.04875100	-0.76908600
C	0.23112900	1.18419700	-0.73221900
H	0.58100700	0.15792000	-0.76460800
S	3.25852700	-2.05428100	-2.36235200
O	3.71185000	-2.10394700	-0.89330000
O	3.19929200	-3.39464200	-2.90356000
O	2.15046800	-1.13639500	-2.57495700
C	4.74705800	-1.26915000	-3.17290200
F	4.37939200	-0.15253800	-3.79833700
F	5.24856300	-2.10734600	-4.06800800
F	5.68360900	-0.97726500	-2.28343700
C	-0.84013900	3.50033900	-0.77439300
C	-1.64947900	4.16242600	0.16308500
C	-0.15379200	4.26366700	-1.72196500
C	-1.73599200	5.54235600	0.16856300
H	-2.20044900	3.57977800	0.89669300
C	-0.24651800	5.65388300	-1.73417400
H	0.44899800	3.75767900	-2.47088400
C	-1.03540300	6.29964500	-0.78027800
H	-2.34528200	6.06801600	0.89579300
H	0.29399100	6.21401300	-2.48763900

O	-1.19281400	7.64075900	-0.69427900
C	-0.49548300	8.44414100	-1.62305800
H	-0.80670000	8.22464400	-2.65134900
H	-0.74844700	9.47548400	-1.37994800
H	0.58824500	8.30313300	-1.53351000

1d
(**R** = CH_3)

Au/Ga stabilized Reactant complex:

E_{elec}(BS1) = -4762.2128371 Hartree E_{ZPE} = 0.630408 Hartree H_{ZPE} = 0.694602 Hartree G_{ZPE} = 0.526466 Hartree

E_{elec}(BS2)= -6686.2604044 Hartree

Low frequencies (cm^{-1}) 16.1846 18.4364 21.2838 22.6204 24.0822 30.9356 34.8994 40.6420 42.4723

C	1.87889800	-1.28071500	2.63913600
C	2.87030700	-0.29094600	2.56519700
C	3.40008700	0.37943900	3.79443100
H	1.57448100	-1.63829900	3.61405800
H	4.48379600	0.23819100	3.83556700
H	3.21642500	1.45451700	3.69106100
O	3.39036800	0.11054800	1.47495900
C	1.35599400	-1.89516900	1.50673100
O	1.59373900	-1.53487100	0.29545700
Ga	2.93495700	-0.35766000	-0.31300900
O	0.23589700	0.64416200	-1.03739700
O	4.40248800	-1.37660700	-0.82341100
S	4.90983600	-2.61331500	-0.05564200
O	6.34122700	-2.74681100	-0.16349100
O	4.24543600	-2.73706200	1.23271400
S	0.65696300	-0.11727100	-2.21665200
O	0.32320100	0.43476600	-3.52087300
O	2.09091700	-0.55408800	-2.09262700
C	-0.27216900	-1.73238100	-2.12089400
C	4.17633800	-3.93579400	-1.09009700
F	-1.10161200	-1.82302700	-3.15473300
F	-1.00908800	-1.76496600	-1.00219500
F	0.54706300	-2.76297700	-2.12644700
F	4.55868100	-5.11840800	-0.62298000
F	2.84783400	-3.85751100	-1.02742400
F	4.56140000	-3.81391000	-2.34926600
H	2.94162500	-0.00105600	4.70825900

C	0.47204800	-3.10134600	1.62375100
H	1.08218500	-3.96929300	1.34687900
H	0.09355400	-3.24384500	2.63814400
H	-0.34723400	-3.03798200	0.90412800
Au	-1.89779000	0.84197000	0.63879200
P	-3.90825600	0.00464400	-0.13869100
N	-2.89620600	3.26699300	-1.33528100
N	-2.55538600	2.55646200	-2.35676900
N	-1.24460200	2.69376900	-2.57863300
H	-0.78433500	2.08675700	-3.25523100
C	-1.76624800	3.88840600	-0.84963000
C	-1.58482600	4.74829100	0.24892200
H	-2.42745900	5.04502000	0.86446500
C	-0.30184600	5.18983800	0.49276100
H	-0.11174200	5.85502500	1.32852000
C	0.79143700	4.79232700	-0.32158100
H	1.78901800	5.14634100	-0.08565100
C	0.63307200	3.94320300	-1.39909300
H	1.47941600	3.63141700	-2.00230900
C	-0.67873200	3.50747100	-1.64936900
C	-3.90093700	-0.43313300	-1.91190000
H	-4.91551400	-0.66858800	-2.24150300
C	-5.22298300	1.26146600	0.02735200
H	-6.12616600	0.97679500	-0.51632600
C	-4.32407300	-1.52096500	0.80092200
C	-3.24862300	-2.18911500	1.40379600
H	-2.24535000	-1.78475600	1.29603100
C	-3.43777700	-3.35270700	2.14004100
H	-2.58525500	-3.85477100	2.58679700
C	-4.72302600	-3.85718900	2.30790400
H	-4.88866900	-4.75782600	2.89064000
C	-5.80043800	-3.20287500	1.72146100
H	-6.80704600	-3.59245100	1.84174800
C	-5.62141100	-2.04812400	0.95343600
C	-6.82778500	-1.42517200	0.33742100
C	-7.10373600	-1.59938900	-1.02111700
C	-8.21418700	-0.98790300	-1.59874600
H	-8.41698200	-1.12547100	-2.65617500
C	-9.06600300	-0.20924800	-0.81845300
C	-8.81669600	-0.06210000	0.54465400
H	-9.48455400	0.53351200	1.15891100
C	-7.70677500	-0.67287500	1.12097100
H	-6.44954100	-2.22577700	-1.62142000
H	-7.50157900	-0.54988500	2.18106700
H	-9.92779800	0.27189900	-1.26951100
H	-5.45767500	1.41128700	1.08423300
H	-4.80510500	2.18533900	-0.38715500
H	-3.52669700	0.43369800	-2.46538900
H	-3.24362100	-1.28767000	-2.07795700

C	-0.36830700	1.22497800	2.52996300
C	0.06918400	1.85151000	1.57798600
H	0.59942100	2.42026400	0.83173100
C	-0.79334900	0.53031100	3.74968800
H	-0.02067800	0.64711300	4.51544900
H	-1.72984400	0.94831000	4.12790900
H	-0.93385200	-0.53711200	3.55916700
S	3.59509200	2.67749800	0.07112900
O	3.15926700	1.46501400	-0.76693200
O	3.80484900	3.81441900	-0.80289100
O	2.77821500	2.85769900	1.26286000
C	5.28882800	2.17685600	0.67697800
F	5.29544000	2.12590200	2.00186100
F	6.16941100	3.08011000	0.27778500
F	5.62676400	0.99270500	0.18603200

TS(C1)

E_{elec}(BS1) = -4762.1679029 Hartree E_{ZPE} = 0.630408 Hartree H_{ZPE} = 0.694602 Hartree G_{ZPE} = 0.526466 Hartree

E_{elec}(BS2)= -6686.2200266Hartree

Low frequencies (cm^{-1}) -359.8557 11.5748 17.7835 21.2724 26.0120 26.5068 29.3219 31.7809 38.3699

C	-1.98216500	-1.50313500	-2.44198500
C	-2.44364000	-0.17027300	-2.60151400
C	-2.37700100	0.50507400	-3.93522400
H	-1.84177800	-2.09281800	-3.33863000
H	-3.34633200	0.96257400	-4.14899400
H	-1.64182300	1.31362500	-3.86647600
O	-2.86744800	0.53157400	-1.64235500
C	-2.17880800	-2.20079400	-1.22348500
O	-2.52527600	-1.64243800	-0.14356700
Ga	-3.39885100	0.04805900	0.16209700
O	-1.09103300	0.31570500	1.49942700
O	-5.20954300	-0.33629900	-0.05950200
S	-5.84620500	-1.33153300	-1.04002300
O	-7.16012400	-0.90655300	-1.45232500
O	-4.87393900	-1.77873700	-2.03035400
S	-1.87961400	-0.35160900	2.53900700
O	-1.78229200	0.10247300	3.91349500
O	-3.30833300	-0.47145300	2.03982900
C	-1.27542500	-2.11427100	2.55593400
C	-6.08013500	-2.76906100	0.07273500
F	-0.63175700	-2.34449500	3.68933900

F	-0.43651200	-2.30963700	1.54059700
F	-2.28915300	-2.95884800	2.44723900
F	-6.58801600	-3.77859400	-0.62429600
F	-4.89998300	-3.14002800	0.56832600
F	-6.89499800	-2.46339300	1.06673700
H	-2.10045300	-0.18434000	-4.73393100
C	-1.95943000	-3.67848300	-1.13881500
H	-2.93977400	-4.13718900	-0.97102000
H	-1.51995800	-4.09534400	-2.04592100
H	-1.33814100	-3.89760000	-0.26698100
Au	2.34618700	0.04713900	-0.59035400
P	4.64345100	0.18621400	-0.13932700
N	2.05338400	1.21749700	2.08932200
N	1.36703800	0.82677700	3.10563300
N	0.48341100	1.77652600	3.42979600
H	-0.25545400	1.52446800	4.07909200
C	1.58604200	2.45308800	1.69531200
C	1.97332800	3.29539500	0.63945500
H	2.77540300	3.01672900	-0.03931200
C	1.28057900	4.47784400	0.48904900
H	1.53684200	5.15118300	-0.32221300
C	0.21938600	4.82641900	1.35664100
H	-0.33047200	5.74330400	1.17451800
C	-0.17138100	4.01444700	2.40134100
H	-1.01280000	4.27300500	3.03322400
C	0.54230900	2.81845000	2.55499800
C	5.07560700	1.21405900	1.30910400
H	6.15950300	1.32922000	1.38209900
C	5.51430000	0.99183400	-1.53855700
H	6.54131500	1.27236900	-1.29662000
C	5.34175900	-1.48248500	0.18549100
C	4.43309000	-2.42023600	0.69739400
H	3.40508400	-2.12022300	0.88895500
C	4.82119900	-3.72819600	0.96551100
H	4.10121000	-4.43179400	1.37001100
C	6.12668000	-4.12690500	0.69885500
H	6.43746500	-5.14960700	0.88788900
C	7.03951800	-3.20592200	0.19678300
H	8.06580600	-3.50300700	0.00074100
C	6.67328200	-1.87862700	-0.04568500
C	7.72487500	-0.93991000	-0.53029800
C	8.29470800	-0.00870500	0.34248900
C	9.24995400	0.89578400	-0.11540300
H	9.68198600	1.61791700	0.57029500
C	9.65478800	0.86655400	-1.44832200
C	9.11916900	-0.08469700	-2.31433200
H	9.44321100	-0.12073900	-3.34975000
C	8.16397800	-0.98772200	-1.85582200
H	7.99171600	-0.00457900	1.38597300

H	7.73496100	-1.72250900	-2.53188200
H	10.39470600	1.57408600	-1.80849900
H	5.50932500	0.32884200	-2.40715900
H	4.93771200	1.88795300	-1.78793500
H	4.60356100	2.19443100	1.20152900
H	4.66492400	0.74866100	2.20651700
C	0.14770500	-1.01318700	-2.04104100
C	0.27665900	-0.14484300	-1.12833800
H	-0.39866300	0.45826500	-0.52845200
C	0.73495600	-1.91435500	-3.05704900
H	0.41567300	-1.63192000	-4.06419500
H	1.82403000	-1.82835500	-3.00330400
H	0.46004500	-2.95741300	-2.87899400
S	-2.63924200	3.02634800	-0.03556300
O	-3.40794100	1.86189500	0.60835600
O	-2.77987400	4.21416400	0.77712700
O	-1.33094700	2.61846600	-0.51760200
C	-3.67367700	3.35537100	-1.55670000
F	-2.93573000	3.18647200	-2.65131100
F	-4.10150100	4.60885900	-1.52735200
F	-4.72236400	2.54537400	-1.61451200

TS(C2)

E_{elec}(BS1) = -4762.1708923 Hartree E_{ZPE} = 0.630014 Hartree H_{ZPE} = 0.693437 Hartree G_{ZPE} = 0.525632 Hartree

E_{elec}(BS2)= -6686.220543 Hartree

Low frequencies (cm^{-1}) -380.6218 13.8734 17.7202 19.2019 23.6851 27.8715 30.6442 31.8993 34.3719

C	2.19853900	-0.53295800	2.57147600
C	3.02823700	0.59296500	2.31792700
C	3.18583100	1.65743200	3.35586600
H	1.94725300	-0.72884100	3.60545500
H	4.23980700	1.93124800	3.43918400
H	2.64489600	2.53900700	2.99264700
O	3.63199100	0.78225100	1.22648800
C	2.11284900	-1.61217100	1.65707900
O	2.42709800	-1.51351800	0.43586700
Ga	3.49912500	-0.18436400	-0.44494100
O	0.97183000	0.33254700	-1.17139300
O	5.17487600	-0.98505600	-0.48912300
S	5.74722700	-1.90931100	0.60455900
O	7.18056200	-1.79109100	0.69494100
O	4.92806400	-1.86985900	1.80879100

S	1.31516000	-0.62965800	-2.22501700
O	0.91862000	-0.36317900	-3.59350400
O	2.77818400	-0.99885500	-2.07886000
C	0.42067600	-2.19197800	-1.74158500
C	5.39587000	-3.54191400	-0.15112100
F	-0.47617700	-2.48987900	-2.67397700
F	-0.22013700	-2.00036500	-0.58710600
F	1.26028200	-3.20377000	-1.60574700
F	5.77238100	-4.49505700	0.69424800
F	4.09052500	-3.65839500	-0.37696200
F	6.05283300	-3.67830700	-1.29000500
H	2.78860300	1.35308100	4.32475300
C	1.59626300	-2.94600300	2.09025400
H	2.47142700	-3.59715900	2.20504400
H	1.05838600	-2.89568200	3.03843900
H	0.96293300	-3.36268100	1.30462800
Au	-2.51586100	0.13910700	1.59569400
P	-4.67455100	0.25510400	0.68805000
N	-2.04829700	1.24047400	-1.11376100
N	-1.67748100	0.76570900	-2.25179100
N	-0.91554700	1.66912500	-2.87359100
H	-0.38722600	1.34972200	-3.67885100
C	-1.48134100	2.48359200	-0.94978800
C	-1.55269500	3.39546100	0.11638500
H	-2.13196200	3.16998500	1.00790000
C	-0.84354500	4.56970900	-0.01777900
H	-0.85698700	5.30038300	0.78440100
C	-0.07874400	4.84362800	-1.17784400
H	0.48908100	5.76687100	-1.22629600
C	-0.00411500	3.96252900	-2.23563300
H	0.61635100	4.16494200	-3.09972100
C	-0.72469700	2.76890600	-2.09320100
C	-5.03634900	1.91744400	0.00950500
H	-6.09934500	2.02167600	-0.21768600
C	-5.95073900	0.02941800	1.98751600
H	-6.94446900	0.33324400	1.65211200
C	-4.91034900	-0.99667000	-0.63073400
C	-3.73772600	-1.52989700	-1.18415700
H	-2.77032800	-1.15583900	-0.86366500
C	-3.78934100	-2.52465100	-2.15480800
H	-2.86562600	-2.90726800	-2.57314100
C	-5.02023000	-3.01932800	-2.56895400
H	-5.07352900	-3.80418800	-3.31708300
C	-6.19168600	-2.49990000	-2.02733000
H	-7.15834400	-2.87162500	-2.35475900
C	-6.15888300	-1.47988500	-1.07350500
C	-7.46004300	-0.95451900	-0.57198500
C	-7.92936900	0.29473400	-0.98714000
C	-9.13224400	0.79667200	-0.49496600

H	-9.48681500	1.76855400	-0.82393300
C	-9.88476900	0.04579000	0.40543000
C	-9.44226500	-1.21724400	0.79394000
H	-10.03396400	-1.81303900	1.48190200
C	-8.23966700	-1.71709800	0.30245300
H	-7.35197700	0.86412500	-1.71055900
H	-7.88448200	-2.69631400	0.61214700
H	-10.82077200	0.43698000	0.79109200
H	-5.97531000	-1.01778000	2.29970400
H	-5.64954000	0.64029100	2.84329300
H	-4.75107000	2.66277500	0.75804600
H	-4.43112000	2.06972200	-0.88610700
C	-0.69904300	-0.17438400	2.73267200
C	0.20458500	0.13292800	1.90079900
H	0.51381700	0.53430400	0.94175200
C	-0.84110400	-0.76821400	4.08966000
H	0.13430900	-0.90922400	4.56821000
H	-1.44981900	-0.12365000	4.72844500
H	-1.34614000	-1.73693500	4.02772200
S	3.09434500	2.83732200	-0.82298000
O	3.59616300	1.47100000	-1.31930200
O	2.96659800	3.74458600	-1.94262600
O	2.01576000	2.72441100	0.14590300
C	4.58048200	3.44203700	0.13189800
F	4.23714700	3.66412500	1.39892200
F	5.00418200	4.58044900	-0.39661700
F	5.56537000	2.55756500	0.10114800

1e
(**R** = C_2H_5)

Au/Ga stabilized Reactant complex:

E_{elec}(BS1) = -4801.5074227 Hartree E_{ZPE} = 0.659123 Hartree H_{ZPE} = 0.724543 Hartree G_{ZPE} = 0.553670 Hartree

E_{elec}(BS2)= -6725.5681325 Hartree

Low frequencies (cm^{-1}) 13.9289 20.0750 22.5631 24.9318 27.9092 29.7512 31.7452 39.3073 43.7739

C	2.00676400	-1.28597500	2.64337400
C	2.98286800	-0.28018500	2.57306500
C	3.49743200	0.39505700	3.80576200
H	1.70711600	-1.65055900	3.61712200
H	4.58580300	0.29485100	3.83840000

H	3.27097900	1.46315600	3.71620000
O	3.49519000	0.13339600	1.48395300
C	1.47811300	-1.89188900	1.51019600
O	1.70573900	-1.52230500	0.29905400
Ga	3.03288500	-0.33103200	-0.30529800
O	0.32077800	0.63221700	-1.05907300
O	4.52764300	-1.30841000	-0.81851800
S	5.04675600	-2.55288100	-0.07119200
O	6.47940400	-2.67033200	-0.18057500
O	4.38227800	-2.70429300	1.21400900
S	0.76376800	-0.12968500	-2.22994000
O	0.43794000	0.41176900	-3.54081900
O	2.20063100	-0.55044800	-2.09029600
C	-0.14966300	-1.75435800	-2.13733600
C	4.32682400	-3.86636800	-1.12641900
F	-0.96436700	-1.85955100	-3.18160500
F	-0.90164900	-1.78996600	-1.02852300
F	0.68034800	-2.77617400	-2.12637700
F	4.72125000	-5.05226900	-0.67791100
F	2.99760700	-3.80249200	-1.06253900
F	4.71034100	-3.72127300	-2.38363100
H	3.05789600	-0.01078300	4.71773400
C	0.59037400	-3.09590700	1.62183000
H	1.17930300	-3.95825100	1.28754100
H	0.25319100	-3.27255700	2.64539400
H	-0.25796200	-3.00084400	0.93955100
Au	-1.90644200	0.84214200	0.45727700
P	-3.90240500	-0.03426400	-0.31418300
N	-2.97735900	3.19406200	-1.55881500
N	-2.56779100	2.48421700	-2.55497400
N	-1.24324300	2.61441800	-2.68032000
H	-0.73652000	2.01502600	-3.33023500
C	-1.88253800	3.80742500	-0.98974400
C	-1.77538000	4.66329600	0.12244600
H	-2.65695200	4.95822200	0.68181300
C	-0.51206300	5.10683400	0.45090800
H	-0.37986400	5.77205200	1.29787100
C	0.63354700	4.71753000	-0.29351400
H	1.61158700	5.07991500	0.00398900
C	0.54858000	3.86855900	-1.37904900
H	1.43196300	3.56529700	-1.93147100
C	-0.74244300	3.42718700	-1.71305700
C	-3.88911200	-0.52559800	-2.07317300
H	-4.88920100	-0.82994200	-2.38956400
C	-5.24812400	1.19209500	-0.17038300
H	-6.14915700	0.87356000	-0.69869800
C	-4.27921900	-1.53139300	0.69087600
C	-3.18312400	-2.15706100	1.30352600
H	-2.18541100	-1.75794800	1.13844700

C	-3.34352100	-3.26795500	2.12281300
H	-2.47482000	-3.73547800	2.57614700
C	-4.62069200	-3.76349600	2.36412500
H	-4.76418100	-4.62069900	3.01437400
C	-5.71746900	-3.15717000	1.76267900
H	-6.71774400	-3.54409400	1.93426800
C	-5.56747600	-2.05689200	0.91193400
C	-6.79343900	-1.48974800	0.28256100
C	-7.06797300	-1.71357600	-1.06911400
C	-8.19668300	-1.15167000	-1.66127600
H	-8.39894700	-1.32808800	-2.71300500
C	-9.06761300	-0.37284400	-0.90255500
C	-8.81918700	-0.17712400	0.45458400
H	-9.50158000	0.41856700	1.05257600
C	-7.69150800	-0.73910100	1.04564800
H	-6.39893300	-2.34081900	-1.65192600
H	-7.48651300	-0.57689600	2.10050900
H	-9.94351400	0.07075500	-1.36477500
H	-5.47694800	1.35954200	0.88547000
H	-4.85689900	2.11628500	-0.60869300
H	-3.56686700	0.34540500	-2.65244900
H	-3.18054900	-1.34221300	-2.22147800
C	-0.46112000	1.01235500	2.44643300
C	0.00082800	1.75904100	1.59672800
H	0.56409800	2.41891500	0.95589000
C	-0.94772900	0.16892400	3.54882200
H	-0.26292700	0.31995700	4.39188500
S	3.56169000	2.72039600	0.10313300
O	3.20341700	1.49698200	-0.75441200
O	3.70933800	3.88071400	-0.75225200
O	2.72845300	2.83565400	1.29207600
C	5.27910000	2.30663300	0.70757800
F	5.28959000	2.25509200	2.03234400
F	6.11122800	3.25497600	0.30812300
F	5.67650600	1.14282200	0.21378700
C	-2.38871000	0.48150800	3.96550500
H	-2.66192000	-0.11857800	4.83694300
H	-2.49938500	1.53899800	4.21828100
H	-3.08312700	0.24463200	3.15269300
H	-0.85513200	-0.88365900	3.25524600

TS(C1)

E_{elec}(BS1) = -4801.478627Hartree E_{ZPE} = 0.658792 Hartree H_{ZPE} = 0.723290 Hartree G_{ZPE} = 0.555007 Hartree

E_{elec}(BS2)= -6725.5402846 Hartree

Low frequencies (cm^{-1}) -334.3058 15.4670 20.4970 23.4195 25.0223 29.5605 33.6641 37.3605 40.9005

C	3.20341500	-0.47171400	2.65812300
C	3.37220200	0.88271600	2.25065200
C	3.70680300	1.95064400	3.24116400
H	3.57839600	-0.73976100	3.63832000
H	4.64993900	2.41897300	2.94349300
H	2.92759200	2.71728300	3.18364900
O	3.19156300	1.26088300	1.06289100
C	3.10399800	-1.51109700	1.69304500
O	2.78546200	-1.31769300	0.48421700
Ga	2.88128100	0.26302100	-0.58523200
O	0.09057300	-0.68532000	-0.57662700
O	4.58956000	0.25831600	-1.29932700
S	5.87071600	-0.22210000	-0.59001500
O	7.02076700	0.53798200	-1.00567100
O	5.61838000	-0.46902200	0.82456400
S	0.69061400	-1.36731300	-1.72280300
O	-0.10655100	-1.51009900	-2.92796700
O	2.08593700	-0.83651400	-1.98259400
C	1.00873600	-3.11175500	-1.13703300
C	6.02132800	-1.88742900	-1.33868000
F	0.29714000	-3.95883500	-1.87199700
F	0.61489200	-3.22330400	0.13213100
F	2.28574100	-3.43311700	-1.22857100
F	7.08320100	-2.49844600	-0.82965400
F	4.93205600	-2.59705900	-1.04334900
F	6.14500100	-1.79887400	-2.64978900
H	3.78784100	1.56366100	4.25734000
C	3.34575300	-2.93899000	2.06605400
H	4.20993400	-3.27313800	1.48146500
H	3.55276900	-3.07275000	3.12815200
H	2.48803700	-3.54306700	1.75752600
Au	-1.64433800	-0.03472900	1.84884100
P	-3.89271500	-0.41931400	1.36496200
N	-4.33270900	1.25449600	-3.34025900
N	-3.56504500	0.24802300	-3.57182400
N	-2.50783000	0.29416500	-2.75014400
H	-1.77786800	-0.41082800	-2.83696400
C	-3.76705700	2.00461000	-2.33302500
C	-4.18612700	3.20654800	-1.73657000
H	-5.10452800	3.68911000	-2.05493200
C	-3.37808500	3.73831800	-0.75113800
H	-3.65857800	4.67002500	-0.27034500
C	-2.17488500	3.10138000	-0.35666400
H	-1.54782700	3.55926700	0.40221400
C	-1.74691400	1.92181100	-0.93640300
H	-0.81268200	1.44881200	-0.65549600

C	-2.57215400	1.38474500	-1.93847000
C	-4.83147000	1.14026900	1.20915300
H	-5.90726600	0.97945400	1.31115300
C	-4.70346300	-1.30988000	2.75013300
H	-5.78617600	-1.34813400	2.61596100
C	-4.06481000	-1.42733500	-0.15562900
C	-2.93037900	-2.15687100	-0.54096200
H	-2.03256600	-2.12491900	0.07175100
C	-2.91693700	-2.89559900	-1.71982900
H	-2.02578100	-3.44353000	-2.00458600
C	-4.03313800	-2.88465900	-2.54869100
H	-4.02105200	-3.42426900	-3.48996600
C	-5.16520200	-2.16902900	-2.17599400
H	-6.03908900	-2.15423700	-2.82009100
C	-5.21114700	-1.45309800	-0.97721400
C	-6.47570400	-0.74468300	-0.63058300
C	-6.87555300	0.37033100	-1.37390300
C	-8.03061000	1.06395400	-1.02340800
H	-8.32460600	1.93800700	-1.59630400
C	-8.80629700	0.64239300	0.05457500
C	-8.44010900	-0.49837700	0.76616000
H	-9.06048100	-0.85370300	1.58343900
C	-7.28306900	-1.19274800	0.41922200
H	-6.26921000	0.69562900	-2.21595900
H	-7.01062900	-2.10136000	0.94961000
H	-9.70375600	1.18865000	0.32739400
H	-4.29996000	-2.32338400	2.81708400
H	-4.47089500	-0.77707400	3.67686300
H	-4.47456300	1.81798300	1.98986400
H	-4.61782800	1.59223700	0.23725700
C	1.06722500	-0.43672300	3.02461400
C	0.45071600	0.24262700	2.14474800
H	0.82190600	0.88090000	1.34809000
C	1.01535300	-1.25634800	4.25904500
H	1.58702300	-0.74939400	5.04509500
S	1.55578100	3.10226900	-0.60156900
O	1.89959500	1.72154400	-1.20046200
O	0.93500200	3.93154000	-1.60390500
O	0.93378500	2.96475400	0.70818500
C	3.24333500	3.84299900	-0.29257100
F	3.40722500	4.06610600	1.00621800
F	3.32727100	4.99290400	-0.93847300
F	4.20147200	3.03141300	-0.72239700
C	-0.42533100	-1.47655800	4.73724900
H	-0.41557700	-2.05617100	5.66415100
H	-0.92204000	-0.52066500	4.92193800
H	-1.00211000	-2.02333800	3.98592900
H	1.49953900	-2.22389300	4.08546900

TS(C2)

E_{elec}(BS1) = -4801.4642022 Hartree E_{ZPE} = 0.658730 Hartree H_{ZPE} = 0.723515 Hartree G_{ZPE} = 0.552235Hartree

E_{elec}(BS2)= -6725.527437 Hartree

Low frequencies (cm^{-1}) -380.2122 13.1121 18.2762 18.9734 20.6065 26.7051 30.8888 32.1837 33.3810

C	2.19668400	-0.50474200	2.52487500
C	3.02802500	0.61820600	2.26439900
C	3.17227100	1.69800600	3.28840600
H	1.93524600	-0.68716000	3.55875300
H	4.22576700	1.96935500	3.38572600
H	2.64106100	2.57579400	2.90249100
O	3.64413500	0.79274500	1.17726600
C	2.12111500	-1.59643200	1.62423400
O	2.44564600	-1.51248800	0.40481500
Ga	3.52846000	-0.19631600	-0.48195700
O	1.00799200	0.31453900	-1.24151000
O	5.20173400	-1.00394800	-0.49577700
S	5.75891800	-1.91362600	0.61787800
O	7.19180800	-1.80006400	0.72068500
O	4.92820200	-1.85188200	1.81332300
S	1.36065900	-0.66340800	-2.27740700
O	0.97714100	-0.41671200	-3.65334500
O	2.82196000	-1.03138300	-2.11220900
C	0.46041500	-2.21768400	-1.77857300
C	5.40798600	-3.55639400	-0.11570600
F	-0.42796500	-2.52914100	-2.71462900
F	-0.19047200	-2.00829600	-0.63295300
F	1.29809400	-3.22795700	-1.61987800
F	5.77086700	-4.49769900	0.74857500
F	4.10472200	-3.67072800	-0.35404500
F	6.07694800	-3.71348400	-1.24488400
H	2.75752400	1.40986600	4.25506000
C	1.60474500	-2.92539200	2.07191800
H	2.48370800	-3.55762900	2.24878300
H	1.02210600	-2.85577500	2.99229600
H	1.01635300	-3.37571900	1.27037200
Au	-2.50294400	0.16352300	1.49172300
P	-4.65565600	0.25690000	0.56851600
N	-2.01739200	1.22637200	-1.22871000
N	-1.63276800	0.73630100	-2.35566500
N	-0.86083800	1.63021800	-2.97880400
H	-0.32480400	1.30044600	-3.77457000

C	-1.45020100	2.47040700	-1.07350100
C	-1.53442100	3.39615900	-0.02026900
H	-2.12654400	3.18324400	0.86594300
C	-0.82131000	4.56731800	-0.16000100
H	-0.84479000	5.30870300	0.63208500
C	-0.03970700	4.82445300	-1.31270900
H	0.53089000	5.74577900	-1.36511700
C	0.04765900	3.92962400	-2.35793000
H	0.68141000	4.11914700	-3.21531500
C	-0.67781700	2.73953300	-2.21021700
C	-5.02109300	1.90820200	-0.13446900
H	-6.08232700	2.00352700	-0.37333200
C	-5.93429100	0.04337700	1.86796100
H	-6.92846100	0.34109700	1.52826200
C	-4.88337300	-1.01207800	-0.73480100
C	-3.70704500	-1.54815700	-1.27755600
H	-2.74187400	-1.16881500	-0.95644400
C	-3.75230100	-2.55307600	-2.23802300
H	-2.82597400	-2.93805200	-2.64838400
C	-4.98027800	-3.05479700	-2.65231500
H	-5.02843700	-3.84746700	-3.39252700
C	-6.15530500	-2.53311800	-2.12055600
H	-7.11966800	-2.91114100	-2.44756500
C	-6.12891200	-1.50354400	-1.17690200
C	-7.43319600	-0.97868400	-0.68272200
C	-7.90974400	0.26264100	-1.11334800
C	-9.11487500	0.76421400	-0.62632000
H	-9.47496700	1.73000100	-0.96702100
C	-9.86250500	0.02077700	0.28426300
C	-9.41293000	-1.23492500	0.68814600
H	-10.00073000	-1.82515600	1.38421300
C	-8.20802900	-1.73431300	0.20189400
H	-7.33619900	0.82600500	-1.84451500
H	-7.84714200	-2.70751300	0.52368500
H	-10.80014200	0.41186700	0.66604500
H	-5.95668800	-1.00040700	2.19165200
H	-5.63549400	0.66430000	2.71759100
H	-4.74719100	2.66504800	0.60674100
H	-4.40811500	2.05175600	-1.02628100
C	-0.70076800	-0.13111600	2.65904500
C	0.21295100	0.15294300	1.82918400
H	0.53013800	0.52992400	0.86283000
C	-0.86551700	-0.67192600	4.04001500
H	0.12385300	-0.86597100	4.47406800
S	3.13415400	2.81996500	-0.90460500
O	3.63775400	1.44631300	-1.37881900
O	3.01782300	3.71332900	-2.03663000
O	2.04661500	2.72168900	0.05576000
C	4.61352200	3.43279900	0.05562700

F	4.25770400	3.67915800	1.31465800
F	5.05013500	4.55907400	-0.48815700
F	5.59340800	2.54221900	0.05130300
C	-1.64854700	0.27698600	4.95165200
H	-1.15067300	1.24820300	5.01797200
H	-2.65839300	0.43929900	4.56216700
H	-1.72765500	-0.14210900	5.95816300
H	-1.38605900	-1.63461000	3.97880100

1f
(**R** = $CH(CH_3)_2$

Au/Ga stabilized Reactant complex:

E_{elec}(BS1) = -4840.8031771 Hartree E_{ZPE} = 0.687413 Hartree H_{ZPE} = 0.754318 Hartree G_{ZPE} = 0.580112 Hartree

E_{elec}(BS2)= -6764.8776929 Hartree

Low frequencies (cm^{-1}) 16.5741 19.9158 23.7928 27.3734 27.5561 31.2210 33.7958 34.4514 38.8808

C	1.83099400	-1.19407700	2.61067200
C	2.80399000	-0.18737100	2.52431900
C	3.28520000	0.54566000	3.73793100
H	1.50600700	-1.52049100	3.59026300
H	4.36472100	0.39867200	3.83576000
H	3.11731300	1.61479500	3.56726000
O	3.35176000	0.17649000	1.43408600
C	1.35787300	-1.86566000	1.48780400
O	1.61792700	-1.54054700	0.27114800
Ga	2.96521200	-0.37437300	-0.34698000
O	0.27165300	0.56742800	-1.22393000
O	4.45441000	-1.40458300	-0.76978300
S	4.94844600	-2.59992200	0.06762200
O	6.38410600	-2.72039400	0.01658600
O	4.24020000	-2.67622300	1.33658500
S	0.74992100	-0.24878900	-2.34277600
O	0.46864300	0.22664500	-3.68823400
O	2.18262900	-0.66025500	-2.13826800

C	-0.17086900	-1.86340900	-2.19436300
C	4.26659100	-3.97489900	-0.93339800
F	-0.98260100	-2.00225800	-3.23668700
F	-0.92490700	-1.85435100	-1.08697400
F	0.65492800	-2.88790300	-2.14369200
F	4.60283000	-5.13112500	-0.37346100
F	2.93787400	-3.88208100	-0.96206300
F	4.73479800	-3.93196900	-2.16940000
H	2.78394500	0.21781600	4.64991300
C	0.51269200	-3.09736800	1.62174300
H	1.15646900	-3.94817600	1.36841100
H	0.12746900	-3.23357400	2.63436800
H	-0.29971400	-3.07769300	0.89106700
Au	-1.86251400	0.82108100	0.46933400
P	-3.85406300	-0.05260700	-0.32917800
N	-2.76872400	3.08624100	-1.71149600
N	-2.38412200	2.37763100	-2.71845700
N	-1.07703600	2.56464900	-2.92347000
H	-0.58570700	1.95182600	-3.57162000
C	-1.67109500	3.75639100	-1.21563300
C	-1.53975200	4.63365200	-0.12394200
H	-2.40362500	4.90884200	0.47223300
C	-0.27666900	5.11885400	0.14083800
H	-0.12494700	5.79834100	0.97294600
C	0.84507100	4.74698400	-0.64598600
H	1.82634500	5.13135300	-0.39019300
C	0.73515200	3.88484900	-1.71919900
H	1.60329400	3.59333600	-2.30113800
C	-0.55688600	3.40614300	-1.99192800
C	-3.81900700	-0.52718300	-2.09237500
H	-4.82637500	-0.78776200	-2.42588600
C	-5.16973100	1.20958900	-0.21222300
H	-6.07141600	0.91274700	-0.75177600
C	-4.28270500	-1.56179300	0.62934700
C	-3.20379600	-2.24013200	1.21316400
H	-2.19822900	-1.85237200	1.07382800
C	-3.39343200	-3.38359600	1.97980600
H	-2.53758200	-3.88961200	2.41606900
C	-4.68299100	-3.85850900	2.19418000
H	-4.84985900	-4.74202100	2.80232600
C	-5.76372400	-3.19811500	1.62013100
H	-6.77330600	-3.56891600	1.77150000
C	-5.58441700	-2.06354400	0.82262700
C	-6.79129700	-1.43972500	0.20980300
C	-7.07405500	-1.62684500	-1.14583700
C	-8.18365700	-1.01582700	-1.72517900
H	-8.39218200	-1.16401700	-2.78004700
C	-9.02720400	-0.22320600	-0.94971300
C	-8.77044200	-0.06186800	0.41034300

H	-9.43185100	0.54468400	1.02087000
C	-7.66168200	-0.67305800	0.98869200
H	-6.42535200	-2.26281700	-1.74208100
H	-7.45083300	-0.53948600	2.04640100
H	-9.88836100	0.25782200	-1.40211700
H	-5.40961000	1.39744300	0.83739500
H	-4.74361700	2.11521500	-0.65762200
H	-3.44930800	0.32966700	-2.66429400
H	-3.14692200	-1.37527900	-2.23179400
C	-0.36088100	1.41380400	2.34049400
C	0.09836700	1.87662200	1.30645300
H	0.64435500	2.31715600	0.48921700
C	-0.80646500	1.00507900	3.68614400
H	0.11707100	0.87790400	4.26820000
S	3.62906700	2.67657800	-0.07339500
O	3.18800100	1.43272800	-0.86366300
O	3.87946700	3.76566500	-0.99617300
O	2.79053400	2.92615200	1.08946400
C	5.29962300	2.17799600	0.59503200
F	5.27187900	2.17403600	1.92049100
F	6.20215000	3.05548200	0.18733500
F	5.63445500	0.97271900	0.15514800
C	-1.64594900	2.12274100	4.31852800
H	-1.92376400	1.84643400	5.33988300
H	-1.09435900	3.06516000	4.34607800
H	-2.56299200	2.27538300	3.73915700
C	-1.56521100	-0.32550800	3.68403200
H	-0.99397600	-1.10606300	3.17294600
H	-1.75508800	-0.64411000	4.71350300
H	-2.52895500	-0.21629700	3.17369700

TS(C1)

E_{elec}(BS1) = -4840.7726555 Hartree E_{ZPE} = 0.687425 Hartree H_{ZPE} = 0.752951 Hartree G_{ZPE} = 0.583366 Hartree

E_{elec}(BS2)= -6764.8465978 Hartree

Low frequencies (cm^{-1}) -373.1721 12.6525 15.4136 24.8236 27.8069 32.4553 35.9889 36.6267 42.6813

C	2.89845800	-0.40090700	2.66432000
C	3.26706700	0.90121900	2.21310500
C	3.61817500	1.98710400	3.17668500
H	3.15548900	-0.63842200	3.68933400
H	4.66374900	2.26821800	3.01376500

H	3.00194200	2.85894200	2.93634400
O	3.27096900	1.21803000	0.99605900
C	2.85605900	-1.48700900	1.74184500
O	2.66114900	-1.34214500	0.50124900
Ga	2.98573000	0.17240200	-0.61868400
O	0.12292700	-0.47625500	-0.76797100
O	4.73956400	-0.09695900	-1.16184800
S	5.88885800	-0.64705100	-0.29563600
O	7.14764800	-0.03539700	-0.63575800
O	5.48247000	-0.76634700	1.10064100
S	0.71814700	-1.26490900	-1.84565300
O	-0.01782100	-1.37515300	-3.09275800
O	2.17316600	-0.88327900	-2.03319200
C	0.82867500	-3.00357300	-1.17423300
C	5.93815700	-2.37211400	-0.91141300
F	0.03047600	-3.79570000	-1.87941200
F	0.41629100	-3.01125800	0.09308600
F	2.06300300	-3.46973600	-1.23292800
F	6.87331900	-3.03903100	-0.24624200
F	4.75862200	-2.94940400	-0.68787800
F	6.20460000	-2.40098000	-2.20400200
H	3.47253200	1.68579700	4.21429700
C	3.06267900	-2.89116100	2.21069200
H	4.13223400	-3.09711500	2.07330900
H	2.81422400	-3.02442900	3.26561300
H	2.50003700	-3.58088700	1.57925500
Au	-1.78194100	0.31046800	1.49434300
P	-4.00284500	-0.31800000	1.13330200
N	-4.34700900	1.33841700	-2.78749800
N	-3.55746300	0.43868600	-3.25946200
N	-2.33491600	0.59921300	-2.73523100
H	-1.59409400	-0.04975400	-2.99412500
C	-3.62942200	2.12597400	-1.91519500
C	-4.01198900	3.24706400	-1.15761200
H	-5.02454200	3.63451500	-1.21997000
C	-3.05379500	3.82325800	-0.34876600
H	-3.30803700	4.69189700	0.25008600
C	-1.72836300	3.32139900	-0.29826600
H	-0.99040100	3.80564700	0.33376800
C	-1.33040900	2.23627300	-1.05527600
H	-0.31945700	1.85142800	-1.02586300
C	-2.31297900	1.64454900	-1.86592400
C	-5.19975700	1.05554400	1.29773300
H	-6.21406000	0.69151900	1.47645800
C	-4.52154700	-1.47368600	2.46482500
H	-5.58761400	-1.70082400	2.38393000
C	-4.20028300	-1.24680400	-0.43291300
C	-3.04055300	-1.86087500	-0.92721400
H	-2.09540400	-1.72832100	-0.40322700

C	-3.07116900	-2.61598700	-2.09551500
H	-2.16005800	-3.07081000	-2.46760200
C	-4.26292400	-2.74284300	-2.79928600
H	-4.29150900	-3.30552900	-3.72673800
C	-5.41868500	-2.13667100	-2.32067900
H	-6.35306300	-2.22803000	-2.86622200
C	-5.41136400	-1.40053800	-1.13522000
C	-6.69611900	-0.81840200	-0.65323300
C	-7.18945800	0.36976500	-1.20086700
C	-8.36824200	0.92315700	-0.70603200
H	-8.74249800	1.85279700	-1.12392000
C	-9.06650900	0.29363900	0.32333700
C	-8.59728500	-0.91027600	0.84497100
H	-9.15058300	-1.41892100	1.62854400
C	-7.41997700	-1.46704900	0.35109200
H	-6.62258300	0.85962800	-1.99007000
H	-7.05813100	-2.41683900	0.73659500
H	-9.98194200	0.73209000	0.70830800
H	-3.94200600	-2.39744200	2.39201500
H	-4.32210100	-1.00472800	3.43308400
H	-4.86431900	1.66530800	2.14203400
H	-5.17836000	1.66956100	0.39674300
C	0.78134200	-0.18053400	2.77553200
C	0.31649800	0.58591000	1.86810000
H	0.79063000	1.22105600	1.12601900
C	0.39792300	-1.07462500	3.91587300
H	1.29935000	-1.34460900	4.47293500
S	2.08616700	3.16563500	-0.86539500
O	2.24359600	1.71253800	-1.36791700
O	1.62159800	4.00386500	-1.94269200
O	1.40873700	3.20980900	0.42315400
C	3.85403800	3.66966300	-0.53250300
F	4.00382200	3.96621100	0.75261400
F	4.13492800	4.73717700	-1.25799700
F	4.68863900	2.68973300	-0.85542100
C	-0.24914700	-2.36865400	3.39930400
H	-1.20099800	-2.13805600	2.90807900
H	0.38427900	-2.87933400	2.67019900
H	-0.44183600	-3.04827200	4.23559900
C	-0.53848800	-0.33752800	4.88355800
H	-0.77087300	-0.98340900	5.73612900
H	-0.08184100	0.58404900	5.25326000
H	-1.47379700	-0.07563300	4.37780000

TS(C2)

E_{elec}(BS1) = -4840.7600001 Hartree E_{ZPE} = 0.687585 Hartree H_{ZPE} = 0.753646

Hartree G_{ZPE} = 0.579661 Hartree

E_{elec}(BS2)= -6764.8370389 Hartree

Low frequencies (cm^{-1}) -382.5349 10.9969 17.1973 17.6330 21.5982 27.3489 28.1021 31.9923 33.3686

C	2.15700600	-0.70804800	2.44844300
C	2.96119300	0.45219300	2.28291300
C	3.06679300	1.45666500	3.38544300
H	1.88500500	-0.97201600	3.46153600
H	4.11538900	1.72509400	3.53271200
H	2.54215800	2.35822600	3.04913400
O	3.58341100	0.72098800	1.21958800
C	2.11569800	-1.72887400	1.46758200
O	2.45413200	-1.54631600	0.26209600
Ga	3.53250800	-0.15253600	-0.50832400
O	1.05379500	0.38375400	-1.27757700
O	5.23125500	-0.90350200	-0.52262900
S	5.78505100	-1.88631500	0.52779700
O	7.20625500	-1.72331000	0.70278800
O	4.90626300	-1.97053800	1.68707800
S	1.42307700	-0.52115500	-2.37371100
O	1.06598400	-0.17909400	-3.73598700
O	2.88151300	-0.89765100	-2.20483000
C	0.50669400	-2.10309100	-2.00577700
C	5.54000600	-3.46329800	-0.37335700
F	-0.35448200	-2.34751200	-2.98578200
F	-0.17660900	-1.96856100	-0.86806500
F	1.33827100	-3.12387200	-1.89091000
F	5.93797200	-4.46836600	0.39859300
F	4.24823900	-3.61883600	-0.65162800
F	6.23530600	-3.46841800	-1.49756300
H	2.62700500	1.09648600	4.31625000
C	1.60798500	-3.09492200	1.79791200
H	2.47432600	-3.76624800	1.77409600
H	1.14044500	-3.14045300	2.78291700
H	0.91029600	-3.41704200	1.02130000
Au	-2.51327400	0.14452600	1.41549900
P	-4.65147300	0.31632100	0.47108800
N	-1.96245600	1.33190400	-1.24561700
N	-1.57250700	0.88809800	-2.38994700
N	-0.78904600	1.80172400	-2.96790000
H	-0.24780400	1.50282300	-3.77248100
C	-1.38778300	2.56423700	-1.03267300
C	-1.47575800	3.44776100	0.05589700
H	-2.07877300	3.20436800	0.92673900
C	-0.75145700	4.61743100	-0.02904600
H	-0.77702800	5.32593400	0.79240000

C	0.04621100	4.91395000	-1.16130500
H	0.62810400	5.82953400	-1.16919200
C	0.13717400	4.06128400	-2.24082500
H	0.78111800	4.27940100	-3.08384000
C	-0.60257000	2.87446100	-2.15015100
C	-4.99339800	1.98562900	-0.19869100
H	-6.05002300	2.09526400	-0.45203200
C	-5.94455900	0.08417400	1.75271900
H	-6.93455400	0.39216300	1.41013600
C	-4.86958200	-0.92289700	-0.86311300
C	-3.68722200	-1.43315000	-1.41810300
H	-2.72666500	-1.04504700	-1.09363300
C	-3.72097400	-2.42265700	-2.39470100
H	-2.79024600	-2.78732900	-2.81409600
C	-4.94312800	-2.93604000	-2.81268300
H	-4.98230300	-3.71835100	-3.56440600
C	-6.12385800	-2.43818700	-2.27086000
H	-7.08382500	-2.82312400	-2.60275000
C	-6.10919200	-1.42222700	-1.31208300
C	-7.41770600	-0.91327700	-0.81351700
C	-7.88993600	0.33903400	-1.21594100
C	-9.09822800	0.82949700	-0.72572700
H	-9.45502100	1.80381400	-1.04493200
C	-9.85294700	0.06417900	0.16069000
C	-9.40703900	-1.20142100	0.53660000
H	-10.00024500	-1.80796200	1.21379500
C	-8.19911200	-1.69010400	0.04665900
H	-7.31002800	0.92001900	-1.92803700
H	-7.84129100	-2.67127300	0.34710200
H	-10.79303600	0.44645700	0.54534100
H	-5.97375900	-0.96522400	2.05772300
H	-5.65025800	0.68838700	2.61591700
H	-4.72471200	2.72247200	0.56429700
H	-4.36488100	2.14506400	-1.07683500
C	-0.73759300	-0.27632100	2.58822100
C	0.18846200	0.00324900	1.77009600
H	0.51765100	0.40435700	0.81763000
C	-0.92283400	-0.86266800	3.95201400
H	0.06998100	-1.15393600	4.32370700
S	3.17417000	2.89254600	-0.73750900
O	3.66411900	1.54458900	-1.29414000
O	3.12885200	3.87198100	-1.80150100
O	2.04429400	2.75028400	0.16605100
C	4.62387600	3.39307600	0.32752300
F	4.22569900	3.53934500	1.58954000
F	5.09760000	4.55436600	-0.10027900
F	5.59080300	2.48932800	0.28228200
C	-1.50197700	0.18482100	4.90850100
H	-0.87295200	1.07849900	4.94536800

H	-2.50299200	0.48430900	4.57790300
H	-1.58094100	-0.23070900	5.91791200
C	-1.80416600	-2.11548000	3.90974200
H	-2.82753600	-1.85215800	3.61941100
H	-1.42626600	-2.84633000	3.18883900
H	-1.83670100	-2.58310700	4.89875000

[XPhosAu(TA)]$^{+}$ Actual system:

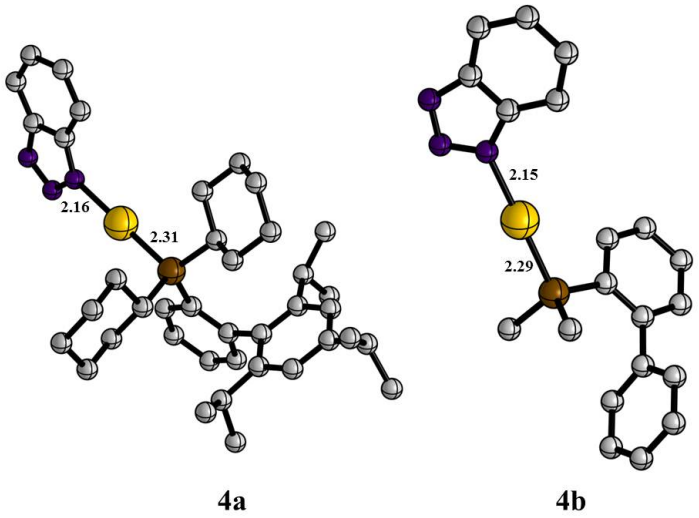

*Figure S3. Optimized geometries of actual catalytic system (**4a**) and the model catalyst (**4b**).*

In the present study we have used a model catalytic system in-lieu of the actual one to make the calculations tractable. As mentioned in the manuscript, the cyclohexyl and isopropyl group has been replaced by methyl and H respectively. The kinetics as well as regioselectivty remains similar. Few calculations have been performed to model the catalyst as shown below.

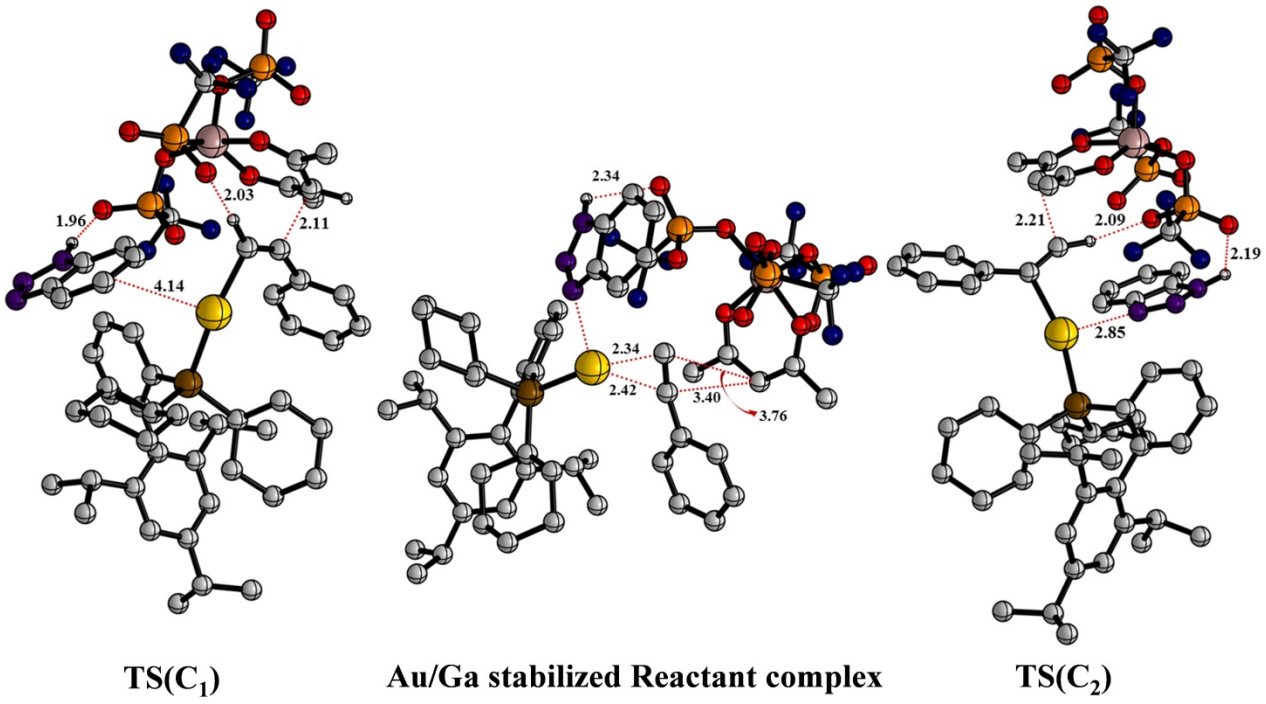

Figure S4. The optimized geometries of transition states for C-C coupling involved in the Au cycle using [XPhosAu(TA)]$^+$ (actual system) as catalyst and R = C_6H_5 in alkyne. Important bond lengths (in Å) are shown.

For quantitative comparison of our model**,** we have computed the reaction profile considering phenylacetylene as alkyne and using both the actual [XPhosAu(TA)]+(**4a**) and the model (**4b**) as catalyst. For **4a** as catalyst, The free energy of activation for the C - C_1 (Ph substituted carbon) coupling is 18.8 kcal/mol while that for the C-C2 coupling is 21.7 kcal/mol, a preference of 2.9 kcal/mol. This trend is in agreement with **4b** which shows a C-C1 preference by 4.9 kcal/mol.

Au/Ga stabilized Reactant complex:

E_{elec}(BS1) = -5698.0624787 Hartree E_{ZPE} = 1.189741 Hartree H_{ZPE} = 1.278966 Hartree G_{ZPE} = 1.054321 Hartree

E_{elec}(BS2)= -7622.4216253 Hartree

Low frequencies (cm^{-1}) 6.9561 10.8813 15.8612 18.7950 19.7312 20.3570 24.3091 26.7028 28.4823

C	2.78863600	-2.50299800	1.53623600
C	4.06672000	-2.14924600	1.99673300
C	4.51093200	-2.57366800	3.36546500
H	2.17219100	-3.13893500	2.15840600
H	5.55363300	-2.89586900	3.32432200
H	4.46093400	-1.70152900	4.02550600
O	4.90613100	-1.45766000	1.33530000
C	2.28314000	-2.07866800	0.31719200
O	2.89612500	-1.29437300	-0.50338100
Ga	4.67414800	-0.71632200	-0.42556500
O	2.88266500	1.68037400	-0.79980300
O	5.91879200	-1.79923200	-1.29354800
S	5.74909800	-3.32445200	-1.41694100
O	7.02291300	-3.99686700	-1.49065600
O	4.70715200	-3.79922500	-0.51917200
S	3.18637700	1.23574200	-2.15644400
O	3.35886700	2.24145700	-3.19240700
O	4.25409100	0.17529900	-2.16766700
C	1.64528500	0.31989300	-2.66968900
C	5.00716200	-3.40838800	-3.09000600
F	0.98217200	1.05292800	-3.57418100
F	0.83695900	0.15573500	-1.62162100
F	1.91169900	-0.85911400	-3.20046100
F	4.74974900	-4.67626800	-3.39311100
F	3.86749400	-2.72250200	-3.09618600
F	5.82904200	-2.90103800	-3.99407600
H	3.88095400	-3.36764200	3.76901000
C	0.92201900	-2.51220400	-0.14472300
H	0.99749500	-2.84594700	-1.18370200
H	0.51696800	-3.30932800	0.48087200
H	0.24133300	-1.65284100	-0.12630600
Au	-0.96194400	1.16499300	0.72376300
P	-3.19985200	0.92471000	0.08854500
N	-0.03058800	3.35416900	-0.40947900
N	0.01185600	3.18242400	-1.69068200
N	1.12406400	3.74794800	-2.16098800
H	1.41425900	3.55255600	-3.11263100
C	1.10679600	4.01825600	-0.01355800
C	1.60167800	4.31199600	1.27020400

H	1.01400800	4.09767300	2.15745900
C	2.87800700	4.82293500	1.33935600
H	3.32897800	5.01880000	2.30571400
C	3.64964200	5.06713800	0.17221800
H	4.66552200	5.42552400	0.29259300
C	3.16915100	4.81099600	-1.09199000
H	3.77339300	4.94558600	-1.98105100
C	1.87638300	4.27009000	-1.15372200
C	-3.20088100	-0.10410800	-1.44345900
C	-2.10071400	0.16407000	-2.27802500
H	-1.36398400	0.90661500	-1.98296900
C	-1.93010000	-0.48229700	-3.49557300
H	-1.06278900	-0.25259700	-4.10494000
C	-2.86906000	-1.42113900	-3.90761100
H	-2.75031700	-1.94392700	-4.85126800
C	-3.96633700	-1.68764700	-3.09821600
H	-4.70863800	-2.41616600	-3.41303600
C	-4.15894300	-1.04392900	-1.86718400
C	-5.39163700	-1.44243500	-1.11578100
C	-6.61372000	-0.79836700	-1.39119600
C	-7.77888300	-1.28400200	-0.79635100
H	-8.72546900	-0.79328100	-1.01137800
C	-7.76514900	-2.38474100	0.06102600
C	-6.54063000	-2.99345400	0.33104800
H	-6.52324200	-3.85080100	1.00017200
C	-5.34901300	-2.54665600	-0.24398600
C	0.65244700	0.07555000	2.16066500
C	1.24114800	0.92378300	1.49765500
H	1.93837300	1.54713100	0.95996900
S	5.26037600	1.57723100	1.48005700
O	5.49145000	0.87691800	0.13690000
O	5.61548800	2.97693400	1.39939800
O	3.99057100	1.18966500	2.08116400
C	6.57945500	0.78740500	2.53707000
F	6.01573200	0.06707200	3.50247000
F	7.31036500	1.74155700	3.09832800
F	7.36622200	0.00723500	1.81555000
C	0.27318300	-0.95968900	3.08742600
C	1.09127100	-1.13174000	4.21408100
C	-0.80843500	-1.82136500	2.87018500
C	0.82454500	-2.15684400	5.11277700
H	1.93602200	-0.46431700	4.35487400
C	-1.07230800	-2.83901200	3.78207300
H	-1.42938000	-1.69292400	1.98548800
C	-0.25801800	-3.00963400	4.89978800
H	1.46236500	-2.29010800	5.98056700
H	-1.91514200	-3.50254500	3.61843400
H	-0.46700900	-3.80766700	5.60479200
C	-4.16140400	0.19375300	1.51534200

C	-3.47833900	0.51172500	2.86247000
C	-5.64031100	0.60317400	1.59072000
H	-4.10676300	-0.89185200	1.35444600
C	-4.18353200	-0.20319700	4.01790300
H	-3.50083100	1.59657100	3.03649800
H	-2.42455700	0.22246900	2.84447900
C	-6.34563300	-0.12577400	2.73934900
H	-5.70459000	1.68675400	1.76605800
H	-6.15499400	0.39213000	0.65269400
C	-5.66805800	0.15570900	4.08001400
H	-3.68268000	0.04694900	4.95915200
H	-4.07315600	-1.28911500	3.88358400
H	-7.39854000	0.17611600	2.76602900
H	-6.32957200	-1.20531700	2.53354500
H	-6.16264700	-0.39894600	4.88430700
H	-5.76967800	1.22331400	4.31955500
C	-4.03472700	2.51520900	-0.37465100
C	-3.76257300	3.57653000	0.70565200
C	-3.58804000	3.02770300	-1.75217000
H	-5.11382800	2.30270100	-0.41426200
C	-4.45780300	4.89770600	0.36515500
H	-2.67657600	3.73947400	0.76179400
H	-4.08773600	3.22536200	1.69158300
C	-4.27998300	4.35390600	-2.08193000
H	-2.49841300	3.17011200	-1.75295400
H	-3.81397500	2.28870200	-2.52806200
C	-4.01415300	5.40713500	-1.00617700
H	-4.23892100	5.63794900	1.14175800
H	-5.54656500	4.74584500	0.36487400
H	-3.93926700	4.70861100	-3.06011500
H	-5.36348900	4.18432400	-2.16318800
H	-4.52777000	6.34263500	-1.25117900
H	-2.93821100	5.62702100	-0.97657000
C	-6.68495600	0.39607300	-2.33276700
C	-7.60482900	1.51044300	-1.82031800
C	-7.12695100	-0.04940800	-3.73308400
H	-5.67523700	0.81539900	-2.41994200
H	-7.37060500	1.79402700	-0.78835200
H	-7.49962800	2.39834900	-2.45192500
H	-8.65783300	1.21211000	-1.85394400
H	-6.43289500	-0.78160200	-4.15490100
H	-8.12065900	-0.50894300	-3.68812900
H	-7.17646400	0.80739900	-4.41275900
C	-9.04743300	-2.90949100	0.67893500
C	-10.06711800	-3.30457300	-0.39509700
C	-9.65141900	-1.89439400	1.65575300
H	-8.78979700	-3.81233500	1.24712400
H	-9.64290300	-4.02865900	-1.09642900
H	-10.95552400	-3.74786600	0.06546000

H	-10.39145500	-2.42946000	-0.96847600
H	-8.95183000	-1.66087400	2.46344700
H	-9.89729300	-0.95895900	1.14041400
H	-10.57229000	-2.28634200	2.09932500
C	-4.04694300	-3.29166400	0.02107900
C	-3.91889400	-4.49426300	-0.92499700
C	-3.89441800	-3.76156900	1.47116300
H	-3.21528700	-2.60827000	-0.19491900
H	-3.94100300	-4.18237800	-1.97211400
H	-2.97861700	-5.02595100	-0.74658000
H	-4.74584900	-5.19363900	-0.75944100
H	-4.03717700	-2.94393500	2.18777700
H	-4.60912600	-4.55287500	1.71899200
H	-2.89077700	-4.17613400	1.61449300

TS(C_1)

E_{elec}(BS1) = -5698.0428295 Hartree E_{ZPE} = 1.190820 Hartree H_{ZPE} = 1.277894 Hartree G_{ZPE} = 1.065045 Hartree

E_{elec}(BS2)= -7622.4014816 Hartree

Low frequencies (cm^{-1}) -387.1622 17.2666 20.1430 24.7476 26.6794 29.3047 29.7082 33.0366 34.7298

C	-3.36869100	-1.85780900	-2.28815400
C	-4.18179000	-0.70663700	-2.50149100
C	-4.52476500	-0.24191100	-3.87860700
H	-3.23471200	-2.52273200	-3.13380800
H	-5.61412300	-0.22852500	-3.98154000
H	-4.17594300	0.79212000	-3.97450500
O	-4.59223300	0.01669000	-1.55759500
C	-3.30738500	-2.45488800	-0.98821900
O	-3.46311400	-1.80055600	0.07799600
Ga	-4.36715300	-0.14206500	0.36506100
O	-1.41785500	0.04051600	1.15258900
O	-6.05864000	-0.73237600	0.85394500
S	-6.78284500	-1.96915900	0.28815000
O	-8.21083100	-1.78333900	0.27288100
O	-6.09672100	-2.48496300	-0.89135000
S	-2.15453200	-0.12479400	2.40504600
O	-1.81178400	0.74510500	3.51969800
O	-3.64672600	-0.20424800	2.15843500
C	-1.77903300	-1.82889000	3.00334700
C	-6.41037400	-3.17723800	1.61717700
F	-0.65861000	-1.79580400	3.71294300

F	-1.60266400	-2.64872500	1.96986600
F	-2.76725900	-2.27899000	3.75447600
F	-6.91419700	-4.35801300	1.27891300
F	-5.09123800	-3.29600000	1.75207400
F	-6.93502800	-2.78290700	2.76307400
H	-4.08301800	-0.86881000	-4.65318700
C	-3.02773800	-3.91382700	-0.84304100
H	-4.00942300	-4.40596200	-0.81841800
H	-2.45316700	-4.30873600	-1.68371200
H	-2.52043200	-4.10279500	0.10389700
P	2.84857400	0.58995900	-0.60890300
N	0.99560400	4.88225800	2.80335800
N	0.55453200	3.89512300	3.49868000
N	-0.25187000	3.13607700	2.73599300
H	-0.75979600	2.35789800	3.15183300
C	0.45907100	4.79171400	1.53814800
C	0.61286000	5.61524400	0.41127600
H	1.21679400	6.51570600	0.46258600
C	-0.03046500	5.22934800	-0.74799400
H	0.05573500	5.84160800	-1.64044300
C	-0.82327600	4.05556400	-0.80128200
H	-1.33656800	3.79816300	-1.72264400
C	-1.00416000	3.24554400	0.30489600
H	-1.62452800	2.35551500	0.27475400
C	-0.34814100	3.64586300	1.47959900
C	2.88330200	0.14850500	1.18347900
C	1.70899300	0.48446900	1.87831000
H	0.86280700	0.90179700	1.33880200
C	1.59139700	0.30427300	3.25257500
H	0.66996300	0.57508400	3.75765700
C	2.65642100	-0.23179700	3.96359000
H	2.58330400	-0.38200000	5.03604300
C	3.82361600	-0.57326500	3.29030400
H	4.66254500	-0.99179200	3.83982500
C	3.96814900	-0.39097500	1.90930000
C	5.28424100	-0.81354100	1.32877900
C	6.36943100	0.08659800	1.30970000
C	7.60248000	-0.36068500	0.83081700
H	8.44605500	0.32521300	0.80378700
C	7.79557100	-1.66349200	0.37573600
C	6.71617300	-2.54277500	0.43307600
H	6.85239600	-3.56721300	0.10015700
C	5.46407700	-2.14721500	0.90728400
C	-1.47020200	-0.94561400	-2.12290600
C	-1.44238400	0.31208300	-1.89373300
H	-2.21047900	1.07842200	-1.82807000
S	-4.36470100	2.83823600	-0.65468800
O	-4.16460100	1.71592800	0.38928900
O	-4.38031600	4.12035600	0.00274200

O	-3.51616500	2.63822100	-1.82277600
C	-6.10626700	2.53158400	-1.25532800
F	-6.08998400	2.22192300	-2.54483400
F	-6.81687200	3.63144800	-1.08333700
F	-6.66463300	1.53859700	-0.57344500
C	-0.60803000	-2.12774700	-2.14605400
C	-0.34183100	-2.83109200	-3.32405900
C	0.00697100	-2.51125300	-0.94515900
C	0.55586400	-3.89518900	-3.30749600
H	-0.81886200	-2.52432400	-4.25079200
C	0.90823100	-3.57074000	-0.93853600
H	-0.21945600	-1.95540800	-0.03830300
C	1.18612700	-4.26112800	-2.11812700
H	0.77509500	-4.43064400	-4.22578700
H	1.39014700	-3.85668000	-0.00830900
H	1.89266000	-5.08606500	-2.11124600
C	3.75754500	-0.67732700	-1.64981700
C	2.95935300	-0.98722400	-2.93195900
C	5.21400600	-0.32039800	-1.99625500
H	3.75769400	-1.58585000	-1.03244300
C	3.64198000	-2.06374700	-3.77956400
H	2.85082800	-0.06642100	-3.52500000
H	1.94761400	-1.31672300	-2.67247400
C	5.86818300	-1.42712700	-2.82959800
H	5.23379900	0.60826500	-2.58168800
H	5.80178200	-0.14267600	-1.09412500
C	5.08627000	-1.69429000	-4.11375800
H	3.05773400	-2.23060600	-4.69208700
H	3.62952100	-3.01230300	-3.22324500
H	6.90401700	-1.14549500	-3.05309400
H	5.91428700	-2.34680500	-2.22960400
H	5.56102600	-2.49211800	-4.69510200
H	5.09547900	-0.79190300	-4.74101400
C	3.72012100	2.21213000	-0.74859200
C	3.54852600	2.80128600	-2.15915900
C	3.15593700	3.20401700	0.27941300
H	4.78708300	2.03415500	-0.55116900
C	4.29277400	4.13562300	-2.27278800
H	2.47443000	2.96715700	-2.33397700
H	3.89067800	2.10614900	-2.93382800
C	3.86209300	4.55794100	0.17706300
H	2.08346800	3.33587900	0.07345000
H	3.23488900	2.81685600	1.30139100
C	3.77564900	5.13490100	-1.23654000
H	4.17803900	4.53838100	-3.28487900
H	5.36745300	3.96292200	-2.11678700
H	3.42280800	5.24524900	0.90823700
H	4.91841800	4.43112300	0.45248800
H	4.33561900	6.07429000	-1.29982700

H	2.72648900	5.36663600	-1.46148500
C	4.35152400	-3.18298300	1.03664000
C	4.47425600	-3.91768700	2.37994900
C	4.32666900	-4.21029900	-0.10024300
H	3.39025800	-2.65283700	1.03171700
H	4.41750700	-3.22477000	3.22257700
H	3.67309200	-4.65625700	2.49068700
H	5.43410300	-4.44347200	2.43541900
H	4.24726200	-3.73765800	-1.08536600
H	5.22167500	-4.84028100	-0.09675900
H	3.47019000	-4.88187700	0.02562900
C	6.24168100	1.50996100	1.83506700
C	7.07290300	2.52321800	1.04032400
C	6.64311900	1.57094000	3.31610400
H	5.18810900	1.80581900	1.76353700
H	6.89748500	2.44763100	-0.03881500
H	6.82373100	3.53923400	1.36046700
H	8.14526600	2.38675600	1.21512000
H	6.00934200	0.92808600	3.93184800
H	7.68237800	1.24521100	3.43879200
H	6.55727300	2.59491000	3.69348000
C	9.17043900	-2.10056000	-0.09561400
C	9.13251000	-3.19274000	-1.16558600
C	10.01266400	-2.55546500	1.10444000
H	9.65544500	-1.21739700	-0.53204800
H	8.47057000	-2.92189300	-1.99412800
H	10.13624800	-3.36053600	-1.56739100
H	8.78661700	-4.14565200	-0.75035400
H	10.09756800	-1.76252300	1.85340700
H	9.54614200	-3.42310900	1.58439700
H	11.02071300	-2.84106500	0.78636800
Au	0.60738900	0.72346300	-1.30887900

TS(C_2)

E_{elec}(BS1) = -5698.0318661 Hartree E_{ZPE} = 1.189956 Hartree H_{ZPE} = 1.277941 Hartree G_{ZPE} = 1.057539 Hartree

E_{elec}(BS2)= -7622.3904899 Hartree

Low frequencies (cm^{-1}) -378.6055 9.0805 9.2781 13.2029 17.0733 20.4373 23.2728 24.8738 26.7966

C	3.42320700	-1.65910400	1.65755400
C	4.39171200	-0.68225400	2.01016900

C	4.54934600	-0.25662600	3.43496300
H	3.01073300	-2.25785200	2.46099700
H	5.61107000	-0.24005800	3.69190100
H	4.17969900	0.77330300	3.50476000
O	5.14053700	-0.10234300	1.17455700
C	3.34883400	-2.18683300	0.34167300
O	3.83746700	-1.61116700	-0.67170300
Ga	5.07289600	-0.13285000	-0.74888800
O	2.84771700	0.95160200	-1.09994900
O	6.67026100	-1.01384500	-1.10803400
S	7.07782500	-2.39246300	-0.55296500
O	8.50068300	-2.47016000	-0.33260100
O	6.15072800	-2.84842400	0.47377700
S	3.05508400	0.62796100	-2.52350200
O	2.76152600	1.62730600	-3.53077500
O	4.42946600	0.00510000	-2.62777200
C	1.87487000	-0.77880300	-2.85458100
C	6.72435200	-3.42526200	-2.02533100
F	1.04077700	-0.43579200	-3.82708200
F	1.16694800	-1.02716400	-1.75300500
F	2.52727500	-1.87289900	-3.20718100
F	7.04898600	-4.68623300	-1.76219200
F	5.42762400	-3.36447900	-2.31498700
F	7.42508000	-2.99897200	-3.06307600
H	3.99913400	-0.90185600	4.12111600
C	2.63946500	-3.47663800	0.08119200
H	3.41568600	-4.24201600	-0.03905200
H	1.97843100	-3.75729900	0.90332900
H	2.08827800	-3.40304400	-0.85851300
Au	-1.19321100	-0.16378900	1.02895000
P	-3.41596600	0.26281200	0.38076000
N	0.07599100	1.94818100	-0.40745800
N	0.36250200	2.10913300	-1.65176800
N	1.15748700	3.17506000	-1.77989200
H	1.62960000	3.29427700	-2.66953400
C	0.71930200	2.91769100	0.32399700
C	0.73010200	3.17161100	1.70571200
H	0.17328100	2.54034800	2.39321800
C	1.48859500	4.23913100	2.13526300
H	1.53827200	4.47217200	3.19386700
C	2.22909300	5.03528300	1.22646200
H	2.83811100	5.84454300	1.61567900
C	2.22778900	4.79920000	-0.13146700
H	2.83043100	5.38782100	-0.81211700
C	1.44771500	3.71751000	-0.56476100
C	-3.57152900	0.13197500	-1.45026800
C	-2.35259300	0.28741000	-2.13023400
H	-1.42588100	0.38455800	-1.57307700
C	-2.29022500	0.35027600	-3.51798000

H	-1.32748900	0.48489100	-3.99805300
C	-3.46020200	0.24104700	-4.25759900
H	-3.43522000	0.28462800	-5.34200600
C	-4.67297900	0.06757200	-3.59802800
H	-5.59060500	-0.03566500	-4.17118800
C	-4.76145700	0.01439200	-2.20133900
C	-6.13341300	-0.20952500	-1.63672400
C	-7.01347000	0.87286700	-1.45252200
C	-8.32284900	0.61408400	-1.03418300
H	-9.01403700	1.44254100	-0.90004300
C	-8.78068200	-0.67654000	-0.79261800
C	-7.88990300	-1.73479000	-0.98244000
H	-8.23704100	-2.75107700	-0.81121000
C	-6.57990400	-1.53104300	-1.41178800
C	0.58909300	-1.06826500	1.93743600
C	1.55359900	-0.52412000	1.32475500
H	1.94389500	0.21800100	0.63800700
S	5.12538900	2.72906300	0.34863000
O	5.48895000	1.70476100	-0.73917000
O	5.21754800	4.07036500	-0.18769800
O	3.95567600	2.35035300	1.12448500
C	6.58196600	2.54250000	1.50146700
F	6.14699100	2.21523800	2.71684700
F	7.22927800	3.69658000	1.58063000
F	7.41668500	1.60619400	1.07813000
C	0.36561100	-2.12803800	2.91607500
C	-0.40356100	-3.25579800	2.59855600
C	0.93777900	-2.02587300	4.19081000
C	-0.57938600	-4.26893500	3.53469700
H	-0.85011700	-3.33221700	1.61018400
C	0.74892200	-3.03908700	5.12629600
H	1.51710400	-1.14167000	4.44051400
C	-0.00676500	-4.16296200	4.80145700
H	-1.16793500	-5.14308800	3.27444900
H	1.19432900	-2.94801100	6.11196200
H	-0.15090700	-4.95155000	5.53262500
C	-3.87608100	2.01129400	0.79147500
C	-3.47945900	2.33927500	2.24158600
C	-3.19670200	3.00332600	-0.16621200
H	-4.96765600	2.09073500	0.68285800
C	-3.86077900	3.77786600	2.60055500
H	-2.38884200	2.22557400	2.33237100
H	-3.92758900	1.63418100	2.95060300
C	-3.55716800	4.44658500	0.19569400
H	-2.10960800	2.86792900	-0.09742700
H	-3.46944100	2.79269200	-1.20566200
C	-3.19142100	4.76691700	1.64549300
H	-3.57528000	3.98757600	3.63695900
H	-4.95295300	3.88937300	2.54069000

H	-3.04571300	5.13173100	-0.48860000
H	-4.63629300	4.59756000	0.05396300
H	-3.47881800	5.79375700	1.89501100
H	-2.10070500	4.69961400	1.76466600
C	-4.59337400	-0.87429700	1.29198300
C	-3.87351300	-1.53264500	2.48647600
C	-5.91052800	-0.22661300	1.75292200
H	-4.83327400	-1.66284600	0.56720800
C	-4.77812200	-2.52638700	3.21810200
H	-3.54375600	-0.75174000	3.18813600
H	-2.96520200	-2.04081900	2.14703900
C	-6.80008400	-1.24476100	2.47432900
H	-5.69167600	0.59473600	2.44876900
H	-6.45331600	0.20160500	0.90736900
C	-6.08285800	-1.87180300	3.66814300
H	-4.23574000	-2.94707700	4.07205400
H	-5.00767600	-3.36489500	2.54519600
H	-7.72326400	-0.75007300	2.79556300
H	-7.09483100	-2.03055900	1.76423400
H	-6.72912600	-2.60454700	4.16306900
H	-5.85945900	-1.09057400	4.40824300
C	-6.59865000	2.30769000	-1.74338800
C	-7.15357500	3.31117900	-0.72581200
C	-7.03458700	2.71528400	-3.15780500
H	-5.50456300	2.35728900	-1.70467100
H	-6.94287400	3.01203100	0.30720800
H	-6.71079600	4.29723000	-0.89652600
H	-8.23785800	3.42603700	-0.82517600
H	-6.58194200	2.07203900	-3.91681800
H	-8.12369400	2.64099900	-3.25416800
H	-6.74240500	3.74957500	-3.36702000
C	-10.21881900	-0.93174500	-0.38326000
C	-10.31129100	-1.62887400	0.97747400
C	-10.95797300	-1.73830000	-1.45773700
H	-10.71123100	0.04525000	-0.29669200
H	-9.84773800	-1.02597500	1.76329000
H	-11.35740300	-1.80344500	1.24905400
H	-9.80509300	-2.60068500	0.95539200
H	-10.90705300	-1.24001600	-2.43015800
H	-10.51763100	-2.73548100	-1.56716800
H	-12.01120900	-1.86522700	-1.18762100
C	-5.69239000	-2.73358800	-1.71087100
C	-5.91555600	-3.20580900	-3.15516800
C	-5.90862400	-3.90904000	-0.75157200
H	-4.64589600	-2.41747700	-1.62412400
H	-5.68330900	-2.41718600	-3.87519200
H	-5.28224200	-4.07049700	-3.37891500
H	-6.96134500	-3.50091800	-3.29697700
H	-5.87889200	-3.59762600	0.29816300

H	-6.87221400	-4.39889500	-0.92681000
H	-5.13097800	-4.66297700	-0.90707200

1a'

R = C_6H_5, Au catalyst without TA ligand

Au/Ga stabilized Reactant complex:

E_{elec}(BS1) = -4558.1479775 Hartree E_{ZPE} = 0.573870 Hartree H_{ZPE} = 0.632401 Hartree G_{ZPE} = 0.474872 Hartree

E_{elec}(BS2)= -6482.1306223 Hartree

Low frequencies (cm^{-1}) -10.9046 -5.8556 13.2142 15.9681 22.5174 24.8810 26.9936 30.8876 32.2926

C	3.81319600	1.67040900	-2.00762000
C	4.40330400	0.40446300	-2.17201500
C	5.37028800	0.15324600	-3.29017400
H	4.08672300	2.45878900	-2.69543200
H	6.35456100	-0.04543900	-2.85392500
H	5.05804700	-0.74731800	-3.82599500
O	4.19335900	-0.59255900	-1.41274900
C	2.93366200	1.96847800	-0.97919700
O	2.51573100	1.12837700	-0.09258900
Ga	3.07413500	-0.62946200	0.14015100
O	-0.02198200	-0.25144100	0.37733000
O	4.48696400	-1.20704200	1.22429800
S	5.68569000	-0.26330800	1.44300900
O	6.94608000	-0.96548300	1.42676800
O	5.50353500	0.95622200	0.66584700
S	0.51272900	-0.23052500	1.73893400
O	-0.28484300	-0.84048700	2.78387400
O	1.96238800	-0.64857000	1.77536500
C	0.57910800	1.58528200	2.16916600
C	5.36900900	0.21884900	3.18223800
F	-0.22916800	1.82109100	3.20050100
F	0.13295400	2.30684800	1.13361000
F	1.79930400	1.98133900	2.47799800
F	6.29735100	1.08615600	3.56911000
F	4.17410100	0.79255100	3.26707000
F	5.40578900	-0.84308400	3.97140100

H	5.43984200	0.99594300	-3.97856800
C	2.36748700	3.34812100	-0.81729100
H	2.55501800	3.68200800	0.20750600
H	2.79842100	4.05608700	-1.52573800
H	1.28207400	3.30388800	-0.95264600
Au	-2.01095100	0.33551000	-1.35208200
P	-3.29150300	-1.11832100	-0.09388300
C	-2.32288200	-2.55798400	0.46696700
H	-2.99491300	-3.32011200	0.87003400
C	-4.68363100	-1.80250600	-1.06834500
H	-5.15627300	-2.65388100	-0.57513000
C	-3.87947000	-0.23964000	1.40846200
C	-3.07235800	0.81717600	1.85070200
H	-2.16007400	1.05521600	1.30997000
C	-3.41236900	1.56254900	2.97287900
H	-2.75513400	2.35807500	3.30673300
C	-4.58925700	1.27610200	3.65665900
H	-4.87344300	1.85950400	4.52663900
C	-5.39452800	0.22422300	3.23456000
H	-6.30263100	-0.02228400	3.77695200
C	-5.04410600	-0.55890100	2.13065600
C	-5.91057300	-1.71866900	1.78003400
C	-5.49221700	-3.01922200	2.07564900
C	-6.27748900	-4.11094900	1.71227700
H	-5.94281700	-5.11757100	1.94284500
C	-7.49277300	-3.90979800	1.06084800
C	-7.93161400	-2.61422100	0.79530800
H	-8.88499900	-2.45348300	0.30177900
C	-7.14715700	-1.52328900	1.15989500
H	-4.55083300	-3.16762100	2.59772500
H	-7.47844100	-0.51100800	0.94373300
H	-8.10204200	-4.76055300	0.77289800
H	-5.42737600	-1.02380300	-1.25269400
H	-4.26169700	-2.12087600	-2.02607900
H	-1.75301800	-2.94811000	-0.37953100
H	-1.62105000	-2.22313100	1.23580200
C	-1.27099200	2.50579300	-2.28825800
C	-0.43221100	1.64898100	-2.53117100
H	0.39797100	0.99267700	-2.75463500
S	1.25880800	-1.86260900	-1.91828000
O	2.01696400	-2.03595500	-0.60697200
O	-0.12145100	-2.30391200	-1.84425700
O	1.54253500	-0.56897000	-2.53548500
C	2.11196000	-3.09333800	-2.97475900
F	3.39213600	-2.77541700	-3.10085500
F	1.54138700	-3.09097800	-4.17418300
F	2.00594500	-4.29964500	-2.44004300
C	-2.20061500	3.56588200	-2.00019100
C	-2.94176200	4.15362300	-3.03226400

C	-2.35016000	4.01013000	-0.67909500
C	-3.82717500	5.18377700	-2.73951400
H	-2.81587900	3.79830600	-4.04967100
C	-3.24050100	5.03837400	-0.39846100
H	-1.76476200	3.54613600	0.10904900
C	-3.97805400	5.62448500	-1.42597800
H	-4.40087000	5.64336400	-3.53756100
H	-3.35920400	5.38319200	0.62336200
H	-4.67249900	6.42816300	-1.20263200

TS(C1)

E_{elec}(BS1) = -4558.11161 Hartree E_{ZPE} = 0.573872 Hartree H_{ZPE} = 0.632818 Hartree G_{ZPE} = 0.474508 Hartree

E_{elec}(BS2)= -6482.0966999 Hartree

Low frequencies (cm^{-1}) -364.2726 9.8731 13.3243 23.1963 26.2294 31.5718 32.5857 35.2033 36.6980

C	2.43252300	-0.57777100	2.47517900
C	2.76242000	0.78163900	2.22573800
C	3.05509100	1.72547300	3.34531600
H	2.59779800	-0.94492400	3.48129900
H	4.06958800	2.11293800	3.20821600
H	2.36713200	2.57353900	3.26567700
O	2.74541100	1.28242300	1.06909600
C	2.52731800	-1.54504800	1.42306000
O	2.41695200	-1.25620600	0.20226400
Ga	2.56166200	0.45882000	-0.67964900
O	-0.22081800	-0.85011500	-0.88662300
O	4.34187000	0.37886800	-1.20886400
S	5.53845000	-0.04879800	-0.33986800
O	6.68998200	0.78536900	-0.57389300
O	5.12251600	-0.35575000	1.02405500
S	0.47725600	-1.15155600	-2.13692900
O	-0.26040700	-1.09760000	-3.37954900
O	1.79600900	-0.39800800	-2.20789400
C	1.05467100	-2.92027600	-1.97898500
C	5.88893400	-1.68281800	-1.08955300
F	0.47744800	-3.64966800	-2.92167400
F	0.69425700	-3.40778000	-0.78922800
F	2.36727900	-3.01034800	-2.09799000
F	6.93569100	-2.22300500	-0.47753100
F	4.83282900	-2.47567700	-0.91959900

F	6.14502300	-1.56202900	-2.38029000
H	2.96573100	1.25102200	4.32255900
C	2.76883300	-2.98197500	1.75184000
H	3.85762400	-3.12151100	1.72858500
H	2.39838800	-3.24435900	2.74548300
H	2.31987400	-3.61574400	0.98614000
Au	-2.12759700	0.65627800	1.12715000
P	-4.29666400	0.88546600	0.29549700
C	-4.63359100	2.64623200	-0.08282800
H	-5.68660200	2.79839200	-0.32985500
C	-5.54230600	0.46277100	1.57380500
H	-6.53512600	0.84671200	1.33006200
C	-4.57116800	-0.05868300	-1.24876200
C	-3.41510400	-0.38737100	-1.97132400
H	-2.43327300	-0.10684400	-1.59606300
C	-3.49352100	-1.08760200	-3.17199100
H	-2.57841800	-1.31493200	-3.70847300
C	-4.73518400	-1.49242500	-3.64834100
H	-4.80901600	-2.05035800	-4.57669900
C	-5.88947500	-1.18062500	-2.93563300
H	-6.86285400	-1.49027300	-3.30529600
C	-5.83021500	-0.45238400	-1.74565600
C	-7.11053400	-0.12731900	-1.05357500
C	-7.67582800	1.14638100	-1.16323600
C	-8.85046500	1.45888600	-0.48250500
H	-9.27892700	2.45230200	-0.57258400
C	-9.47943300	0.49472600	0.30229400
C	-8.94288500	-0.78870800	0.38479300
H	-9.43826200	-1.54823200	0.98162800
C	-7.76814200	-1.09898100	-0.29443700
H	-7.19482100	1.88806100	-1.79537900
H	-7.33866400	-2.09466200	-0.22226400
H	-10.39192500	0.73878800	0.83677200
H	-5.58896300	-0.62138400	1.70047500
H	-5.19461300	0.90752400	2.51085400
H	-4.37127600	3.24585100	0.79324000
H	-4.00352700	2.95864000	-0.91902300
C	0.28806700	-0.42430000	2.35688600
C	-0.11563500	0.63978700	1.78151600
H	0.41313600	1.52178300	1.42417900
S	1.55247900	3.44803200	-0.60365700
O	1.79058900	2.06879200	-1.24352700
O	1.16457200	4.39954800	-1.61598700
O	0.77117500	3.34712300	0.62080500
C	3.26850300	3.94524100	-0.05966400
F	3.32559600	4.01004200	1.26555800
F	3.54830100	5.13749700	-0.55842900
F	4.16993000	3.07099700	-0.48988000
C	-0.07281900	-1.74701300	2.84602700

C	0.10177900	-2.11489000	4.18480600
C	-0.56897400	-2.67375400	1.91947400
C	-0.21378000	-3.40522500	4.59355600
H	0.48589100	-1.38776900	4.89461700
C	-0.88552500	-3.96244200	2.33973300
H	-0.68450400	-2.36779100	0.88329800
C	-0.70302600	-4.33084200	3.67055700
H	-0.07999300	-3.69040700	5.63209900
H	-1.26717000	-4.68104900	1.62135300
H	-0.94275500	-5.33945800	3.99211300

TS(C2)

E_{elec}(BS1) = -4558.1154049 Hartree E_{ZPE} = 0.573872 Hartree H_{ZPE} = 0.632818 Hartree G_{ZPE} = 0.474508 Hartree

E_{elec}(BS2)=-6482.0977771 Hartree

Low frequencies (cm^{-1}) -391.9828 11.9812 16.6678 24.4672 26.5647 29.2277 31.9564 33.4624 37.5391

C	2.75318200	1.22029600	-1.85360400
C	3.06259000	-0.13113700	-2.18103400
C	3.54764600	-0.49179900	-3.54866700
H	3.02267500	1.98501600	-2.57136700
H	4.33403300	-1.24427300	-3.45578900
H	2.71504100	-0.94919200	-4.09497700
O	2.85525200	-1.08900100	-1.38481300
C	2.63904100	1.62807400	-0.49165900
O	2.40327400	0.83052700	0.46005300
Ga	2.43287800	-1.08072800	0.52278800
O	-0.26825500	-0.36978800	0.76719900
O	4.12203200	-1.52080500	1.14975000
S	5.42098700	-0.75021600	0.83653100
O	6.55874300	-1.63298500	0.79638300
O	5.20868300	0.22503400	-0.22575100
S	0.15607300	-0.35839500	2.17239900
O	-0.72625700	-0.89226200	3.18113500
O	1.58483100	-0.87168700	2.25778800
C	0.35037000	1.45346300	2.58312100
C	5.56600400	0.24473300	2.36870100
F	-0.53410800	1.78899800	3.51636700
F	0.09951400	2.18777100	1.49318900
F	1.56523400	1.73165400	3.01794500
F	6.62831200	1.03440000	2.27042100

F	4.47804200	0.99788200	2.50773700
F	5.69462700	-0.54190000	3.42231800
H	3.91171600	0.37594200	-4.09877500
C	2.80581400	3.06447300	-0.11388700
H	3.79535200	3.14488500	0.35356000
H	2.75027400	3.73496600	-0.97262400
H	2.05767000	3.33315700	0.63417200
Au	-1.88042400	0.97300900	-1.31429000
P	-3.59635100	-0.33867700	-0.44739800
C	-2.93835400	-2.02080600	-0.16666800
H	-3.74535200	-2.72989500	0.03167900
C	-4.97287400	-0.54415500	-1.63986700
H	-5.62987400	-1.37724800	-1.38215200
C	-4.20641100	0.30821400	1.15617200
C	-3.31436400	1.12942600	1.85908900
H	-2.32617800	1.31621000	1.44544300
C	-3.67152900	1.71038800	3.07016400
H	-2.95715400	2.32816500	3.60186400
C	-4.94665200	1.49937200	3.58304700
H	-5.24391900	1.96150100	4.51918600
C	-5.83852500	0.67892600	2.90171400
H	-6.82818000	0.48959900	3.30751600
C	-5.47933700	0.05616300	1.70348300
C	-6.45873800	-0.86728700	1.06618100
C	-6.24740400	-2.24868600	1.10214500
C	-7.13671300	-3.11398700	0.46962000
H	-6.96132000	-4.18483400	0.49941800
C	-8.25227100	-2.60541800	-0.19266800
C	-8.48792500	-1.23206400	-0.20050700
H	-9.36377300	-0.83311000	-0.70275400
C	-7.59888000	-0.36771300	0.43214400
H	-5.38585400	-2.63977400	1.63656200
H	-7.77083700	0.70528300	0.41683600
H	-8.94304400	-3.27896600	-0.68997400
H	-5.55520200	0.37867700	-1.69778200
H	-4.51274700	-0.72807100	-2.61498500
H	-2.37581700	-2.32899600	-1.05209000
H	-2.24292100	-1.98658700	0.67594000
C	-0.08576000	2.03747600	-1.99525700
C	0.64369300	0.99400000	-1.96152500
H	0.64187200	-0.08422700	-1.84332800
S	0.62915800	-3.12221100	-0.96240700
O	1.45551600	-2.65531700	0.23878900
O	-0.29123400	-4.16430000	-0.57277800
O	0.12698100	-2.00789100	-1.76068300
C	1.93325700	-3.93376900	-2.01934100
F	2.14924100	-3.20473800	-3.10995900
F	1.50221600	-5.13101000	-2.38591300
F	3.06781900	-4.06044600	-1.35100400

C	0.11845400	3.47507300	-2.11366200
C	-0.42758800	4.34924600	-1.16625800
C	0.91811400	3.98833500	-3.14346900
C	-0.14282700	5.70880900	-1.22565900
H	-1.05696200	3.94908000	-0.37588400
C	1.18700600	5.35184900	-3.20603400
H	1.31528600	3.31014500	-3.89307400
C	0.66625200	6.21326000	-2.24200100
H	-0.55766700	6.37837800	-0.47899000
H	1.80503000	5.74224500	-4.00858500
H	0.88165300	7.27580800	-2.28930700

1f'

R = $CH(CH_3)_2$, Au catalyst without TA ligand

Au/Ga stabilized Reactant complex:

E_{elec}(BS1) = -4445.0857293 Hartree E_{ZPE} = 0.577547 Hartree H_{ZPE} = 0.637507Hartree G_{ZPE} = 0.477392 Hartree

E_{elec}(BS2)= -6369.0322662 Hartree

Low frequencies (cm^{-1}) 16.2468 21.3531 21.6288 24.7925 28.5682 31.5221 35.3353 36.1455 38.0122

C	3.74835600	0.66904400	2.51750800
C	3.97916800	1.59199100	1.48138900
C	5.14265900	2.53012000	1.53842600
H	4.41014500	0.68257500	3.37275200
H	5.88886300	2.14716700	0.83171300
H	4.83413900	3.51784500	1.19193300
O	3.28019600	1.65923500	0.41649000
C	2.80005500	-0.33803500	2.43274000
O	1.95485900	-0.48304200	1.46375700
Ga	1.99661100	0.35271400	-0.18267000
O	-0.14333200	-2.49247100	0.83179300
O	3.11179300	-0.26434400	-1.54877300
S	4.65341000	-0.25467200	-1.42919100
O	5.25591500	0.89168400	-2.07180300
O	5.06214400	-0.62592900	-0.08255300

S	0.13719000	-2.23166300	-0.57619700
O	-0.85936200	-2.63353100	-1.55364800
O	0.58273500	-0.80476100	-0.84189400
C	1.67053800	-3.16474600	-0.95443200
C	5.02010200	-1.69810400	-2.50398200
F	1.46482000	-4.45935000	-0.75419100
F	2.64385700	-2.74753400	-0.14830700
F	2.02173000	-2.96041000	-2.21343400
F	6.32303600	-1.70415500	-2.75708600
F	4.69497900	-2.82704200	-1.88943400
F	4.35171200	-1.60604100	-3.64242500
H	5.58271500	2.58987200	2.53420200
C	2.69123900	-1.40016300	3.48408000
H	2.94143100	-2.35879800	3.01741900
H	3.35464700	-1.21798700	4.32996700
H	1.65248400	-1.46536300	3.82002400
Au	-1.54327200	0.15144500	1.38559900
P	-2.83155200	0.42621300	-0.51934500
C	-1.90204900	0.54636200	-2.08193400
H	-2.55057600	0.95494300	-2.86018500
C	-3.73926300	2.00704300	-0.36986500
H	-4.22474400	2.28539500	-1.30738400
C	-4.01673500	-0.97720700	-0.60462900
C	-3.62210300	-2.16443000	0.02956500
H	-2.62674400	-2.24310900	0.45836700
C	-4.47584700	-3.25922300	0.10509100
H	-4.13868400	-4.16844300	0.59189900
C	-5.75341000	-3.17629400	-0.43792100
H	-6.43453800	-4.01877400	-0.37180400
C	-6.15157900	-2.01192600	-1.08490400
H	-7.13680800	-1.94602200	-1.53726300
C	-5.29302300	-0.91399100	-1.19869300
C	-5.76859000	0.26752700	-1.96939100
C	-5.20084000	0.57150300	-3.21001900
C	-5.61619300	1.69615400	-3.91888000
H	-5.16579900	1.92599000	-4.87935100
C	-6.61326500	2.51888100	-3.39885200
C	-7.20928100	2.20065400	-2.17995200
H	-7.99482300	2.83241100	-1.77754800
C	-6.79391800	1.07649200	-1.47215400
H	-4.43875700	-0.08598400	-3.61914800
H	-7.24466800	0.83300200	-0.51382800
H	-6.93295100	3.39905400	-3.94725800
H	-4.48637900	1.92750900	0.42396200
H	-2.99642700	2.76133200	-0.09727200
H	-1.04829600	1.20730800	-1.91162900
H	-1.53246900	-0.44381100	-2.35785900
C	-1.12145800	-0.52348800	3.75654800
C	-0.35289800	0.37092100	3.43907700

H	0.34607000	1.16514900	3.24354600
C	-2.00531300	-1.59812700	4.24210000
H	-1.86962100	-1.61230100	5.33180500
S	0.48544800	2.91158400	0.37225400
O	0.79644900	1.76315700	-0.59014100
O	-0.83078100	3.44794300	0.08656800
O	0.82834100	2.55644900	1.74402200
C	1.70806600	4.22249300	-0.14095500
F	2.59336900	4.40537800	0.82870900
F	1.05113300	5.35453200	-0.34272900
F	2.32645100	3.86804200	-1.25124900
C	-3.47917000	-1.28920400	3.94274000
H	-4.11197500	-2.04031900	4.42376900
H	-3.76462000	-0.30037200	4.31111300
H	-3.66548500	-1.32817200	2.86321700
C	-1.58813400	-2.95870700	3.66996400
H	-0.54481500	-3.18713800	3.90090200
H	-2.22304800	-3.74009000	4.09776400
H	-1.69228800	-2.96747200	2.58172300

TS(C1)

E_{elec}(BS1) = -4445.0338306 Hartree E_{ZPE} = 0.576589 Hartree H_{ZPE} = 0.635703 Hartree G_{ZPE} = 0.475291 Hartree

E_{elec}(BS2)= -6368.9840604 Hartree

Low frequencies (cm^{-1}) -325.8027 8.2185 13.6848 14.6034 20.1646 26.2653 28.4824 29.3155 32.6873

C	-2.75285400	-1.00436800	2.35415000
C	-2.97705700	-1.93144200	1.29814000
C	-3.27484700	-3.36867700	1.58844800
H	-3.05978300	-1.30209100	3.34909100
H	-4.13145000	-3.68226000	0.98708800
H	-2.41304900	-3.96095500	1.26187100
O	-2.87227000	-1.62029500	0.08060700
C	-2.66424200	0.38722900	2.08248400
O	-2.44041500	0.86274900	0.93350000
Ga	-2.70262600	0.11209900	-0.81158800
O	0.17507600	0.64568800	-0.88779300
O	-4.47811800	0.48601600	-1.20493300
S	-5.63544300	0.63578200	-0.20183800
O	-6.90027400	0.29780000	-0.80233100
O	-5.26984300	0.09091000	1.10025300

S	-0.42797800	1.94060800	-1.20424100
O	0.18454100	2.80771300	-2.18408400
O	-1.92568600	1.77941600	-1.40841100
C	-0.31092000	2.88464400	0.39731800
C	-5.61926600	2.45510400	0.02345400
F	0.68582800	3.76209200	0.29810300
F	-0.02113400	2.05548300	1.40410700
F	-1.43135300	3.52855600	0.67675600
F	-6.53916700	2.78894700	0.92067700
F	-4.42310100	2.83182700	0.47301700
F	-5.87078700	3.06783600	-1.11888900
H	-3.46949100	-3.54669700	2.64648400
C	-2.78706700	1.40150900	3.17553600
H	-3.63142500	2.04840000	2.91662900
H	-2.95728000	0.95542500	4.15569300
H	-1.88684100	2.02330800	3.18237200
Au	2.02278500	-0.80352000	1.05549000
P	4.26387000	-0.30829200	0.64894900
C	5.16286800	-1.77794100	0.02631700
H	6.24605300	-1.65925700	0.09767400
C	5.11407800	0.09513000	2.22349800
H	6.19639900	0.14380900	2.08922100
C	4.47125300	1.10284600	-0.49677800
C	3.33452600	1.89709600	-0.70037300
H	2.40890600	1.65044600	-0.18798800
C	3.35463700	2.97770900	-1.57718100
H	2.45076100	3.55669500	-1.72939200
C	4.51954800	3.26338400	-2.27886200
H	4.54477900	4.09073700	-2.98078700
C	5.65531300	2.48086800	-2.09094300
H	6.56808400	2.70028000	-2.63717000
C	5.65603200	1.40628300	-1.19959700
C	6.91355400	0.61979200	-1.04999400
C	7.30125200	-0.28068700	-2.04686900
C	8.45816800	-1.04067900	-1.89916100
H	8.74257500	-1.74607800	-2.67347400
C	9.24677700	-0.89970800	-0.75866400
C	8.88724800	0.02186000	0.22234600
H	9.51308200	0.15618100	1.09913300
C	7.73017300	0.78341700	0.07226800
H	6.67628300	-0.39623900	-2.92812900
H	7.46017000	1.52365200	0.82063200
H	10.14627500	-1.49554100	-0.64191900
H	4.74010500	1.05092400	2.59864800
H	4.87140600	-0.68524700	2.95055900
H	4.84288600	-2.63231300	0.62939100
H	4.87969000	-1.96315200	-1.01279100
C	-0.56241200	-1.14583200	2.52352900
C	-0.04016600	-1.21574400	1.36935500

H	-0.47030500	-1.33544900	0.37750500
C	-0.39883000	-1.15220000	4.00013900
H	-1.09401200	-0.42698000	4.43746500
S	-1.37842900	-2.15225700	-2.48161100
O	-2.02791900	-0.77119700	-2.30186200
O	-0.86065000	-2.28929900	-3.82003400
O	-0.54893200	-2.51299600	-1.34206500
C	-2.86976000	-3.27317000	-2.39392300
F	-2.77028600	-4.08104000	-1.34117600
F	-2.92201700	-4.01208500	-3.49102300
F	-3.98987900	-2.57022600	-2.29200400
C	1.02696100	-0.69998400	4.35970900
H	1.76156800	-1.42055700	3.98716100
H	1.25056000	0.27882900	3.92577900
H	1.11892300	-0.63727500	5.44824600
C	-0.68975900	-2.54134800	4.58027400
H	-0.57335100	-2.52700300	5.66774600
H	-1.70577700	-2.87344500	4.34900600
H	0.00896800	-3.27197400	4.16201200

TS(C2)

E_{elec}(BS1) = -4445.0338306 Hartree E_{ZPE} = 0.577167 Hartree H_{ZPE} = 0.636002 Hartree G_{ZPE} = 0.478697 Hartree

E_{elec}(BS2)= -4445.039944 Hartree

Low frequencies (cm^{-1}) -393.3061 13.2879 15.5714 22.9479 25.1542 28.4957 31.4714 33.1450 36.4103

C	2.72247900	-0.20239100	2.43372100
C	3.01880500	1.12955000	2.01276700
C	3.40261900	2.17369700	3.01155000
H	2.95455000	-0.46432900	3.45899100
H	4.17310300	2.81505400	2.57897200
H	2.51961600	2.79581800	3.19731300
O	2.87902600	1.51075200	0.81913500
C	2.68072200	-1.26285700	1.48300000
O	2.45845600	-1.08538300	0.25246400
Ga	2.51668200	0.49722600	-0.82108700
O	-0.21865200	-0.25365100	-0.74718900
O	4.23304400	0.54338600	-1.51786900
S	5.48929200	-0.01955000	-0.82083800
O	6.67497300	0.69110100	-1.22527900
O	5.23095300	-0.27973900	0.59039700

S	0.27626100	-1.03011700	-1.89026500
O	-0.54665600	-1.16630500	-3.06673200
O	1.71196400	-0.61943800	-2.18626300
C	0.47731000	-2.75932000	-1.21495100
C	5.55734800	-1.67630400	-1.60373200
F	-0.39515600	-3.56430900	-1.81184800
F	0.21308700	-2.76275100	0.09528800
F	1.69818000	-3.22677100	-1.40925900
F	6.57326800	-2.35641900	-1.08683200
F	4.42575900	-2.32764300	-1.34884500
F	5.71709700	-1.56489600	-2.91017100
H	3.74569100	1.73966000	3.95059600
C	2.91040100	-2.67582400	1.91047900
H	3.97156100	-2.88214000	1.72033600
H	2.70639800	-2.82919900	2.97148400
H	2.31778800	-3.35036000	1.29167500
Au	-1.88610000	-0.19398100	1.77208000
P	-3.54394500	0.42975000	0.25742500
C	-2.85735800	1.70120900	-0.86120300
H	-3.64473300	2.15689400	-1.46555100
C	-4.96872100	1.23653400	1.08165900
H	-5.59749000	1.78944400	0.38112000
C	-4.10267500	-0.98629600	-0.76599800
C	-3.21298600	-2.06655400	-0.85103700
H	-2.25477800	-2.00901500	-0.34009300
C	-3.53490900	-3.20943000	-1.57446700
H	-2.82259500	-4.02376000	-1.63738800
C	-4.77121400	-3.29912000	-2.20411700
H	-5.03966500	-4.19207500	-2.75950700
C	-5.66098400	-2.23310800	-2.13352500
H	-6.62060500	-2.28557400	-2.63947500
C	-5.33693700	-1.06356300	-1.44044000
C	-6.31515400	0.05978700	-1.46381800
C	-6.06753900	1.19216800	-2.24516500
C	-6.96083000	2.26090000	-2.24040800
H	-6.75678400	3.13747800	-2.84714600
C	-8.11700000	2.19981900	-1.46490400
C	-8.38810500	1.05836100	-0.71278300
H	-9.29479000	1.00115500	-0.11873100
C	-7.49465800	-0.00917200	-0.71761500
H	-5.17497700	1.22482800	-2.86368800
H	-7.69472900	-0.89605800	-0.12238400
H	-8.81104900	3.03412000	-1.45683100
H	-5.57017500	0.48815000	1.60336900
H	-4.55036900	1.92580800	1.82074900
H	-2.35828500	2.46496600	-0.25878900
H	-2.10424200	1.23376800	-1.50039600
C	-0.14335000	-0.71047200	3.00136500
C	0.65075600	-0.01437600	2.29078600

H	0.68200000	0.68460800	1.46504500
C	-0.09879400	-1.71114700	4.10559500
H	0.94599000	-1.79266500	4.44364600
S	0.69447300	2.99597600	-0.67776600
O	1.54464400	1.97113300	-1.43741800
O	-0.19676000	3.68424700	-1.58113600
O	0.15786000	2.45447100	0.56591000
C	1.98960000	4.23755900	-0.16476100
F	2.11545000	4.23518900	1.15908000
F	1.60765800	5.44344800	-0.55447600
F	3.16005500	3.95044100	-0.71124600
C	-0.95882500	-1.25486800	5.28753300
H	-0.63678200	-0.27884800	5.66000000
H	-2.00660200	-1.17318200	4.97810300
H	-0.89410300	-1.97988500	6.10468900
C	-0.55793600	-3.07971000	3.58974100
H	-1.60740400	-3.03003500	3.27792500
H	0.03292200	-3.40100300	2.72738600
H	-0.46777400	-3.83195300	4.37947300