## Supporting Information

# DFT Insights into Cycloisomerization of ω-Alkynylfuran Catalyzed by Planar Gold Clusters: Mechanism and Selectivity, as Compared to Au(I)-Catalysis

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**Supporting Information**

## S1. Figures

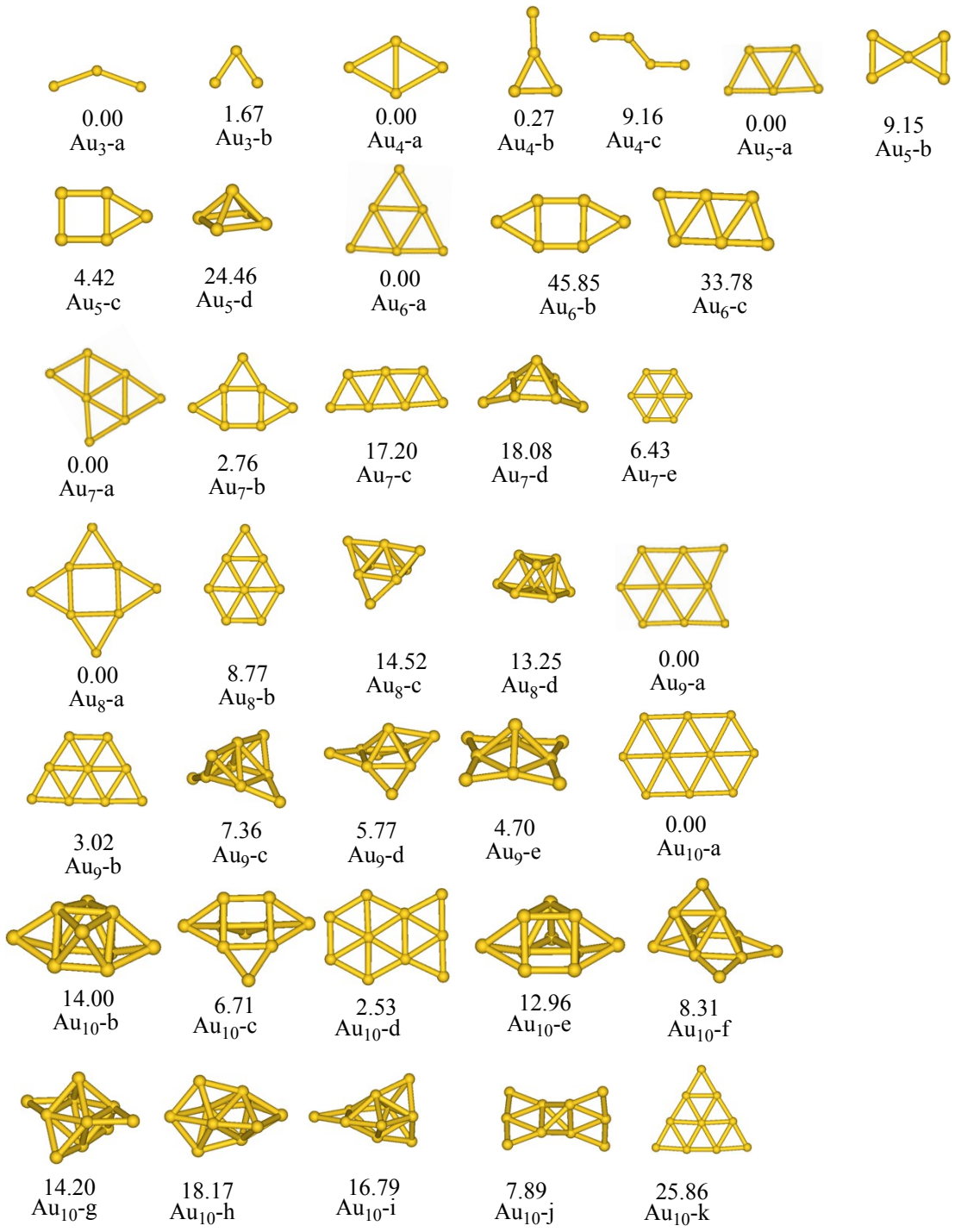



**Figure S1.** The optimized structures and relative energies of $Au_{3\text{-}10}$. The relative energy is in kcal/mol.

**Table S1** The adsorption energies ($\Delta E_{ad}$, kcal/mol) of substrate on the $Au_3$ clusters and the energy barriers ($\Delta_r E_a$, kcal/mol) of three steps in the gas phase and acetonitrile solvent (parentheses).

| | $E_{ad}$ | $\Delta_r E_a$(**TS1/2**) | $\Delta_r E_a$(**TS2/3**) | $\Delta_r E_a$(**TS3/4**) | $\Delta_r E$(Sub-**IM5**) | $\Delta_r E$(Sub-**P1**) |
|---|---|---|---|---|---|---|
| TPSSh | -32.84(-29.05) | 19.06(15.87) | 8.48(8.44) | 12.21(16.99) | -14.78(-14.38) | -55.86(-57.17) |
| PBE | -34.84(-30.42) | 15.46(13.30) | 6.24(4.73) | 9.38(12.97) | -16.41(-15.26) | -59.33(-60.15) |

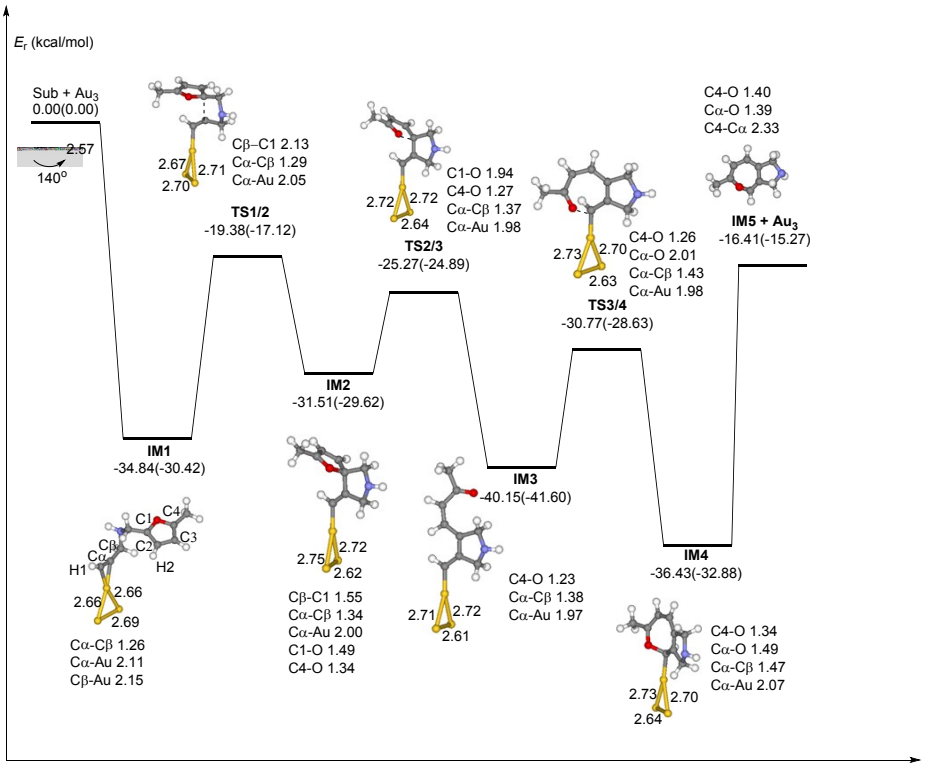



**Figure S2.** The optimized structures, related parameters, and potential energy profile of the 5-*exo* FCT pathway catalyzed by $Au_3$ cluster at the PBE/def2-TZVP levels in the gas phase and acetonitrile solvent (parentheses). The bond length is in Å.

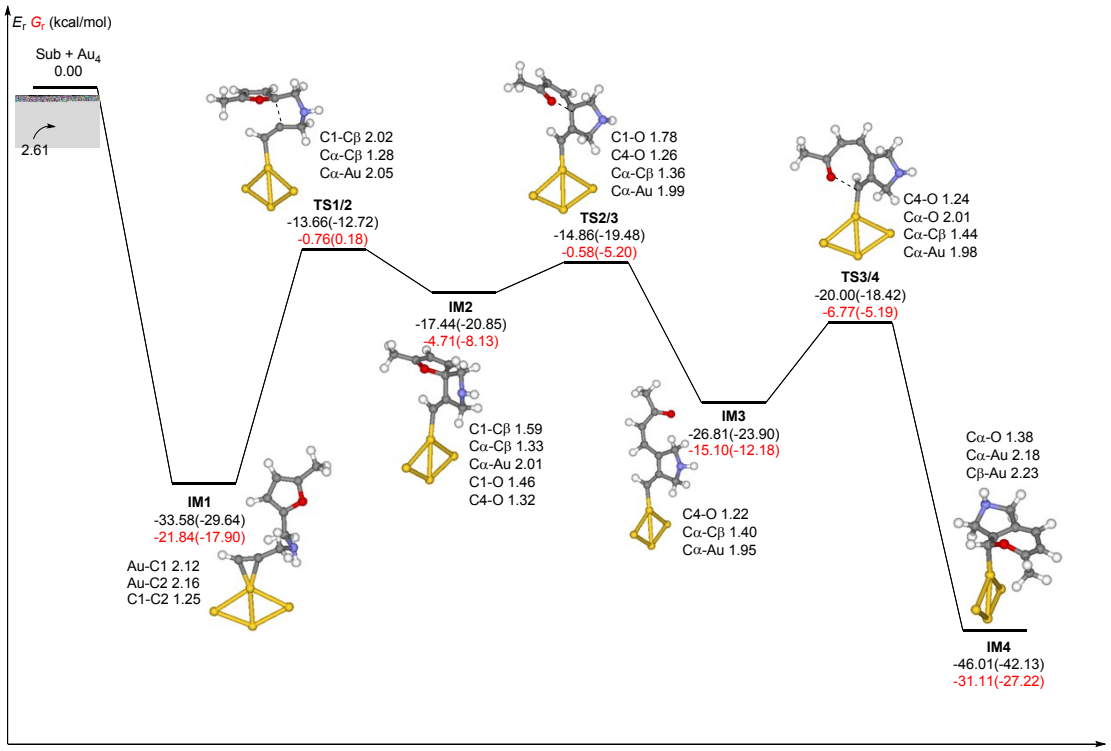



**Figure S3.** The optimized structures, related parameters, potential energy profile, and relative Gibbs free energies (colored by red, 298.15 K and 1 atm) of the 5-*exo* FCT pathway catalyzed by $Au_4$ cluster in the gas phase and acetonitrile solvent (parentheses). The bond length is in Å.

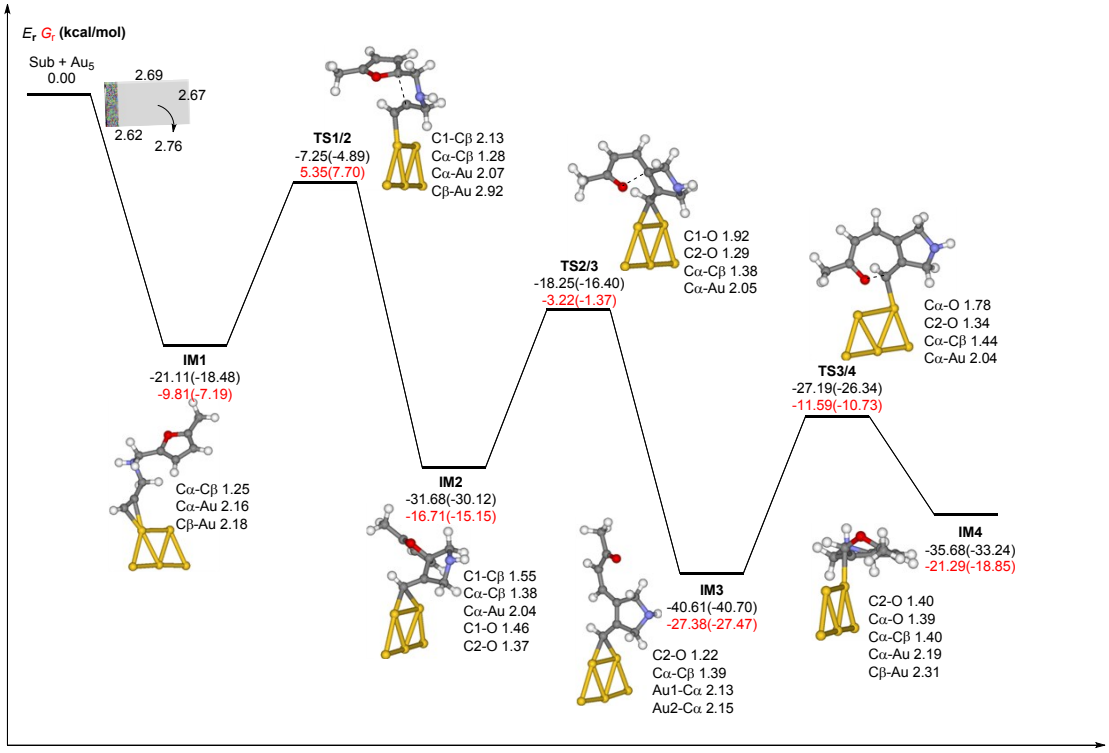



**Figure S4.** The optimized structures, related parameters, potential energy profile, and relative Gibbs free energies (colored by red, 298.15 K and 1 atm) of the 5-*exo* FCT pathway catalyzed by $Au_5$ cluster in the gas phase and acetonitrile solvent (parentheses). The bond length is in Å.

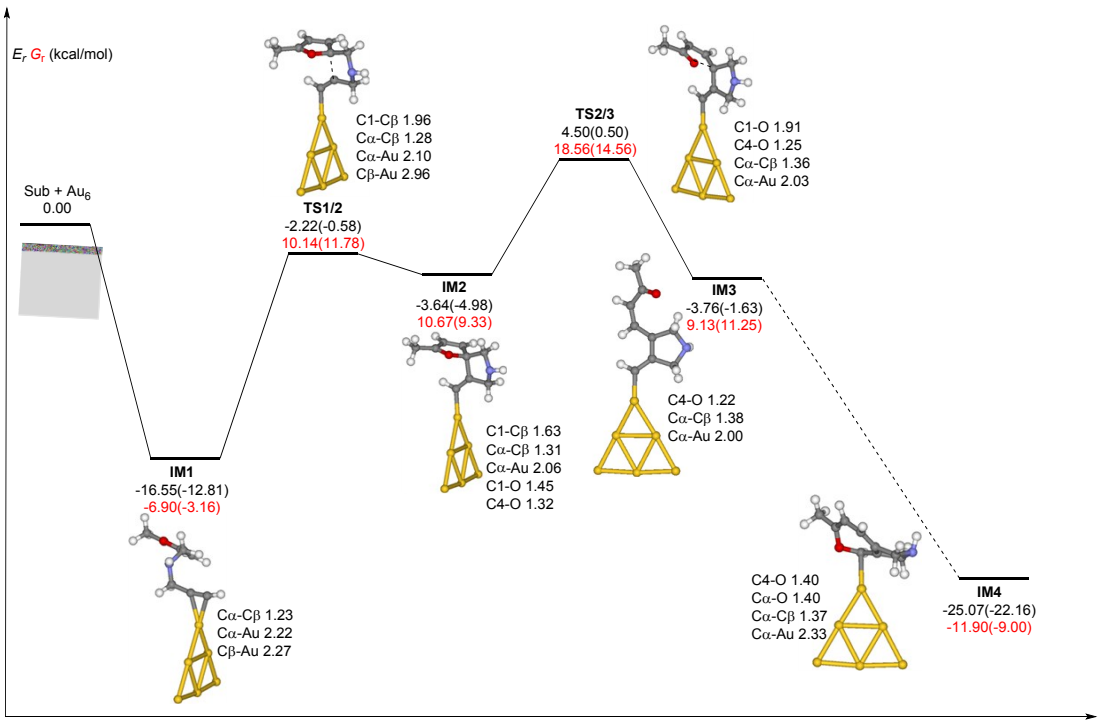



**Figure S5.** The optimized structures, related parameters, potential energy profile, and relative Gibbs free energies (colored by red, 298.15 K and 1 atm) of the 5-*exo* FCT pathway catalyzed by $Au_6$ cluster in the gas phase and acetonitrile solvent (parentheses). The bond length is in Å.

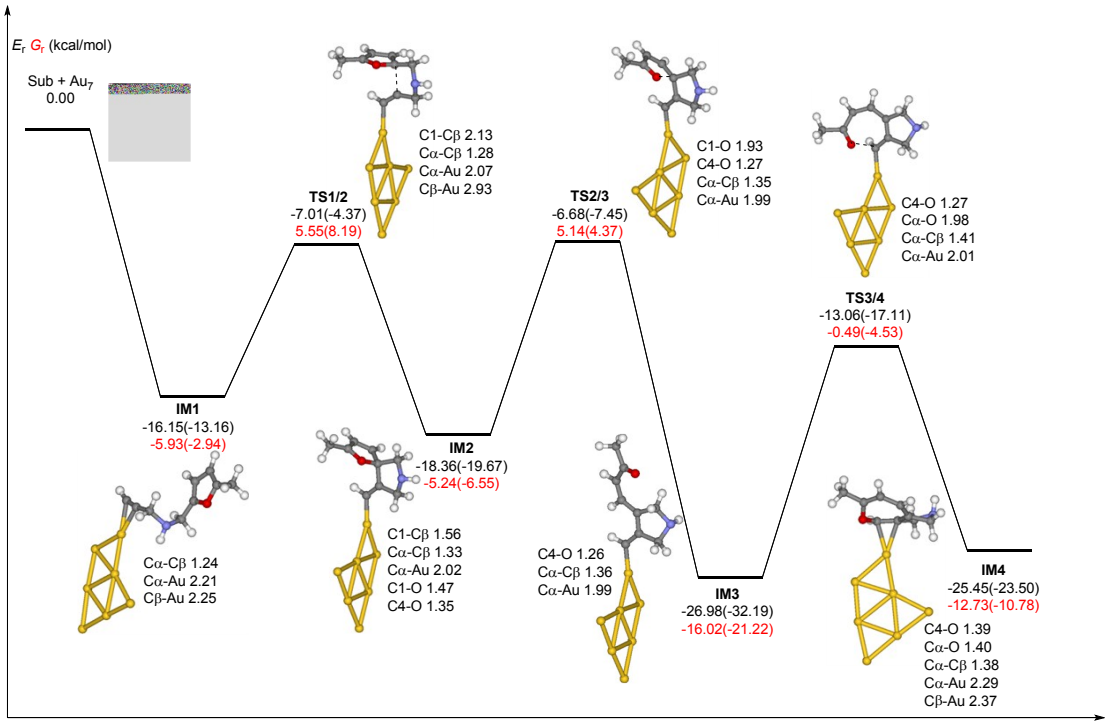



**Figure S6.** The optimized structures, related parameters, potential energy profile, and relative Gibbs free energies (colored by red, 298.15 K and 1 atm) of the 5-*exo* FCT pathway catalyzed by $Au_7$ cluster in the gas phase and acetonitrile solvent (parentheses). The bond length is in Å.

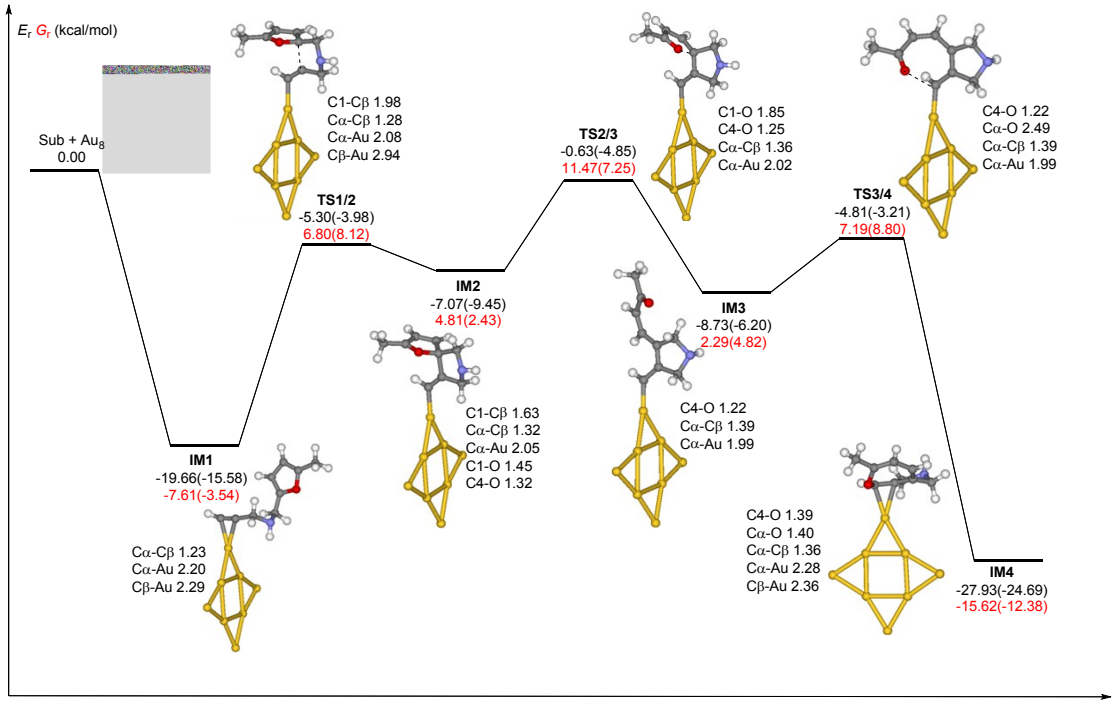



**Figure S7.** The optimized structures, related parameters, potential energy profile, and relative Gibbs free energies (colored by red, 298.15 K and 1 atm) of the 5-*exo* FCT pathway catalyzed by $Au_8$ cluster in the gas phase and acetonitrile solvent (parentheses). The bond length is in Å.

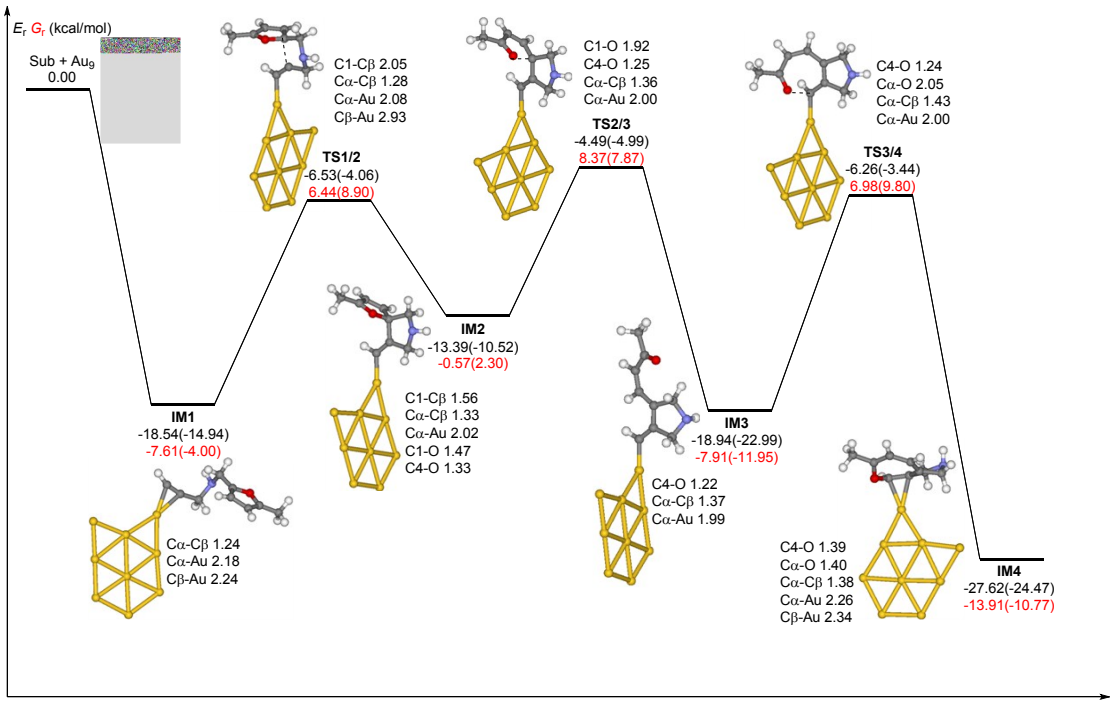



**Figure S8.** The optimized structures, related parameters, potential energy profile, and relative Gibbs free energies (colored by red, 298.15 K and 1 atm) of the 5-*exo* FCT pathway catalyzed by $Au_9$ cluster in the gas phase and acetonitrile solvent (parentheses). The bond length is in Å.

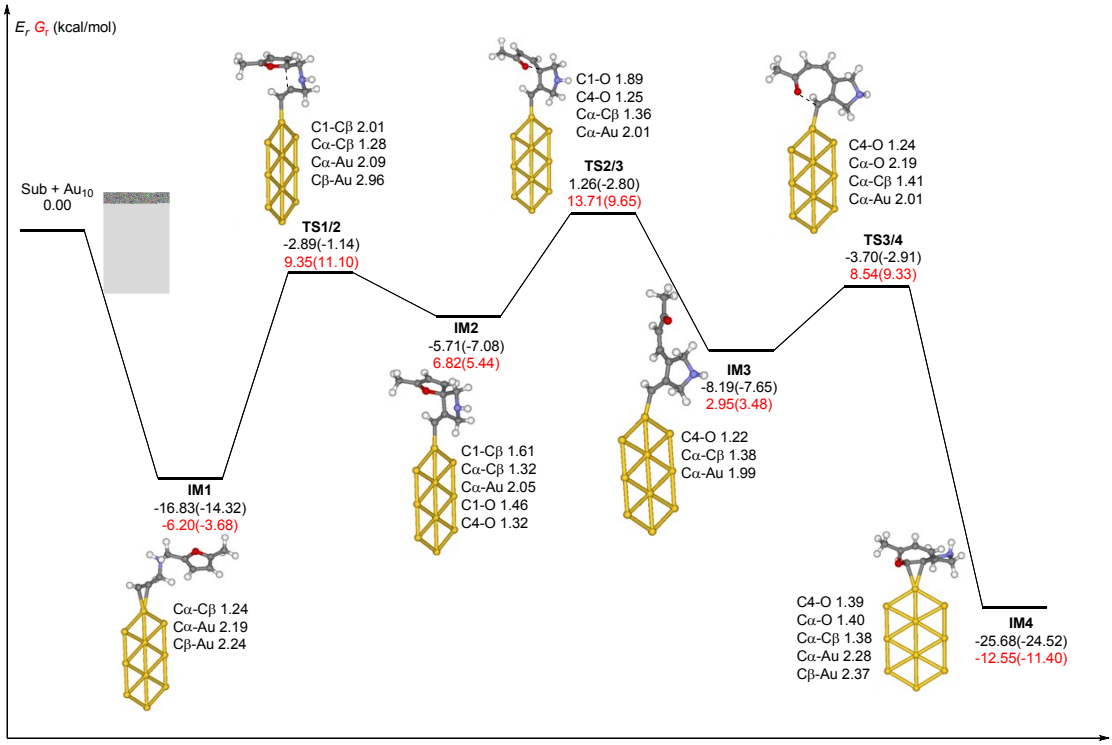



**Figure S9.** The optimized structures, related parameters, potential energy profile, and relative Gibbs free energies (colored by red, 298.15 K and 1 atm) of the 5-*exo* FCT pathway catalyzed by $Au_{10}$ cluster in the gas phase and acetonitrile solvent (parentheses). The bond length is in Å.

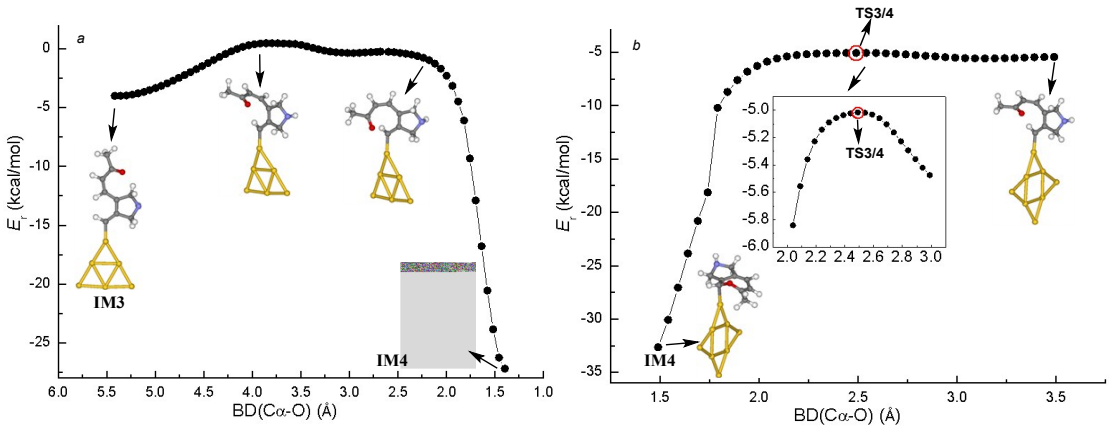



**Figure S10.** The scan potential energy profiles with the Cα-O bond and some optimized structures of intermediate: (a) $Au_6$ cluster, (b) $Au_8$ cluster. The insert indicates an enlarged view near **TS3/4**

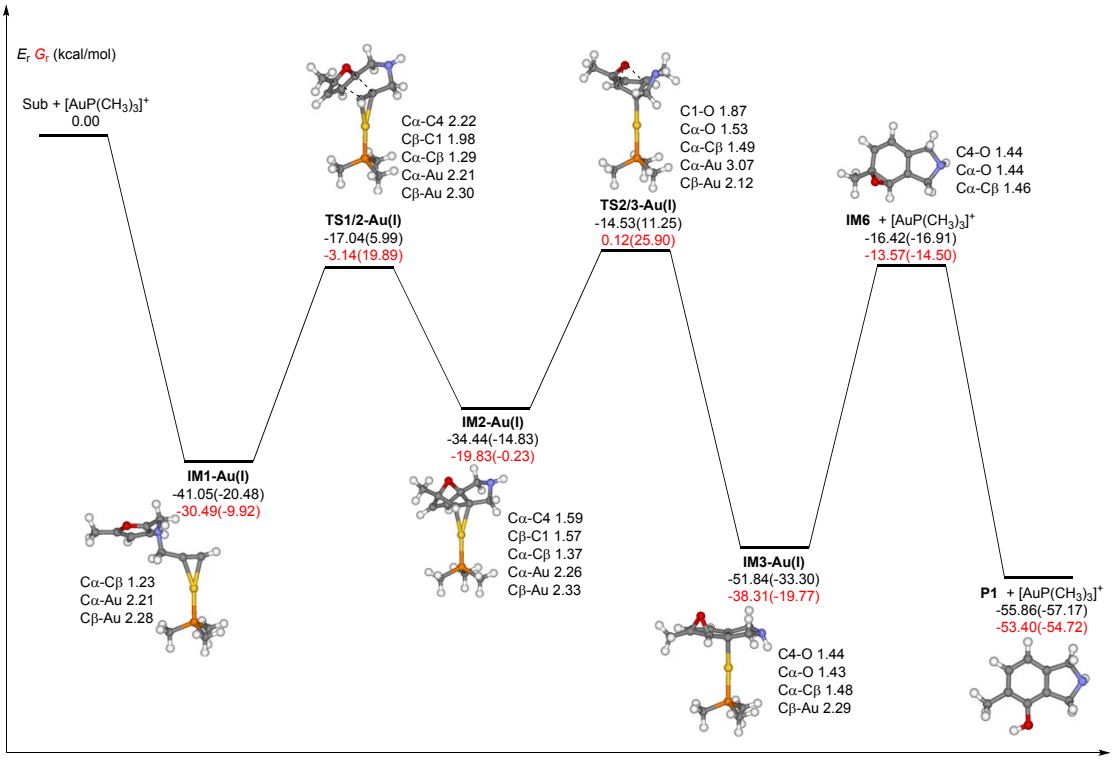



**Figure S11.** The optimized structures, related parameters, potential energy profile, and relative Gibbs free energies (colored by red, 298.15 K and 1 atm) of the DDA pathway catalyzed by the $[AuP(CH_3)_3]^+$ complex in the gas phase and acetonitrile solvent (parentheses). The bond length is in Å.

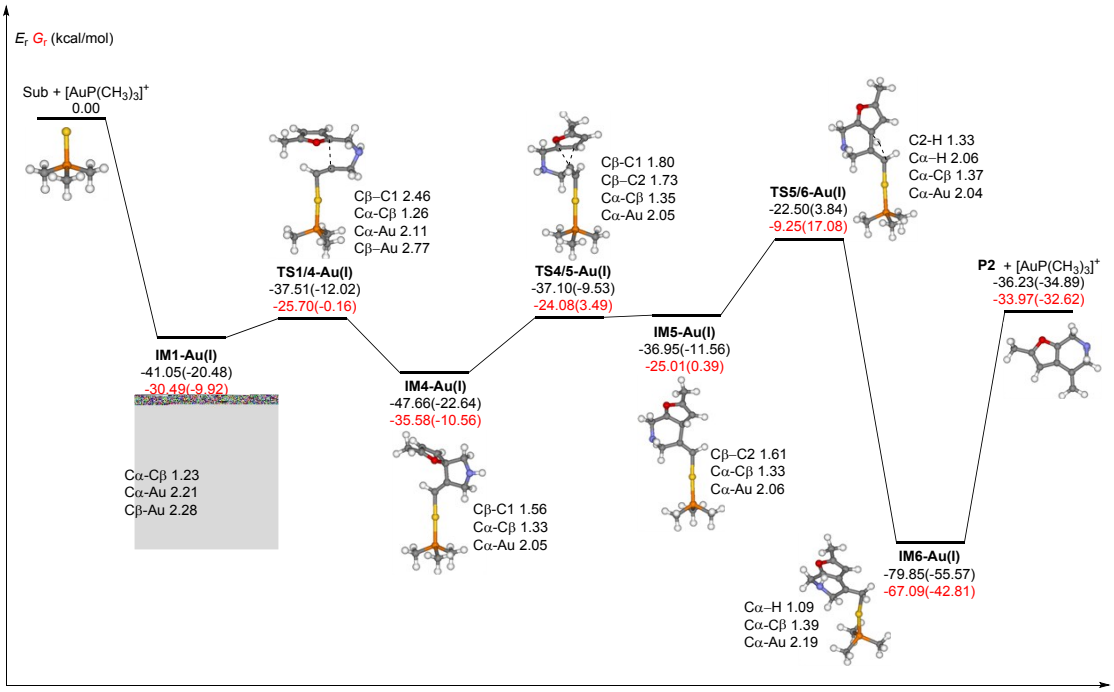



**Figure S12.** The optimized structures, related parameters, potential energy profile, and relative Gibbs free energies (colored by red, 298.15 K and 1 atm) of the 5-*exo* FCT pathway toward the the β-alkenylated furan (**P2**) catalyzed by $[AuP(CH_3)_3]^+$ in the gas phase and acetonitrile solvent (parentheses). The bond length is in Å.

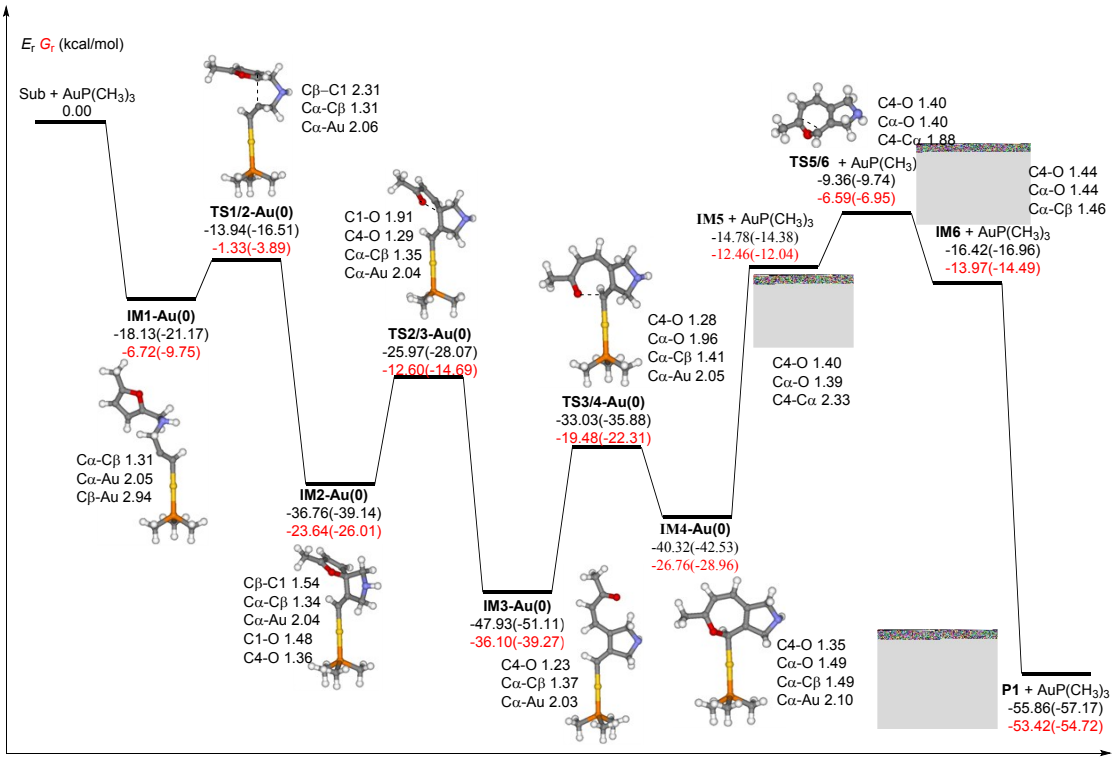



**Figure S13.** The optimized structures, related parameters, potential energy profile, and relative Gibbs free energies (colored by red, 298.15 K and 1 atm) of the 5-*exo* FCT pathway catalyzed by $AuP(CH_3)_3$ in the gas phase and acetonitrile solvent (parentheses). The bond length is in Å.

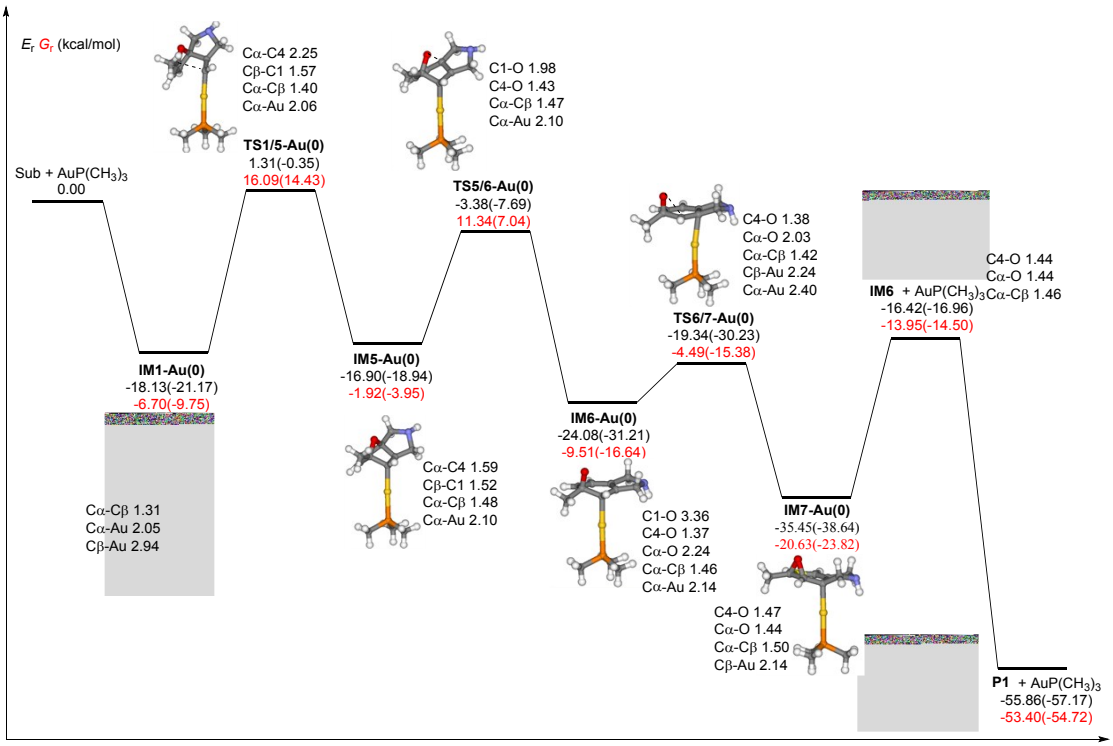



**Figure S14.** The optimized structures, related parameters, potential energy profile, and relative Gibbs free energies (colored by red, 298.15 K and 1 atm) of the DDA pathway catalyzed by $AuP(CH_3)_3$ in the gas phase and acetonitrile solvent (parentheses). The bond length is in Å.

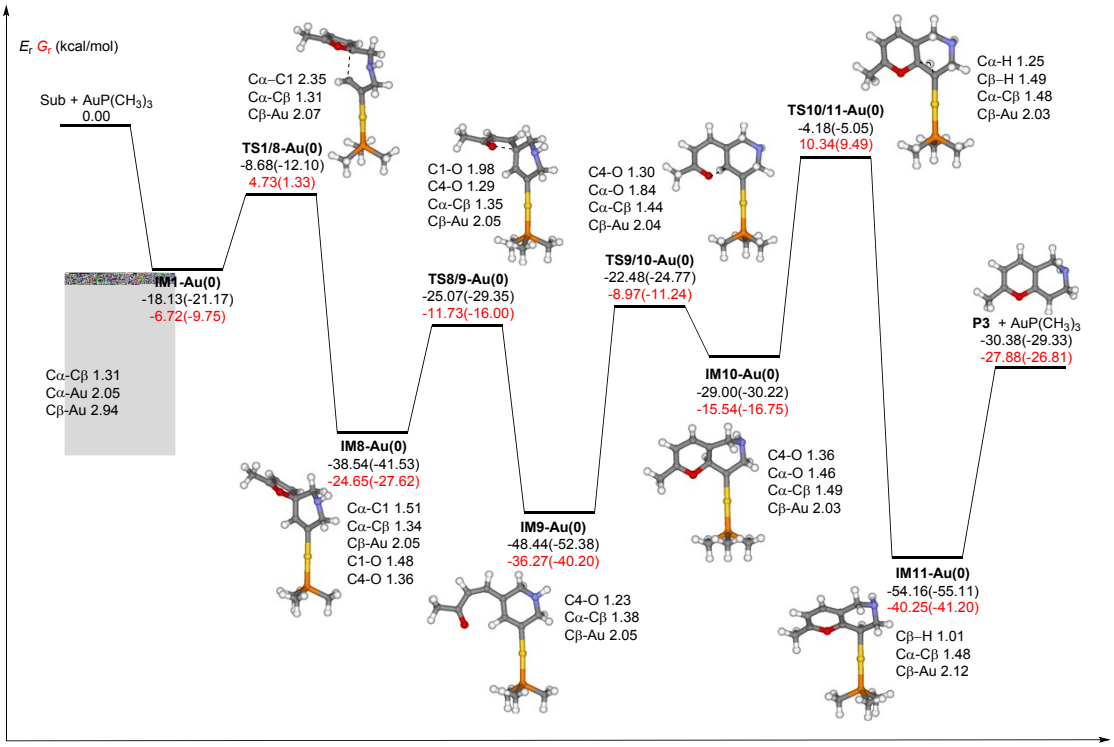
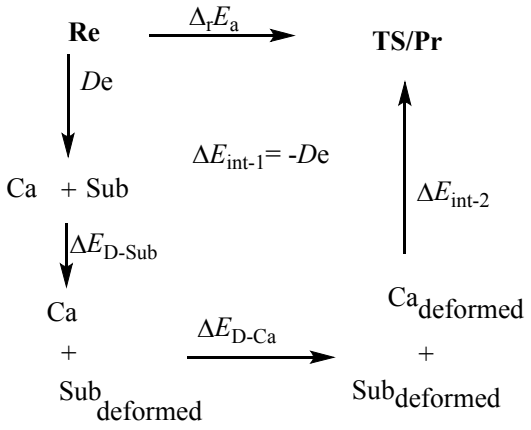



**Figure S15.** The optimized structures, related parameters, potential energy profile, and relative Gibbs free energies (colored by red, 298.15 K and 1 atm) of the 6-*endo* FCT pathway toward the pyran derivative **P3** catalyzed by $AuP(CH_3)_3$ in the gas phase and acetonitrile solvent (parentheses). The bond length is in Å.

## S2. Details for Energy Decomposition Analysis




$$\Delta_r E_a = \Delta E_{int-2} - \Delta E_{int-1} + \Delta E_{D-Sub} + \Delta E_{D-Ca}$$

$$= \Delta E_B + \Delta E_{D-Sub} + \Delta E_{D-Ca}$$

**Scheme S1.** General framework of energy decomposition analysis "**Re → TS/Pr**" [Ca = $Au_{3\sim10}$].

To further explore the possible reasons for energy barrier variation, we carried out an energy decomposition analysis (EDA)[1-3] (Scheme S1) on the energy barriers and reaction energies of the related elementary reactions. In Scheme 1, $D_e$ represented the energy required to dissociate the reactants into two fragments. $\Delta E_D$ referred to the energy needed to deform the two fragments to the geometries they have in the transition states. The interaction energies between the two fragments in the reactants and transition states were represented by $\Delta E_{int-1}$ ($\Delta E_{int-1} = -D_e$) and $\Delta E_{int-2}$, respectively. $\Delta E_B$ represented the change in interaction energy between the Sub and Ca fragments from reactants to transition states. The results of the energy decomposition analysis were

presented in Table S2-S9.

**Table S2** Energy barriers ($\Delta_r E_a$) and their energy components for 5-*exo* cyclization and ring-closing of dienone steps catalyzed by $Au_3$ cluster (units in kcal/mol)

| Reactions | $\Delta E_{int\text{-}1}$ | $\Delta E_{int\text{-}2}$ | $\Delta E_B$ | $\Delta E_{D\text{-}Sub}$ | $\Delta E_{D\text{-}Ca}$ | $\Delta_r E_a/\Delta_r E$ |
|---|---|---|---|---|---|---|
| **IM1→TS1/2** | -45.92 | -49.49 | -3.57 | 23.20 | -0.04 | 19.59 |
| **IM1→IM2** | -45.92 | -82.84 | -36.92 | 44.31 | -0.64 | 6.75 |
| **IM3→TS3/4** | -94.87 | -77.24 | 17.63 | -5.61 | 0.34 | 12.36 |
| **IM3→IM4** | -94.87 | -44.27 | 50.60 | -63.90 | 0.59 | -12.71 |

**Table S3** Energy barriers ($\Delta_r E_a$) and their energy components for 5-*exo* cyclization and ring-closing of dienone steps catalyzed by $Au_4$ cluster (units in kcal/mol)

| Reactions | $\Delta E_{int\text{-}1}$ | $\Delta E_{int\text{-}2}$ | $\Delta E_B$ | $\Delta E_{D\text{-}Sub}$ | $\Delta E_{D\text{-}Ca}$ | $\Delta_r E_a/\Delta_r E$ |
|---|---|---|---|---|---|---|
| **IM1→TS1/2** | -45.04 | -48.60 | -3.56 | 23.42 | 0.34 | 20.20 |
| **IM1→IM2** | -45.04 | -66.74 | -21.70 | 36.97 | 0.36 | 15.63 |
| **IM3→TS3/4** | -83.80 | -70.13 | 13.67 | -7.15 | -0.02 | 6.50 |
| **IM3→IM4** | -83.80 | -42.66 | 41.14 | -62.54 | 0.07 | -21.33 |

**Table S4** Energy barriers ($\Delta_r E_a$) and their energy components for 5-*exo* cyclization and ring-closing of dienone steps catalyzed by $Au_5$ cluster (units in kcal/mol)

| Reactions | $\Delta E_{int\text{-}1}$ | $\Delta E_{int\text{-}2}$ | $\Delta E_B$ | $\Delta E_{D\text{-}Sub}$ | $\Delta E_{D\text{-}Ca}$ | $\Delta_r E_a/\Delta_r E$ |
|---|---|---|---|---|---|---|
| **IM1→TS1/2** | -30.56 | -37.67 | -7.11 | 21.94 | -0.38 | 14.45 |
| **IM1→IM2** | -30.56 | -94.84 | -64.28 | 50.81 | 2.65 | -10.82 |
| **IM3→TS3/4** | -98.80 | -76.59 | 22.21 | -11.57 | 2.86 | 13.50 |
| **IM3→IM4** | -98.80 | -30.28 | 68.52 | -65.70 | 0.28 | 3.10 |

**Table S5** Energy barriers ($\Delta_r E_a$) and their energy components for 5-*exo* cyclization and ring-closing of dienone steps catalyzed by $Au_6$ cluster (units in kcal/mol)

| Reactions | $\Delta E_{int\text{-}1}$ | $\Delta E_{int\text{-}2}$ | $\Delta E_B$ | $\Delta E_{D\text{-}Sub}$ | $\Delta E_{D\text{-}Ca}$ | $\Delta_r E_a/\Delta_r E$ |
|---|---|---|---|---|---|---|
| **IM1→TS1/2** | -21.50 | -37.78 | -16.28 | 30.67 | 0.09 | 14.48 |
| **IM1→IM2** | -21.50 | -49.47 | -27.97 | 40.04 | 0.32 | 12.39 |
| **IM3→IM4** | -54.48 | -15.18 | 39.30 | -61.86 | -0.64 | -23.20 |

**Table S6** Energy barriers ($\Delta_r E_a$) and their energy components for 5-*exo* cyclization and ring-closing of dienone steps catalyzed by $Au_7$ cluster (units in kcal/mol)

| Reactions | $\Delta E_{int\text{-}1}$ | $\Delta E_{int\text{-}2}$ | $\Delta E_B$ | $\Delta E_{D\text{-}Sub}$ | $\Delta E_{D\text{-}Ca}$ | $\Delta_r E_a/\Delta_r E$ |
|---|---|---|---|---|---|---|
| **IM1→TS1/2** | -21.62 | -37.26 | -15.64 | 25.59 | -0.48 | 9.47 |
| **IM1→IM2** | -21.62 | -71.00 | -49.38 | 47.06 | -0.28 | -2.60 |
| **IM3→TS3/4** | -85.65 | -62.30 | 23.35 | -9.75 | 0.05 | 13.65 |
| **IM3→IM4** | -85.65 | -16.88 | 68.77 | -69.17 | -0.18 | -0.58 |

**Table S7** Energy barriers ($\Delta_r E_a$) and their energy components for 5-*exo* cyclization and ring-closing of dienone steps catalyzed by $Au_8$ cluster (units in kcal/mol)

| Reactions | $\Delta E_{int\text{-}1}$ | $\Delta E_{int\text{-}2}$ | $\Delta E_B$ | $\Delta E_{D\text{-}Sub}$ | $\Delta E_{D\text{-}Ca}$ | $\Delta_r E_a/\Delta_r E$ |
|---|---|---|---|---|---|---|
| **IM1→TS1/2** | -24.44 | -40.37 | -15.93 | 30.26 | 0.12 | 14.45 |
| **IM1→IM2** | -24.44 | -53.52 | -29.08 | 40.64 | 0.37 | 11.93 |
| **IM3→TS3/4** | -61.36 | -58.91 | 2.45 | 1.94 | -0.23 | 4.16 |
| **IM3→IM4** | -61.36 | -19.50 | 41.86 | -61.53 | -1.26 | -20.93 |

**Table S8** Energy barriers ($\Delta_r E_a$) and their energy components for 5-*exo* cyclization and ring-closing of dienone steps catalyzed by $Au_9$ cluster (units in kcal/mol)

| Reactions | $\Delta E_{int\text{-}1}$ | $\Delta E_{int\text{-}2}$ | $\Delta E_B$ | $\Delta E_{D\text{-}Sub}$ | $\Delta E_{D\text{-}Ca}$ | $\Delta_r E_a/\Delta_r E$ |
|---|---|---|---|---|---|---|
| **IM1→TS1/2** | -24.95 | -39.18 | -14.23 | 26.67 | -0.18 | 12.26 |
| **IM1→IM2** | -24.95 | -65.83 | -40.88 | 45.30 | 0.28 | 4.70 |
| **IM3→TS3/4** | -79.47 | -61.00 | 18.47 | -6.03 | -0.15 | 12.29 |
| **IM3→IM4** | -79.47 | -19.67 | 59.80 | -70.00 | -0.82 | -11.02 |

**Table S9** Energy barriers ($\Delta_r E_a$) and their energy components for 5-*exo* cyclization and ring-closing of dienone steps catalyzed by $Au_{10}$ cluster (units in kcal/mol)

| Reactions | $\Delta E_{int\text{-}1}$ | $\Delta E_{int\text{-}2}$ | $\Delta E_B$ | $\Delta E_{D\text{-}Sub}$ | $\Delta E_{D\text{-}Ca}$ | $\Delta_r E_a/\Delta_r E$ |
|---|---|---|---|---|---|---|
| **IM1→TS1/2** | -24.07 | -37.17 | -13.10 | 27.35 | -0.04 | 14.21 |
| **IM1→IM2** | -24.07 | -53.60 | -29.53 | 39.72 | 0.34 | 10.53 |
| **IM3→TS3/4** | -59.73 | -54.23 | 5.50 | -1.01 | 0.08 | 4.57 |
| **IM3→IM4** | -59.73 | -17.80 | 41.93 | -60.70 | -0.40 | -19.17 |

## S3. Cartesian coordinates, single point electronic energies (in the gas phase and acetonitrile), zero-point, and free energy correction for all of the stationary points and imaginary frequencies of transition structures

**S3.1 $Au_3$**

Sub

| | | | |
|---|---|---|---|
| C | 4.10272800 | 0.95290000 | -0.10857600 |
| C | 3.20846500 | 0.25593600 | -0.51564600 |
| C | 2.11418200 | -0.62265500 | -0.95579000 |
| N | 1.46095200 | -1.38145700 | 0.11398100 |
| C | 0.79520200 | -0.53938000 | 1.12156200 |
| C | -0.42816300 | 0.12009600 | 0.59077300 |
| C | -0.74637700 | 1.41538700 | 0.32454200 |
| C | -2.09168900 | 1.41815300 | -0.16106700 |
| C | -2.50857200 | 0.12293400 | -0.15925500 |
| O | -1.50210600 | -0.68119500 | 0.29909500 |
| C | -3.77689400 | -0.54959500 | -0.53757400 |
| H | 4.89557200 | 1.57124300 | 0.23898400 |
| H | 1.34991300 | -0.02151400 | -1.45717400 |
| H | 2.49664100 | -1.33379900 | -1.69296700 |
| H | 2.15256500 | -1.96104700 | 0.58036700 |
| H | 0.52614100 | -1.19726300 | 1.95296600 |
| H | 1.45139100 | 0.24980600 | 1.51647400 |
| H | -0.09599400 | 2.26594400 | 0.45874400 |
| H | -4.49670200 | 0.19263300 | -0.88377100 |
| H | -3.61667500 | -1.27711700 | -1.33890200 |
| H | -4.21238100 | -1.08383100 | 0.31223400 |
| H | -2.67357100 | 2.27204200 | -0.47139700 |

SCF energy: -479.662612 hartree

SCF energy in acetonitrile: -479.678099 hartree

zero-point correction: + 0.179981 hartree

free energy correction: +0.141542 hartree

$Au_3$

| | | | |
|---|---|---|---|
| Au | 2.38564000 | -0.31247700 | 0.00000000 |
| Au | 0.00000000 | 0.62495000 | 0.00000000 |
| Au | -2.38564000 | -0.31247300 | 0.00000000 |

SCF energy: -407.109726 hartree

SCF energy in acetonitrile: -407.116804 hartree
zero-point correction: +0.000718 hartree
free energy correction: -0.036169 hartree

**IM1**

| | | | |
|---|---|---|---|
| Au | 1.57661600 | 1.59614900 | -0.39472000 |
| Au | 0.33153900 | -0.72774900 | -0.23282800 |
| Au | 2.81907200 | -0.54534600 | 0.63432200 |
| C | -1.06071400 | -2.31656700 | -0.32086000 |
| C | -1.64962900 | -1.32071000 | -0.80446600 |
| C | -2.74495000 | -0.52112400 | -1.42393000 |
| N | -3.97630500 | -1.26509900 | -1.63395700 |
| C | -4.65110100 | -1.72452600 | -0.40951200 |
| C | -5.20016900 | -0.59821800 | 0.39116800 |
| C | -4.87256200 | -0.06949000 | 1.60069800 |
| C | -5.78280100 | 1.00704000 | 1.83869200 |
| C | -6.60830300 | 1.06561200 | 0.75855100 |
| O | -6.26377300 | 0.08856500 | -0.13445200 |
| C | -7.75009400 | 1.93640300 | 0.38237300 |
| H | -0.92761700 | -3.33168000 | -0.00425900 |
| H | -2.95677700 | 0.33856500 | -0.78369900 |
| H | -2.39455200 | -0.12997000 | -2.38145900 |
| H | -3.81309100 | -2.05203500 | -2.25378400 |
| H | -5.46394100 | -2.38192800 | -0.73059100 |
| H | -3.99229000 | -2.30756500 | 0.25005400 |
| H | -4.07607300 | -0.40751300 | 2.24561100 |
| H | -7.92534600 | 2.67172900 | 1.16793600 |
| H | -7.55136100 | 2.46851300 | -0.55257800 |
| H | -8.66519000 | 1.35302400 | 0.24362000 |
| H | -5.81844600 | 1.65421200 | 2.70097500 |

SCF energy: -886.825842 hartree
SCF energy in acetonitrile: -886.842365 hartree
zero-point correction: + 0.181867 hartree
free energy correction: + 0.126199 hartree

**TS1/2**

| | | | |
|---|---|---|---|
| Au | 2.11898700 | 1.28395400 | 0.52738500 |
| Au | -0.08265100 | -0.14953000 | -0.06972900 |
| Au | 2.31531200 | -1.23509500 | -0.39525300 |
| C | -2.09911400 | -0.46981100 | -0.20005400 |
| C | -2.81142100 | 0.49141700 | -0.66207100 |
| C | -2.83880700 | 1.82865900 | -1.30238800 |
| N | -3.97642200 | 2.54771200 | -0.73358000 |

| | | | |
|---|---|---|---|
| C | -5.16181800 | 1.71736000 | -0.92189100 |
| C | -4.84706400 | 0.32878700 | -0.44273300 |
| C | -5.07638600 | -0.89020000 | -1.09063000 |
| C | -5.12849800 | -1.88199600 | -0.10598900 |
| C | -5.03158000 | -1.23447400 | 1.11088400 |
| O | -4.94166000 | 0.09525000 | 0.92829500 |
| C | -5.02977200 | -1.72273000 | 2.50977500 |
| H | -2.47258700 | -1.41957100 | 0.17271800 |
| H | -1.91046300 | 2.35061300 | -1.06619900 |
| H | -2.89907700 | 1.71081600 | -2.39901200 |
| H | -4.09261800 | 3.45736100 | -1.16927800 |
| H | -6.00142900 | 2.13186900 | -0.35952800 |
| H | -5.46649700 | 1.62242200 | -1.97713700 |
| H | -5.11638500 | -1.02344600 | -2.16065300 |
| H | -5.13914200 | -2.80629300 | 2.53004400 |
| H | -4.09657100 | -1.45003000 | 3.01016300 |
| H | -5.85054600 | -1.27134200 | 3.07423900 |
| H | -5.21991800 | -2.94747400 | -0.24597700 |

SCF energy: -886.794630 hartree

SCF energy in acetonitrile: -886.816238 hartree

zero-point correction: + 0.181027 hartree

free energy correction: + 0.126881 hartree

imaginary frequency: -388.74 *i* $cm^{-1}$

**IM2**

| | | | |
|---|---|---|---|
| Au | -2.18474100 | 1.38299400 | 0.05139300 |
| Au | 0.07141000 | -0.14459700 | -0.15590200 |
| Au | -2.41639200 | -1.19988800 | -0.12077500 |
| C | 2.06357800 | -0.38355000 | -0.30324300 |
| C | 2.95515600 | -0.23724200 | 0.68050600 |
| C | 2.70342000 | 0.05778300 | 2.14284900 |
| N | 4.03435500 | 0.41481500 | 2.65036000 |
| C | 4.97030700 | -0.45990500 | 1.95603200 |
| C | 4.47728200 | -0.40091500 | 0.49984400 |
| C | 4.91123200 | -1.49563900 | -0.40038500 |
| C | 5.57866400 | -0.95731000 | -1.47529300 |
| C | 5.64947000 | 0.42381700 | -1.28420700 |
| O | 5.04718400 | 0.80203100 | -0.15145900 |
| C | 6.27472100 | 1.49008700 | -2.09887000 |
| H | 2.45129500 | -0.63484800 | -1.29069400 |
| H | 2.00133200 | 0.88271200 | 2.27578900 |
| H | 2.27764700 | -0.83275500 | 2.63580400 |
| H | 4.10268100 | 0.32293800 | 3.65798900 |

| | | | |
|---|---|---|---|
| H | 5.99981000 | -0.10999200 | 2.04784600 |
| H | 4.92428900 | -1.51501800 | 2.27771600 |
| H | 4.67700800 | -2.53370000 | -0.22021000 |
| H | 6.74899000 | 1.06722600 | -2.98401000 |
| H | 5.52328700 | 2.22244400 | -2.41162300 |
| H | 7.02656800 | 2.03028000 | -1.51417900 |
| H | 5.99433200 | -1.48414300 | -2.32126900 |

SCF energy: -886.815096 hartree

SCF energy in acetonitrile: -886.840902 hartree

zero-point correction: + 0.182058 hartree

free energy correction: + 0.128260 hartree

**TS2/3**

| | | | |
|---|---|---|---|
| Au | -2.12890200 | 1.38448800 | 0.37293600 |
| Au | 0.04334000 | -0.09885300 | -0.22336500 |
| Au | -2.44509500 | -1.12418600 | -0.35227700 |
| C | 2.00589200 | -0.29663500 | -0.44986000 |
| C | 2.92759300 | -0.59250600 | 0.51022100 |
| C | 2.65673900 | -0.87021700 | 1.97518300 |
| N | 4.00348600 | -0.94548800 | 2.56207400 |
| C | 4.90267300 | -1.42918400 | 1.52308700 |
| C | 4.33647200 | -0.78853700 | 0.27368800 |
| C | 4.89275600 | -1.12179800 | -1.04109200 |
| C | 5.54772600 | -0.13407300 | -1.69071000 |
| C | 5.69435200 | 1.02124000 | -0.84167500 |
| O | 5.13179900 | 0.95040700 | 0.28245400 |
| C | 6.48055500 | 2.23813100 | -1.20837400 |
| H | 2.41239700 | -0.15496000 | -1.45373600 |
| H | 2.07783800 | -0.06985100 | 2.44106600 |
| H | 2.08209000 | -1.80424600 | 2.07555800 |
| H | 4.03629600 | -1.52171100 | 3.39477300 |
| H | 5.93952100 | -1.14348000 | 1.71437400 |
| H | 4.87892200 | -2.52473500 | 1.35705700 |
| H | 4.77666400 | -2.12899100 | -1.42390700 |
| H | 7.28352700 | 1.99989600 | -1.90748100 |
| H | 5.80947500 | 2.95332100 | -1.69750300 |
| H | 6.88087500 | 2.71237600 | -0.31282300 |
| H | 5.99702100 | -0.21544100 | -2.67055400 |

SCF energy: -886.799524 hartree

SCF energy in acetonitrile: -886.825382 hartree

zero-point correction: + 0.179994 hartree

free energy correction: + 0.126002 hartree

imaginary frequency: -609.88 *i* $cm^{-1}$

**IM3**

| | | | |
|---|---|---|---|
| Au | 2.42873800 | 1.34038800 | -0.16483300 |
| Au | 0.12934200 | -0.00819200 | 0.27329100 |
| Au | 2.52840300 | -1.23171200 | 0.15916300 |
| C | -1.83531200 | -0.06411000 | 0.54113800 |
| C | -2.79369200 | -0.22507900 | -0.43677900 |
| C | -2.50929700 | -0.42303000 | -1.91829300 |
| N | -3.75350000 | -0.95117500 | -2.49243300 |
| C | -4.82622100 | -0.39338400 | -1.64999200 |
| C | -4.20637700 | -0.20668500 | -0.27916000 |
| C | -4.84218200 | -0.08347000 | 0.97964900 |
| C | -6.15350400 | 0.07711100 | 1.34545900 |
| C | -7.33847300 | 0.34770000 | 0.51838400 |
| O | -7.28761200 | 0.64314500 | -0.66826000 |
| C | -8.66815300 | 0.27729300 | 1.24661000 |
| H | -2.18425700 | 0.04952700 | 1.56761500 |
| H | -2.27202300 | 0.54369000 | -2.38017000 |
| H | -1.66678900 | -1.09075800 | -2.10037100 |
| H | -3.75129400 | -1.96018000 | -2.36823600 |
| H | -5.15102400 | 0.57418500 | -2.04629300 |
| H | -5.70494000 | -1.03616600 | -1.64789100 |
| H | -4.15746000 | -0.16184100 | 1.82154700 |
| H | -8.69347700 | 1.01120000 | 2.05853400 |
| H | -9.47892100 | 0.47819500 | 0.54883100 |
| H | -8.80594100 | -0.70839600 | 1.70190000 |
| H | -6.35139600 | 0.03729700 | 2.41347100 |

SCF energy: -886.829828 hartree

SCF energy in acetonitrile: -886.861221 hartree

zero-point correction: + 0.181174 hartree

free energy correction: + 0.125758 hartree

**TS3/4**

| | | | |
|---|---|---|---|
| Au | -2.08409200 | -1.30374900 | 0.14065400 |
| Au | 0.32227000 | -0.29655900 | -0.47299300 |
| Au | -1.72466900 | 1.29601800 | 0.21107800 |
| C | 2.17790100 | -0.53813000 | -1.07763800 |
| C | 3.27353700 | -0.96060500 | -0.27691200 |
| C | 4.09589800 | -2.21516500 | -0.58420200 |
| N | 5.21937200 | -2.18498800 | 0.36362000 |
| C | 4.80156300 | -1.31971300 | 1.47683700 |
| C | 3.70505400 | -0.43366500 | 0.90515200 |
| C | 3.20184400 | 0.71593600 | 1.58845400 |

| | | | |
|---|---|---|---|
| C | 2.70449900 | 1.88116200 | 1.09055900 |
| C | 2.76204700 | 2.37562100 | -0.28788800 |
| O | 3.00537000 | 1.69130400 | -1.28173000 |
| C | 2.52850800 | 3.86412000 | -0.44570600 |
| H | 2.33435300 | -0.59987000 | -2.15509000 |
| H | 3.47766400 | -3.10423600 | -0.41400400 |
| H | 4.44800400 | -2.25315000 | -1.61797300 |
| H | 6.00909900 | -1.74330500 | -0.09555500 |
| H | 4.39953000 | -1.92512500 | 2.30272800 |
| H | 5.65578500 | -0.76360800 | 1.86929600 |
| H | 3.27274200 | 0.66380800 | 2.67523700 |
| H | 2.68784100 | 4.15637600 | -1.48177400 |
| H | 1.49461300 | 4.09106600 | -0.15941700 |
| H | 3.18114200 | 4.44272300 | 0.21345400 |
| H | 2.38835700 | 2.62136700 | 1.81925300 |

SCF energy: -886.810126 hartree

SCF energy in acetonitrile: -886.833908 hartree

zero-point correction: + 0.180933 hartree

free energy correction: + 0.127900 hartree

imaginary frequency: -70.29 *i* $cm^{-1}$

**IM4**

| | | | |
|---|---|---|---|
| Au | 1.47790400 | -1.47036900 | -0.54022400 |
| Au | -0.48330300 | 0.07169700 | 0.36237000 |
| Au | 1.99155600 | 1.01242200 | 0.33985700 |
| C | -2.32133600 | 1.00142400 | 1.04179000 |
| C | -2.65487100 | -0.30570200 | 0.63797700 |
| C | -2.90622200 | -1.46615200 | 1.61600800 |
| N | -4.18543000 | -2.03894100 | 1.17026000 |
| C | -4.14593000 | -1.91726600 | -0.30027400 |
| C | -3.42043100 | -0.61284900 | -0.57681500 |
| C | -3.47499900 | 0.12667000 | -1.70090900 |
| C | -2.73591100 | 1.35351100 | -1.92959300 |
| C | -2.33848900 | 2.23575700 | -0.99934500 |
| O | -2.72570600 | 2.12794700 | 0.34470500 |
| C | -1.55194900 | 3.47628600 | -1.24446100 |
| H | -2.17415000 | 1.23843600 | 2.09133900 |
| H | -2.13393900 | -2.23319500 | 1.52908900 |
| H | -2.95580300 | -1.14362000 | 2.65662800 |
| H | -4.93868100 | -1.44783900 | 1.51528700 |
| H | -3.58291700 | -2.76765000 | -0.70273300 |
| H | -5.15076500 | -1.94878100 | -0.72219200 |
| H | -4.05279800 | -0.25226400 | -2.53995200 |

| | | | |
|---|---|---|---|
| H | -2.10621600 | 4.34940600 | -0.88641400 |
| H | -0.60637900 | 3.43842100 | -0.69374900 |
| H | -1.33682600 | 3.59832700 | -2.30593500 |
| H | -2.46354400 | 1.58139600 | -2.95531400 |

SCF energy: -886.8500719 hartree

SCF energy in acetonitrile: -886.866651 hartree

zero-point correction: + 0.184926hartree

free energy correction: + 0.134314 hartree

**IM5**

| | | | |
|---|---|---|---|
| C | 0.33505400 | -1.40549500 | 0.12980300 |
| C | -0.75293100 | -0.67396800 | -0.12405500 |
| C | -2.11517500 | -1.16795600 | -0.57204400 |
| N | -3.05956900 | -0.25081300 | 0.09918600 |
| C | -2.37557100 | 1.05949900 | 0.12677800 |
| C | -0.88350500 | 0.75782600 | 0.09175100 |
| C | 0.13260500 | 1.64534200 | 0.05520000 |
| C | 1.51548300 | 1.29505200 | -0.20032400 |
| C | 2.10403600 | 0.11313600 | 0.04513700 |
| O | 1.45346100 | -0.88801500 | 0.77981200 |
| C | 3.50835900 | -0.25347300 | -0.29976800 |
| H | 0.41151900 | -2.46999400 | -0.07116600 |
| H | -2.23729300 | -1.06355200 | -1.65639400 |
| H | -2.32447500 | -2.20405500 | -0.30458100 |
| H | -3.16187700 | -0.56832700 | 1.05949200 |
| H | -2.66949900 | 1.63614500 | -0.75817800 |
| H | -2.68095700 | 1.62986800 | 1.00645000 |
| H | -0.09790800 | 2.70691500 | 0.10195700 |
| H | 4.05479600 | -0.53391500 | 0.60661400 |
| H | 3.52903500 | -1.11958400 | -0.96868100 |
| H | 4.02422400 | 0.57573300 | -0.78492300 |
| H | 2.13160700 | 2.05080300 | -0.67826100 |

SCF energy: -479.688980 hartree

SCF energy in acetonitrile: -479.703825 hartree

zero-point correction: + 0.182791 hartree

free energy correction: + 0.148059 hartree

**TS5/6**

| | | | |
|---|---|---|---|
| C | 0.58384000 | -1.19936400 | 0.10920500 |
| C | -0.67276300 | -0.63613000 | -0.02628200 |
| C | -1.95855100 | -1.27937000 | -0.51489200 |
| N | -3.01956000 | -0.36514900 | -0.04457500 |
| C | -2.40216400 | 0.97316400 | 0.06259400 |

| | | | |
|---|---|---|---|
| C | -0.90821100 | 0.72444600 | 0.17198300 |
| C | 0.09819900 | 1.68229400 | 0.05076500 |
| C | 1.42318900 | 1.34348800 | -0.20990200 |
| C | 1.96223100 | 0.07598200 | 0.01474400 |
| O | 1.44950800 | -0.67566800 | 1.08015800 |
| C | 3.31758400 | -0.35546000 | -0.46147600 |
| H | 0.85163600 | -2.18913400 | -0.24909200 |
| H | -1.97884400 | -1.33466500 | -1.61108800 |
| H | -2.12966300 | -2.28655300 | -0.13016200 |
| H | -3.28473800 | -0.66069100 | 0.88970900 |
| H | -2.62807200 | 1.55979200 | -0.83686800 |
| H | -2.81730200 | 1.51474800 | 0.91613700 |
| H | -0.19277700 | 2.72370800 | -0.05298000 |
| H | 4.05326700 | -0.22174600 | 0.33920000 |
| H | 3.31935100 | -1.41276400 | -0.73317600 |
| H | 3.63182000 | 0.22466400 | -1.33027100 |
| H | 2.05605100 | 2.06972000 | -0.71107600 |

SCF energy: -479.679359 hartree

SCF energy in acetonitrile: -479.695449 hartree

zero-point correction: + 0.181815 hartree

free energy correction: + 0.147792 hartree

imaginary frequency: -423.18 *i* $cm^{-1}$

**IM6**

| | | | |
|---|---|---|---|
| C | 0.73373900 | -1.05430200 | -0.03755400 |
| C | -0.64345500 | -0.57145600 | -0.07132400 |
| C | -1.90002100 | -1.36441100 | -0.31572800 |
| N | -2.99965500 | -0.40192200 | -0.07910000 |
| C | -2.41744000 | 0.95790600 | -0.04256600 |
| C | -0.92700500 | 0.74204000 | 0.05552800 |
| C | 0.10747100 | 1.74420600 | 0.05931400 |
| C | 1.40753900 | 1.39140600 | -0.03292500 |
| C | 1.83506000 | -0.01871800 | -0.01721100 |
| O | 1.47683800 | -0.77011300 | 1.16222100 |
| C | 3.20355100 | -0.34585400 | -0.55839300 |
| H | 0.95766900 | -2.03383000 | -0.45602800 |
| H | -1.93078300 | -1.74319400 | -1.34802600 |
| H | -2.00105100 | -2.23391700 | 0.34208300 |
| H | -3.40848900 | -0.60141900 | 0.82547500 |
| H | -2.66613700 | 1.51059800 | -0.95922700 |
| H | -2.82771200 | 1.53064500 | 0.79506000 |
| H | -0.17015300 | 2.79363600 | 0.05659700 |
| H | 3.97636900 | 0.12743800 | 0.05408100 |

| | | | |
|---|---|---|---|
| H | 3.37025100 | -1.42392400 | -0.54591300 |
| H | 3.31049300 | 0.01565900 | -1.58456000 |
| H | 2.17579400 | 2.14777200 | -0.15845100 |

SCF energy: -479.691943 hartree
SCF energy in acetonitrile: -479.708293 hartree
zero-point correction: + 0.183141 hartree
free energy correction: + 0.148617 hartree

**P1**

| | | | |
|---|---|---|---|
| C | -0.83005200 | -0.72257400 | 0.02357600 |
| C | 0.52945900 | -0.44108900 | 0.04360800 |
| C | 1.71368700 | -1.37638100 | 0.10398800 |
| N | 2.88469200 | -0.52071800 | -0.19533100 |
| C | 2.48523600 | 0.86976500 | 0.11375800 |
| C | 0.97275700 | 0.87704700 | 0.04228400 |
| C | 0.07047900 | 1.93271100 | 0.01625500 |
| C | -1.29100000 | 1.63682200 | -0.02171200 |
| C | -1.76542700 | 0.32336100 | -0.01927100 |
| O | -1.20923700 | -2.04118000 | 0.03947300 |
| C | -3.24075800 | 0.01954700 | -0.06309400 |
| H | -2.17393000 | -2.09217700 | 0.01663000 |
| H | 1.81315500 | -1.80910800 | 1.10753400 |
| H | 1.65241800 | -2.20875900 | -0.59989900 |
| H | 3.05619200 | -0.57605400 | -1.19420300 |
| H | 2.81843000 | 1.13369500 | 1.12586600 |
| H | 2.96279800 | 1.56849500 | -0.57695100 |
| H | 0.40530500 | 2.96412300 | 0.01762200 |
| H | -3.82216500 | 0.94163700 | -0.09383000 |
| H | -3.51325400 | -0.56616200 | -0.94993600 |
| H | -3.57017000 | -0.54241800 | 0.81984200 |
| H | -2.01401900 | 2.44593900 | -0.05749500 |

SCF energy: -479.755529 hartree
SCF energy in acetonitrile: -479.773109 hartree
zero-point correction: + 0.183886 hartree
free energy correction: + 0.149334 hartree

**TS1/7**

| | | | |
|---|---|---|---|
| Au | 1.70835500 | -1.39558900 | 0.33009300 |
| Au | -0.34350400 | 0.09883900 | -0.43995000 |
| Au | 2.01340200 | 1.23923600 | -0.05635300 |
| C | -2.24685300 | 0.84834200 | -1.02859200 |
| C | -2.39174600 | -0.43865100 | -0.84133700 |
| C | -2.80602800 | -1.77305600 | -1.37222800 |

| | | | |
|---|---|---|---|
| N | -4.15418600 | -2.04122100 | -0.85957500 |
| C | -4.18020600 | -1.84485400 | 0.59475600 |
| C | -3.58183000 | -0.50414800 | 0.85353400 |
| C | -2.67126700 | -0.05751400 | 1.84460500 |
| C | -2.56852700 | 1.30071500 | 1.68002500 |
| C | -3.43250400 | 1.64427800 | 0.60607900 |
| O | -4.29606000 | 0.59116800 | 0.41770800 |
| C | -3.93458500 | 2.98855400 | 0.20258500 |
| H | -2.29072500 | 1.59060300 | -1.80905300 |
| H | -2.83670100 | -1.76066400 | -2.46524500 |
| H | -2.06466100 | -2.52290700 | -1.05721900 |
| H | -4.45395200 | -2.97889500 | -1.10873600 |
| H | -5.21605800 | -1.89699100 | 0.93970500 |
| H | -3.58812700 | -2.58601000 | 1.15482600 |
| H | -2.05665300 | -0.69668000 | 2.46021400 |
| H | -3.11637800 | 3.70948400 | 0.22668000 |
| H | -4.35237400 | 2.96129100 | -0.80502400 |
| H | -4.71640000 | 3.33225700 | 0.88703400 |
| H | -1.86095400 | 1.96932700 | 2.14618400 |

SCF energy: -886.785116 hartree

SCF energy in acetonitrile: -886.800175 hartree

zero-point correction: + 0.181498 hartree

free energy correction: + 0.131478 hartree

imaginary frequency: -472.63 *i* $cm^{-1}$

**IM7**

| | | | |
|---|---|---|---|
| Au | -1.68094200 | 1.41123600 | 0.28158000 |
| Au | 0.39609400 | -0.11256600 | -0.31910000 |
| Au | -1.99424300 | -1.22135400 | -0.09917800 |
| C | 2.31590700 | -0.94341900 | -0.82110500 |
| C | 2.47293100 | 0.43480200 | -0.61153900 |
| C | 2.77832200 | 1.64270600 | -1.46187600 |
| N | 4.08984000 | 2.06729000 | -0.93542800 |
| C | 4.09043200 | 1.84460700 | 0.52043600 |
| C | 3.38940100 | 0.51528700 | 0.66133500 |
| C | 2.61950600 | 0.03748800 | 1.87875500 |
| C | 2.44267600 | -1.26810400 | 1.67848100 |
| C | 3.13900900 | -1.59402800 | 0.35351300 |
| O | 4.22753500 | -0.63201200 | 0.39342900 |
| C | 3.63080500 | -2.99912800 | 0.12137100 |
| H | 2.23574100 | -1.44454700 | -1.77837100 |
| H | 2.84893500 | 1.40368300 | -2.52543300 |
| H | 1.99476800 | 2.40354900 | -1.33086100 |

| | | | |
|---|---|---|---|
| H | 4.29058600 | 3.03312400 | -1.17153400 |
| H | 5.11183400 | 1.81676000 | 0.90288800 |
| H | 3.52078300 | 2.60150200 | 1.08368400 |
| H | 2.20679900 | 0.66797800 | 2.65353000 |
| H | 2.78534000 | -3.68975300 | 0.08154400 |
| H | 4.17847400 | -3.06210500 | -0.82102100 |
| H | 4.29407200 | -3.30467200 | 0.93229300 |
| H | 1.85782400 | -1.96974900 | 2.25670800 |

SCF energy: -886.824589 hartree
SCF energy in acetonitrile: -886.841776 hartree
zero-point correction: + 0.184655 hartree
free energy correction: + 0.135736 hartree

**TS7/8**

| | | | |
|---|---|---|---|
| Au | 1.69830600 | -1.37718600 | 0.24843000 |
| Au | -0.43540000 | 0.13520000 | -0.31687200 |
| Au | 1.92179900 | 1.25569600 | -0.05855400 |
| C | -2.38021400 | 0.89552600 | -0.80039300 |
| C | -2.56615700 | -0.50016800 | -0.60391300 |
| C | -2.88613700 | -1.64298200 | -1.55346900 |
| N | -3.14172900 | -2.80772500 | -0.68773100 |
| C | -3.68005000 | -2.25294300 | 0.57222200 |
| C | -3.12143700 | -0.86236700 | 0.68213700 |
| C | -2.78388000 | -0.09673900 | 1.86418100 |
| C | -2.69329100 | 1.22819400 | 1.66149800 |
| C | -3.20837900 | 1.61895000 | 0.28284500 |
| O | -4.46576400 | 0.98930500 | 0.14761300 |
| C | -3.34981000 | 3.12414600 | 0.07824300 |
| H | -2.37048800 | 1.31857400 | -1.79990700 |
| H | -3.80745600 | -1.38633300 | -2.09176900 |
| H | -2.11121800 | -1.86140500 | -2.28639900 |
| H | -2.24629900 | -3.24139700 | -0.47770800 |
| H | -4.77414200 | -2.19167100 | 0.51079400 |
| H | -3.43702100 | -2.89211300 | 1.42437300 |
| H | -2.57609700 | -0.59269100 | 2.80551800 |
| H | -2.37465600 | 3.61371600 | 0.14103500 |
| H | -3.78482600 | 3.32933100 | -0.90157800 |
| H | -4.00882000 | 3.53973000 | 0.84230200 |
| H | -2.36631200 | 1.95110800 | 2.39911200 |

SCF energy: -886.769678 hartree
SCF energy in acetonitrile: -886.798026 hartree
zero-point correction: + 0.181447 hartree
free energy correction: + 0.131797 hartree

imaginary frequency: -292.74 *i* $cm^{-1}$

**IM8**

| | | | |
|---|---|---|---|
| Au | 2.26448800 | -1.12443500 | -0.59575800 |
| Au | -0.10263100 | -0.19273000 | 0.07030400 |
| Au | 1.93590300 | 1.38002100 | 0.54919200 |
| C | -2.90129100 | -0.56255300 | 0.21908500 |
| C | -3.57501400 | 0.58972900 | -0.36219500 |
| C | -2.98251500 | 1.81805000 | -1.00373200 |
| N | -4.14553300 | 2.55496300 | -1.54219400 |
| C | -5.35002900 | 2.02378000 | -0.86616400 |
| C | -4.92090600 | 0.68913600 | -0.30071600 |
| C | -5.74864200 | -0.38707800 | 0.17539900 |
| C | -5.19955600 | -1.55107000 | 0.58649100 |
| C | -3.74331700 | -1.72463800 | 0.70866900 |
| O | -3.07131400 | -0.81105200 | 1.60827800 |
| C | -3.18776500 | -3.12353500 | 0.72977700 |
| H | -1.89427500 | -0.87028400 | -0.19464900 |
| H | -2.45750100 | 2.42584100 | -0.25426300 |
| H | -2.25740900 | 1.59502400 | -1.79309200 |
| H | -4.22090600 | 2.34560200 | -2.53136300 |
| H | -5.66086000 | 2.69864500 | -0.05773700 |
| H | -6.18723000 | 1.95280100 | -1.56584900 |
| H | -6.82801200 | -0.29129100 | 0.11624800 |
| H | -3.51376200 | -3.68076600 | -0.15182000 |
| H | -2.09705700 | -3.10310900 | 0.75142000 |
| H | -3.53847500 | -3.65174100 | 1.62042700 |
| H | -5.82403100 | -2.41361900 | 0.79487300 |

SCF energy: -886.806491 hartree

SCF energy in acetonitrile: -886.828356 hartree

zero-point correction: + 0.183117 hartree

free energy correction: + 0.126253 hartree

**TS1/9**

| | | | |
|---|---|---|---|
| Au | 1.69815900 | 1.52897400 | -0.49000400 |
| Au | 0.26310900 | -0.68882900 | -0.35592100 |
| Au | 2.59506700 | -0.61743000 | 0.87202700 |
| C | -1.30881800 | -2.18865200 | -0.45551100 |
| C | -1.70585700 | -1.16278400 | -1.18385600 |
| C | -2.80521900 | -0.27748200 | -1.73985200 |
| N | -4.07564200 | -0.93255800 | -1.94162500 |
| C | -4.66287600 | -1.57626800 | -0.75687100 |
| C | -5.00284200 | -0.59669000 | 0.30817300 |

| | | | |
|---|---|---|---|
| C | -4.52032100 | -0.38423500 | 1.56198400 |
| C | -5.26648600 | 0.70548000 | 2.10919800 |
| C | -6.15644300 | 1.08826800 | 1.15366000 |
| O | -6.00704900 | 0.29919900 | 0.04591600 |
| C | -7.20188100 | 2.13968700 | 1.08434100 |
| H | -1.28638700 | -2.08779300 | -1.85224500 |
| H | -2.92090300 | 0.52348100 | -1.00501900 |
| H | -2.46879900 | 0.17652200 | -2.67136600 |
| H | -4.03951200 | -1.58446600 | -2.71795800 |
| H | -5.56492800 | -2.09064900 | -1.09960800 |
| H | -3.99485300 | -2.32928400 | -0.31158500 |
| H | -3.72956000 | -0.94185700 | 2.03995100 |
| H | -7.22522400 | 2.69618200 | 2.02146500 |
| H | -7.00429600 | 2.84187700 | 0.26908400 |
| H | -8.19118000 | 1.70455700 | 0.91492000 |
| H | -5.15454500 | 1.14737600 | 3.08678200 |

SCF energy: -886.750094 hartree
SCF energy in acetonitrile: -886.772728 hartree
zero-point correction: + 0.177754 hartree
free energy correction: + 0.122236 hartree
imaginary frequency: -407.35 *i* $cm^{-1}$

**IM9**

| | | | |
|---|---|---|---|
| Au | -1.23326200 | -1.62408300 | -0.22321800 |
| Au | -0.34092000 | 0.87402000 | -0.22755600 |
| Au | -2.87595900 | 0.36659600 | 0.36891600 |
| C | 1.07962000 | 2.10623300 | -0.47369200 |
| C | 2.08277900 | 2.90530200 | -0.65332700 |
| C | 3.52030400 | 2.42415500 | -0.97644600 |
| N | 4.39687800 | 2.39960200 | 0.17191400 |
| C | 4.09582200 | 1.35245000 | 1.15833300 |
| C | 4.48532800 | -0.00288400 | 0.68574400 |
| C | 3.77331400 | -1.10710200 | 0.33476900 |
| C | 4.72565300 | -2.11180100 | -0.02417400 |
| C | 5.95766600 | -1.55562300 | 0.13142500 |
| O | 5.82607300 | -0.26578100 | 0.56675900 |
| C | 7.34239200 | -2.05179600 | -0.06888500 |
| H | 1.94664500 | 3.98070900 | -0.53568900 |
| H | 3.47561100 | 1.42119600 | -1.39940200 |
| H | 3.93167400 | 3.09789400 | -1.73080100 |
| H | 4.44507900 | 3.30702700 | 0.62260400 |
| H | 4.64783700 | 1.60236100 | 2.06846400 |
| H | 3.02530900 | 1.31990600 | 1.41144700 |

| | | | |
|---|---|---|---|
| H | 2.69741000 | -1.19181800 | 0.33145800 |
| H | 7.31511400 | -3.08638400 | -0.41181200 |
| H | 7.87430800 | -1.45357000 | -0.81472300 |
| H | 7.91781900 | -2.01025700 | 0.86076100 |
| H | 4.52038400 | -3.11772600 | -0.35554500 |

SCF energy: -886.809877 hartree
SCF energy in acetonitrile: -886.829728 hartree
zero-point correction: + 0.181941 hartree
free energy correction: + 0.126188 hartree

**TS9/10**

| | | | |
|---|---|---|---|
| Au | -2.17826300 | 1.20839600 | -0.35009800 |
| Au | 0.21882500 | 0.08406700 | -0.11651900 |
| Au | -1.98970000 | -1.34349500 | 0.30567900 |
| C | 2.13250900 | 0.21751200 | -0.23212700 |
| C | 3.14902100 | 0.05834300 | -1.14196500 |
| C | 3.63769800 | -1.27035500 | -1.67899800 |
| N | 5.08708500 | -1.13181900 | -1.85407700 |
| C | 5.72108400 | -0.74819600 | -0.57622600 |
| C | 4.78962600 | 0.17496400 | 0.14275600 |
| C | 4.79201900 | 1.57475300 | 0.35341300 |
| C | 3.76761500 | 1.83423800 | 1.23176800 |
| C | 3.18506300 | 0.58091400 | 1.56224700 |
| O | 4.07635900 | -0.39815000 | 1.18250500 |
| C | 2.30182100 | 0.25272200 | 2.71699600 |
| H | 3.31551300 | 0.89300000 | -1.82310300 |
| H | 3.34136200 | -2.07203100 | -0.98682500 |
| H | 3.19291900 | -1.47750600 | -2.65618900 |
| H | 5.49426100 | -1.99153200 | -2.21151400 |
| H | 5.90785300 | -1.60642900 | 0.08402900 |
| H | 6.67601100 | -0.26000300 | -0.78385300 |
| H | 5.37582600 | 2.28549500 | -0.21279200 |
| H | 2.87245400 | 0.25688900 | 3.65097600 |
| H | 1.50687100 | 0.99560700 | 2.79271000 |
| H | 1.84579500 | -0.72889700 | 2.58693800 |
| H | 3.37379700 | 2.79556500 | 1.52506200 |

SCF energy: -886.764362 hartree
SCF energy in acetonitrile: -886.781381 hartree
zero-point correction: + 0.181726 hartree
free energy correction: + 0.130742 hartree
imaginary frequency: -495.52 *i* $cm^{-1}$

**IM10**

| | | | |
|---|---|---|---|
| Au | 2.10093900 | -1.22147000 | -0.42385700 |
| Au | -0.25475900 | -0.05733700 | 0.04329300 |
| Au | 2.03012200 | 1.31213800 | 0.27059000 |
| C | -2.19486700 | -0.15734600 | 0.13577000 |
| C | -3.19091500 | 0.11397500 | -0.95177400 |
| C | -3.46315000 | 1.57157500 | -1.35182000 |
| N | -4.86477500 | 1.49290800 | -1.79744400 |
| C | -5.61045600 | 0.58628300 | -0.89638700 |
| C | -4.53130700 | -0.23418800 | -0.22302500 |
| C | -4.53636300 | -1.72798500 | 0.02736000 |
| C | -3.59349300 | -1.93434100 | 0.94950900 |
| C | -3.05860800 | -0.55283600 | 1.33806200 |
| O | -4.22067800 | 0.27757100 | 1.09098300 |
| C | -2.50483500 | -0.35955600 | 2.72521600 |
| H | -3.00868300 | -0.48236300 | -1.84837300 |
| H | -3.30611000 | 2.23132100 | -0.48853000 |
| H | -2.82384000 | 1.90279200 | -2.17188200 |
| H | -5.29540400 | 2.40877900 | -1.85339800 |
| H | -6.19087400 | 1.10821100 | -0.12678600 |
| H | -6.29545000 | -0.03954700 | -1.47589000 |
| H | -5.10437500 | -2.45971000 | -0.53076100 |
| H | -3.25280000 | -0.63441100 | 3.47120500 |
| H | -1.62091200 | -0.98557500 | 2.86056600 |
| H | -2.21520200 | 0.68184100 | 2.87408100 |
| H | -3.19135800 | -2.86890300 | 1.31446800 |

SCF energy: -886.807608 hartree

SCF energy in acetonitrile: -886.826579 hartree

zero-point correction: + 0.184935 hartree

free energy correction: + 0.134716 hartree

**TS10/7**

| | | | |
|---|---|---|---|
| Au | -2.14980900 | 1.28963200 | -0.15977600 |
| Au | 0.22505500 | 0.08755000 | 0.05442100 |
| Au | -1.99748800 | -1.37334300 | -0.00669400 |
| C | 2.23169800 | 0.10128100 | 0.18004700 |
| C | 3.25034800 | 0.04190600 | -0.77402300 |
| C | 3.47446700 | -0.17372600 | -2.23344100 |
| N | 4.94581400 | -0.09023900 | -2.31002700 |
| C | 5.50596300 | -0.68622300 | -1.08003200 |
| C | 4.59188100 | -0.08829100 | -0.02689900 |
| C | 4.86419900 | 1.23897600 | 0.67595000 |
| C | 3.93850900 | 1.30444200 | 1.62976900 |
| C | 3.11821700 | 0.01593700 | 1.51764800 |

| | | | |
|---|---|---|---|
| O | 4.14351100 | -0.91061400 | 1.05686900 |
| C | 2.40014100 | -0.49825800 | 2.73512400 |
| H | 2.50387300 | 1.16033000 | -0.44889400 |
| H | 3.06043900 | -1.16112300 | -2.49673300 |
| H | 3.00018300 | 0.56848800 | -2.87963000 |
| H | 5.31526600 | -0.51708800 | -3.15210600 |
| H | 5.42788500 | -1.78205000 | -1.03219300 |
| H | 6.55149300 | -0.39725000 | -0.96849100 |
| H | 5.59965000 | 1.96804000 | 0.36820500 |
| H | 3.10424700 | -0.62481600 | 3.55962400 |
| H | 1.62525400 | 0.21073700 | 3.03250600 |
| H | 1.92318200 | -1.45472400 | 2.51813400 |
| H | 3.72427000 | 2.10650900 | 2.32187100 |

SCF energy: -886.755362 hartree

SCF energy in acetonitrile: -886.774574 hartree

zero-point correction: + 0.180175 hartree

free energy correction: + 0.130296 hartree

imaginary frequency: -972.20 *i* $cm^{-1}$

**TS1/11**

| | | | |
|---|---|---|---|
| Au | 2.45808500 | 1.07267200 | 0.15513300 |
| Au | -0.04225800 | 0.22102600 | -0.05788500 |
| Au | 1.95881300 | -1.55472900 | -0.09387300 |
| C | -2.65689700 | -0.01800600 | -0.35101200 |
| C | -1.93795100 | 1.01184000 | -0.10218900 |
| C | -2.31605700 | 2.44386100 | 0.08526900 |
| N | -3.72606200 | 2.53618100 | 0.44698500 |
| C | -4.62759700 | 1.94344800 | -0.52396800 |
| C | -4.67091500 | 0.43622500 | -0.46275200 |
| C | -5.04051900 | -0.44053700 | -1.48430600 |
| C | -5.53982400 | -1.60526400 | -0.87810400 |
| C | -5.54492400 | -1.37363300 | 0.47911800 |
| O | -5.08476800 | -0.13041400 | 0.73955000 |
| C | -5.92637400 | -2.20644800 | 1.64473300 |
| H | -2.67842600 | -1.08525600 | -0.46503700 |
| H | -1.71934000 | 2.88177100 | 0.88650900 |
| H | -2.06352100 | 2.98408800 | -0.84403900 |
| H | -3.98206900 | 3.50176800 | 0.61528500 |
| H | -5.63489300 | 2.31813400 | -0.32059500 |
| H | -4.38369800 | 2.20016000 | -1.56883800 |
| H | -4.88112500 | -0.26517100 | -2.53720200 |
| H | -6.32004200 | -3.16436300 | 1.30622200 |
| H | -5.06274300 | -2.38946600 | 2.29055200 |

| | | | |
|---|---|---|---|
| H | -6.68769700 | -1.70376700 | 2.24769100 |
| H | -5.85605300 | -2.51535900 | -1.36323300 |

SCF energy: -886.792872 hartree
SCF energy in acetonitrile: -886.811392 hartree
zero-point correction: + 0.181070 hartree
free energy correction: + 0.127090 hartree
imaginary frequency: -445.26 *i* $cm^{-1}$

**IM11**

| | | | |
|---|---|---|---|
| Au | -2.44521100 | -1.03337100 | -0.50797700 |
| Au | 0.02299900 | -0.22342100 | 0.21253200 |
| Au | -2.14990600 | 1.44211400 | 0.23398500 |
| C | 2.92830300 | -0.10467200 | -0.30367800 |
| C | 1.98657000 | -0.63873600 | 0.48938700 |
| C | 2.36881800 | -1.55008700 | 1.62606500 |
| N | 3.79080600 | -1.42955900 | 1.94798400 |
| C | 4.61827500 | -1.62118900 | 0.77628800 |
| C | 4.40221500 | -0.45576300 | -0.19894200 |
| C | 5.00939500 | -0.68098200 | -1.54095600 |
| C | 5.92350600 | 0.31220900 | -1.79983800 |
| C | 5.99385800 | 1.13179400 | -0.67116600 |
| O | 5.15843200 | 0.73112500 | 0.29046300 |
| C | 6.83264900 | 2.31789100 | -0.38290700 |
| H | 2.67990100 | 0.57119000 | -1.11412400 |
| H | 1.79277200 | -1.28764100 | 2.51586100 |
| H | 2.07814800 | -2.58149000 | 1.35008300 |
| H | 4.04942400 | -2.08442700 | 2.67806600 |
| H | 5.67057100 | -1.65272100 | 1.06481800 |
| H | 4.38758600 | -2.54843100 | 0.22064800 |
| H | 4.71052200 | -1.48902600 | -2.19169100 |
| H | 7.47657300 | 2.54755400 | -1.23138800 |
| H | 6.20472200 | 3.18774000 | -0.16487800 |
| H | 7.45499900 | 2.14161400 | 0.50057800 |
| H | 6.50749900 | 0.45037100 | -2.69774200 |

SCF energy: -886.819710 hartree
SCF energy in acetonitrile: -886.845400 hartree
zero-point correction: + 0.182846 hartree
free energy correction: + 0.129851 hartree

**TS11/12**

| | | | |
|---|---|---|---|
| Au | -2.41021500 | -1.07181300 | -0.56822800 |
| Au | -0.00459400 | -0.19219400 | 0.26143300 |
| Au | -2.16352200 | 1.43065000 | 0.20676500 |

| | | | |
|---|---|---|---|
| C | 2.91557100 | -0.22573200 | -0.28404100 |
| C | 1.93681900 | -0.51496000 | 0.63306000 |
| C | 2.32721200 | -1.16239900 | 1.93157500 |
| N | 3.75232000 | -1.01068400 | 2.21967200 |
| C | 4.58154800 | -1.46138900 | 1.12673600 |
| C | 4.26971100 | -0.65315200 | -0.11099100 |
| C | 5.02926500 | -0.98670400 | -1.32935500 |
| C | 5.89379800 | -0.05249600 | -1.78802600 |
| C | 6.02039800 | 1.03223800 | -0.85048900 |
| O | 5.27883300 | 0.97136900 | 0.16604100 |
| C | 6.98028900 | 2.16892600 | -1.00430700 |
| H | 2.66529600 | 0.24050400 | -1.22982700 |
| H | 1.75976100 | -0.71201000 | 2.74828700 |
| H | 2.00490900 | -2.22048800 | 1.87300100 |
| H | 4.00187900 | -1.48866200 | 3.07847400 |
| H | 5.63517500 | -1.34728800 | 1.38820400 |
| H | 4.42704700 | -2.52444800 | 0.84489800 |
| H | 4.86886300 | -1.94994800 | -1.79992400 |
| H | 7.77627800 | 1.93143400 | -1.71067500 |
| H | 6.43617000 | 3.04262500 | -1.37910100 |
| H | 7.40077300 | 2.43620800 | -0.03407400 |
| H | 6.48739600 | -0.13487500 | -2.68788800 |

SCF energy: -886.806124 hartree

SCF energy in acetonitrile: -886.831949 hartree

zero-point correction: + 0.180869 hartree

free energy correction: + 0.126735 hartree

imaginary frequency: -475.42 *i* $cm^{-1}$

**IM12**

| | | | |
|---|---|---|---|
| Au | 2.11398000 | 0.47811100 | 1.28144500 |
| Au | -0.05662700 | -0.54980300 | 0.03402800 |
| Au | 2.16652900 | 0.18764700 | -1.29654000 |
| C | -3.01347600 | -0.44811900 | -0.08015900 |
| C | -1.90860200 | -1.28662500 | 0.02580800 |
| C | -2.12774000 | -2.76097900 | 0.19868200 |
| N | -3.44930600 | -3.15860800 | -0.27917200 |
| C | -4.51244400 | -2.39571400 | 0.35313700 |
| C | -4.32099100 | -0.91843500 | 0.10415600 |
| C | -5.50933500 | -0.13641600 | 0.15698500 |
| C | -5.81685200 | 1.19960700 | 0.03461600 |
| C | -5.00678100 | 2.39729400 | -0.21686100 |
| O | -3.79422300 | 2.41037800 | -0.39728000 |
| C | -5.79561600 | 3.69618600 | -0.24595900 |

| | | | |
|---|---|---|---|
| H | -2.88269100 | 0.61207400 | -0.24880500 |
| H | -1.37361800 | -3.32328100 | -0.35592300 |
| H | -1.96324100 | -2.99078700 | 1.27173000 |
| H | -3.59188700 | -4.15192300 | -0.12811800 |
| H | -5.47063700 | -2.71849500 | -0.06327700 |
| H | -4.57015000 | -2.55517700 | 1.45032500 |
| H | -6.39307300 | -0.74717200 | 0.34134200 |
| H | -6.31299800 | 3.85221500 | 0.70588300 |
| H | -5.12013000 | 4.52806000 | -0.43603500 |
| H | -6.56257300 | 3.65971400 | -1.02606500 |
| H | -6.87564900 | 1.42081000 | 0.14329800 |

SCF energy: -886.831571 hartree

SCF energy in acetonitrile: -886.864235 hartree

zero-point correction: + 0.181705 hartree

free energy correction: + 0.126644 hartree

**TS12/13**

| | | | |
|---|---|---|---|
| Au | -2.25253400 | -1.03381700 | -0.63085300 |
| Au | 0.15220100 | -0.22802900 | 0.26668400 |
| Au | -1.98565100 | 1.38149200 | 0.33009200 |
| C | 3.09993700 | -0.26051700 | -0.33585500 |
| C | 2.06154700 | -0.51571000 | 0.64674000 |
| C | 2.57729400 | -1.16823900 | 1.89260000 |
| N | 3.10411400 | -2.46256000 | 1.41716600 |
| C | 4.29393400 | -2.32567800 | 0.57665400 |
| C | 4.27270700 | -1.10171300 | -0.31707300 |
| C | 5.34753600 | -0.65075700 | -1.03879900 |
| C | 5.43462100 | 0.70095700 | -1.45263900 |
| C | 4.74170200 | 1.67315800 | -0.72226700 |
| O | 3.69602300 | 1.45170000 | -0.00610500 |
| C | 5.29755000 | 3.06999300 | -0.60540000 |
| H | 2.78489100 | 0.07059200 | -1.32068400 |
| H | 3.39882800 | -0.61261500 | 2.35666600 |
| H | 1.80679400 | -1.34517800 | 2.64011600 |
| H | 2.36676700 | -2.95799000 | 0.92149100 |
| H | 5.16132900 | -2.27782200 | 1.24783200 |
| H | 4.40077000 | -3.24081900 | -0.01315400 |
| H | 6.22797400 | -1.27911200 | -1.16325000 |
| H | 4.50426200 | 3.80513200 | -0.75425600 |
| H | 5.69867200 | 3.21564600 | 0.40181200 |
| H | 6.09491300 | 3.23745900 | -1.32975700 |
| H | 6.28958600 | 1.02802700 | -2.02985700 |

SCF energy: -886.794065 hartree

SCF energy in acetonitrile: -886.818281 hartree
zero-point correction: + 0.182393 hartree
free energy correction: + 0.130179 hartree
imaginary frequency: -463.59 *i* $cm^{-1}$

**IM13**

| | | | |
|---|---|---|---|
| Au | 2.15985400 | 0.22219500 | 1.17123600 |
| Au | -0.23244900 | -0.44261200 | 0.18621200 |
| Au | 1.82887700 | 0.07355100 | -1.43192100 |
| C | -3.22020100 | 0.00313800 | 0.50917900 |
| C | -2.09862100 | -0.96656600 | 0.45029600 |
| C | -2.53458600 | -2.39876200 | 0.61411600 |
| N | -3.95727100 | -2.68674100 | 0.39367800 |
| C | -4.49313700 | -1.85227500 | -0.69191500 |
| C | -4.41062900 | -0.39451200 | -0.35145200 |
| C | -5.29408800 | 0.57497400 | -0.62562800 |
| C | -5.00593500 | 1.94508800 | -0.25297600 |
| C | -3.74679800 | 2.28123200 | 0.09460500 |
| O | -2.76828600 | 1.33518800 | 0.21981800 |
| C | -3.21197000 | 3.66033200 | 0.27203800 |
| H | -3.55690200 | 0.00289300 | 1.57198500 |
| H | -1.94095800 | -3.01454200 | -0.07191700 |
| H | -2.25492600 | -2.73996800 | 1.61940500 |
| H | -4.48945000 | -2.51630200 | 1.24260600 |
| H | -3.89627500 | -2.07978600 | -1.58498900 |
| H | -5.52257100 | -2.14734600 | -0.90659400 |
| H | -6.20055600 | 0.35804300 | -1.18352600 |
| H | -2.39536700 | 3.83376000 | -0.43580300 |
| H | -3.99364300 | 4.39985100 | 0.09960800 |
| H | -2.80221200 | 3.79464700 | 1.27710200 |
| H | -5.75050600 | 2.72099400 | -0.36829800 |

SCF energy: -886.814008 hartree
SCF energy in acetonitrile: -886.835026 hartree
zero-point correction: + 0.183612 hartree
free energy correction: + 0.132162 hartree

**TS13/14**

| | | | |
|---|---|---|---|
| Au | -1.99081500 | 0.83126000 | -1.07924100 |
| Au | 0.20355100 | -0.39819700 | -0.16615900 |
| Au | -2.07794100 | -0.55590700 | 1.19459700 |
| C | 3.21509500 | -0.00553100 | -0.05752700 |
| C | 2.12068300 | -0.87275000 | -0.39713500 |
| C | 2.55630000 | -2.19720100 | -1.00511800 |

| | | | |
|---|---|---|---|
| N | 3.96702300 | -2.37626800 | -1.33996200 |
| C | 4.85442800 | -1.89052100 | -0.28313600 |
| C | 4.61668200 | -0.44093600 | 0.04370400 |
| C | 5.54356000 | 0.48063400 | 0.37574100 |
| C | 5.15503800 | 1.82700400 | 0.70009100 |
| C | 3.84636900 | 2.12622200 | 0.81909400 |
| O | 2.88076500 | 1.18336600 | 0.58016100 |
| C | 3.24860200 | 3.41067500 | 1.27085400 |
| H | 2.88211900 | 0.10447400 | -1.23900400 |
| H | 2.27335400 | -2.94688100 | -0.25311800 |
| H | 1.95441700 | -2.42083900 | -1.88674900 |
| H | 4.18311500 | -1.91479400 | -2.21897500 |
| H | 4.66230000 | -2.50437500 | 0.60602200 |
| H | 5.89358100 | -2.05835500 | -0.57273700 |
| H | 6.59062500 | 0.20071100 | 0.43713100 |
| H | 2.63532600 | 3.24578300 | 2.16145600 |
| H | 4.03141400 | 4.13142900 | 1.50410500 |
| H | 2.59389000 | 3.82398200 | 0.49881700 |
| H | 5.89524500 | 2.58489500 | 0.91548900 |

SCF energy: -886.801466 hartree

SCF energy in acetonitrile: -886.821657 hartree

zero-point correction: + 0.181213 hartree

free energy correction: + 0.129844 hartree

imaginary frequency: -811.29 *i* $cm^{-1}$

**IM14**

| | | | |
|---|---|---|---|
| Au | -2.30608300 | 0.77763800 | 0.35082900 |
| Au | 0.32689700 | 0.48692200 | 0.23014800 |
| Au | -1.23165100 | -1.51077000 | -0.57335800 |
| C | 2.69936900 | 0.49834500 | 0.33320300 |
| C | 2.04078000 | 1.69332900 | 0.70945700 |
| C | 2.20279900 | 2.91829100 | -0.21690000 |
| N | 3.12849600 | 2.71526100 | -1.33189600 |
| C | 2.93358200 | 1.40815300 | -1.96437600 |
| C | 3.20400000 | 0.28428800 | -0.99728000 |
| C | 3.89733500 | -0.85187100 | -1.25932000 |
| C | 4.07911200 | -1.83251200 | -0.23198700 |
| C | 3.67419200 | -1.56190100 | 1.02707800 |
| O | 3.10812300 | -0.35507400 | 1.33361900 |
| C | 3.80106600 | -2.43381900 | 2.22497000 |
| H | 1.98561500 | 1.89255800 | 1.77596400 |
| H | 1.23684000 | 3.22654700 | -0.62171200 |
| H | 2.57728000 | 3.75381700 | 0.38059200 |

| | | | |
|---|---|---|---|
| H | 4.08409400 | 2.76914400 | -0.98833500 |
| H | 1.89619900 | 1.36173700 | -2.31651000 |
| H | 3.58460000 | 1.32002400 | -2.83673100 |
| H | 4.29697900 | -1.03266600 | -2.25141400 |
| H | 2.81327800 | -2.66824500 | 2.63146900 |
| H | 4.30755200 | -3.36206600 | 1.96326800 |
| H | 4.36876700 | -1.92621200 | 3.01018300 |
| H | 4.54705900 | -2.78410600 | -0.44344000 |

SCF energy: -886.875650 hartree
SCF energy in acetonitrile: -886.891551 hartree
zero-point correction: + 0.185853 hartree
free energy correction: + 0.134485 hartree

**TS12/15**

| | | | |
|---|---|---|---|
| Au | 2.47093300 | -1.33216100 | 0.04701100 |
| Au | 0.12518400 | -0.03751100 | 0.10014000 |
| Au | 2.45785800 | 1.28256200 | -0.20309500 |
| C | -2.79038500 | -0.04025700 | -0.77868600 |
| C | -1.90044500 | -0.05085300 | 0.26896200 |
| C | -2.59141700 | 0.33144600 | 1.66325000 |
| N | -3.95700200 | 0.73792800 | 1.54857200 |
| C | -4.30094700 | 1.39614900 | 0.30098200 |
| C | -4.10632100 | 0.31879800 | -0.78467300 |
| C | -5.11735200 | -0.32011300 | -1.56186400 |
| C | -6.45450900 | -0.49297300 | -1.35013000 |
| C | -7.19762300 | -0.31417000 | -0.10549200 |
| O | -6.66370600 | -0.11296200 | 0.98612100 |
| C | -8.70344300 | -0.45681800 | -0.20212300 |
| H | -2.23861100 | -1.17230700 | -0.21300500 |
| H | -2.48390000 | -0.47482000 | 2.38705100 |
| H | -1.97579100 | 1.17419300 | 1.99076300 |
| H | -4.64875300 | 0.01695100 | 1.73625700 |
| H | -5.32601000 | 1.75272200 | 0.33462000 |
| H | -3.62273200 | 2.23416600 | 0.12753700 |
| H | -4.73376600 | -0.73460600 | -2.49108100 |
| H | -9.11343200 | 0.29556300 | -0.88307100 |
| H | -8.96686500 | -1.43644000 | -0.61278200 |
| H | -9.14907100 | -0.34224600 | 0.78428100 |
| H | -7.02171900 | -0.92050500 | -2.17128700 |

SCF energy: -886.737715 hartree
SCF energy in acetonitrile: -886.762272 hartree
zero-point correction: + 0.176258 hartree
free energy correction: + 0.121683 hartree

imaginary frequency: -1194.46 *i* $cm^{-1}$

**IM15**

| | | | |
|---|---|---|---|
| Au | 2.06347200 | 0.87866500 | 1.03639500 |
| Au | -0.09398100 | -0.45418200 | 0.18007100 |
| Au | 2.25631300 | -0.34074100 | -1.24146200 |
| C | -2.01677500 | -1.02586200 | 0.54298600 |
| C | -2.26112600 | -2.36477900 | 0.64020000 |
| C | -3.65321800 | -2.93689700 | 0.55853000 |
| N | -4.72346600 | -1.95534000 | 0.57659700 |
| C | -4.34590500 | -0.71258500 | 1.24948600 |
| C | -3.13318300 | -0.13577000 | 0.55817900 |
| C | -3.06396700 | 1.15381400 | -0.00742700 |
| C | -4.04854300 | 1.98641900 | -0.49099600 |
| C | -5.41383300 | 1.63711400 | -0.87504200 |
| O | -5.84069700 | 0.48311200 | -0.91437400 |
| C | -6.29886800 | 2.79459900 | -1.30124100 |
| H | -1.45929800 | -3.07987000 | 0.79604300 |
| H | -3.75693100 | -3.56971900 | -0.32905000 |
| H | -3.76527200 | -3.61485700 | 1.42208400 |
| H | -5.05105400 | -1.72089400 | -0.35625500 |
| H | -5.19392500 | -0.03600100 | 1.24320500 |
| H | -4.08798000 | -0.94566300 | 2.28809200 |
| H | -2.04660200 | 1.53844100 | -0.08647200 |
| H | -5.85250400 | 3.32267600 | -2.14968100 |
| H | -7.28173100 | 2.42032700 | -1.58210800 |
| H | -6.39858900 | 3.52040900 | -0.48819700 |
| H | -3.74223300 | 2.99570100 | -0.75223100 |

SCF energy: -886.826658 hartree

SCF energy in acetonitrile: -886.858462 hartree

zero-point correction: + 0.181312 hartree

free energy correction: + 0.123980 hartree

**TS15/14**

| | | | |
|---|---|---|---|
| Au | 2.27223500 | -0.88827700 | 0.25625700 |
| Au | -0.34472400 | -0.49807900 | 0.20043500 |
| Au | 1.26591300 | 1.46747300 | -0.53204300 |
| C | -2.46918200 | -0.62949400 | 0.24305400 |
| C | -1.94476100 | -1.84766300 | 0.66912800 |
| C | -2.30007200 | -2.94630600 | -0.35192000 |
| N | -3.74210500 | -2.90301100 | -0.59525400 |
| C | -4.22014400 | -1.64116500 | -1.13818000 |
| C | -3.43837700 | -0.38898000 | -0.66988700 |

| | | | |
|---|---|---|---|
| C | -3.73980600 | 0.89459100 | -1.16825600 |
| C | -3.46239500 | 2.06048400 | -0.49361800 |
| C | -3.04621300 | 2.07800900 | 0.88017400 |
| O | -2.51739700 | 1.11699900 | 1.48154000 |
| C | -3.37591500 | 3.31258400 | 1.69260900 |
| H | -1.93529700 | -2.11588500 | 1.72169900 |
| H | -1.78120900 | -2.78042900 | -1.29608400 |
| H | -2.02668800 | -3.93196500 | 0.02589800 |
| H | -4.24073600 | -3.12976400 | 0.25876700 |
| H | -4.13084000 | -1.66027200 | -2.23265300 |
| H | -5.28330800 | -1.55503200 | -0.90086300 |
| H | -4.34043600 | 0.96085000 | -2.07403800 |
| H | -2.68499500 | 3.40252400 | 2.52969800 |
| H | -3.33123900 | 4.20984000 | 1.07198100 |
| H | -4.39241900 | 3.22773000 | 2.08977500 |
| H | -3.81820900 | 2.99689400 | -0.90558900 |

SCF energy: -886.811843 hartree

SCF energy in acetonitrile: -886.831073 hartree

zero-point correction: + 0.182046 hartree

free energy correction: + 0.130592 hartree

imaginary frequency: -209.90 *i* $cm^{-1}$

**P3**

| | | | |
|---|---|---|---|
| C | -0.19906100 | -0.57902400 | -0.08115100 |
| C | -1.17051200 | -1.50826000 | -0.10039400 |
| C | -2.62019200 | -1.09222500 | -0.04272200 |
| N | -2.83106100 | 0.28541500 | 0.41839400 |
| C | -1.92106900 | 1.21081500 | -0.26126200 |
| C | -0.46569300 | 0.84441500 | -0.09981200 |
| C | 0.55785800 | 1.71939200 | -0.00652500 |
| C | 1.91429200 | 1.23603600 | 0.07057800 |
| C | 2.14748800 | -0.08968200 | 0.03352100 |
| O | 1.13128800 | -0.99703300 | -0.04561000 |
| C | 3.47551200 | -0.76314800 | 0.06313900 |
| H | -0.91723100 | -2.56200700 | -0.13210500 |
| H | -3.09605900 | -1.19270400 | -1.02855100 |
| H | -3.17379500 | -1.75591300 | 0.62861900 |
| H | -2.63395700 | 0.31980100 | 1.41592400 |
| H | -2.18057900 | 1.19351100 | -1.32736500 |
| H | -2.10125800 | 2.22649100 | 0.09940000 |
| H | 0.37054300 | 2.78845800 | -0.01588600 |
| H | 3.61774700 | -1.36702000 | -0.83817200 |
| H | 4.27388500 | -0.02414800 | 0.12482000 |

| | | | |
|---|---|---|---|
| H | 3.54606800 | -1.43745400 | 0.92179600 |
| H | 2.75002400 | 1.91942400 | 0.13539800 |

SCF energy: -479.714662 hartree
SCF energy in acetonitrile: -479.728467 hartree
zero-point correction: + 0.183614 hartree
free energy correction: + 0.149160 hartree

**S3.2 $Au_4$**

$Au_4$

| | | | |
|---|---|---|---|
| Au | 2.35094800 | 0.00000800 | 0.00000000 |
| Au | 0.00000000 | -1.30718400 | 0.00000000 |
| Au | -2.35094800 | 0.00000000 | 0.00000000 |
| Au | 0.00000000 | 1.30717600 | 0.00000000 |

SCF energy: -542.858837 hartree
SCF energy in acetonitrile: -542.868824 hartree
zero-point correction: + 0.001397 hartree
free energy correction: -0.038612 hartree

**IM1**

| | | | |
|---|---|---|---|
| Au | 0.10261200 | 0.51441300 | -0.46910300 |
| Au | 0.15422200 | -2.23928800 | -0.12940100 |
| Au | 2.24451900 | -0.73021600 | 0.42555700 |
| Au | 2.42703600 | 1.87806800 | 0.15864200 |
| C | -1.26290700 | 2.00244300 | -1.10289700 |
| C | -1.89602900 | 0.92637300 | -1.18998000 |
| C | -3.01571600 | -0.03486700 | -1.40348900 |
| N | -3.37063000 | -0.86140500 | -0.26330700 |
| C | -3.79401800 | -0.11006900 | 0.92925300 |
| C | -5.09488500 | 0.58376100 | 0.72978900 |
| C | -5.45129300 | 1.89548300 | 0.67309800 |
| C | -6.86732600 | 1.93004200 | 0.47622000 |
| C | -7.28460600 | 0.63587800 | 0.42577900 |
| O | -6.21127100 | -0.19737900 | 0.58023100 |
| C | -8.60862200 | -0.01168100 | 0.24851800 |
| H | -1.09294100 | 3.05674900 | -1.17751800 |
| H | -3.89074800 | 0.55882900 | -1.68857700 |
| H | -2.76152500 | -0.68668100 | -2.24147400 |
| H | -2.57694900 | -1.45408000 | -0.02120400 |
| H | -3.88204900 | -0.83849900 | 1.73989500 |
| H | -3.06101000 | 0.64769000 | 1.24308400 |
| H | -4.78261400 | 2.73732700 | 0.76663600 |
| H | -9.37834900 | 0.75190100 | 0.13374100 |
| H | -8.62114400 | -0.65309500 | -0.63763900 |

| | | | |
|---|---|---|---|
| H | -8.86437600 | -0.63402300 | 1.11122500 |
| H | -7.49413600 | 2.80336300 | 0.38542800 |

SCF energy: -1022.575815 hartree
SCF energy in acetonitrile: -1022.595015 hartree
zero-point correction: + 0.182229 hartree
free energy correction: +0.122491 hartree

**TS1/2**

| | | | |
|---|---|---|---|
| Au | -0.25441700 | -0.15024900 | -0.03884500 |
| Au | 1.48904800 | -2.31266500 | -0.23137200 |
| Au | 2.35922000 | 0.16173500 | 0.06067500 |
| Au | 0.94103200 | 2.37319200 | 0.28754300 |
| C | -2.27488700 | -0.50858200 | -0.12829100 |
| C | -3.03378100 | 0.35530200 | -0.69353600 |
| C | -3.11012800 | 1.64400600 | -1.42323000 |
| N | -4.29210400 | 2.33943600 | -0.91910900 |
| C | -5.42612400 | 1.43222700 | -1.05691100 |
| C | -5.03030600 | 0.10114600 | -0.48104500 |
| C | -5.18848900 | -1.17248800 | -1.04379500 |
| C | -5.18970300 | -2.09458500 | 0.00398100 |
| C | -5.13664500 | -1.35913400 | 1.17514400 |
| O | -5.12709400 | -0.04487000 | 0.90366000 |
| C | -5.11493200 | -1.75251000 | 2.60348800 |
| H | -2.59976100 | -1.44349900 | 0.32092900 |
| H | -2.20756000 | 2.21645000 | -1.20060300 |
| H | -3.14314600 | 1.45552800 | -2.51075900 |
| H | -4.45253500 | 3.20826300 | -1.41901600 |
| H | -6.29468700 | 1.83224900 | -0.52916300 |
| H | -5.71448300 | 1.24467000 | -2.10439600 |
| H | -5.20901800 | -1.38053900 | -2.10245400 |
| H | -4.20386500 | -1.38907200 | 3.08629300 |
| H | -5.96595000 | -1.31489100 | 3.13273900 |
| H | -5.15785200 | -2.83682800 | 2.69606900 |
| H | -5.21545200 | -3.17069100 | -0.06206200 |

SCF energy: -1022.543630 hartree
SCF energy in acetonitrile: -1022.567609 hartree
zero-point correction: + 0.181795 hartree
free energy correction: + 0.123904 hartree
imaginary frequency: -318.88 *i* $cm^{-1}$

**IM2**

| | | | |
|---|---|---|---|
| Au | 0.27236200 | -0.00212700 | -0.11970900 |
| Au | -1.21113000 | -2.34910200 | -0.10807800 |

| | | | |
|---|---|---|---|
| Au | -2.38304900 | 0.01715300 | 0.01139600 |
| Au | -1.21234200 | 2.36434500 | 0.02141600 |
| C | 2.26518700 | -0.23447300 | -0.24971300 |
| C | 3.13116500 | -0.26640400 | 0.75680800 |
| C | 2.91824800 | -0.24117800 | 2.24900400 |
| N | 4.11602900 | 0.45383000 | 2.73079400 |
| C | 5.22955100 | -0.14069100 | 2.00755100 |
| C | 4.71210900 | -0.26837400 | 0.56981600 |
| C | 5.02651300 | -1.44108800 | -0.23341500 |
| C | 5.30717100 | -1.03324800 | -1.51557800 |
| C | 5.35051300 | 0.36751200 | -1.48729900 |
| O | 5.11158600 | 0.84675200 | -0.28075100 |
| C | 5.65469200 | 1.34308800 | -2.55697300 |
| H | 2.65448900 | -0.32229800 | -1.26737100 |
| H | 2.01237900 | 0.31401600 | 2.49185600 |
| H | 2.81700600 | -1.26448600 | 2.65152900 |
| H | 4.23486500 | 0.37905100 | 3.73560600 |
| H | 6.12461900 | 0.48196100 | 2.05100000 |
| H | 5.49358300 | -1.15572700 | 2.34855400 |
| H | 4.92747000 | -2.45206300 | 0.13204300 |
| H | 4.78244500 | 1.97854100 | -2.73706200 |
| H | 6.47332500 | 1.99742300 | -2.24472300 |
| H | 5.92506500 | 0.83344300 | -3.48007100 |
| H | 5.47751600 | -1.64284500 | -2.38904100 |

SCF energy: -1022.550896 hartree

SCF energy in acetonitrile: -1022.581817 hartree

zero-point correction: + 0.183041 hartree

free energy correction: + 0.124873 hartree

**TS2/3**

| | | | |
|---|---|---|---|
| Au | 0.21998000 | -0.07224600 | -0.21696800 |
| Au | -0.94689300 | 2.42344400 | 0.17511900 |
| Au | -2.41001000 | 0.23765400 | 0.09535400 |
| Au | -1.56877400 | -2.22569400 | -0.25237000 |
| C | 2.17747500 | -0.28519500 | -0.47156900 |
| C | 3.09795600 | -0.68054900 | 0.45026600 |
| C | 2.85458100 | -1.09672800 | 1.89340700 |
| N | 3.87064500 | -2.13057600 | 2.15367800 |
| C | 5.04815600 | -1.70850900 | 1.41633400 |
| C | 4.51479100 | -0.87009600 | 0.19883900 |
| C | 5.06374600 | -1.09114600 | -1.13727300 |
| C | 5.89019900 | -0.13167300 | -1.60262500 |
| C | 5.97391100 | 0.92241500 | -0.62416200 |

| | | | |
|---|---|---|---|
| O | 5.34996400 | 0.68384300 | 0.44607500 |
| C | 6.68378800 | 2.21769000 | -0.80907700 |
| H | 2.56996000 | -0.07262600 | -1.46885400 |
| H | 3.01128000 | -0.25994000 | 2.58356400 |
| H | 1.84663600 | -1.48114300 | 2.04299700 |
| H | 3.53295700 | -3.01060800 | 1.77393100 |
| H | 5.66657900 | -1.05069700 | 2.03047000 |
| H | 5.65599400 | -2.55567700 | 1.09687500 |
| H | 4.77941400 | -1.97838300 | -1.69021700 |
| H | 7.71977200 | 2.03662600 | -1.10755100 |
| H | 6.20675700 | 2.77591400 | -1.62142200 |
| H | 6.65321600 | 2.80864900 | 0.10364900 |
| H | 6.38563500 | -0.11559200 | -2.56232700 |

SCF energy: -1022.545847 hartree

SCF energy in acetonitrile: -1022.578684 hartree

zero-point correction: + 0.182090 hartree

free energy correction: + 0.126404 hartree

imaginary frequency: -364.89 *i* $cm^{-1}$

**IM3**

| | | | |
|---|---|---|---|
| Au | 1.24805600 | 2.34686800 | -0.01954600 |
| Au | 2.60216100 | 0.09991500 | 0.08385800 |
| Au | 1.48558600 | -2.27549200 | -0.11373600 |
| Au | -0.07799500 | -0.03988900 | -0.23932700 |
| C | -2.00520400 | -0.19724100 | -0.49656900 |
| C | -2.98485100 | -0.28713900 | 0.50189100 |
| H | -2.37118900 | -0.20985000 | -1.52372300 |
| C | -2.68381800 | -0.34311500 | 1.97959700 |
| N | -3.96279800 | -0.77967700 | 2.54746600 |
| C | -5.02804100 | -0.28113200 | 1.67117200 |
| C | -4.36905900 | -0.25535200 | 0.32417200 |
| C | -4.99212500 | -0.23197100 | -0.96584800 |
| O | -7.44936800 | 0.70645800 | 0.56432300 |
| C | -7.49140100 | 0.24552700 | -0.56459500 |
| C | -6.28447400 | -0.08382600 | -1.35636100 |
| C | -8.80943000 | 0.00989500 | -1.27209500 |
| H | -4.29616500 | -0.40092800 | -1.78272500 |
| H | -6.47109300 | -0.20712800 | -2.42009600 |
| H | -8.86942200 | 0.63590300 | -2.16839600 |
| H | -8.88670300 | -1.03019400 | -1.60366200 |
| H | -9.63412600 | 0.24938100 | -0.60380500 |
| H | -5.90637200 | -0.92980500 | 1.70059000 |
| H | -5.38477700 | 0.73303500 | 1.91087500 |

| | | | |
|---|---|---|---|
| H | -1.88318000 | -1.05185100 | 2.20493200 |
| H | -2.35181400 | 0.65308500 | 2.31829600 |
| H | -4.08698500 | -0.47026600 | 3.50403500 |

SCF energy: -1022.564851 hartree
SCF energy in acetonitrile: -1022.585686 hartree
zero-point correction: + 0.182057 hartree
free energy correction: + 0.122277 hartree

**TS3/4**

| | | | |
|---|---|---|---|
| Au | 0.37403800 | 0.06547500 | -0.14477500 |
| Au | -1.01852400 | -2.31161100 | -0.47310200 |
| Au | -2.27798600 | -0.05529000 | 0.07303100 |
| Au | -1.16871800 | 2.29643600 | 0.40845000 |
| C | 2.32510400 | -0.16427300 | -0.38406800 |
| C | 3.19831100 | -0.80971800 | 0.55778800 |
| C | 2.76263800 | -1.55129200 | 1.80676200 |
| N | 3.93305800 | -2.34499400 | 2.21662100 |
| C | 5.10710600 | -1.70147300 | 1.60388500 |
| C | 4.55800800 | -0.88947000 | 0.44498800 |
| C | 5.35593600 | -0.33028600 | -0.59703900 |
| C | 5.11149700 | 0.78842100 | -1.34244700 |
| C | 4.15469100 | 1.83477500 | -1.02169200 |
| O | 3.12260900 | 1.68009300 | -0.34536600 |
| C | 4.49853100 | 3.22942900 | -1.48707800 |
| H | 2.67541900 | -0.24272500 | -1.41601000 |
| H | 2.49838000 | -0.81991000 | 2.58266400 |
| H | 1.88595200 | -2.17941600 | 1.64424000 |
| H | 3.83598200 | -3.27542000 | 1.82367600 |
| H | 5.59272300 | -1.03400200 | 2.32817700 |
| H | 5.85331400 | -2.44092700 | 1.29921600 |
| H | 6.29629300 | -0.84169200 | -0.79742900 |
| H | 4.55410900 | 3.23643900 | -2.58088900 |
| H | 3.73453300 | 3.92935700 | -1.15616700 |
| H | 5.47753700 | 3.53624400 | -1.11048900 |
| H | 5.85654800 | 1.06368800 | -2.08178300 |

SCF energy: -1022.554487 hartree
SCF energy in acetonitrile: -1022.577437 hartree
zero-point correction: + 0.182538 hartree
free energy correction: + 0.125179 hartree
imaginary frequency: -172.35 *i* $cm^{-1}$

**IM4**

| | | | |
|---|---|---|---|
| Au | 1.73673900 | -1.00116300 | -0.17936200 |
| Au | -0.50825800 | -2.36641900 | -0.27189900 |
| Au | -0.48231500 | 0.35360300 | 0.29468400 |
| Au | 2.03824500 | 1.55406700 | 0.36291500 |
| C | -1.78525100 | 2.04213500 | 0.75684900 |
| C | -2.59680300 | 0.89293400 | 0.73089900 |
| C | -3.10573200 | 0.18851200 | 2.00178200 |
| N | -4.55605600 | 0.07760200 | 1.79058700 |
| C | -4.69416300 | -0.18210300 | 0.34433100 |
| C | -3.59537800 | 0.62921600 | -0.31642300 |
| C | -3.54869200 | 1.04945700 | -1.59361900 |
| C | -2.45958800 | 1.80616300 | -2.17980300 |
| C | -1.64917200 | 2.66541200 | -1.54308900 |
| O | -1.85519500 | 3.03273500 | -0.20386800 |
| C | -0.51990100 | 3.42258900 | -2.14778700 |
| H | -1.42635800 | 2.44920100 | 1.69659500 |
| H | -2.68802300 | -0.81605600 | 2.08916800 |
| H | -2.87767200 | 0.73947500 | 2.91493900 |
| H | -4.98151400 | 0.97981100 | 1.99250900 |
| H | -4.54344900 | -1.25416300 | 0.17039400 |
| H | -5.69280000 | 0.07926200 | -0.00650300 |
| H | -4.34355900 | 0.74251700 | -2.26841800 |
| H | -0.66882000 | 4.49740800 | -2.00597400 |
| H | 0.42052000 | 3.15138400 | -1.65291900 |
| H | -0.43239500 | 3.20861500 | -3.21291200 |
| H | -2.27236800 | 1.66462300 | -3.23957800 |

SCF energy: -1022.598855 hartree

SCF energy in acetonitrile: -1022.618142 hartree

zero-point correction: + 0.185461 hartree

free energy correction: + 0.130765 hartree

**S3.3 $Au_5$**

$Au_5$

| | | | |
|---|---|---|---|
| Au | 0.00089900 | -0.99129300 | -0.00007900 |
| Au | -2.62140000 | -0.92777300 | -0.00006000 |
| Au | -1.34540500 | 1.42204900 | 0.00019600 |
| Au | 1.34229300 | 1.42190900 | -0.00019800 |
| Au | 2.62361300 | -0.92489300 | 0.00014100 |

SCF energy: -678.600716 hartree

SCF energy in acetonitrile: -678.609301 hartree

zero-point correction: + 0.001931 hartree

free energy correction: -0.043816 hartree

**IM1**

| | | | |
|---|---|---|---|
| Au | -1.93994400 | 0.07950400 | 0.25879500 |
| Au | -1.71154300 | 2.66107200 | 0.41876800 |
| Au | 0.44551100 | 1.19083600 | -0.37280700 |
| Au | 0.11727300 | -1.55041300 | -0.50916100 |
| Au | -2.33121500 | -2.51463600 | 0.14721400 |
| C | 2.09001000 | 2.52951400 | -0.76194800 |
| C | 2.52019600 | 1.38242000 | -1.00235900 |
| C | 3.46848600 | 0.30343300 | -1.40203700 |
| N | 4.79330400 | 0.77944500 | -1.75888300 |
| C | 5.55902400 | 1.39716500 | -0.66500500 |
| C | 5.93663200 | 0.41544700 | 0.38635300 |
| C | 5.56157900 | 0.24971800 | 1.68313900 |
| C | 6.28521100 | -0.87918800 | 2.17919200 |
| C | 7.05604700 | -1.32981400 | 1.15241100 |
| O | 6.85376600 | -0.54605700 | 0.04973800 |
| C | 8.02201500 | -2.44729800 | 1.00571000 |
| H | 2.07058600 | 3.59458800 | -0.66298500 |
| H | 3.55617800 | -0.40520100 | -0.57498800 |
| H | 3.03927400 | -0.24088900 | -2.24584300 |
| H | 4.74327700 | 1.41428600 | -2.54897500 |
| H | 6.45982100 | 1.82142300 | -1.11739000 |
| H | 5.01715000 | 2.21671200 | -0.17096300 |
| H | 4.85225900 | 0.85974700 | 2.22098300 |
| H | 8.09047900 | -2.99840200 | 1.94388000 |
| H | 7.70959500 | -3.13997700 | 0.21876700 |
| H | 9.01916000 | -2.07909500 | 0.74670500 |
| H | 6.23719700 | -1.30189300 | 3.17045600 |

SCF energy: -1158.297721 hartree

SCF energy in acetonitrile: -1158.317612 hartree

zero-point correction: + 0.182666 hartree

free energy correction: + 0.116478 hartree

**TS1/2**

| | | | |
|---|---|---|---|
| Au | -1.74389000 | 0.80587700 | -0.02994900 |
| Au | -0.05683900 | 2.76990500 | -0.10261900 |
| Au | 0.94741900 | 0.22536500 | -0.06954900 |
| Au | -0.86679900 | -1.80920000 | -0.00645500 |
| Au | -3.47266500 | -1.18261200 | 0.04909400 |
| C | 2.82198500 | -0.65186400 | -0.13908700 |
| C | 3.60686500 | -0.54091200 | 0.86395700 |
| C | 3.78115900 | -0.10178200 | 2.26276900 |
| N | 5.14930200 | 0.39715600 | 2.39678700 |

| | | | |
|---|---|---|---|
| C | 6.06176200 | -0.64901100 | 1.94179800 |
| C | 5.63860600 | -1.11282300 | 0.57994900 |
| C | 5.51397200 | -2.41604100 | 0.09633400 |
| C | 5.58431100 | -2.34563800 | -1.30309300 |
| C | 5.84593500 | -1.03055600 | -1.62178500 |
| O | 5.95542400 | -0.29129500 | -0.49541700 |
| C | 6.03719800 | -0.32228400 | -2.90947600 |
| H | 3.03487200 | -1.13522200 | -1.08657400 |
| H | 3.07225200 | 0.70188800 | 2.47716100 |
| H | 3.55655500 | -0.94522100 | 2.93978400 |
| H | 5.34898800 | 0.65808600 | 3.35756000 |
| H | 7.08023200 | -0.25444700 | 1.90821200 |
| H | 6.06046000 | -1.54198600 | 2.58872500 |
| H | 5.31291600 | -3.28627000 | 0.70152500 |
| H | 5.28499500 | 0.46160000 | -3.03578900 |
| H | 7.02046600 | 0.15568500 | -2.94589000 |
| H | 5.95630800 | -1.02473200 | -3.73841900 |
| H | 5.46177000 | -3.15119500 | -2.00998100 |

SCF energy: -1158.274703 hartree

SCF energy in acetonitrile: -1158.295019 hartree

zero-point correction: + 0.181731 hartree

free energy correction: + 0.117623 hartree

imaginary frequency: -335.99 *i* $cm^{-1}$

**IM2**

| | | | |
|---|---|---|---|
| Au | -1.56682700 | -0.76896300 | -0.02514700 |
| Au | -3.08068300 | 1.37685000 | -0.08962400 |
| Au | -0.45723800 | 1.78988100 | -0.16109400 |
| Au | 1.22797800 | -0.66343900 | 0.11362300 |
| Au | -0.06569900 | -2.93820200 | -0.00114900 |
| C | 1.56458300 | 1.54132400 | -0.28596800 |
| C | 2.42946300 | 1.19840900 | 0.73635200 |
| C | 2.23322700 | 1.43899400 | 2.22009600 |
| N | 3.45667800 | 2.19264400 | 2.52059800 |
| C | 4.54322400 | 1.44287800 | 1.88612200 |
| C | 3.94935800 | 0.99848300 | 0.52836200 |
| C | 4.30732400 | -0.38466300 | 0.07029600 |
| C | 4.89438900 | -0.28385000 | -1.18183300 |
| C | 4.95447800 | 1.05252700 | -1.53150300 |
| O | 4.41976800 | 1.84794000 | -0.55828000 |
| C | 5.48908000 | 1.74995100 | -2.72275600 |
| H | 2.00821000 | 1.56576200 | -1.28133900 |
| H | 1.33733300 | 2.02801900 | 2.41425300 |

| | | | |
|---|---|---|---|
| H | 2.16396800 | 0.48987900 | 2.77843500 |
| H | 3.60108500 | 2.30564900 | 3.51876900 |
| H | 5.42601000 | 2.06546900 | 1.73713400 |
| H | 4.83570200 | 0.54209800 | 2.44854200 |
| H | 4.19683400 | -1.26343800 | 0.68701600 |
| H | 4.70523300 | 2.32848800 | -3.22371000 |
| H | 6.27851500 | 2.45488500 | -2.44043600 |
| H | 5.89855200 | 1.02881500 | -3.43011900 |
| H | 5.25800600 | -1.09603800 | -1.79366100 |

SCF energy: -1158.314969 hartree

SCF energy in acetonitrile: -1158.336558 hartree

zero-point correction: + 0.183073 hartree

free energy correction: + 0.122742 hartree

**TS2/3**

| | | | |
|---|---|---|---|
| Au | -1.45412200 | 0.90569400 | 0.03781500 |
| Au | 0.30189600 | 2.86401800 | 0.16141000 |
| Au | 1.27562300 | 0.41392200 | 0.03306200 |
| Au | -0.64945000 | -1.76033800 | -0.26009300 |
| Au | -3.20370300 | -1.04547000 | -0.10865800 |
| C | 1.39104700 | -1.79052400 | -0.40426600 |
| C | 2.30015900 | -1.80995800 | 0.63440800 |
| C | 1.99285700 | -1.96643500 | 2.10964000 |
| N | 3.22495300 | -1.49877600 | 2.74579500 |
| C | 4.31835600 | -1.98637100 | 1.90802200 |
| C | 3.77254500 | -1.88770300 | 0.50029400 |
| C | 4.45114900 | -2.58270200 | -0.57461400 |
| C | 4.76123900 | -1.82220500 | -1.67749400 |
| C | 4.60737900 | -0.44550000 | -1.39881400 |
| O | 4.06236500 | -0.15492500 | -0.26816900 |
| C | 5.08731700 | 0.67264200 | -2.26681000 |
| H | 1.82332900 | -1.85182500 | -1.40344700 |
| H | 1.12590800 | -1.38636600 | 2.42836400 |
| H | 1.77621500 | -3.03272700 | 2.30563100 |
| H | 3.31008400 | -1.80970300 | 3.70675000 |
| H | 5.22248200 | -1.38788100 | 2.03828400 |
| H | 4.58787100 | -3.04633700 | 2.08384900 |
| H | 4.79565300 | -3.60023500 | -0.42717500 |
| H | 4.23805100 | 1.27860500 | -2.59868400 |
| H | 5.74851300 | 1.32887800 | -1.69464700 |
| H | 5.61663700 | 0.29584400 | -3.14241400 |
| H | 5.24006100 | -2.19319100 | -2.57318900 |

SCF energy: -1158.291263 hartree

SCF energy in acetonitrile: -1158.312382 hartree
zero-point correction: + 0.180761 hartree
free energy correction: + 0.120527 hartree
imaginary frequency: -562.24 *i* $cm^{-1}$

**IM3**

| | | | |
|---|---|---|---|
| Au | -2.09963800 | 0.01546100 | 0.03412800 |
| Au | -1.93259300 | 2.63788700 | 0.03018300 |
| Au | 0.37320800 | 1.35563800 | -0.20322500 |
| Au | 0.35037400 | -1.35111200 | -0.20958200 |
| Au | -1.96656800 | -2.61261600 | 0.00698900 |
| C | 2.00172500 | 0.00370900 | -0.44184700 |
| C | 2.98280600 | -0.03093800 | 0.54830000 |
| C | 2.72333500 | 0.02616300 | 2.04725300 |
| N | 3.93818000 | -0.50322300 | 2.67381200 |
| C | 5.02607500 | -0.11940000 | 1.75688400 |
| C | 4.39401000 | -0.10124100 | 0.37723000 |
| C | 5.00662000 | -0.20451300 | -0.89251900 |
| C | 6.31827700 | -0.16787400 | -1.29411000 |
| C | 7.52790100 | 0.16520200 | -0.52513800 |
| O | 7.50319800 | 0.64226900 | 0.60108500 |
| C | 8.84211500 | -0.08435600 | -1.23978600 |
| H | 2.36383600 | -0.02363700 | -1.46865500 |
| H | 2.58503600 | 1.07175600 | 2.35022500 |
| H | 1.83341200 | -0.52601700 | 2.34965000 |
| H | 3.87323500 | -1.51809500 | 2.68097000 |
| H | 5.39731600 | 0.87712400 | 2.01523800 |
| H | 5.87292200 | -0.79833300 | 1.83876300 |
| H | 4.30330700 | -0.37546000 | -1.70469500 |
| H | 8.89515600 | 0.51914500 | -2.15166600 |
| H | 9.67120300 | 0.17366700 | -0.58369000 |
| H | 8.92141100 | -1.13239800 | -1.54478200 |
| H | 6.49533000 | -0.37919100 | -2.34530700 |

SCF energy: -1158.328679 hartree
SCF energy in acetonitrile: -1158.352898 hartree
zero-point correction: + 0.182549 hartree
free energy correction: + 0.119446 hartree

**TS3/4**

| | | | |
|---|---|---|---|
| Au | -1.00085500 | 1.18591300 | -0.32372600 |
| Au | 1.02355500 | 2.92037100 | -0.20640200 |
| Au | 1.69715900 | 0.43531800 | 0.08457400 |
| Au | 2.41318300 | -2.07980900 | 0.41255500 |

| | | | |
|---|---|---|---|
| Au | -0.10862000 | -1.62585600 | -0.02691800 |
| C | -2.73054500 | 0.12415100 | -0.49747800 |
| C | -3.83541600 | 0.30809100 | 0.40926000 |
| H | -3.04192300 | -0.02515000 | -1.53198500 |
| C | -3.92641600 | 1.35951700 | 1.47724500 |
| N | -5.15691900 | 1.00135500 | 2.19700900 |
| C | -6.00359900 | 0.18235400 | 1.31864200 |
| C | -5.00257600 | -0.42591900 | 0.36143800 |
| C | -5.26953000 | -1.53766200 | -0.44947600 |
| O | -2.26940500 | -1.58403100 | -0.26766700 |
| C | -2.97979300 | -2.44246500 | -1.01908700 |
| C | -4.35544800 | -2.35914600 | -1.13662500 |
| C | -2.17907000 | -3.50464300 | -1.70229900 |
| H | -6.31032600 | -1.84194500 | -0.52788400 |
| H | -4.79268400 | -3.12475400 | -1.76856000 |
| H | -2.82038700 | -4.19303100 | -2.25345600 |
| H | -1.46252600 | -3.05104400 | -2.39642300 |
| H | -1.59974200 | -4.07671500 | -0.96833800 |
| H | -6.54378400 | -0.57194300 | 1.89976200 |
| H | -6.75359700 | 0.76499600 | 0.75508400 |
| H | -3.05555700 | 1.33741200 | 2.14352200 |
| H | -3.95560700 | 2.36550500 | 1.02435000 |
| H | -5.64513000 | 1.81482900 | 2.54999000 |

SCF energy: -1158.307164 hartree

SCF energy in acetonitrile: -1158.329874 hartree

zero-point correction: + 0.182412 hartree

free energy correction: + 0.123095 hartree

imaginary frequency: -316.88 *i* $cm^{-1}$

**IM4**

| | | | |
|---|---|---|---|
| Au | -1.11320700 | -1.08841600 | 0.14315600 |
| Au | 1.15077700 | -2.35326600 | 0.25277000 |
| Au | 1.18271700 | 0.33063500 | -0.28919600 |
| Au | -1.26144900 | 1.58354800 | -0.42603900 |
| Au | -3.46309500 | 0.08561300 | 0.05522800 |
| C | 2.50327300 | 2.02885500 | -0.71076200 |
| C | 3.37897400 | 0.93259700 | -0.70057800 |
| C | 3.89639400 | 0.22080600 | -1.95787500 |
| N | 5.33561500 | 0.05492400 | -1.70318300 |
| C | 5.42870000 | -0.19326500 | -0.25167500 |
| C | 4.31751000 | 0.63392500 | 0.37207800 |
| C | 4.20704400 | 1.00457000 | 1.66702500 |
| C | 3.10444200 | 1.75154600 | 2.23045900 |

| | | | |
|---|---|---|---|
| C | 2.30803700 | 2.62379400 | 1.58766200 |
| O | 2.54432800 | 3.01519500 | 0.26385000 |
| C | 1.16843600 | 3.37256000 | 2.18131600 |
| H | 2.14220500 | 2.43893000 | -1.64813500 |
| H | 3.44369100 | -0.76729500 | -2.06976800 |
| H | 3.71769900 | 0.78552600 | -2.87368700 |
| H | 5.79911700 | 0.93842700 | -1.90272500 |
| H | 5.26604500 | -1.26222100 | -0.06946300 |
| H | 6.41942400 | 0.06365000 | 0.12444100 |
| H | 4.95843000 | 0.65181100 | 2.36852000 |
| H | 1.03950000 | 3.12482700 | 3.23467600 |
| H | 1.33366100 | 4.44969400 | 2.07935600 |
| H | 0.24427300 | 3.13078700 | 1.64154800 |
| H | 2.89147200 | 1.59646700 | 3.28327300 |

SCF energy: -1158.323743 hartree

SCF energy in acetonitrile: -1158.343929 hartree

zero-point correction: + 0.185466 hartree

free energy correction: + 0.124216 hartree

**S3.4 $Au_6$**

$Au_6$

| | | | |
|---|---|---|---|
| Au | -1.53517900 | -0.47711500 | -0.00032100 |
| Au | -0.66913900 | -2.96257100 | 0.00011700 |
| Au | 1.18046000 | -1.09053000 | 0.00009700 |
| Au | 0.35433100 | 1.56794400 | 0.00016500 |
| Au | 2.90069300 | 0.90147600 | -0.00014000 |
| Au | -2.23116600 | 2.06079600 | 0.00008200 |

SCF energy: -814.374678 hartree

SCF energy in acetonitrile: -814.385867 hartree

zero-point correction: + 0.002616 hartree

free energy correction: -0.046424 hartree

**IM1**

| | | | |
|---|---|---|---|
| Au | 0.01321500 | -1.05163400 | -0.52557500 |
| Au | -1.73333300 | 0.92554000 | -0.92383200 |
| Au | 0.73135000 | 1.49210100 | -0.07222500 |
| Au | 2.62403000 | -0.53527100 | 0.38227400 |
| Au | 3.19024800 | 1.99889600 | 0.79216200 |
| Au | 1.78974600 | -2.98000900 | -0.10589000 |
| C | -3.52890300 | 1.61093600 | -2.03866000 |
| C | -3.91233400 | 1.57189400 | -0.86657300 |
| C | -4.68080100 | 1.64352500 | 0.40279900 |
| N | -6.05519900 | 2.08569200 | 0.23019600 |

| | | | |
|---|---|---|---|
| C | -6.91509100 | 1.17633700 | -0.54483000 |
| C | -7.16830700 | -0.10468200 | 0.16623900 |
| C | -6.81038600 | -1.39350100 | -0.08108500 |
| C | -7.37346100 | -2.18466500 | 0.96829000 |
| C | -8.03880000 | -1.32715300 | 1.78896800 |
| O | -7.92252500 | -0.05131400 | 1.30932800 |
| C | -8.82312200 | -1.49951500 | 3.03724900 |
| H | -3.45206700 | 1.73461500 | -3.09743900 |
| H | -4.68461800 | 0.65457600 | 0.86775500 |
| H | -4.16799700 | 2.32249600 | 1.08724200 |
| H | -6.07991500 | 3.01569700 | -0.17540900 |
| H | -7.85820800 | 1.70603000 | -0.70602900 |
| H | -6.49922600 | 0.92951500 | -1.53244600 |
| H | -6.21646100 | -1.73852300 | -0.91348600 |
| H | -8.84231800 | -2.55341500 | 3.31543600 |
| H | -8.38420900 | -0.93103400 | 3.86239300 |
| H | -9.85380900 | -1.15597400 | 2.90906500 |
| H | -7.29252700 | -3.25264700 | 1.09633900 |

SCF energy: -1294.064118 hartree

SCF energy in acetonitrile: -1294.084834 hartree

zero-point correction: + 0.183055 hartree

free energy correction: + 0.110951 hartree

**TS1/2**

| | | | |
|---|---|---|---|
| Au | -0.34023800 | -1.38387000 | -0.11476100 |
| Au | -2.74809900 | -2.52676800 | -0.04618700 |
| Au | -2.71082100 | 0.09886000 | 0.03783300 |
| Au | -0.18342300 | 1.30049000 | -0.03459500 |
| Au | -2.44119700 | 2.71204000 | 0.11075600 |
| Au | 2.04737400 | -0.17931300 | -0.14796400 |
| C | 4.13070800 | -0.32897000 | -0.31190900 |
| C | 4.85626700 | -0.44025500 | 0.73951500 |
| H | 4.49489900 | -0.30983300 | -1.33704100 |
| C | 4.80018800 | -0.52857600 | 2.22258800 |
| N | 5.92699300 | 0.26078700 | 2.71498700 |
| C | 7.12047400 | -0.22162600 | 2.02902700 |
| C | 6.80387900 | -0.29938000 | 0.55767300 |
| C | 7.12567300 | -1.34555700 | -0.32788400 |
| O | 6.91109200 | 0.89352400 | -0.16901400 |
| C | 7.04177500 | 0.56946400 | -1.46387600 |
| C | 7.19572000 | -0.80084000 | -1.60757900 |
| C | 7.04273100 | 1.68265200 | -2.44178600 |
| H | 7.18699700 | -2.38718000 | -0.05255100 |

| | | | |
|---|---|---|---|
| H | 7.33729800 | -1.32123100 | -2.54167200 |
| H | 7.17098900 | 1.29683900 | -3.45222700 |
| H | 6.10433500 | 2.24090300 | -2.38896700 |
| H | 7.85461500 | 2.38203100 | -2.22217800 |
| H | 7.95973700 | 0.45426800 | 2.20573700 |
| H | 7.42298000 | -1.23655600 | 2.33541300 |
| H | 3.85634000 | -0.10577300 | 2.57050600 |
| H | 4.84150900 | -1.58825000 | 2.53139400 |
| H | 6.02407000 | 0.18590200 | 3.72260500 |

SCF energy: -1294.041036 hartree

SCF energy in acetonitrile: -1294.065105 hartree

zero-point correction: + 0.182812 hartree

free energy correction: + 0.115023 hartree

imaginary frequency: -320.31 *i* $cm^{-1}$

**IM2**

| | | | |
|---|---|---|---|
| Au | -0.21403300 | 1.31864100 | -0.04796200 |
| Au | 2.06169400 | -0.11072700 | -0.17476300 |
| Au | -0.30793900 | -1.36385400 | -0.11480000 |
| Au | -2.70881400 | 0.06175400 | 0.03744600 |
| Au | -2.69443800 | -2.56351800 | -0.03378900 |
| Au | -2.51085600 | 2.68088400 | 0.09821200 |
| C | 4.11456200 | -0.25298600 | -0.28898700 |
| C | 4.92745300 | -0.34977800 | 0.73951200 |
| C | 4.68644900 | -0.37637600 | 2.22710400 |
| N | 5.85874000 | 0.31972000 | 2.76174100 |
| C | 7.00038500 | -0.24647400 | 2.06070900 |
| C | 6.55494900 | -0.31950500 | 0.59756200 |
| C | 6.99538000 | -1.40488700 | -0.26100900 |
| C | 7.26981100 | -0.89012000 | -1.50361100 |
| C | 7.17228200 | 0.50512200 | -1.39263800 |
| O | 6.88630500 | 0.87338000 | -0.15392800 |
| C | 7.39151500 | 1.57656300 | -2.38938400 |
| H | 4.52371200 | -0.26111900 | -1.30327800 |
| H | 3.76417400 | 0.14786800 | 2.47520700 |
| H | 4.60290200 | -1.41855900 | 2.58310700 |
| H | 5.94553000 | 0.22289100 | 3.76798900 |
| H | 7.89340400 | 0.37038900 | 2.17218900 |
| H | 7.24579200 | -1.27662600 | 2.36889900 |
| H | 6.96537600 | -2.44428200 | 0.02919300 |
| H | 6.48972700 | 2.18690800 | -2.48979400 |
| H | 8.19696700 | 2.23910700 | -2.05819300 |
| H | 7.64962400 | 1.15259200 | -3.35838300 |

| | | | |
|---|---|---|---|
| H | 7.52090700 | -1.42482400 | -2.40642800 |

SCF energy: -1294.044375 hartree
SCF energy in acetonitrile: -1294.073189 hartree
zero-point correction: + 0.183877 hartree
free energy correction: + 0.119212 hartree

**TS2/3**

| | | | |
|---|---|---|---|
| Au | -0.17710900 | 1.21951500 | 0.02923600 |
| Au | 2.03214200 | -0.32222400 | 0.28467600 |
| Au | -0.42813900 | -1.42357900 | 0.12214600 |
| Au | -2.76052700 | 0.13169400 | -0.12065300 |
| Au | -2.88345200 | -2.48891000 | -0.02195400 |
| Au | -2.37321100 | 2.73097900 | -0.19826600 |
| C | 4.05156800 | -0.49086000 | 0.39709900 |
| C | 4.97720500 | 0.50930600 | 0.39232700 |
| C | 4.70239800 | 2.00156200 | 0.33504700 |
| N | 6.04466400 | 2.58776600 | 0.19756500 |
| C | 6.98034300 | 1.69304600 | 0.85989000 |
| C | 6.40128900 | 0.33076100 | 0.53668700 |
| C | 7.01891900 | -0.89073300 | 1.06114600 |
| C | 7.69493800 | -1.65884600 | 0.19276400 |
| C | 7.69395400 | -1.05099200 | -1.13034500 |
| O | 7.12928900 | 0.05845200 | -1.20393900 |
| C | 8.31159800 | -1.68188600 | -2.33192000 |
| H | 4.47732800 | -1.49792200 | 0.43523300 |
| H | 4.07688100 | 2.26880000 | -0.51845700 |
| H | 4.17736400 | 2.31314500 | 1.25043100 |
| H | 6.10048500 | 3.53438100 | 0.55446700 |
| H | 8.00327200 | 1.82461900 | 0.50019400 |
| H | 6.99702000 | 1.76547500 | 1.96522000 |
| H | 6.88250700 | -1.14017500 | 2.10709900 |
| H | 7.81070000 | -2.63409600 | -2.53450300 |
| H | 8.22506500 | -1.02885100 | -3.19725000 |
| H | 9.36286400 | -1.90884900 | -2.13262300 |
| H | 8.17967300 | -2.59713300 | 0.42293200 |

SCF energy: -1294.029831 hartree
SCF energy in acetonitrile: -1294.062877 hartree
zero-point correction: + 0.182309 hartree
free energy correction: + 0.117229 hartree
imaginary frequency: -314.41 *i* $cm^{-1}$

**IM3**

| | | | |
|---|---|---|---|
| Au | 0.51961800 | 1.44931500 | -0.02525700 |

| | | | |
|---|---|---|---|
| Au | -1.91145600 | 0.36678700 | -0.43792700 |
| Au | 0.23987000 | -1.21608600 | -0.08733600 |
| Au | 2.81508600 | -0.14396900 | 0.09912500 |
| Au | 2.41746700 | -2.74181200 | 0.02452600 |
| Au | 2.96814700 | 2.47913000 | 0.15484500 |
| C | -3.86720100 | 0.60258700 | -0.08361600 |
| C | -4.75910300 | -0.38627500 | 0.28404500 |
| C | -4.46278200 | -1.87933700 | 0.37347300 |
| N | -5.69212600 | -2.46960300 | 0.90988000 |
| C | -6.77445700 | -1.59953600 | 0.42110200 |
| C | -6.15186400 | -0.21895000 | 0.38849100 |
| C | -6.77612400 | 1.05898600 | 0.50072600 |
| C | -8.08243900 | 1.43190800 | 0.42101800 |
| C | -9.24442600 | 0.64240000 | -0.03746500 |
| O | -9.13530400 | -0.43280100 | -0.60679900 |
| C | -10.59907600 | 1.27350300 | 0.20626600 |
| H | -4.17959800 | 1.63088900 | 0.12212800 |
| H | -4.25825100 | -2.27721100 | -0.62772800 |
| H | -3.60001500 | -2.10071400 | 1.00209100 |
| H | -5.66265100 | -2.41014200 | 1.92424900 |
| H | -7.07886500 | -1.90508800 | -0.58399100 |
| H | -7.66029300 | -1.66188500 | 1.05185000 |
| H | -6.08278600 | 1.86275000 | 0.74374000 |
| H | -10.66366500 | 2.23395700 | -0.31532300 |
| H | -11.38434000 | 0.61035000 | -0.15103900 |
| H | -10.74085500 | 1.47922900 | 1.27187600 |
| H | -8.30637700 | 2.45988500 | 0.69313300 |

SCF energy: -1294.043625 hartree

SCF energy in acetonitrile: -1294.066919 hartree

zero-point correction: + 0.182946 hartree

free energy correction: + 0.115999 hartree

imaginary frequency: -316.88 *i* $cm^{-1}$

**IM4**

| | | | |
|---|---|---|---|
| Au | -0.11556000 | -1.31244600 | -0.20521000 |
| Au | -2.44480500 | -2.56523000 | -0.04222500 |
| Au | -2.53232400 | 0.06184600 | 0.11420900 |
| Au | -0.04568800 | 1.37396100 | -0.05438500 |
| Au | -2.34351500 | 2.67612600 | 0.24413300 |
| Au | 2.20784900 | 0.01850700 | -0.33439200 |
| C | 4.43263200 | 0.12136600 | -1.00229000 |
| C | 4.45452100 | -0.93148800 | -0.12473900 |
| C | 4.19937100 | -2.41179300 | -0.45305300 |

| | | | |
|---|---|---|---|
| N | 4.58664400 | -3.15851200 | 0.76095000 |
| C | 4.47159400 | -2.19491200 | 1.87745700 |
| C | 4.91444600 | -0.88816600 | 1.25827600 |
| C | 5.84767500 | -0.03402100 | 1.72734500 |
| C | 6.49556200 | 1.01319700 | 0.96654300 |
| C | 6.04006700 | 1.63416200 | -0.13497200 |
| O | 4.74977900 | 1.43258100 | -0.63047300 |
| C | 6.75884200 | 2.70023900 | -0.88860300 |
| H | 4.36379200 | -0.01622000 | -2.07796700 |
| H | 3.14202700 | -2.59255300 | -0.66806600 |
| H | 4.77754600 | -2.74876200 | -1.31564200 |
| H | 5.56748500 | -3.41141200 | 0.67574200 |
| H | 3.42495000 | -2.15072700 | 2.19738200 |
| H | 5.07952400 | -2.50935800 | 2.72569200 |
| H | 6.23259600 | -0.20024000 | 2.73000000 |
| H | 7.72001200 | 2.92774500 | -0.42774500 |
| H | 6.92564100 | 2.39489900 | -1.92628900 |
| H | 6.14890300 | 3.60868700 | -0.91550500 |
| H | 7.47392300 | 1.32705200 | 1.31545000 |

SCF energy: -1294.080592 hartree

SCF energy in acetonitrile: -1294.102639 hartree

zero-point correction: + 0.185954 hartree

free energy correction: + 0.119449 hartree

**S3.5 $Au_7$**

$Au_7$

| | | | |
|---|---|---|---|
| Au | -0.94143700 | 0.59329800 | -0.00000600 |
| Au | -1.72187000 | -1.98832600 | -0.00016100 |
| Au | 0.89241000 | -1.62684000 | -0.00016100 |
| Au | 1.75870600 | 1.00699700 | -0.00000300 |
| Au | 3.46633100 | -1.00134500 | 0.00021000 |
| Au | 0.08265900 | 3.02654500 | -0.00011900 |
| Au | -3.53680000 | -0.01032900 | 0.00024100 |

SCF energy: -950.091334 hartree

SCF energy in acetonitrile: -950.103481 hartree

zero-point correction: + 0.003052 hartree

free energy correction: -0.052164 hartree

**IM1**

| | | | |
|---|---|---|---|
| Au | -0.11629300 | 0.17954900 | 0.29907900 |
| Au | 0.06127000 | -2.48426300 | 0.06673700 |
| Au | 2.37903400 | -1.28817600 | -0.28305300 |
| Au | 2.33417600 | 1.45523700 | -0.05330000 |

| | | | |
|---|---|---|---|
| Au | 4.57738000 | 0.16734100 | -0.59006300 |
| Au | 0.16059800 | 2.80895200 | 0.47749600 |
| Au | -2.33506600 | -1.18131300 | 0.55868800 |
| C | -4.16110400 | -2.42529800 | 0.68524100 |
| C | -4.55299600 | -1.28001400 | 0.93206500 |
| C | -5.29465500 | -0.02059700 | 1.19870400 |
| N | -5.14243200 | 1.01933400 | 0.19366100 |
| C | -5.62523800 | 0.65381300 | -1.14785500 |
| C | -7.10374800 | 0.49755700 | -1.19295300 |
| C | -7.92068400 | -0.56815700 | -1.41152600 |
| C | -9.26245000 | -0.07753700 | -1.35356100 |
| C | -9.17822500 | 1.25737700 | -1.10306000 |
| O | -7.86381200 | 1.62211700 | -1.00321200 |
| C | -10.18270000 | 2.33620800 | -0.92805500 |
| H | -4.11438000 | -3.48011900 | 0.51990200 |
| H | -6.35548300 | -0.28259600 | 1.27351700 |
| H | -4.98023600 | 0.37541000 | 2.16653000 |
| H | -4.16821900 | 1.30409900 | 0.13875900 |
| H | -5.31525100 | 1.45993400 | -1.81825700 |
| H | -5.18268000 | -0.27962800 | -1.52541000 |
| H | -7.60245900 | -1.58221200 | -1.59877900 |
| H | -11.18664600 | 1.92156200 | -1.02157500 |
| H | -10.09170200 | 2.80665200 | 0.05536300 |
| H | -10.05959100 | 3.11895700 | -1.68238300 |
| H | -10.17189400 | -0.64315400 | -1.48269700 |

SCF energy: -1429.779986 hartree

SCF energy in acetonitrile: -950.103481 hartree

zero-point correction: + 0.183334 hartree

free energy correction: +0.105967 hartree

**TS1/2**

| | | | |
|---|---|---|---|
| Au | 0.63675000 | -2.04875000 | 0.05601000 |
| Au | -1.95994600 | -1.59328000 | -0.03174400 |
| Au | -0.01776800 | 0.53611800 | 0.08497100 |
| Au | -2.74000100 | 1.06033800 | 0.00252000 |
| Au | 2.58284800 | -0.16765300 | 0.09875600 |
| Au | -0.97193700 | 3.00019900 | 0.10494400 |
| Au | -4.52235200 | -0.87580800 | -0.09864900 |
| C | 4.61221600 | 0.23739600 | 0.23569300 |
| C | 5.32746300 | 0.30834800 | -0.82146000 |
| C | 5.35738000 | 0.25037000 | -2.29637900 |
| N | 6.61848300 | -0.38129400 | -2.68302100 |
| C | 7.71014900 | 0.34812600 | -2.04303300 |

| | | | |
|---|---|---|---|
| C | 7.44087900 | 0.44221100 | -0.57092200 |
| C | 7.59595500 | 1.53654000 | 0.28225500 |
| C | 7.71723900 | 1.03004200 | 1.58511100 |
| C | 7.73356900 | -0.34384200 | 1.47831800 |
| O | 7.64377900 | -0.71033200 | 0.17936300 |
| C | 7.84819600 | -1.43396600 | 2.47591300 |
| H | 4.94455400 | 0.37184900 | 1.26033600 |
| H | 4.51694600 | -0.35242100 | -2.65117200 |
| H | 5.24125600 | 1.27197100 | -2.70027500 |
| H | 6.72850600 | -0.38610200 | -3.69233900 |
| H | 8.65180300 | -0.17619200 | -2.22383600 |
| H | 7.81809900 | 1.38355600 | -2.40713100 |
| H | 7.53788100 | 2.57116600 | -0.01791300 |
| H | 6.96689700 | -2.08110500 | 2.44775000 |
| H | 8.72200400 | -2.05849700 | 2.26811500 |
| H | 7.94541000 | -1.01553500 | 3.47728400 |
| H | 7.78886400 | 1.58967400 | 2.50461000 |

SCF energy: -1294.029831 hartree

SCF energy in acetonitrile: -1429.788327 hartree

zero-point correction: + 0.182810 hartree

free energy correction: + 0.109171 hartree

imaginary frequency: -339.13 *i* $cm^{-1}$

**IM2**

| | | | |
|---|---|---|---|
| Au | 0.33440900 | -2.33784900 | -0.19185000 |
| Au | -2.13435700 | -1.41250700 | -0.02612300 |
| Au | 0.04515600 | 0.33337800 | -0.10818500 |
| Au | -2.55217700 | 1.32867100 | 0.06699200 |
| Au | 2.51806200 | -0.77358800 | -0.21846200 |
| Au | -0.46496100 | 2.92068100 | -0.01023100 |
| Au | -4.56205300 | -0.37606000 | 0.13858000 |
| C | 4.51485800 | -0.51282300 | -0.32339200 |
| C | 5.32471700 | -0.33104000 | 0.71136000 |
| C | 4.98860500 | -0.30977800 | 2.18470800 |
| N | 6.16902300 | 0.30970300 | 2.79525800 |
| C | 7.31333700 | -0.19483700 | 2.04627900 |
| C | 6.85930200 | -0.08154000 | 0.58181800 |
| C | 7.59791700 | -0.89411500 | -0.41663000 |
| C | 8.07553800 | -0.05457600 | -1.40025000 |
| C | 7.73807800 | 1.25134700 | -1.05707300 |
| O | 7.07234100 | 1.29499000 | 0.11679200 |
| C | 7.99214300 | 2.54700800 | -1.72735000 |
| H | 4.92068900 | -0.51601700 | -1.33296700 |

| | | | |
|---|---|---|---|
| H | 4.08868400 | 0.27281000 | 2.39003500 |
| H | 4.81230700 | -1.34237600 | 2.53288000 |
| H | 6.24088000 | 0.10816200 | 3.78654000 |
| H | 8.21140600 | 0.39623700 | 2.23129800 |
| H | 7.54087900 | -1.25755800 | 2.23942400 |
| H | 7.66565300 | -1.97040000 | -0.37453100 |
| H | 7.05015800 | 3.05366500 | -1.96234500 |
| H | 8.56470200 | 3.21656800 | -1.07654700 |
| H | 8.54935200 | 2.39288300 | -2.65135700 |
| H | 8.62413100 | -0.33509000 | -2.28736500 |

SCF energy: -1429.784132 hartree

SCF energy in acetonitrile: -1429.813855 hartree

zero-point correction: + 0.183957 hartree

free energy correction: + 0.111208 hartree

**TS2/3**

| | | | |
|---|---|---|---|
| Au | 0.37265900 | -2.32017400 | -0.21385600 |
| Au | -2.08002200 | -1.39840300 | -0.02607800 |
| Au | 0.03956200 | 0.39810800 | -0.11299700 |
| Au | -2.62474300 | 1.31282300 | 0.09613800 |
| Au | 2.48682700 | -0.67816100 | -0.30760200 |
| Au | -0.60690100 | 2.97067200 | 0.02084400 |
| Au | -4.54721300 | -0.50164600 | 0.16197900 |
| C | 4.47019500 | -0.54460400 | -0.46000800 |
| C | 5.35911800 | -0.56427700 | 0.56015900 |
| C | 5.06422200 | -0.77492300 | 2.03071700 |
| N | 6.35517000 | -0.51034100 | 2.68204900 |
| C | 7.40322100 | -0.85643000 | 1.72722200 |
| C | 6.79859200 | -0.43654200 | 0.40047900 |
| C | 7.48119600 | -0.64733100 | -0.87148400 |
| C | 8.23374300 | 0.38911700 | -1.33446100 |
| C | 8.04206400 | 1.56091400 | -0.53989900 |
| O | 7.35213000 | 1.40474400 | 0.51440900 |
| C | 8.52388900 | 2.92972100 | -0.90817700 |
| H | 4.85495900 | -0.35614300 | -1.46155500 |
| H | 4.29847400 | -0.08953100 | 2.40155100 |
| H | 4.69739500 | -1.80304200 | 2.18163700 |
| H | 6.45443000 | -1.01508600 | 3.55520200 |
| H | 8.34140700 | -0.34631900 | 1.95087100 |
| H | 7.60807600 | -1.94137100 | 1.65721000 |
| H | 7.30116900 | -1.55408300 | -1.43702900 |
| H | 9.05916600 | 2.92254600 | -1.85793500 |
| H | 7.67097800 | 3.61039300 | -0.97622100 |

| | | | |
|---|---|---|---|
| H | 9.18502000 | 3.31674800 | -0.12754200 |
| H | 8.79495900 | 0.38210900 | -2.25881800 |

SCF energy: -1429.763612 hartree

SCF energy in acetonitrile:-1429.792471 hartree

zero-point correction: + 0.182047 hartree

free energy correction: + 0.107233 hartree

imaginary frequency: -514.67 *i* $cm^{-1}$

**IM3**

| | | | |
|---|---|---|---|
| Au | 0.20327900 | -2.38558200 | -0.14400700 |
| Au | -2.22126200 | -1.35078100 | 0.03232300 |
| Au | -0.04941900 | 0.32901800 | -0.14342300 |
| Au | -2.62695900 | 1.39302000 | 0.05415000 |
| Au | 2.36933500 | -0.84416200 | -0.34256200 |
| Au | -0.50797400 | 2.92967700 | -0.11470600 |
| Au | -4.63259900 | -0.31982500 | 0.21605200 |
| C | 4.32443100 | -0.51147800 | -0.53278700 |
| C | 5.19092100 | -0.30266000 | 0.49871800 |
| C | 4.82425700 | -0.30899600 | 1.97829400 |
| N | 6.09008500 | -0.48131000 | 2.69874200 |
| C | 7.10369700 | 0.15552300 | 1.83952900 |
| C | 6.59521100 | -0.01460700 | 0.41949100 |
| C | 7.30569800 | 0.02296600 | -0.79400400 |
| C | 8.60000400 | 0.37636100 | -1.10743000 |
| C | 9.62624500 | 1.01688300 | -0.28057800 |
| O | 9.41750600 | 1.47595300 | 0.83674200 |
| C | 11.00199800 | 1.12215800 | -0.91597800 |
| H | 4.67792700 | -0.47939200 | -1.56162100 |
| H | 4.37841600 | 0.65623600 | 2.24888500 |
| H | 4.10631800 | -1.08902800 | 2.23326400 |
| H | 6.29492000 | -1.47633000 | 2.74008700 |
| H | 7.18429600 | 1.21947200 | 2.08408500 |
| H | 8.08930600 | -0.27578500 | 2.00320000 |
| H | 6.72894700 | -0.32213300 | -1.64995200 |
| H | 10.94882900 | 1.70378200 | -1.84185300 |
| H | 11.68875500 | 1.60417600 | -0.22253700 |
| H | 11.38045700 | 0.13026500 | -1.18200100 |
| H | 8.89881500 | 0.19563100 | -2.13664700 |

SCF energy: -1429.796874 hartree

SCF energy in acetonitrile: -1429.832804 hartree

zero-point correction: + 0.182958 hartree

free energy correction: + 0.106778 hartree

**TS3/4**

| | | | |
|---|---|---|---|
| Au | 0.12475100 | 0.31375000 | -0.00226600 |
| Au | 0.48447500 | -2.34395600 | -0.29194300 |
| Au | -2.00341000 | -1.42883100 | -0.13425600 |
| Au | -2.47067400 | 1.30226600 | 0.18741900 |
| Au | -4.44359800 | -0.43917500 | 0.05645700 |
| Au | -0.37631300 | 2.88433400 | 0.29631200 |
| Au | 2.61881400 | -0.75458900 | -0.28132800 |
| C | 4.57919400 | -0.32163800 | -0.35501700 |
| C | 5.43852700 | -0.48326400 | 0.75085200 |
| C | 5.10058400 | -1.07211100 | 2.11122000 |
| N | 6.40252500 | -1.40285100 | 2.71682100 |
| C | 7.37874700 | -0.49761500 | 2.08510000 |
| C | 6.76566800 | -0.09530800 | 0.75341300 |
| C | 7.45714200 | 0.60024100 | -0.25814300 |
| C | 6.95408000 | 1.39373800 | -1.28022200 |
| C | 5.64642300 | 1.94301200 | -1.41776500 |
| O | 4.63739300 | 1.62309700 | -0.71543900 |
| C | 5.42329800 | 3.04195000 | -2.43252100 |
| H | 5.01837600 | -0.47516700 | -1.33907800 |
| H | 4.57973800 | -0.32300400 | 2.72327600 |
| H | 4.45886200 | -1.95268700 | 2.05752500 |
| H | 6.63590300 | -2.35251500 | 2.44296500 |
| H | 7.51727900 | 0.39094000 | 2.71483900 |
| H | 8.35575100 | -0.97896100 | 1.98685400 |
| H | 8.54361800 | 0.54556800 | -0.20774100 |
| H | 4.67374000 | 2.71385000 | -3.15866200 |
| H | 5.02139300 | 3.92679100 | -1.93214200 |
| H | 6.33934200 | 3.31275200 | -2.95809700 |
| H | 7.68756900 | 1.80343900 | -1.96652100 |

SCF energy: -1429.775120 hartree

SCF energy in acetonitrile: -1429.809200 hartree

zero-point correction: + 0.183386 hartree

free energy correction: + 0.109775 hartree

imaginary frequency: -345.53 *i* $cm^{-1}$

**IM4**

| | | | |
|---|---|---|---|
| Au | 0.77679900 | -2.04252600 | 0.27861600 |
| Au | -1.81644700 | -1.63468800 | 0.06525900 |
| Au | 0.20266000 | 0.54835600 | 0.08303800 |
| Au | -2.51660800 | 1.02373000 | -0.15803300 |
| Au | 2.73731100 | -0.11602600 | 0.33972400 |
| Au | -0.78482800 | 2.99007000 | -0.15217300 |

| | | | |
|---|---|---|---|
| Au | -4.35498700 | -0.86696400 | -0.17067300 |
| C | 4.86774500 | -0.91123000 | 0.57063500 |
| C | 5.02976300 | 0.45685100 | 0.53268200 |
| C | 5.05417700 | 1.40316400 | 1.74853700 |
| N | 5.52911900 | 2.70170700 | 1.22871400 |
| C | 5.23368300 | 2.69099000 | -0.22034400 |
| C | 5.46718000 | 1.24944800 | -0.61245800 |
| C | 6.24290000 | 0.78846100 | -1.61412500 |
| C | 6.72337900 | -0.56933800 | -1.76382900 |
| C | 6.21817100 | -1.69818600 | -1.23716300 |
| O | 5.01548200 | -1.75164100 | -0.53373200 |
| C | 6.78076400 | -3.06406100 | -1.43727400 |
| H | 4.83887900 | -1.45573700 | 1.51040700 |
| H | 4.05858900 | 1.52382400 | 2.18251500 |
| H | 5.71836600 | 1.03758900 | 2.53438200 |
| H | 6.53941000 | 2.73300800 | 1.33380000 |
| H | 4.18799500 | 2.98180000 | -0.36987000 |
| H | 5.86912900 | 3.39974800 | -0.75103700 |
| H | 6.63066700 | 1.50840100 | -2.32993600 |
| H | 7.65775000 | -3.03695900 | -2.08359100 |
| H | 7.05867400 | -3.51123000 | -0.47770500 |
| H | 6.02296800 | -3.71350400 | -1.88659200 |
| H | 7.61521400 | -0.69650200 | -2.36835700 |

SCF energy: -1429.797805 hartree

SCF energy in acetonitrile: -1429.822319 hartree

zero-point correction: + 0.186330 hartree

free energy correction: + 0.112945 hartree

**S3.6 $Au_8$**

$Au_8$

| | | | |
|---|---|---|---|
| Au | 2.55315700 | -2.55315700 | 0.00000000 |
| Au | 0.00000000 | -1.94787800 | -0.00033900 |
| Au | 1.94787800 | 0.00000000 | 0.00033900 |
| Au | -1.94787800 | 0.00000000 | 0.00033900 |
| Au | 0.00000000 | 1.94787800 | -0.00033900 |
| Au | 2.55315700 | 2.55315700 | 0.00000000 |
| Au | -2.55315700 | 2.55315700 | 0.00000000 |
| Au | -2.55315700 | -2.55315700 | 0.00000000 |

SCF energy: -1085.855893 hartree

SCF energy in acetonitrile: -1085.871822 hartree

zero-point correction: + 0.003619 hartree

free energy correction: -0.055024 hartree

**IM1**

| | | | |
|---|---|---|---|
| Au | -2.50915500 | -1.02858400 | -0.96079600 |
| Au | -0.73213900 | 0.90133300 | -0.54683900 |
| Au | -0.01779200 | -1.65954300 | -0.30678700 |
| Au | 1.82791300 | 1.73811700 | 0.09986700 |
| Au | 2.56924900 | -0.90813500 | 0.35133400 |
| Au | 1.85775500 | -3.43307600 | 0.22921900 |
| Au | 4.27728000 | 1.04845200 | 0.74988000 |
| Au | -0.08710900 | 3.45476100 | -0.43869700 |
| C | -4.40945500 | -1.57187200 | -1.93204800 |
| C | -4.70852600 | -1.61149400 | -0.73606400 |
| C | -5.29258300 | -1.66297700 | 0.62699900 |
| N | -5.15370300 | -0.44914800 | 1.41489600 |
| C | -5.80602400 | 0.73831400 | 0.84026000 |
| C | -7.28884700 | 0.62049100 | 0.83375600 |
| C | -8.21244200 | 0.54933200 | -0.16273700 |
| C | -9.49345800 | 0.47089300 | 0.46791200 |
| C | -9.26904300 | 0.49859900 | 1.80975600 |
| O | -7.92539500 | 0.59091400 | 2.04708700 |
| C | -10.15289700 | 0.45222500 | 3.00146100 |
| H | -4.44471200 | -1.62460000 | -2.99924000 |
| H | -6.35869500 | -1.88469800 | 0.50922200 |
| H | -4.83898500 | -2.49262300 | 1.17331200 |
| H | -4.17022000 | -0.25377000 | 1.57922400 |
| H | -5.50114600 | 1.58713000 | 1.45823800 |
| H | -5.48682400 | 0.94835400 | -0.19112400 |
| H | -8.00403000 | 0.55887300 | -1.22158600 |
| H | -11.19352300 | 0.38199200 | 2.68407700 |
| H | -9.92324800 | -0.41169700 | 3.63205900 |
| H | -10.03758200 | 1.35032200 | 3.61528100 |
| H | -10.45642700 | 0.40372600 | -0.01362600 |

SCF energy: -1565.550297 hartree

SCF energy in acetonitrile: -1565.575221 hartree

zero-point correction: + 0.184068 hartree

free energy correction: +0.106178 hartree

**TS1/2**

| | | | |
|---|---|---|---|
| Au | 2.77680300 | -0.23062100 | -0.12202900 |
| Au | 0.39898100 | -1.42728700 | -0.11234400 |
| Au | 0.55329700 | 1.23974000 | -0.08383100 |
| Au | -2.35264700 | -1.27454800 | 0.00850300 |
| Au | -2.19405800 | 1.47436600 | 0.03882300 |
| Au | -0.64581000 | 3.59826500 | -0.02784900 |

| | | | |
|---|---|---|---|
| Au | -4.50676700 | 0.22827500 | 0.14800500 |
| Au | -1.11753600 | -3.59464300 | -0.10606000 |
| C | 4.84925000 | -0.39517000 | -0.25312100 |
| C | 5.55779100 | -0.43331100 | 0.81429500 |
| C | 5.50262400 | -0.44481400 | 2.29861000 |
| N | 6.60160300 | 0.40387200 | 2.75261600 |
| C | 7.81644300 | -0.08163500 | 2.10684000 |
| C | 7.52108300 | -0.25264500 | 0.64023800 |
| C | 7.84952800 | -1.34551500 | -0.18079900 |
| C | 7.91535300 | -0.87741400 | -1.49143600 |
| C | 7.74399600 | 0.49649600 | -1.42892400 |
| O | 7.60525700 | 0.89458900 | -0.15624800 |
| C | 7.72782700 | 1.54899300 | -2.47161700 |
| H | 5.22916300 | -0.43292500 | -1.27187200 |
| H | 4.54442100 | -0.03256900 | 2.61917200 |
| H | 5.57303200 | -1.48485700 | 2.66332700 |
| H | 6.69025400 | 0.39125100 | 3.76373500 |
| H | 8.63287100 | 0.62878000 | 2.25263300 |
| H | 8.14571900 | -1.06729800 | 2.47471500 |
| H | 7.92530000 | -2.36774700 | 0.15671200 |
| H | 6.77838300 | 2.09051800 | -2.45468500 |
| H | 8.52490500 | 2.27590900 | -2.29134200 |
| H | 7.86755000 | 1.10597400 | -3.45670700 |
| H | 8.06309500 | -1.45103300 | -2.39269900 |

SCF energy: -1565.527286 hartree

SCF energy in acetonitrile: -1565.556603 hartree

zero-point correction: + 0.183931 hartree

free energy correction: + 0.106142 hartree

imaginary frequency: -315.60 *i* $cm^{-1}$

**IM2**

| | | | |
|---|---|---|---|
| Au | 2.78939200 | 0.06276200 | 0.16314600 |
| Au | 0.48283700 | 1.40190300 | 0.11576100 |
| Au | 0.46114900 | -1.26115500 | 0.09136000 |
| Au | -2.25493200 | 1.29744800 | -0.00724900 |
| Au | -2.29346800 | -1.45314800 | -0.03493300 |
| Au | -0.78504000 | -3.60305100 | 0.02339400 |
| Au | -4.51364700 | -0.05074700 | -0.13310800 |
| Au | -0.98172500 | 3.60692600 | 0.08252700 |
| C | 4.82747500 | 0.23792000 | 0.24086500 |
| C | 5.63042600 | 0.27699700 | -0.80248200 |
| C | 5.36808100 | 0.22241600 | -2.28609400 |
| N | 6.54178300 | -0.48830700 | -2.79824700 |

| | | | |
|---|---|---|---|
| C | 7.68471700 | 0.12764400 | -2.14379200 |
| C | 7.25148100 | 0.27093900 | -0.68158700 |
| C | 7.66921700 | 1.41246200 | 0.11297800 |
| C | 7.97674900 | 0.97525000 | 1.37661900 |
| C | 7.92107100 | -0.42732200 | 1.33994700 |
| O | 7.62218800 | -0.87090700 | 0.13272200 |
| C | 8.18784700 | -1.43402200 | 2.39082300 |
| H | 5.25101000 | 0.31461200 | 1.24623100 |
| H | 4.44912800 | -0.32594100 | -2.49035100 |
| H | 5.26539500 | 1.24206900 | -2.69731300 |
| H | 6.61504700 | -0.44673400 | -3.80934100 |
| H | 8.58421800 | -0.48352200 | -2.23232000 |
| H | 7.91386400 | 1.14305800 | -2.50825900 |
| H | 7.60774400 | 2.43296400 | -0.23407600 |
| H | 7.29551800 | -2.04355600 | 2.55901800 |
| H | 8.98616700 | -2.10908100 | 2.06893000 |
| H | 8.47537800 | -0.95085500 | 3.32297400 |
| H | 8.22358900 | 1.56456300 | 2.24586200 |

SCF energy: -1565.531286 hartree

SCF energy in acetonitrile: -1565.566507 hartree

zero-point correction: + 0.185120 hartree

free energy correction: + 0.106971 hartree

**TS2/3**

| | | | |
|---|---|---|---|
| Au | 2.76521100 | -0.30879000 | -0.26270800 |
| Au | 0.31858800 | -1.40647800 | -0.18034000 |
| Au | 0.56321200 | 1.21523400 | -0.13502800 |
| Au | -2.43150100 | -1.24723400 | 0.02178100 |
| Au | -2.17309500 | 1.49165000 | 0.06734100 |
| Au | -0.59330200 | 3.59920200 | -0.01150900 |
| Au | -4.52951200 | 0.32812700 | 0.22703200 |
| Au | -1.20993300 | -3.57487500 | -0.13710700 |
| C | 4.77407500 | -0.45119900 | -0.36886700 |
| C | 5.64881100 | -0.54183600 | 0.66992500 |
| C | 5.31073900 | -0.56754300 | 2.14970300 |
| N | 6.62987100 | -0.50258000 | 2.79863700 |
| C | 7.58287700 | -1.14656500 | 1.90949300 |
| C | 7.08198900 | -0.71261600 | 0.54419400 |
| C | 7.71932700 | -1.21019600 | -0.67952700 |
| C | 8.44702700 | -0.32445100 | -1.37746500 |
| C | 8.45608500 | 0.95535600 | -0.68684300 |
| O | 7.84402700 | 0.96866300 | 0.40260200 |
| C | 9.12728100 | 2.18060400 | -1.20229900 |

| | | | |
|---|---|---|---|
| H | 5.23738300 | -0.45060300 | -1.35974100 |
| H | 4.69620100 | 0.28510900 | 2.44324800 |
| H | 4.75048800 | -1.48538200 | 2.38235200 |
| H | 6.63469600 | -0.90993700 | 3.72643800 |
| H | 8.61077300 | -0.83731900 | 2.11221500 |
| H | 7.55292600 | -2.25353300 | 1.91030000 |
| H | 7.55726900 | -2.23828900 | -0.98107700 |
| H | 9.03291000 | 3.00039800 | -0.49403000 |
| H | 10.18205000 | 1.96926100 | -1.40009600 |
| H | 8.67197500 | 2.46091600 | -2.15771300 |
| H | 8.95909400 | -0.51110600 | -2.31052000 |

SCF energy: -1565.519703 hartree

SCF energy in acetonitrile: -1565.557851 hartree

zero-point correction: + 0.183798 hartree

free energy correction: + 0.106000 hartree

imaginary frequency: -325.72 *i* $cm^{-1}$

**IM3**

| | | | |
|---|---|---|---|
| Au | -2.66070500 | -0.18731200 | -0.36483800 |
| Au | -0.15620700 | -1.13672100 | -0.15092400 |
| Au | -0.56703600 | 1.45242700 | -0.20017000 |
| Au | 2.57392400 | -1.53085100 | 0.08145600 |
| Au | 2.14145800 | 1.19079900 | 0.03420900 |
| Au | 0.99671200 | 3.57962500 | -0.08082900 |
| Au | 4.56497100 | 0.16049800 | 0.25844000 |
| Au | 0.90872000 | -3.55365000 | -0.05925400 |
| C | -4.62496400 | 0.08136000 | -0.50431000 |
| C | -5.50677300 | 0.24335300 | 0.55284800 |
| C | -5.13115900 | 0.26141600 | 2.02958800 |
| N | -6.36609000 | 0.63936100 | 2.72368100 |
| C | -7.45133500 | 0.11693700 | 1.87791600 |
| C | -6.90851400 | 0.21582200 | 0.46712500 |
| C | -7.61524400 | 0.32460200 | -0.76890400 |
| C | -8.92645600 | 0.13437700 | -1.07691400 |
| C | -10.00101200 | -0.45379900 | -0.24874400 |
| O | -9.78511400 | -1.05640100 | 0.79113200 |
| C | -11.40411900 | -0.29835900 | -0.79592900 |
| H | -5.02263900 | 0.29580300 | -1.49984800 |
| H | -4.81164200 | -0.73968700 | 2.34334300 |
| H | -4.31621600 | 0.95171400 | 2.24770400 |
| H | -6.42851300 | 1.65382400 | 2.73932100 |
| H | -7.65731600 | -0.92744700 | 2.13018400 |
| H | -8.38072800 | 0.66528000 | 2.02678100 |

| | | | |
|---|---|---|---|
| H | -6.99584200 | 0.66532500 | -1.59653800 |
| H | -11.48102100 | -0.78837200 | -1.77202500 |
| H | -12.11976100 | -0.74260800 | -0.10704700 |
| H | -11.64143900 | 0.75884900 | -0.95045400 |
| H | -9.22897300 | 0.41828700 | -2.08136800 |

SCF energy: -1565.533128 hartree

SCF energy in acetonitrile: -1565.560510 hartree

zero-point correction: + 0.184309 hartree

free energy correction: + 0.104788 hartree

**TS3/4**

| | | | |
|---|---|---|---|
| Au | 2.83274900 | 0.03059600 | -0.14863600 |
| Au | 0.38765300 | 1.13076400 | 0.00200700 |
| Au | 0.63304600 | -1.47571200 | -0.18061600 |
| Au | -2.35167300 | 1.54707700 | 0.11902000 |
| Au | -2.08338600 | -1.18931300 | -0.06566600 |
| Au | -0.95980600 | -3.58036500 | -0.27079000 |
| Au | -4.44725900 | -0.02463000 | 0.10740000 |
| Au | -0.66180500 | 3.55146300 | 0.17926200 |
| C | 4.77638600 | -0.38159800 | -0.19285300 |
| C | 5.56793600 | -0.70654800 | 0.90868800 |
| C | 5.07037000 | -0.99284500 | 2.32622100 |
| N | 6.22711600 | -1.56610400 | 3.02338900 |
| C | 7.40695900 | -1.01476700 | 2.34463000 |
| C | 6.94924200 | -0.72433300 | 0.92664800 |
| C | 7.86226000 | -0.53616200 | -0.15761900 |
| C | 7.79689800 | 0.27174200 | -1.25060600 |
| C | 6.91647800 | 1.43404600 | -1.49921200 |
| O | 5.94337200 | 1.72799600 | -0.81579300 |
| C | 7.34046200 | 2.31783600 | -2.65391000 |
| H | 5.21122200 | -0.62810600 | -1.16463200 |
| H | 4.76782100 | -0.04979300 | 2.79792500 |
| H | 4.21432700 | -1.66643700 | 2.35239200 |
| H | 6.21684000 | -2.57240500 | 2.88608700 |
| H | 7.71430800 | -0.07976800 | 2.83149300 |
| H | 8.25934400 | -1.69821400 | 2.39132100 |
| H | 8.76787700 | -1.13751200 | -0.07385000 |
| H | 7.35363000 | 1.73503200 | -3.58114800 |
| H | 6.64785500 | 3.15105400 | -2.75277000 |
| H | 8.35555100 | 2.69564400 | -2.49883500 |
| H | 8.62054300 | 0.18440100 | -1.95379700 |

SCF energy: -1565.526499 hartree

SCF energy in acetonitrile: -1565.555353 hartree

zero-point correction: + 0.183921 hartree
free energy correction: + 0.105971 hartree
imaginary frequency: -26.65 *i* $cm^{-1}$

**IM4**

| | | | |
|---|---|---|---|
| Au | 2.89469600 | 0.44632000 | -0.22725100 |
| Au | 0.46586600 | 1.50110100 | -0.14175100 |
| Au | 0.76769400 | -1.13703300 | -0.03287300 |
| Au | -2.28181400 | 1.19194000 | 0.01295700 |
| Au | -1.96971300 | -1.54933500 | 0.11079600 |
| Au | -0.27392800 | -3.55553200 | 0.11780300 |
| Au | -4.34421800 | -0.42979700 | 0.17876800 |
| Au | -1.16870800 | 3.56800600 | -0.14545000 |
| C | 5.00727900 | 1.27262200 | 0.00005400 |
| C | 5.17759000 | 0.12886800 | -0.74808600 |
| C | 5.19121300 | 0.04053000 | -2.28691000 |
| N | 5.68416200 | -1.31598200 | -2.60006400 |
| C | 5.39787100 | -2.13575000 | -1.40263600 |
| C | 5.62778700 | -1.17261800 | -0.25989100 |
| C | 6.40956400 | -1.35750200 | 0.82230400 |
| C | 6.88418200 | -0.32313900 | 1.71800900 |
| C | 6.37054200 | 0.90059600 | 1.93105600 |
| O | 5.16614200 | 1.34195300 | 1.38606600 |
| C | 6.92614300 | 1.90850900 | 2.87858800 |
| H | 4.95672900 | 2.25446300 | -0.46305700 |
| H | 4.18964200 | 0.17124700 | -2.70266100 |
| H | 5.84017600 | 0.79752000 | -2.73184800 |
| H | 6.69415800 | -1.26833800 | -2.70304400 |
| H | 4.35499900 | -2.46802200 | -1.44427000 |
| H | 6.04047200 | -3.01546700 | -1.37185600 |
| H | 6.80573500 | -2.35391600 | 0.99935900 |
| H | 7.80579400 | 1.52161900 | 3.39248300 |
| H | 7.19699500 | 2.82753400 | 2.34956000 |
| H | 6.16582600 | 2.17636600 | 3.61889100 |
| H | 7.77801400 | -0.55729300 | 2.28652300 |

SCF energy: -1565.566473 hartree
SCF energy in acetonitrile: -1565.592714 hartree
zero-point correction: + 0.187051 hartree
free energy correction: + 0.109588 hartree

**S3.7 $Au_9$**

$Au_9$

| | | | |
|---|---|---|---|
| Au | 0.00000000 | 0.93020800 | 0.00000000 |

| | | | |
|---|---|---|---|
| Au | 2.31319900 | -0.44384200 | 0.00000000 |
| Au | 0.00000900 | -1.97789400 | 0.00000000 |
| Au | 2.37180900 | 2.23134000 | 0.00000000 |
| Au | 0.00000300 | 3.61317800 | 0.00000000 |
| Au | -2.31322200 | -0.44380400 | 0.00000000 |
| Au | -2.37179000 | 2.23137200 | 0.00000000 |
| Au | -2.41586200 | -3.07025500 | 0.00000000 |
| Au | 2.41585600 | -3.07030300 | 0.00000000 |

SCF energy: -1221.580883 hartree

SCF energy in acetonitrile: -1221.595552 hartree

zero-point correction: + 0.004176 hartree

free energy correction: -0.059885 hartree

**IM1**

| | | | |
|---|---|---|---|
| Au | -1.41190300 | -0.68639500 | -0.02352800 |
| Au | -2.43313800 | 1.80312000 | 0.31971200 |
| Au | 0.34120400 | 1.62005200 | -0.11769800 |
| Au | -4.04329400 | -0.32872900 | 0.40231900 |
| Au | -2.98523800 | -2.85648000 | 0.05638300 |
| Au | 1.23340800 | -0.89993100 | -0.44034200 |
| Au | -0.28515900 | -3.13226600 | -0.37081000 |
| Au | 2.92143500 | 1.17549100 | -0.55479500 |
| Au | -0.88407300 | 3.93142800 | 0.24901900 |
| C | 4.77502800 | 2.31071900 | -0.73268000 |
| C | 5.12436300 | 1.14059300 | -0.94538100 |
| C | 5.91027600 | -0.08554500 | -1.24386200 |
| N | 7.33722800 | 0.15564200 | -1.38083700 |
| C | 8.02244300 | 0.60303400 | -0.15703900 |
| C | 8.03418000 | -0.44396800 | 0.89850500 |
| C | 7.43912700 | -0.54142000 | 2.11774100 |
| C | 7.84227300 | -1.79593900 | 2.67227000 |
| C | 8.65801800 | -2.38363900 | 1.75526200 |
| O | 8.78500100 | -1.56682600 | 0.66529200 |
| C | 9.39748000 | -3.66986600 | 1.71167300 |
| H | 4.79267400 | 3.37269600 | -0.60428700 |
| H | 5.75255800 | -0.81039900 | -0.44174800 |
| H | 5.53052700 | -0.53096900 | -2.16585000 |
| H | 7.51818000 | 0.80617200 | -2.13854800 |
| H | 9.04679100 | 0.84985100 | -0.44993200 |
| H | 7.57425900 | 1.50675000 | 0.28040600 |
| H | 6.79050800 | 0.19430000 | 2.56790600 |
| H | 9.21470300 | -4.22920500 | 2.62934500 |
| H | 9.07806300 | -4.28181800 | 0.86304300 |

| | | | |
|---|---|---|---|
| H | 10.47466000 | -3.50514000 | 1.61492800 |
| H | 7.56133100 | -2.20790900 | 3.62876200 |

SCF energy: -1701.273581 hartree
SCF energy in acetonitrile: -1701.298000 hartree
zero-point correction: + 0.184700 hartree
free energy correction: + 0.099623 hartree

**TS1/2**

| | | | |
|---|---|---|---|
| Au | -1.61958700 | -0.40692300 | 0.00408100 |
| Au | -1.68412200 | 2.30909800 | 0.00269300 |
| Au | 0.83470100 | 1.09419200 | 0.09790100 |
| Au | -3.96405400 | 0.91590700 | -0.09317100 |
| Au | -3.90080100 | -1.83471900 | -0.08086700 |
| Au | 0.76526100 | -1.62148600 | 0.09740100 |
| Au | -1.48810900 | -3.12292900 | 0.01925100 |
| Au | 3.09856200 | -0.33765300 | 0.12129300 |
| Au | 0.53216100 | 3.73303000 | 0.09803500 |
| C | 5.17201000 | -0.24586500 | 0.24494000 |
| C | 5.86532700 | -0.24683100 | -0.82926700 |
| C | 5.83959600 | -0.24386100 | -2.30990300 |
| N | 6.92097200 | -1.12146600 | -2.75130700 |
| C | 8.15208800 | -0.65911900 | -2.11654900 |
| C | 7.89312400 | -0.49178000 | -0.64622400 |
| C | 8.23667500 | 0.58399300 | 0.18226200 |
| C | 8.28245400 | 0.10097500 | 1.49261600 |
| C | 8.07293300 | -1.26377200 | 1.41856200 |
| O | 7.92305500 | -1.64489800 | 0.13706900 |
| C | 8.01891300 | -2.32771700 | 2.44848900 |
| H | 5.54961100 | -0.20826100 | 1.26320100 |
| H | 4.87639000 | -0.63360700 | -2.64595200 |
| H | 5.93909200 | 0.79316000 | -2.67629700 |
| H | 7.00748400 | -1.12085900 | -3.76282400 |
| H | 8.95157300 | -1.38451100 | -2.28286800 |
| H | 8.49368200 | 0.32180600 | -2.48570800 |
| H | 8.34590700 | 1.60619100 | -0.14568000 |
| H | 7.05118700 | -2.83602300 | 2.42679200 |
| H | 8.79048500 | -3.08034300 | 2.26260500 |
| H | 8.17284900 | -1.90041000 | 3.43854200 |
| H | 8.44487200 | 0.66333800 | 2.39849500 |

SCF energy: -1701.254047 hartree
SCF energy in acetonitrile: -1701.280279 hartree
zero-point correction: + 0.184310 hartree
free energy correction: + 0.102470 hartree

imaginary frequency: -336.01 *i* $cm^{-1}$

**IM2**

| | | | |
|---|---|---|---|
| Au | -1.66631900 | -0.26725400 | -0.01290900 |
| Au | -1.27253200 | 2.43038400 | 0.07119200 |
| Au | 0.95407800 | 0.77463600 | -0.11190300 |
| Au | -3.75692200 | 1.45162900 | 0.16656800 |
| Au | -4.14983900 | -1.26547300 | 0.07364000 |
| Au | 0.44312600 | -1.89116700 | -0.19156000 |
| Au | -2.06732700 | -2.98112600 | -0.09583300 |
| Au | 2.96184300 | -1.00190800 | -0.25166900 |
| Au | 1.16608100 | 3.42718700 | -0.01915600 |
| C | 4.98312400 | -0.98564000 | -0.36867100 |
| C | 5.81587300 | -1.15592900 | 0.64994100 |
| C | 5.49932400 | -1.37903700 | 2.11247200 |
| N | 6.76323100 | -1.06560800 | 2.78618800 |
| C | 7.81161200 | -1.58680800 | 1.92288200 |
| C | 7.37430900 | -1.12430400 | 0.52356200 |
| C | 7.96900000 | -1.81674600 | -0.63716000 |
| C | 8.54768200 | -0.88897000 | -1.46442200 |
| C | 8.41120100 | 0.36570500 | -0.85553100 |
| O | 7.79480100 | 0.27294400 | 0.32226400 |
| C | 8.83423500 | 1.71432800 | -1.29442500 |
| H | 5.38881800 | -0.83463700 | -1.36806300 |
| H | 4.69789300 | -0.72387400 | 2.45710000 |
| H | 5.17702000 | -2.42336700 | 2.26364700 |
| H | 6.81113200 | -1.45034900 | 3.72326500 |
| H | 8.79326200 | -1.19159900 | 2.18879100 |
| H | 7.86789200 | -2.68887100 | 1.89554700 |
| H | 7.87778000 | -2.87976200 | -0.80132400 |
| H | 7.96440900 | 2.37120500 | -1.39561600 |
| H | 9.49755500 | 2.16949000 | -0.55215900 |
| H | 9.35242900 | 1.66026900 | -2.25108900 |
| H | 9.02959300 | -1.06416300 | -2.41452000 |

SCF energy: -1701.266088 hartree
SCF energy in acetonitrile: -1701.291664 hartree
zero-point correction: + 0.185406 hartree
free energy correction: + 0.103336 hartree

**TS2/3**

| | | | |
|---|---|---|---|
| Au | -1.67434600 | -0.28560700 | -0.01215400 |
| Au | -1.39349800 | 2.43295200 | 0.07727800 |
| Au | 0.92031900 | 0.84518800 | -0.12334500 |

| | | | |
|---|---|---|---|
| Au | -3.82446500 | 1.33803900 | 0.17970500 |
| Au | -4.10854000 | -1.39990300 | 0.08022400 |
| Au | 0.49257000 | -1.82183100 | -0.19803900 |
| Au | -1.94072900 | -3.02819400 | -0.10030500 |
| Au | 2.98527600 | -0.85779300 | -0.28172000 |
| Au | 1.01077300 | 3.50071000 | -0.02493500 |
| C | 4.97552000 | -1.04320300 | -0.40111200 |
| C | 5.85216800 | -1.18105700 | 0.63031700 |
| C | 5.52133300 | -1.26524300 | 2.10755400 |
| N | 6.84334200 | -1.25672100 | 2.75333600 |
| C | 7.79290600 | -1.84521300 | 1.81886700 |
| C | 7.27575000 | -1.35737500 | 0.48150300 |
| C | 7.91644300 | -1.74833700 | -0.77880000 |
| C | 8.73346300 | -0.84708600 | -1.35760300 |
| C | 8.75783700 | 0.38831700 | -0.60224700 |
| O | 8.11811700 | 0.36927900 | 0.47581400 |
| C | 9.45310300 | 1.62936800 | -1.05728200 |
| H | 5.41969200 | -0.98602800 | -1.39680400 |
| H | 4.92414400 | -0.41535300 | 2.44416900 |
| H | 4.94269100 | -2.18172100 | 2.29968000 |
| H | 6.84341400 | -1.73084600 | 3.64873800 |
| H | 8.81880200 | -1.53203900 | 2.02341000 |
| H | 7.77631900 | -2.95147300 | 1.77703300 |
| H | 7.68138700 | -2.71224600 | -1.21491800 |
| H | 9.04319800 | 1.95038700 | -2.02022300 |
| H | 9.33275300 | 2.42437600 | -0.32457100 |
| H | 10.51632500 | 1.42405500 | -1.21250200 |
| H | 9.26027800 | -0.98855700 | -2.29109400 |

SCF energy: -1701.250252 hartree
SCF energy in acetonitrile: -1701.281202 hartree
zero-point correction: + 0.183755 hartree
free energy correction: + 0.101751 hartree
imaginary frequency: -429.04 *i* $cm^{-1}$

**IM3**

| | | | |
|---|---|---|---|
| Au | -1.73048200 | -0.22146700 | -0.00412300 |
| Au | -1.19057400 | 2.44704600 | 0.02516800 |
| Au | 0.91661000 | 0.65321800 | -0.16230100 |
| Au | -3.73329100 | 1.63154000 | 0.16879800 |
| Au | -4.23800700 | -1.06866400 | 0.14826000 |
| Au | 0.24515600 | -1.99378900 | -0.17134300 |
| Au | -2.32529400 | -2.93814700 | -0.02253300 |
| Au | 2.79478800 | -1.21519600 | -0.35279600 |

| | | | |
|---|---|---|---|
| Au | 1.28777300 | 3.29775600 | -0.11215900 |
| C | 4.77444700 | -1.04704200 | -0.52157400 |
| C | 5.65082600 | -0.92165000 | 0.51944100 |
| C | 5.27380500 | -0.92970600 | 1.99655500 |
| N | 6.51000000 | -1.25389900 | 2.71556500 |
| C | 7.59288600 | -0.71440600 | 1.87694100 |
| C | 7.07265800 | -0.76741100 | 0.45210900 |
| C | 7.78581800 | -0.72878000 | -0.76359500 |
| C | 9.10476100 | -0.48248000 | -1.06618400 |
| C | 10.20114500 | -0.01652300 | -0.20882200 |
| O | 10.05128800 | 0.36478200 | 0.94551100 |
| C | 11.57158500 | 0.00410600 | -0.86172900 |
| H | 5.13870100 | -0.98906500 | -1.54613300 |
| H | 4.92911700 | 0.06962200 | 2.29011300 |
| H | 4.47626900 | -1.63623400 | 2.22718700 |
| H | 6.60486300 | -2.26561300 | 2.74159900 |
| H | 7.80121400 | 0.32404800 | 2.15507300 |
| H | 8.52053200 | -1.26433800 | 2.02318200 |
| H | 7.17657700 | -0.96117400 | -1.63442800 |
| H | 11.56690000 | 0.67242200 | -1.72884200 |
| H | 12.31411800 | 0.34602900 | -0.14312800 |
| H | 11.83990400 | -0.99212600 | -1.22677300 |
| H | 9.37621700 | -0.61261800 | -2.11049100 |

SCF energy: -1701.273494 hartree

SCF energy in acetonitrile: -1701.310094 hartree

zero-point correction: + 0.183967 hartree

free energy correction: + 0.099051 hartree

**TS3/4**

| | | | |
|---|---|---|---|
| Au | -1.57881700 | -0.29811300 | -0.01650400 |
| Au | -1.37611300 | 2.42224700 | 0.15616400 |
| Au | 0.98373000 | 0.87933400 | -0.04828000 |
| Au | -3.78019600 | 1.26974200 | 0.18342800 |
| Au | -3.97152000 | -1.47059800 | -0.00165500 |
| Au | 0.60858000 | -1.79320300 | -0.21392500 |
| Au | -1.78318100 | -3.06432000 | -0.19397100 |
| Au | 3.07153600 | -0.78817400 | -0.24135500 |
| Au | 1.00241900 | 3.53335200 | 0.13067700 |
| C | 5.04970900 | -1.05257300 | -0.35109400 |
| C | 5.89116000 | -1.48762600 | 0.72003100 |
| H | 5.48551700 | -1.20112200 | -1.33870500 |
| C | 5.42117800 | -2.02122200 | 2.04487800 |
| N | 6.67478300 | -2.20006100 | 2.79047800 |

| | | | |
|---|---|---|---|
| C | 7.78608300 | -2.32731400 | 1.84108500 |
| C | 7.25328000 | -1.60461600 | 0.62829500 |
| C | 8.06721800 | -1.14544900 | -0.44604500 |
| O | 5.76125700 | 0.86268400 | -0.53065800 |
| C | 6.84530800 | 0.95999400 | -1.13389800 |
| C | 7.83626100 | -0.09195700 | -1.28989700 |
| C | 7.21591300 | 2.31071300 | -1.70353500 |
| H | 9.02642100 | -1.64623600 | -0.56558200 |
| H | 8.61782700 | 0.13541200 | -2.00746300 |
| H | 8.10370600 | 2.70715800 | -1.20335700 |
| H | 7.46048500 | 2.20461300 | -2.76515000 |
| H | 6.38611500 | 3.00358600 | -1.58281600 |
| H | 8.69463100 | -1.86844400 | 2.24492900 |
| H | 8.03771300 | -3.36928600 | 1.57011500 |
| H | 4.75360200 | -1.31604000 | 2.55085900 |
| H | 4.85205000 | -2.95239400 | 1.89146900 |
| H | 6.63311000 | -2.96915200 | 3.44692700 |

SCF energy: -1701.253899 hartree

SCF energy in acetonitrile: -1701.279570 hartree

zero-point correction: + 0.184585 hartree

free energy correction: + 0.103192 hartree

imaginary frequency: -207.55 *i* $cm^{-1}$

**IM4**

| | | | |
|---|---|---|---|
| Au | -1.54392200 | -0.30691900 | -0.00165800 |
| Au | 0.69564700 | -1.77382900 | 0.23737600 |
| Au | 1.08920200 | 0.89520100 | 0.09636000 |
| Au | -1.70039400 | -3.00905200 | 0.16152400 |
| Au | -3.96514100 | -1.46517500 | -0.07876700 |
| Au | -1.27836400 | 2.38830900 | -0.14971700 |
| Au | -3.70625000 | 1.27580800 | -0.24550400 |
| Au | 1.09299800 | 3.53507100 | -0.05003900 |
| Au | 3.15449400 | -0.77353200 | 0.32559900 |
| C | 5.16167900 | -1.81958400 | 0.37516900 |
| C | 5.46687700 | -0.48970400 | 0.59243200 |
| C | 5.59814900 | 0.19824700 | 1.96636500 |
| N | 6.21993000 | 1.50971800 | 1.69241800 |
| C | 5.91738900 | 1.81214200 | 0.27680600 |
| C | 5.99010800 | 0.45659900 | -0.38944200 |
| C | 6.71267100 | 0.11628500 | -1.47538600 |
| C | 7.04233300 | -1.22956100 | -1.89590500 |
| C | 6.42248900 | -2.38103700 | -1.58506400 |
| O | 5.23052800 | -2.45340800 | -0.86699800 |

| | | | |
|---|---|---|---|
| C | 6.83129600 | -3.73025200 | -2.06929700 |
| H | 5.08118900 | -2.52488000 | 1.19788200 |
| H | 4.62292300 | 0.34719200 | 2.43536000 |
| H | 6.21485900 | -0.38398500 | 2.65412400 |
| H | 7.22751200 | 1.40403900 | 1.77358900 |
| H | 4.90891600 | 2.23539600 | 0.21435600 |
| H | 6.62449300 | 2.53766600 | -0.12472200 |
| H | 7.17580200 | 0.91554000 | -2.04788800 |
| H | 7.69987600 | -3.66585000 | -2.72417400 |
| H | 7.06729500 | -4.38736000 | -1.22647200 |
| H | 6.00314200 | -4.19299200 | -2.61511200 |
| H | 7.90902700 | -1.32904000 | -2.54068200 |

SCF energy: -1701.291049 hartree
SCF energy in acetonitrile: -1701.316193 hartree
zero-point correction: + 0.187700 hartree
free energy correction: + 0.1070381 hartree

**S3.8 $Au_{10}$**

$Au_{10}$

| | | | |
|---|---|---|---|
| Au | -0.00002600 | 1.37007200 | 0.00000000 |
| Au | 2.36372700 | 0.00011800 | 0.00000000 |
| Au | 0.00002600 | -1.37007200 | 0.00000000 |
| Au | 2.35636200 | 2.69208200 | 0.00000000 |
| Au | 0.00002900 | 4.05847100 | 0.00000000 |
| Au | -2.36372700 | -0.00011800 | 0.00000000 |
| Au | -2.35636200 | 2.69190500 | 0.00000000 |
| Au | -2.35636200 | -2.69208200 | 0.00000000 |
| Au | 2.35636200 | -2.69190500 | 0.00000000 |
| Au | -0.00002900 | -4.05847100 | 0.00000000 |

SCF energy: -1357.343805 hartree
SCF energy in acetonitrile: -1357.359339 hartree
zero-point correction: + 0.004780 hartree
free energy correction: -0.061920 hartree

**IM1**

| | | | |
|---|---|---|---|
| Au | -2.11037000 | -0.26499700 | 0.06341800 |
| Au | -1.33877900 | 2.32943200 | 0.22629000 |
| Au | 0.60060700 | 0.43601400 | -0.21486400 |
| Au | -3.92660300 | 1.63384900 | 0.48513100 |
| Au | -4.77910400 | -0.95508500 | 0.34100000 |
| Au | -0.23770600 | -2.17585800 | -0.37280000 |
| Au | -2.83786000 | -2.82046800 | -0.09778300 |
| Au | 2.38064400 | -1.52653500 | -0.64516300 |

| | | | |
|---|---|---|---|
| Au | 1.26756400 | 3.03013400 | -0.03000200 |
| Au | 3.19536800 | 1.10824100 | -0.47462200 |
| C | 5.10360300 | 2.18585100 | -0.59153800 |
| C | 5.40722400 | 0.99835300 | -0.77984300 |
| C | 6.17289700 | -0.24957700 | -1.04267600 |
| N | 7.60752500 | -0.04806400 | -1.15795600 |
| C | 8.27966900 | 0.41044600 | 0.06865000 |
| C | 8.25992700 | -0.61839800 | 1.14199100 |
| C | 7.63948600 | -0.69111100 | 2.35028900 |
| C | 8.02077100 | -1.93960700 | 2.93325800 |
| C | 8.84994800 | -2.54878200 | 2.04271600 |
| O | 9.00569700 | -1.75101800 | 0.94245900 |
| C | 9.58009000 | -3.84105000 | 2.03521500 |
| H | 5.17211200 | 3.24608200 | -0.47343600 |
| H | 5.98091000 | -0.95676200 | -0.23181600 |
| H | 5.79839500 | -0.70215300 | -1.96351900 |
| H | 7.81751000 | 0.58257300 | -1.92490900 |
| H | 9.31238200 | 0.63699900 | -0.21086300 |
| H | 7.83784700 | 1.32827300 | 0.48281900 |
| H | 6.98827200 | 0.05734100 | 2.77497100 |
| H | 9.37516400 | -4.38373500 | 2.95823400 |
| H | 9.27283900 | -4.46479100 | 1.19066800 |
| H | 10.66022400 | -3.68597900 | 1.95711100 |
| H | 7.71733800 | -2.33334600 | 3.89057700 |

SCF energy: -1837.033862 hartree

SCF energy in acetonitrile: -1837.060870 hartree

zero-point correction: + 0.185379 hartree

free energy correction: + 0.097184 hartree

**TS1/2**

| | | | |
|---|---|---|---|
| Au | 2.15724200 | -0.04499900 | -0.00095900 |
| Au | 0.88746100 | 2.36153700 | -0.01440600 |
| Au | -0.64951900 | 0.08419800 | -0.04601000 |
| Au | 3.57675200 | 2.21181600 | 0.02601800 |
| Au | 4.91041300 | -0.17291800 | 0.04071800 |
| Au | 0.66998500 | -2.32407000 | -0.02686000 |
| Au | 3.36006500 | -2.42507000 | 0.01227300 |
| Au | -2.02262000 | -2.21288900 | -0.06651500 |
| Au | -1.80599000 | 2.49522700 | -0.05234000 |
| Au | -3.36765400 | 0.20820100 | -0.07125300 |
| C | -5.45213300 | 0.33849100 | -0.16955300 |
| C | -6.17784900 | 0.15126800 | 0.86775000 |
| C | -6.16314900 | -0.14269200 | 2.32098600 |

| | | | |
|---|---|---|---|
| N | -7.26394200 | -1.07225700 | 2.56538700 |
| C | -8.47194700 | -0.46969400 | 2.01032000 |
| C | -8.16692200 | -0.01854900 | 0.60808300 |
| C | -8.49870000 | 1.20295200 | 0.00216100 |
| C | -8.52707700 | 0.98895400 | -1.37631400 |
| C | -8.32733000 | -0.36700700 | -1.57052900 |
| O | -8.20359900 | -0.99555000 | -0.38955400 |
| C | -8.26837700 | -1.20623300 | -2.79038700 |
| H | -5.81203900 | 0.57032700 | -1.16926400 |
| H | -5.20969800 | -0.60897500 | 2.57783500 |
| H | -6.25290600 | 0.79903900 | 2.89104100 |
| H | -7.37243600 | -1.26686800 | 3.55584600 |
| H | -9.28776200 | -1.19575300 | 2.00994700 |
| H | -8.80595100 | 0.42617200 | 2.55909500 |
| H | -8.60459100 | 2.14152200 | 0.52394600 |
| H | -7.30746900 | -1.72351500 | -2.85548900 |
| H | -9.05216300 | -1.96883200 | -2.76770800 |
| H | -8.40044300 | -0.58946800 | -3.67839600 |
| H | -8.67191300 | 1.72005100 | -2.15597000 |

SCF energy: -1837.011222 hartree

SCF energy in acetonitrile: -1837.039446 hartree

zero-point correction: + 0.184954 hartree

free energy correction: + 0.09932 hartree

imaginary frequency: -319.42 *i* $cm^{-1}$

**IM2**

| | | | |
|---|---|---|---|
| Au | 2.16840400 | -0.03153600 | 0.00317600 |
| Au | 0.85360500 | 2.34934300 | -0.05665300 |
| Au | -0.65535000 | 0.05363200 | -0.09893400 |
| Au | 3.54420500 | 2.24644000 | 0.04352300 |
| Au | 4.92577800 | -0.11725200 | 0.11012100 |
| Au | 0.70624300 | -2.32715100 | -0.03373000 |
| Au | 3.39577900 | -2.39245300 | 0.06606900 |
| Au | -1.98537100 | -2.25968700 | -0.12747700 |
| Au | -1.83815600 | 2.44202800 | -0.15033900 |
| Au | -3.39048000 | 0.13583300 | -0.14469500 |
| C | -5.43236100 | 0.26088900 | -0.18043400 |
| C | -6.22862200 | 0.21217300 | 0.87000900 |
| C | -5.92857300 | 0.06131900 | 2.34070700 |
| N | -7.10097800 | -0.65946300 | 2.84189900 |
| C | -8.24666700 | -0.00444200 | 2.23218500 |
| C | -7.83524900 | 0.18239600 | 0.76659700 |
| C | -8.34403600 | 1.31889700 | 0.00938200 |

| | | | |
|---|---|---|---|
| C | -8.71182700 | 0.88661400 | -1.23871100 |
| C | -8.59661600 | -0.51320900 | -1.23319300 |
| O | -8.20097600 | -0.96389700 | -0.05542000 |
| C | -8.88743100 | -1.51251000 | -2.28463500 |
| H | -5.86830400 | 0.37989800 | -1.17488300 |
| H | -5.01470500 | -0.51332900 | 2.49132500 |
| H | -5.79807200 | 1.05259800 | 2.80947500 |
| H | -7.15789700 | -0.65887700 | 3.85489300 |
| H | -9.15402300 | -0.60421900 | 2.31764900 |
| H | -8.45179200 | 1.00213300 | 2.63433300 |
| H | -8.30413000 | 2.33630500 | 0.36824200 |
| H | -7.98685900 | -2.08958500 | -2.51372900 |
| H | -9.64450200 | -2.21997400 | -1.93292500 |
| H | -9.24266200 | -1.02498900 | -3.19099900 |
| H | -9.04201600 | 1.47809800 | -2.07858300 |

SCF energy: -1837.017089 hartree

SCF energy in acetonitrile: -1837.050302 hartree

zero-point correction: + 0.186335 hartree

free energy correction: + 0.101159 hartree

**TS2/3**

| | | | |
|---|---|---|---|
| Au | 2.17842300 | -0.07619000 | 0.01678300 |
| Au | 0.95105000 | 2.34355600 | -0.08976900 |
| Au | -0.65187500 | 0.11433100 | -0.14475900 |
| Au | 3.63442200 | 2.13189700 | 0.06538700 |
| Au | 4.96737300 | -0.26106400 | 0.18168700 |
| Au | 0.64169000 | -2.31171000 | -0.02931300 |
| Au | 3.33042700 | -2.45670300 | 0.12663200 |
| Au | -2.05538900 | -2.15405400 | -0.18409500 |
| Au | -1.74586300 | 2.54724200 | -0.25046400 |
| Au | -3.37333800 | 0.29700700 | -0.23070000 |
| C | -5.38578700 | 0.33920300 | -0.29007600 |
| C | -6.24724600 | 0.37753400 | 0.76405000 |
| C | -5.88000300 | 0.42443400 | 2.23558500 |
| N | -7.17773600 | 0.28502600 | 2.91341700 |
| C | -8.18914300 | 0.85841100 | 2.03964600 |
| C | -7.68566700 | 0.46415600 | 0.66484900 |
| C | -8.39115900 | 0.90276300 | -0.54360800 |
| C | -9.08585700 | -0.03069700 | -1.21439600 |
| C | -9.00022400 | -1.31018200 | -0.52982100 |
| O | -8.36338200 | -1.29324300 | 0.54548300 |
| C | -9.60920800 | -2.57117900 | -1.04116400 |
| H | -5.85968500 | 0.30127200 | -1.27392900 |

| | | | |
|---|---|---|---|
| H | -5.21099800 | -0.39148600 | 2.51590400 |
| H | -5.36704400 | 1.37314300 | 2.45535000 |
| H | -7.18724800 | 0.70178300 | 3.83690100 |
| H | -9.18842100 | 0.47583900 | 2.25866800 |
| H | -8.23954500 | 1.96470200 | 2.04429900 |
| H | -8.30041400 | 1.93469300 | -0.86199600 |
| H | -9.44593600 | -3.38865800 | -0.34265700 |
| H | -10.68038300 | -2.42490400 | -1.20741100 |
| H | -9.16494400 | -2.81805700 | -2.01082400 |
| H | -9.63511400 | 0.12515400 | -2.13212200 |

SCF energy: -1837.004315 hartree
SCF energy in acetonitrile: -1837.041796 hartree
zero-point correction: + 0.184663 hartree
free energy correction: + 0.099364 hartree
imaginary frequency: -366.09 *i* $cm^{-1}$

**IM3**

| | | | |
|---|---|---|---|
| Au | -0.57693700 | -0.21113900 | -0.17736800 |
| Au | 0.59437700 | 2.28511100 | -0.13844600 |
| Au | 2.21205400 | 0.11815500 | 0.02756000 |
| Au | -2.08009700 | 1.98737100 | -0.34429800 |
| Au | -3.27622900 | -0.52689800 | -0.32331800 |
| Au | 1.07887700 | -2.36063500 | -0.00814500 |
| Au | -1.60978200 | -2.69238700 | -0.21098800 |
| Au | 3.73835800 | -2.05084200 | 0.19369800 |
| Au | 3.27285400 | 2.55933400 | 0.06732000 |
| Au | 4.95037700 | 0.41799300 | 0.24270100 |
| C | -5.19277300 | 0.00787500 | -0.41503100 |
| C | -5.99201200 | 0.35333400 | 0.66072600 |
| C | -5.56460000 | 0.35843600 | 2.12350600 |
| N | -6.70171400 | 0.93874800 | 2.84458500 |
| C | -7.88371400 | 0.56127400 | 2.05180400 |
| C | -7.38541400 | 0.53925400 | 0.62124400 |
| C | -8.11259300 | 0.72612300 | -0.59039400 |
| C | -9.44987300 | 0.73243100 | -0.84854200 |
| C | -10.56569600 | 0.32271500 | 0.02733800 |
| O | -10.40359400 | -0.28443500 | 1.07536700 |
| C | -11.95161800 | 0.66829900 | -0.47688800 |
| H | -5.58049500 | 0.23991400 | -1.40972900 |
| H | -5.38893700 | -0.66973800 | 2.46223400 |
| H | -4.64762700 | 0.92415500 | 2.29159800 |
| H | -6.61124400 | 1.95106600 | 2.82402300 |
| H | -8.23430500 | -0.43170000 | 2.34764500 |

| | | | |
|---|---|---|---|
| H | -8.71353700 | 1.24860000 | 2.21179300 |
| H | -7.48068900 | 0.95133300 | -1.44792900 |
| H | -12.12943000 | 0.19024200 | -1.44563400 |
| H | -12.69850300 | 0.33149700 | 0.23929500 |
| H | -12.04507600 | 1.74774100 | -0.63214600 |
| H | -9.74405700 | 1.04366600 | -1.84733300 |

SCF energy: -1837.020028 hartree
SCF energy in acetonitrile: -1837.050200 hartree
zero-point correction: + 0.185326 hartree
free energy correction: + 0.097930 hartree

**TS3/4**

| | | | |
|---|---|---|---|
| Au | -2.10945000 | -0.02494300 | 0.00151500 |
| Au | -0.66865300 | -2.31122700 | -0.20866900 |
| Au | 0.71035400 | 0.07271500 | -0.09334000 |
| Au | -3.36410800 | -2.36771100 | -0.10171700 |
| Au | -4.87527700 | -0.10547700 | 0.10983600 |
| Au | -0.78035600 | 2.34728000 | 0.11715400 |
| Au | -3.46502300 | 2.24918100 | 0.21402800 |
| Au | 1.92788100 | 2.45941200 | 0.02543800 |
| Au | 2.02737000 | -2.23839400 | -0.32525600 |
| Au | 3.42652900 | 0.15908800 | -0.14472900 |
| C | 5.36367900 | -0.35854100 | -0.17493700 |
| C | 6.06594600 | -0.87177900 | 0.93546300 |
| C | 5.45258900 | -1.26309100 | 2.27761300 |
| N | 6.49969300 | -2.02521300 | 2.96834100 |
| C | 7.77432600 | -1.56355400 | 2.39870400 |
| C | 7.42825800 | -1.04894900 | 1.01257300 |
| C | 8.39419000 | -0.83354500 | -0.01226400 |
| C | 8.38547600 | 0.05818200 | -1.04775200 |
| C | 7.55808500 | 1.25356200 | -1.18772200 |
| O | 6.50900800 | 1.46715300 | -0.56789200 |
| C | 8.09686500 | 2.32294500 | -2.11296900 |
| H | 5.75635600 | -0.65989100 | -1.14877100 |
| H | 5.20694800 | -0.35129900 | 2.83750500 |
| H | 4.53514700 | -1.84383500 | 2.17853500 |
| H | 6.38208900 | -3.00713300 | 2.73846800 |
| H | 8.18079600 | -0.74633300 | 3.00878000 |
| H | 8.52224200 | -2.36135700 | 2.38924400 |
| H | 9.27752400 | -1.46757900 | 0.05690300 |
| H | 8.19008300 | 1.91494600 | -3.12513400 |
| H | 7.42269000 | 3.17673000 | -2.12337200 |
| H | 9.09521400 | 2.64094300 | -1.80034500 |

| | | | |
|---|---|---|---|
| H | 9.23247300 | 0.01872800 | -1.72585700 |

SCF energy: -1837.012736 hartree

SCF energy in acetonitrile: -1837.042502 hartree

zero-point correction: + 0.185189 hartree

free energy correction: + 0.099552 hartree

imaginary frequency: -105.18 *i* $cm^{-1}$

**IM4**

| | | | |
|---|---|---|---|
| Au | 2.02653700 | -0.01980600 | -0.03670500 |
| Au | 0.73561600 | 2.36360400 | 0.12165800 |
| Au | -0.77434500 | 0.06747300 | 0.09531300 |
| Au | 3.42276300 | 2.25312100 | -0.00101300 |
| Au | 4.77943700 | -0.10777800 | -0.16127300 |
| Au | 0.57647900 | -2.31626800 | -0.05790400 |
| Au | 3.26444400 | -2.37801300 | -0.18760300 |
| Au | -2.12306100 | -2.25880500 | 0.09488500 |
| Au | -1.96571700 | 2.46876200 | 0.22260100 |
| Au | -3.45806500 | 0.15281500 | 0.26013500 |
| C | -5.60759400 | 0.89662800 | 0.38264700 |
| C | -5.73561100 | -0.47262600 | 0.49953400 |
| C | -5.75778100 | -1.27868300 | 1.81130800 |
| N | -6.14714900 | -2.65242900 | 1.42595600 |
| C | -5.86367100 | -2.77396700 | -0.01968600 |
| C | -6.15272200 | -1.39218800 | -0.55405900 |
| C | -6.95617900 | -1.06480100 | -1.58666600 |
| C | -7.48210400 | 0.25342100 | -1.86859500 |
| C | -6.99263100 | 1.44326600 | -1.47789500 |
| O | -5.77005800 | 1.58573000 | -0.82408700 |
| C | -7.59117100 | 2.76866700 | -1.80548300 |
| H | -5.62635600 | 1.54857700 | 1.25155500 |
| H | -4.77758100 | -1.29483800 | 2.29260600 |
| H | -6.47397600 | -0.86504600 | 2.52508100 |
| H | -7.15096100 | -2.74520300 | 1.55050800 |
| H | -4.80203000 | -3.03184700 | -0.15105900 |
| H | -6.46661400 | -3.56193200 | -0.47067900 |
| H | -7.32885900 | -1.86867400 | -2.21595400 |
| H | -8.48549500 | 2.65561300 | -2.41793800 |
| H | -7.85171500 | 3.31190400 | -0.89175800 |
| H | -6.86107100 | 3.37983500 | -2.34532700 |
| H | -8.39088700 | 0.29118300 | -2.46004500 |

SCF energy: -1837.050567 hartree

SCF energy in acetonitrile: -1837.079752 hartree

zero-point correction: + 0.187993 hartree

free energy correction: + 0.103772 hartree

**S3.9 $AuP(CH_3)_3^+$**

$AuP(CH_3)_3^+$

| | | | |
|---|---|---|---|
| C | 0.00000000 | 1.69198400 | -1.95342000 |
| H | 0.00000000 | 1.65246200 | -3.04649000 |
| H | -0.88916000 | 2.22193600 | -1.61036900 |
| H | 0.88916000 | 2.22193600 | -1.61036900 |
| C | -1.46530100 | -0.84599200 | -1.95342000 |
| H | -1.43107400 | -0.82623100 | -3.04649000 |
| H | -1.47967300 | -1.88100300 | -1.61036900 |
| H | -2.36883300 | -0.34093300 | -1.61036900 |
| C | 1.46530100 | -0.84599200 | -1.95342000 |
| H | 1.47967300 | -1.88100300 | -1.61036900 |
| H | 1.43107400 | -0.82623100 | -3.04649000 |
| H | 2.36883300 | -0.34093300 | -1.61036900 |
| P | 0.00000000 | 0.00000000 | -1.30833000 |
| Au | 0.00000000 | 0.00000000 | 0.93149600 |

SCF energy: -596.688578 hartree

SCF energy in acetonitrile: -596.791967 hartree

zero-point correction: + 0.114500 hartree

free energy correction: + 0.081243 hartree

**IM1-Au(I)**

| | | | |
|---|---|---|---|
| C | 2.65846100 | 2.54154600 | -1.03207400 |
| H | 3.49027600 | 3.24395500 | -1.12413700 |
| H | 2.31001100 | 2.26493000 | -2.02801300 |
| H | 1.84012200 | 3.02118400 | -0.49347700 |
| C | 4.63979500 | 0.42027900 | -1.04721900 |
| H | 5.40182400 | 1.19867600 | -1.13019800 |
| H | 5.05996600 | -0.44016500 | -0.52455400 |
| H | 4.33386600 | 0.10714700 | -2.04637300 |
| C | 3.85267900 | 1.65331500 | 1.45859200 |
| H | 4.26367900 | 0.81902000 | 2.02886300 |
| H | 4.63930000 | 2.39118200 | 1.28427800 |
| H | 3.04989400 | 2.11195700 | 2.03751000 |
| P | 3.20120800 | 1.05479200 | -0.13194100 |
| Au | 1.51129300 | -0.48934400 | 0.11055500 |
| C | 0.19999100 | -2.16904800 | 0.68029100 |
| C | -0.47265400 | -1.57919700 | -0.16939300 |
| C | -1.52301200 | -1.11216900 | -1.12405400 |
| N | -2.73114200 | -1.89251600 | -1.02699200 |
| C | -3.51242200 | -1.76171300 | 0.21472800 |

| | | | |
|---|---|---|---|
| C | -3.95948100 | -0.36540700 | 0.45446400 |
| C | -3.71385900 | 0.53110400 | 1.44880900 |
| C | -4.47638500 | 1.70043400 | 1.14348300 |
| C | -5.13836100 | 1.44363900 | -0.01829400 |
| O | -4.82865600 | 0.18216900 | -0.45083700 |
| C | -6.08603000 | 2.22023100 | -0.85518300 |
| H | 0.55523100 | -2.86289400 | 1.41447600 |
| H | -1.75675500 | -0.06730800 | -0.90531600 |
| H | -1.12490900 | -1.16839400 | -2.13921000 |
| H | -2.58359500 | -2.86422500 | -1.27639900 |
| H | -4.37435400 | -2.42402500 | 0.09625900 |
| H | -2.96200800 | -2.09178100 | 1.10696200 |
| H | -3.08274800 | 0.36974400 | 2.30956500 |
| H | -6.24932000 | 3.20181200 | -0.41077000 |
| H | -5.69992500 | 2.35685000 | -1.86924600 |
| H | -7.05015600 | 1.71040100 | -0.93348100 |
| H | -4.53573700 | 2.61043100 | 1.71930000 |

SCF energy: -1076.417576 hartree

SCF energy in acetonitrile: -1076.503672 hartree

zero-point correction: + 0.295450 hartree

free energy correction: + 0.240564 hartree

**TS1/2-Au(I)**

| | | | |
|---|---|---|---|
| C | 4.01780200 | -0.16000900 | -1.14789000 |
| H | 5.05706800 | -0.12972600 | -0.81225800 |
| H | 3.82610300 | -1.11322100 | -1.64244000 |
| H | 3.84777100 | 0.64459700 | -1.86474800 |
| C | 3.36324000 | -1.28479500 | 1.44012200 |
| H | 4.42669800 | -1.21046100 | 1.67933000 |
| H | 2.78166900 | -1.19122100 | 2.35828100 |
| H | 3.16280900 | -2.26054900 | 0.99554900 |
| C | 3.39599000 | 1.58897400 | 1.07495800 |
| H | 2.81691000 | 1.73745800 | 1.98746400 |
| H | 4.45916500 | 1.55711900 | 1.32436100 |
| H | 3.21037500 | 2.42782400 | 0.40260800 |
| P | 2.89446200 | 0.03286900 | 0.27229000 |
| Au | 0.66864500 | -0.03120800 | -0.32845300 |
| C | -1.30028300 | 0.42476100 | -1.22643800 |
| C | -1.50166000 | -0.71769900 | -0.65445700 |
| C | -1.74562500 | -2.19166300 | -0.73310000 |
| N | -3.10185500 | -2.37399600 | -0.22950500 |
| C | -3.24708200 | -1.70353400 | 1.06557900 |
| C | -2.67640800 | -0.33264200 | 0.88629500 |

| | | | |
|---|---|---|---|
| C | -1.84396100 | 0.43661500 | 1.75580700 |
| C | -1.77900200 | 1.68689700 | 1.20650000 |
| C | -2.61543300 | 1.66793500 | 0.05127800 |
| O | -3.41824100 | 0.56837100 | 0.14040200 |
| C | -3.13036900 | 2.80791300 | -0.75529300 |
| H | -1.14764800 | 0.84537300 | -2.20848400 |
| H | -1.68194200 | -2.54225800 | -1.76554800 |
| H | -0.97145600 | -2.71279700 | -0.14204500 |
| H | -3.36486700 | -3.35290100 | -0.19123700 |
| H | -4.30363100 | -1.66468300 | 1.33671500 |
| H | -2.69455500 | -2.19137900 | 1.88396800 |
| H | -1.27522200 | 0.04014200 | 2.58371400 |
| H | -2.33944000 | 3.54031300 | -0.91843700 |
| H | -3.50783100 | 2.46501600 | -1.71891600 |
| H | -3.95057300 | 3.30155200 | -0.22522600 |
| H | -1.15558000 | 2.51667800 | 1.50396800 |

SCF energy: -1076.378876 hartree

SCF energy in acetonitrile: -1076.461057 hartree

zero-point correction: + 0.295015 hartree

free energy correction: + 0.245452 hartree

imaginary frequency: -454.58 *i* $cm^{-1}$

**IM2-Au(I)**

| | | | |
|---|---|---|---|
| C | 3.62614200 | 1.59125600 | 0.16871500 |
| H | 4.69257200 | 1.51194600 | 0.39261400 |
| H | 3.49948700 | 2.03296800 | -0.82066800 |
| H | 3.15135600 | 2.24017300 | 0.90588700 |
| C | 3.81884700 | -1.07461700 | -0.95412900 |
| H | 4.87661000 | -1.05732800 | -0.68100100 |
| H | 3.45828400 | -2.10396300 | -0.93244100 |
| H | 3.70167800 | -0.68499500 | -1.96630400 |
| C | 3.22240100 | -0.72909900 | 1.86392100 |
| H | 2.84999400 | -1.75182100 | 1.93807900 |
| H | 4.30054500 | -0.72662900 | 2.04051500 |
| H | 2.73138100 | -0.12109800 | 2.62498700 |
| P | 2.85732100 | -0.05904300 | 0.21056200 |
| Au | 0.59497700 | 0.00505000 | -0.27324000 |
| C | -1.44318700 | 0.58724700 | -1.05979300 |
| C | -1.62789600 | -0.64319500 | -0.49556000 |
| C | -1.77141700 | -2.08742700 | -0.87657500 |
| N | -3.09706900 | -2.37359700 | -0.31325500 |
| C | -3.20411900 | -1.71283100 | 0.99773900 |
| C | -2.52992800 | -0.37921300 | 0.76165300 |

| | | | |
|---|---|---|---|
| C | -1.74969300 | 0.41237500 | 1.80175900 |
| C | -1.56985800 | 1.61252400 | 1.25061200 |
| C | -2.26592000 | 1.55989800 | -0.11656800 |
| O | -3.35521900 | 0.65142600 | 0.18923300 |
| C | -2.74552100 | 2.84197500 | -0.74478300 |
| H | -1.21066100 | 0.82605500 | -2.09109400 |
| H | -1.75652000 | -2.25108700 | -1.95531900 |
| H | -0.95646500 | -2.68019100 | -0.42365600 |
| H | -3.29894800 | -3.36650300 | -0.27780600 |
| H | -4.24971800 | -1.60134200 | 1.28495100 |
| H | -2.67008200 | -2.24088500 | 1.80348600 |
| H | -1.38882000 | 0.02872100 | 2.74563200 |
| H | -1.89888500 | 3.49557400 | -0.96636500 |
| H | -3.28360000 | 2.63747800 | -1.67169900 |
| H | -3.41677700 | 3.36174200 | -0.06017400 |
| H | -1.03231300 | 2.46833200 | 1.63490000 |

SCF energy: -1076.409892 hartree

SCF energy in acetonitrile: -1076.497527 hartree

zero-point correction: + 0.298307 hartree

free energy correction: + 0.249863 hartree

**TS2/3-Au(I)**

| | | | |
|---|---|---|---|
| C | 3.64037400 | 1.33677600 | -1.19720000 |
| H | 4.71711900 | 1.46256500 | -1.06144100 |
| H | 3.44962800 | 0.92486900 | -2.18934900 |
| H | 3.15348500 | 2.31059400 | -1.12678400 |
| C | 3.96972600 | -1.29918700 | -0.07216900 |
| H | 5.03301600 | -1.06393500 | 0.01507500 |
| H | 3.69197400 | -2.00256800 | 0.71425900 |
| H | 3.78444400 | -1.76995300 | -1.03885000 |
| C | 3.48089800 | 0.95904700 | 1.65849200 |
| H | 3.19700800 | 0.30336800 | 2.48308400 |
| H | 4.56295300 | 1.10872400 | 1.67562900 |
| H | 2.98389300 | 1.92104100 | 1.79246600 |
| P | 2.96422100 | 0.21607500 | 0.07405100 |
| Au | 0.69066500 | -0.15884000 | -0.12063700 |
| C | -2.16449600 | 0.51297000 | -1.02356200 |
| C | -1.37536700 | -0.56698500 | -0.37679600 |
| C | -1.64491100 | -1.98172800 | -0.96124800 |
| N | -2.87395900 | -2.42688600 | -0.28724700 |
| C | -2.84347400 | -1.89304600 | 1.06645700 |
| C | -2.27175900 | -0.54252600 | 0.84553200 |
| C | -2.05806200 | 0.55673100 | 1.79524700 |

| | | | |
|---|---|---|---|
| C | -2.20702900 | 1.74906400 | 1.21683300 |
| C | -2.70411700 | 1.62849000 | -0.17831000 |
| O | -3.47944400 | 0.36261600 | -0.25995100 |
| C | -3.38246300 | 2.79702500 | -0.83373400 |
| H | -2.27346500 | 0.59550600 | -2.10027200 |
| H | -1.78921700 | -1.96659000 | -2.04417400 |
| H | -0.78753600 | -2.63177400 | -0.74602400 |
| H | -3.01228800 | -3.43055600 | -0.31893100 |
| H | -3.82934200 | -1.87640700 | 1.53494600 |
| H | -2.14384200 | -2.40231800 | 1.76183500 |
| H | -1.76341500 | 0.37311500 | 2.82042600 |
| H | -2.65787800 | 3.60205300 | -0.97892200 |
| H | -3.79315600 | 2.51929800 | -1.80461200 |
| H | -4.19076900 | 3.16853300 | -0.20147400 |
| H | -2.04114400 | 2.70912800 | 1.68576900 |

SCF energy: -1076.378876 hartree

SCF energy in acetonitrile: -1076.454485 hartree

zero-point correction: + 0.296836 hartree

free energy correction: + 0.248467 hartree

imaginary frequency: -257.64 *i* $cm^{-1}$

**IM3-Au(I)**

| | | | |
|---|---|---|---|
| C | 3.85878400 | -0.87647500 | 0.31549000 |
| H | 4.88576200 | -0.50524100 | 0.27991300 |
| H | 3.66016300 | -1.28722900 | 1.30638600 |
| H | 3.73835400 | -1.66929300 | -0.42409000 |
| C | 3.08378800 | 1.78265800 | 1.17447900 |
| H | 4.13995500 | 2.05379800 | 1.10530600 |
| H | 2.47264700 | 2.66430800 | 0.97663800 |
| H | 2.86919400 | 1.42703600 | 2.18312100 |
| C | 3.20211200 | 1.14889500 | -1.65236700 |
| H | 2.59407300 | 2.02033600 | -1.89897000 |
| H | 4.25435600 | 1.44143100 | -1.62127200 |
| H | 3.06195400 | 0.39318300 | -2.42642200 |
| P | 2.69643400 | 0.47944600 | -0.03637900 |
| Au | 0.49018100 | -0.18119500 | 0.00050900 |
| C | -2.30865400 | 0.57643700 | -1.05730200 |
| C | -1.66925200 | -0.66903200 | -0.58128200 |
| C | -1.62996500 | -2.00307900 | -1.32028100 |
| N | -1.14309400 | -2.97053800 | -0.32858700 |
| C | -1.48142200 | -2.42494800 | 0.99290800 |
| C | -1.60639200 | -0.92642400 | 0.78687800 |
| C | -1.93712700 | 0.08162500 | 1.77768300 |

| | | | |
|---|---|---|---|
| C | -2.42530700 | 1.27528100 | 1.38700700 |
| C | -2.72378100 | 1.59148400 | -0.03131300 |
| O | -3.67557000 | 0.70009800 | -0.64809600 |
| C | -2.88190800 | 3.04068800 | -0.40622300 |
| H | -2.11934300 | 0.90760100 | -2.07437300 |
| H | -2.66143100 | -2.24742000 | -1.60923900 |
| H | -1.02313700 | -2.01816900 | -2.22562200 |
| H | -0.13630700 | -3.07177900 | -0.41139500 |
| H | -2.46865400 | -2.78958600 | 1.30904300 |
| H | -0.76288800 | -2.73085000 | 1.75420300 |
| H | -1.76683200 | -0.13463200 | 2.82613200 |
| H | -1.98097600 | 3.60580000 | -0.15386000 |
| H | -3.07431400 | 3.14030800 | -1.47462700 |
| H | -3.72321200 | 3.47801700 | 0.13666300 |
| H | -2.60918900 | 2.05539400 | 2.11875900 |

SCF energy: -1076.438403 hartree

SCF energy in acetonitrile: -1076.527738 hartree

zero-point correction: + 0.299083 hartree

free energy correction: + 0.248936 hartree

**TS1/4-Au(I)**

| | | | |
|---|---|---|---|
| C | -4.03088300 | 0.60530200 | -1.67195900 |
| H | -5.12229500 | 0.56561500 | -1.70819400 |
| H | -3.70533200 | 1.64201900 | -1.76805300 |
| H | -3.62211900 | 0.03256900 | -2.50560600 |
| C | -4.28099900 | 0.86981700 | 1.19999100 |
| H | -5.36305600 | 0.81831000 | 1.05719200 |
| H | -4.02764400 | 0.46621800 | 2.18129300 |
| H | -3.96233600 | 1.91233200 | 1.15902100 |
| C | -4.15254400 | -1.75643600 | -0.00633100 |
| H | -3.90674000 | -2.21334800 | 0.95330300 |
| H | -5.23860900 | -1.70164200 | -0.11162800 |
| H | -3.74464000 | -2.37878500 | -0.80400700 |
| P | -3.43054300 | -0.08680000 | -0.09657200 |
| Au | -1.14395900 | -0.09715600 | 0.10659500 |
| C | 0.94697500 | -0.28341000 | 0.34869500 |
| C | 1.47469000 | 0.81938800 | 0.06515000 |
| C | 1.64534600 | 2.22524400 | -0.38575000 |
| N | 2.94318300 | 2.81216200 | -0.09739600 |
| C | 4.02980400 | 1.93268300 | -0.53833500 |
| C | 3.92164200 | 0.54590800 | 0.01946500 |
| C | 3.99080200 | 0.04916600 | 1.30187100 |
| C | 3.98646500 | -1.35874900 | 1.20028700 |

| | | | |
|---|---|---|---|
| C | 3.95358800 | -1.65905600 | -0.14051400 |
| O | 3.93424900 | -0.51087000 | -0.86438900 |
| C | 3.97232100 | -2.93266100 | -0.89903800 |
| H | 1.33554500 | -1.24951100 | 0.65061900 |
| H | 1.48558300 | 2.25007300 | -1.46890600 |
| H | 0.86878400 | 2.83432000 | 0.08346700 |
| H | 3.02766600 | 3.00665700 | 0.89579500 |
| H | 4.01751600 | 1.87432600 | -1.62946600 |
| H | 4.97292300 | 2.39702000 | -0.24315800 |
| H | 4.02735300 | 0.63548500 | 2.20736200 |
| H | 3.11532200 | -3.00256000 | -1.57408500 |
| H | 4.87783500 | -3.00276100 | -1.50819000 |
| H | 3.95075800 | -3.77637900 | -0.21035300 |
| H | 4.02488400 | -2.07402000 | 2.00687100 |

SCF energy: -1076.411496 hartree

SCF energy in acetonitrile: -1076.489714 hartree

zero-point correction: + 0.295015 hartree

free energy correction: + 0.242165 hartree

imaginary frequency: -136.30 *i* $cm^{-1}$

**IM4-Au(I)**

| | | | |
|---|---|---|---|
| C | 4.29852600 | -1.68050900 | -0.32360300 |
| H | 5.37911700 | -1.60241300 | -0.18244500 |
| H | 3.91304800 | -2.49300500 | 0.29428300 |
| H | 4.08855400 | -1.91328100 | -1.36875100 |
| C | 4.03651200 | 0.20291200 | 1.84062800 |
| H | 5.12788600 | 0.20885800 | 1.88959000 |
| H | 3.65644800 | 1.16873700 | 2.17710700 |
| H | 3.65075300 | -0.57009800 | 2.50709300 |
| C | 4.32381200 | 1.15008200 | -0.86369500 |
| H | 3.95587000 | 2.13996100 | -0.58926800 |
| H | 5.40316900 | 1.10925000 | -0.69910800 |
| H | 4.11466500 | 0.98618900 | -1.92193700 |
| P | 3.47024400 | -0.11885700 | 0.13448500 |
| Au | 1.16740500 | -0.15955200 | -0.12430900 |
| C | -0.86779100 | -0.25266500 | -0.37547500 |
| C | -1.75183100 | 0.72034400 | -0.15783400 |
| C | -1.52237700 | 2.14941700 | 0.29798800 |
| N | -2.83626500 | 2.54828000 | 0.80213500 |
| C | -3.79783600 | 2.01005800 | -0.13862500 |
| C | -3.29379100 | 0.56560300 | -0.31392300 |
| C | -3.73330000 | -0.19169800 | -1.48669500 |
| C | -4.31271000 | -1.35653700 | -1.10768400 |

| | | | |
|---|---|---|---|
| C | -4.34157900 | -1.34372200 | 0.31856800 |
| O | -3.81407700 | -0.26981600 | 0.80655200 |
| C | -4.88849500 | -2.35361000 | 1.24590300 |
| H | -1.27269600 | -1.20800600 | -0.71694200 |
| H | -0.77021200 | 2.19781600 | 1.08609000 |
| H | -1.17851200 | 2.76298400 | -0.55112000 |
| H | -2.93834800 | 3.54844900 | 0.93552700 |
| H | -4.81922200 | 2.05082600 | 0.24256700 |
| H | -3.77266000 | 2.47300900 | -1.13976500 |
| H | -3.55691300 | 0.14971800 | -2.49717200 |
| H | -4.34168300 | -3.29334300 | 1.11612100 |
| H | -4.80965500 | -2.02118400 | 2.27849000 |
| H | -5.93282500 | -2.55775600 | 0.99212700 |
| H | -4.70379300 | -2.14672700 | -1.72998700 |

SCF energy: -1076.429739 hartree

SCF energy in acetonitrile: -1076.508743 hartree

zero-point correction: + 0.297085 hartree

free energy correction: + 0.244607 hartree

**TS4/5-Au(I)**

| | | | |
|---|---|---|---|
| C | 4.27200700 | -1.35273000 | -0.77679900 |
| H | 5.34481400 | -1.26457000 | -0.59026900 |
| H | 3.93655900 | -2.34827200 | -0.48234900 |
| H | 4.08065300 | -1.22491300 | -1.84332500 |
| C | 3.88180300 | -0.33470800 | 1.89730000 |
| H | 4.97049400 | -0.28853800 | 1.97516300 |
| H | 3.44233200 | 0.43968100 | 2.52784000 |
| H | 3.53703000 | -1.30687500 | 2.25276800 |
| C | 4.10698900 | 1.49454400 | -0.32655800 |
| H | 3.67700800 | 2.30490900 | 0.26412800 |
| H | 5.18813100 | 1.47198400 | -0.17170700 |
| H | 3.90015500 | 1.68622100 | -1.38064100 |
| P | 3.35317200 | -0.09142000 | 0.16818900 |
| Au | 1.05009300 | -0.19132300 | -0.12165600 |
| C | -0.97538600 | -0.34313000 | -0.36060300 |
| C | -1.85702700 | 0.65447200 | -0.55929100 |
| C | -1.60335500 | 2.13740300 | -0.59116100 |
| N | -2.21917000 | 2.66904300 | 0.62650300 |
| C | -3.52267000 | 2.03495000 | 0.84979300 |
| C | -3.48232400 | 0.67390800 | 0.21640100 |
| C | -3.43900200 | 0.29756400 | -1.16475700 |
| C | -3.82673500 | -1.10034100 | -1.17354900 |
| C | -4.04132100 | -1.47159700 | 0.10513200 |

| | | | |
|---|---|---|---|
| O | -3.83902300 | -0.39723700 | 0.96417200 |
| C | -4.44729600 | -2.73822000 | 0.75325100 |
| H | -1.40951800 | -1.34458800 | -0.33748100 |
| H | -0.52751800 | 2.31477900 | -0.57107800 |
| H | -2.00418200 | 2.57638200 | -1.51969700 |
| H | -2.30479300 | 3.67965700 | 0.60209400 |
| H | -3.72388500 | 1.92397300 | 1.91705300 |
| H | -4.36079600 | 2.58339200 | 0.39601900 |
| H | -3.58321900 | 0.97757900 | -1.99270400 |
| H | -3.67791300 | -3.08162500 | 1.44933500 |
| H | -5.36874100 | -2.59263300 | 1.32287200 |
| H | -4.61282300 | -3.50623400 | -0.00072400 |
| H | -3.90644700 | -1.73260400 | -2.04312500 |

SCF energy: -1076.412607 hartree

SCF energy in acetonitrile: -1076.487546 hartree

zero-point correction: + 0.296776 hartree

free energy correction: + 0.245807 hartree

imaginary frequency: -193.10 *i* $cm^{-1}$

**IM5-Au(I)**

| | | | |
|---|---|---|---|
| C | 4.66939700 | -0.64863000 | -1.01764100 |
| H | 5.71572400 | -0.52653600 | -0.72770200 |
| H | 4.46471400 | -1.70648600 | -1.18949000 |
| H | 4.48802000 | -0.10718300 | -1.94737600 |
| C | 4.08153500 | -0.90630200 | 1.79261200 |
| H | 5.15310100 | -0.78132400 | 1.96528700 |
| H | 3.53116500 | -0.52404400 | 2.65372900 |
| H | 3.85671300 | -1.96843100 | 1.68406100 |
| C | 4.12662100 | 1.70001500 | 0.56119700 |
| H | 3.57877900 | 2.13815700 | 1.39696600 |
| H | 5.19643900 | 1.72286200 | 0.78177800 |
| H | 3.93178700 | 2.29719400 | -0.33098000 |
| P | 3.56104500 | -0.01439700 | 0.28691600 |
| Au | 1.30973300 | -0.22464100 | -0.20817100 |
| C | -0.67519700 | -0.48668800 | -0.69244100 |
| C | -1.69414400 | 0.28295800 | -0.33356900 |
| C | -1.66754700 | 1.54285300 | 0.50956300 |
| N | -2.55359200 | 2.60802700 | 0.03810500 |
| C | -3.96830700 | 2.26321300 | 0.08687800 |
| C | -4.12999200 | 0.80638100 | -0.13856900 |
| C | -3.18194900 | -0.03748900 | -0.85498200 |
| C | -3.72035300 | -1.39788200 | -0.57663900 |
| C | -4.77245100 | -1.29667000 | 0.23525100 |

| | | | |
|---|---|---|---|
| O | -4.99273900 | 0.10180100 | 0.52271200 |
| C | -5.72084500 | -2.21580300 | 0.89584500 |
| H | -0.89992800 | -1.36375200 | -1.30129100 |
| H | -1.97098500 | 1.30911700 | 1.53902700 |
| H | -0.64792300 | 1.92580800 | 0.54669600 |
| H | -2.27661400 | 2.94071200 | -0.87953600 |
| H | -4.41062400 | 2.52429000 | 1.05473400 |
| H | -4.51696600 | 2.82579800 | -0.67601900 |
| H | -3.14510000 | 0.23163900 | -1.91855200 |
| H | -5.47423000 | -3.24192400 | 0.62544300 |
| H | -5.66917400 | -2.11515400 | 1.98294600 |
| H | -6.74723000 | -2.00630100 | 0.58411700 |
| H | -3.30581600 | -2.31817500 | -0.95555200 |

SCF energy: -1076.412421 hartree

SCF energy in acetonitrile: -1076.490830 hartree

zero-point correction: + 0.296828 hartree

free energy correction: + 0.244146 hartree

**TS5/6-Au(I)**

| | | | |
|---|---|---|---|
| C | 4.11580100 | 1.24948100 | 1.41047900 |
| H | 5.20206500 | 1.33155700 | 1.49124500 |
| H | 3.70235700 | 2.22133000 | 1.13643100 |
| H | 3.70498600 | 0.95906100 | 2.37867700 |
| C | 4.51878100 | 0.54994500 | -1.36261100 |
| H | 5.58962400 | 0.65923000 | -1.17621000 |
| H | 4.36487800 | -0.18529700 | -2.15385500 |
| H | 4.11244900 | 1.50643400 | -1.69492700 |
| C | 4.53101000 | -1.50875000 | 0.66328100 |
| H | 4.37786400 | -2.28903200 | -0.08378200 |
| H | 5.60134500 | -1.31809000 | 0.77026800 |
| H | 4.13121200 | -1.85872800 | 1.61622000 |
| P | 3.65796000 | 0.00971600 | 0.15279700 |
| Au | 1.36513700 | -0.28046500 | -0.11674000 |
| C | -0.63354000 | -0.60381700 | -0.36015300 |
| C | -1.66447000 | 0.25999500 | -0.10979000 |
| C | -1.54939600 | 1.71363400 | 0.34020700 |
| N | -2.54580100 | 2.61236300 | -0.23151400 |
| C | -3.93429200 | 2.27098400 | 0.05676600 |
| C | -4.13367600 | 0.79693900 | 0.00288900 |
| C | -3.14843500 | -0.16719600 | -0.12936500 |
| C | -3.81546100 | -1.44702500 | -0.07427700 |
| C | -5.12594900 | -1.17666800 | 0.12469500 |
| O | -5.31876100 | 0.20543800 | 0.17972200 |

| | | | |
|---|---|---|---|
| C | -6.33942300 | -2.00598000 | 0.29488800 |
| H | -0.94608300 | -1.58320800 | -0.73055100 |
| H | -1.65695900 | 1.73432400 | 1.43035400 |
| H | -0.55541800 | 2.08743800 | 0.09388800 |
| H | -2.39807200 | 2.74559500 | -1.22580600 |
| H | -4.21101700 | 2.63173200 | 1.05670900 |
| H | -4.58834700 | 2.78681800 | -0.65029900 |
| H | -2.37474100 | 0.14669200 | -1.16082400 |
| H | -6.07485400 | -3.06091700 | 0.23390800 |
| H | -6.80885400 | -1.81567200 | 1.26338200 |
| H | -7.07368800 | -1.78230800 | -0.48349400 |
| H | -3.36895400 | -2.42530800 | -0.14004000 |

SCF energy: -1076.386438 hartree

SCF energy in acetonitrile: -1076.463347 hartree

zero-point correction: + 0.293880 hartree

free energy correction: + 0.243272 hartree

imaginary frequency: -844.57 *i* $cm^{-1}$

**IM6-Au(I)**

| | | | |
|---|---|---|---|
| C | -4.32567500 | 0.72681600 | -0.55090500 |
| H | -5.19455400 | 1.12068100 | -0.01837000 |
| H | -4.06828200 | 1.40158000 | -1.36848600 |
| H | -4.57239800 | -0.24988300 | -0.96951400 |
| C | -2.68567900 | 2.23134400 | 1.30086800 |
| H | -3.61333800 | 2.56904800 | 1.76921900 |
| H | -1.89255500 | 2.20614600 | 2.04936900 |
| H | -2.40288600 | 2.93394600 | 0.51577800 |
| C | -3.51460400 | -0.46582700 | 1.95847100 |
| H | -2.74738100 | -0.54119200 | 2.73022500 |
| H | -4.41770100 | -0.02829000 | 2.39072700 |
| H | -3.74124200 | -1.46765600 | 1.59106200 |
| P | -2.91226700 | 0.57074600 | 0.58688200 |
| Au | -1.04086000 | -0.26315700 | -0.45436100 |
| C | 0.56457300 | -1.07228400 | -1.71211000 |
| C | 1.45422400 | -1.07840400 | -0.63809500 |
| C | 1.55172900 | -2.28456500 | 0.30297600 |
| N | 2.89242000 | -2.57114900 | 0.79371500 |
| C | 3.52690000 | -1.43240400 | 1.45819200 |
| C | 3.30212500 | -0.19252100 | 0.66475200 |
| C | 2.36092800 | -0.01871500 | -0.32607600 |
| C | 2.57745600 | 1.31024200 | -0.84522200 |
| C | 3.59756400 | 1.84278300 | -0.13354800 |
| O | 4.04924800 | 0.90815800 | 0.80103700 |

| | | | |
|---|---|---|---|
| C | 4.31185700 | 3.13946400 | -0.14716100 |
| H | 0.67108000 | -0.31546400 | -2.48459400 |
| H | 0.91045900 | -2.09565100 | 1.17236500 |
| H | 1.16272200 | -3.17337200 | -0.19647800 |
| H | 3.48111200 | -2.89536800 | 0.03209900 |
| H | 3.09900400 | -1.31995200 | 2.46349000 |
| H | 4.59257400 | -1.63017900 | 1.58769000 |
| H | 0.14440500 | -2.02025300 | -2.03715800 |
| H | 3.88321500 | 3.78674500 | -0.91162800 |
| H | 4.23458700 | 3.64066100 | 0.82136800 |
| H | 5.37367600 | 2.99771500 | -0.36528500 |
| H | 2.04015400 | 1.80613100 | -1.63771400 |

SCF energy: -1076.483242 hartree
SCF energy in acetonitrile: -1076.563417 hartree
zero-point correction: + 0.299282 hartree
free energy correction: + 0.247895 hartree

**S3.10 $AuP(CH_3)_3^+ \rightarrow AuP(CH_3)_3$**

$TfO^-$

S -0.9345 -0.0001 0.0001
O -1.2427 -1.3685 0.3875
O -1.2431 0.3486 -1.3786
C 0.9356 0.0001 -0.0001
O -1.2429 1.0196 0.9912
F 1.4509 -0.3070 1.2153
F 1.4504 1.2063 -0.3418
F 1.4507 -0.8991 -0.8737
SCF energy: -961.849651798 hartree
SCF energy in acetonitrile: -961.9280766 hartree
zero-point correction: +0.026954 hartree
free energy correction: -0.005538 hartree

TfOH

S 0.8628 -0.1392 -0.0000
O 1.2705 -0.7048 -1.2484
O 1.2705 -0.7049 1.2483
C -0.9997 -0.0010 0.0000
O 1.1000 1.4414 0.0000
H 2.0541 1.6319 0.0001
F -1.4231 0.6402 -1.0865
F -1.4231 0.6399 1.0866
F -1.4858 -1.2415 -0.0001
SCF energy: -962.338481229 hartree

SCF energy in acetonitrile: -962.3474261
zero-point correction: +0.037655 hartree
free energy correction: +0.004906 hartree

**IM-TfO**

Au 0.7385 -1.0923 -0.1115
P 2.6535 -2.2709 0.3448
C 2.3718 -4.0002 0.8638
C 3.7638 -2.3790 -1.0909
C 3.6466 -1.5294 1.6720
H 4.5505 -2.1215 1.8369
H 3.9054 -0.5133 1.3743
H 3.0597 -1.4847 2.5901
H 4.6767 -2.9167 -0.8224
H 3.2620 -2.8983 -1.9087
H 4.0055 -1.3605 -1.4000
H 3.3263 -4.4957 1.0585
H 1.7664 -4.0196 1.7712
H 1.8407 -4.5397 0.0783
C -0.7560 0.4404 -0.7054
C -1.4200 -0.5875 -0.5906
C -2.4788 -1.6173 -0.5353
H -0.2355 1.3758 -0.8662
H -2.2725 -2.3625 -1.3072
H -2.4184 -2.1296 0.4386
O 3.5820 0.8640 -0.8327
S 2.5547 1.7391 -0.2806
O 1.5830 2.2502 -1.2387
O 1.9683 1.2525 0.9715
C 3.5027 3.2492 0.2491
F 2.6893 4.1597 0.8067
F 4.4438 2.9256 1.1557
F 4.1170 3.8243 -0.7955
N -3.7803 -1.0206 -0.8053
H -4.4249 -1.7414 -1.1140
C -4.3492 -0.2991 0.3324
H -4.4741 -0.9308 1.2275
H -3.6463 0.4972 0.6047
C -5.6740 0.2722 -0.0407
C -6.2296 0.6806 -1.2109
O -6.5605 0.4604 0.9855
C -7.5422 1.1542 -0.8905
H -5.7549 0.6556 -2.1785

C -7.7002 1.0070 0.4515
H -8.2741 1.5549 -1.5744
C -8.8024 1.3024 1.4005
H -9.6490 1.7230 0.8572
H -9.1382 0.3981 1.9169
H -8.4892 2.0228 2.1622
SCF energy: -2038.38735834 hartree
SCF energy in acetonitrile: -2038.38735834 hartree
zero-point correction: +0.323160 hartree
free energy correction: +0.252804 hartree

**TS-TfO**

Au 1.1513 1.3119 -0.3116
P 2.9427 2.4457 0.5061
C 2.8689 4.2697 0.5276
C 3.2980 1.9605 2.2252
C 4.4601 2.0409 -0.4165
H 5.3324 2.4975 0.0583
H 4.5709 0.9550 -0.4435
H 4.3720 2.4046 -1.4416
H 4.2298 2.4163 2.5694
H 2.4775 2.2766 2.8714
H 3.3717 0.8723 2.2667
H 3.7887 4.6870 0.9449
H 2.7339 4.6419 -0.4891
H 2.0196 4.5949 1.1304
C -0.3051 -0.0062 -0.9880
C -1.4678 0.0089 -1.3888
C -2.8364 -0.0452 -1.8652
H 0.4602 -1.0430 -0.8181
H -2.9280 -0.9707 -2.4658
H -3.0056 0.7833 -2.5642
O 2.3374 -1.3631 1.3659
S 2.5035 -1.9369 0.0468
O 1.2058 -2.1216 -0.6893
O 3.5635 -1.3993 -0.7766
C 2.9584 -3.7195 0.3354
F 3.1051 -4.3744 -0.8225
F 4.1194 -3.7789 1.0048
F 2.0218 -4.3439 1.0603
N -3.8150 0.0497 -0.7838
H -3.5969 -0.6324 -0.0629
C -5.1819 -0.1494 -1.2589

H -5.3441 -1.1310 -1.7357
H -5.3754 0.6064 -2.0319
C -6.1429 0.0019 -0.1300
C -6.0968 0.6384 1.0685
O -7.3602 -0.6053 -0.2877
C -7.3653 0.4136 1.6938
H -5.2609 1.2009 1.4519
C -8.1016 -0.3414 0.8364
H -7.6856 0.7678 2.6612
C -9.4712 -0.9122 0.8778
H -9.4505 -2.0043 0.8137
H -9.9554 -0.6317 1.8135
H -10.0823 -0.5427 0.0487
SCF energy: -2038.36994522 hartree
SCF energy in acetonitrile: -2038.402335 hartree
zero-point correction: +0.318142 hartree
free energy correction: +0.248527 hartree
imaginary frequency: 637.5187*i* $cm^{-1}$

**IMx**

Au -1.8986 -0.3277 0.0325
P -3.8171 0.9065 -0.0633
C -4.4035 1.5579 1.5427
C -3.7152 2.4035 -1.1108
C -5.2819 0.0309 -0.7224
H -6.1566 0.6860 -0.7416
H -5.0695 -0.3194 -1.7338
H -5.4946 -0.8388 -0.0985
H -4.6611 2.9512 -1.1080
H -2.9202 3.0516 -0.7384
H -3.4671 2.1141 -2.1333
H -5.3167 2.1462 1.4204
H -4.5966 0.7260 2.2219
H -3.6263 2.1839 1.9840
C -0.2149 -1.3849 0.1160
C 0.8283 -2.0141 0.1558
C 2.0748 -2.7721 0.2373
H 1.9956 -3.6757 -0.3759
H 2.2158 -3.1040 1.2820
N 3.2295 -2.0100 -0.2634
H 4.0388 -2.6247 -0.2862
C 3.5386 -0.8412 0.5530
H 3.7994 -1.0870 1.5977

H 2.6306 -0.2286 0.5941
C 4.6619 -0.0744 -0.0567
C 5.1809 -0.0021 -1.3098
O 5.3480 0.7708 0.7769
C 6.2518 0.9479 -1.2517
H 4.8282 -0.5534 -2.1662
C 6.3161 1.3937 0.0303
H 6.8930 1.2582 -2.0625
C 7.1841 2.3634 0.7447
H 7.9036 2.7928 0.0466
H 6.5983 3.1790 1.1803
H 7.7377 1.8833 1.5578
SCF energy: -1076.01987592 hartree
SCF energy in acetonitrile: -1076.050666 hartree
zero-point correction: + 0.284812 hartree
free energy correction: +0.230621 hartree

**S3.11 AuP($CH_3$)$_3$**

AuP($CH_3$)$_3$

| | | | |
|---|---|---|---|
| C | 0.00000000 | 1.65565500 | -2.12973500 |
| H | 0.00000000 | 1.58169000 | -3.22119200 |
| H | -0.88348600 | 2.20802500 | -1.80478100 |
| H | 0.88348600 | 2.20802500 | -1.80478100 |
| C | -1.43384000 | -0.82782800 | -2.12973500 |
| H | -1.36978300 | -0.79084500 | -3.22119200 |
| H | -1.47046300 | -1.86913400 | -1.80478100 |
| H | -2.35394900 | -0.33889100 | -1.80478100 |
| C | 1.43384000 | -0.82782800 | -2.12973500 |
| H | 1.47046300 | -1.86913400 | -1.80478100 |
| H | 1.36978300 | -0.79084500 | -3.22119200 |
| H | 2.35394900 | -0.33889100 | -1.80478100 |
| P | 0.00000000 | 0.00000000 | -1.34526200 |
| Au | 0.00000000 | 0.00000000 | 1.00008100 |

SCF energy: -596.889476 hartree
SCF energy in acetonitrile: -596.894565 hartree
zero-point correction: + 0.113093 hartree
free energy correction: + 0.077685 hartree

**IM1-Au(0)**

| | | | |
|---|---|---|---|
| C | -4.30661300 | 1.52757900 | 1.61705300 |
| H | -5.33298600 | 1.90320700 | 1.64172200 |
| H | -4.13427200 | 0.88940700 | 2.48542300 |
| H | -3.61252800 | 2.36800700 | 1.67089700 |

| | | | |
|---|---|---|---|
| C | -5.33371000 | -0.66497100 | 0.08250800 |
| H | -6.31230700 | -0.18589500 | 0.17142000 |
| H | -5.29500600 | -1.23793700 | -0.84552700 |
| H | -5.19277700 | -1.35673400 | 0.91467900 |
| C | -4.47956500 | 1.73136500 | -1.23790600 |
| H | -4.41920500 | 1.22444100 | -2.20249000 |
| H | -5.49771700 | 2.09910500 | -1.08543500 |
| H | -3.78853800 | 2.57582000 | -1.25461600 |
| P | -3.98308500 | 0.57126900 | 0.08909600 |
| Au | -1.85083500 | -0.27795300 | -0.10068500 |
| C | 0.06043700 | -1.00851100 | -0.23726200 |
| C | 0.90152600 | -0.86950800 | 0.75406100 |
| C | 2.29457600 | -1.18732400 | 1.16252300 |
| N | 3.15007800 | -1.76783400 | 0.11101300 |
| C | 3.50543500 | -0.82496100 | -0.96080800 |
| C | 4.52283000 | 0.17028700 | -0.52468400 |
| C | 4.48547200 | 1.51574800 | -0.32907000 |
| C | 5.79640400 | 1.90971900 | 0.08698400 |
| C | 6.55066200 | 0.77784000 | 0.11737400 |
| O | 5.78601500 | -0.29189900 | -0.25637200 |
| C | 7.96754700 | 0.49507900 | 0.45955100 |
| H | 0.35872200 | -1.51782700 | -1.16643000 |
| H | 2.79465400 | -0.28453800 | 1.52789000 |
| H | 2.27461900 | -1.88889700 | 2.00300800 |
| H | 2.67129200 | -2.56373800 | -0.30068200 |
| H | 3.90977100 | -1.41805900 | -1.78712100 |
| H | 2.64108700 | -0.26477700 | -1.34335700 |
| H | 3.62136300 | 2.14810700 | -0.46242300 |
| H | 8.46685700 | 1.42012000 | 0.74976000 |
| H | 8.04124900 | -0.21346300 | 1.29007400 |
| H | 8.50504000 | 0.06451700 | -0.39097100 |
| H | 6.13425700 | 2.90432200 | 0.33378800 |

SCF energy: -1076.581742 hartree

SCF energy in acetonitrile: -1076.607166 hartree

zero-point correction: + 0.293834 hartree

free energy correction: + 0.238176 hartree

**TS1/2-Au(0)**

| | | | |
|---|---|---|---|
| C | -4.47327400 | -1.00546400 | 1.21427800 |
| H | -5.55350100 | -0.93009400 | 1.06410100 |
| H | -4.17966200 | -2.05655500 | 1.20186900 |
| H | -4.21452200 | -0.59214600 | 2.19063900 |
| C | -4.23788200 | -0.80599100 | -1.63530300 |

| | | | |
|---|---|---|---|
| H | -5.32905000 | -0.74016800 | -1.65597400 |
| H | -3.82736100 | -0.26462900 | -2.48942800 |
| H | -3.93706700 | -1.85162900 | -1.72036200 |
| C | -4.29711200 | 1.56960000 | -0.03189500 |
| H | -3.88603300 | 2.17530600 | -0.84137800 |
| H | -5.38501200 | 1.52562400 | -0.13012500 |
| H | -4.03907200 | 2.04742400 | 0.91476400 |
| P | -3.55431200 | -0.10330600 | -0.08769200 |
| Au | -1.25107900 | -0.17877100 | 0.10416200 |
| C | 0.80094400 | -0.25889200 | 0.26456200 |
| C | 1.61333600 | 0.70861400 | -0.07849100 |
| C | 1.58532600 | 2.10930600 | -0.55729900 |
| N | 2.75440600 | 2.86294500 | -0.07419800 |
| C | 3.96037300 | 2.07184000 | -0.33180500 |
| C | 3.91085700 | 0.63562200 | 0.14223900 |
| C | 4.11533000 | 0.07643100 | 1.39688600 |
| C | 4.45501700 | -1.28323000 | 1.19453400 |
| C | 4.52747700 | -1.48485300 | -0.15579600 |
| O | 4.25212400 | -0.31451000 | -0.80831100 |
| C | 4.83202900 | -2.66401600 | -1.00243900 |
| H | 1.22608800 | -1.19082500 | 0.64426000 |
| H | 1.61116100 | 2.13499600 | -1.65410400 |
| H | 0.67609700 | 2.63275500 | -0.23641200 |
| H | 2.65674400 | 2.98055200 | 0.93213200 |
| H | 4.12832800 | 2.04944700 | -1.41270800 |
| H | 4.80886700 | 2.58951400 | 0.12315700 |
| H | 3.96989100 | 0.57826500 | 2.34098900 |
| H | 5.68315800 | -2.47073900 | -1.66387100 |
| H | 5.07476700 | -3.51877900 | -0.36991100 |
| H | 3.97914800 | -2.93320900 | -1.63439100 |
| H | 4.63461700 | -2.03093100 | 1.95238600 |

SCF energy: -1076.5744424hartree

SCF energy in acetonitrile: -1076.599115 hartree

zero-point correction: + 0.293219 hartree

free energy correction: + 0.239459 hartree

imaginary frequency: -277.43 *i* $cm^{-1}$

**IM2-Au(0)**

| | | | |
|---|---|---|---|
| C | 4.36375600 | -1.66154800 | -0.28509500 |
| H | 5.43935500 | -1.56710800 | -0.11389300 |
| H | 3.97371000 | -2.48517100 | 0.31534800 |
| H | 4.18433300 | -1.89325900 | -1.33637600 |
| C | 4.03727700 | 0.19721400 | 1.87169500 |

| | | | |
|---|---|---|---|
| H | 5.12827000 | 0.21474100 | 1.93686100 |
| H | 3.63971400 | 1.15549100 | 2.21032700 |
| H | 3.64817500 | -0.58249000 | 2.52870400 |
| C | 4.37015500 | 1.15845200 | -0.80624100 |
| H | 3.98529900 | 2.14429100 | -0.53961300 |
| H | 5.44546200 | 1.12576100 | -0.61197600 |
| H | 4.18998500 | 1.00068300 | -1.87097600 |
| P | 3.47929300 | -0.11981400 | 0.15662300 |
| Au | 1.18797700 | -0.17901600 | -0.14354400 |
| C | -0.83275000 | -0.26889600 | -0.41147300 |
| C | -1.73453500 | 0.67509900 | -0.12636300 |
| C | -1.47676500 | 2.06950300 | 0.40719900 |
| N | -2.81730800 | 2.58338700 | 0.72057000 |
| C | -3.72206800 | 1.99053500 | -0.26357600 |
| C | -3.24904200 | 0.53042700 | -0.33704300 |
| C | -3.70603700 | -0.26674200 | -1.51502100 |
| C | -4.45919400 | -1.33519900 | -1.05889400 |
| C | -4.52059600 | -1.27530600 | 0.32336900 |
| O | -3.83713500 | -0.20087200 | 0.80687900 |
| C | -5.16819900 | -2.14890000 | 1.32995600 |
| H | -1.24317100 | -1.19136800 | -0.82790300 |
| H | -0.84966400 | 2.06069000 | 1.30304300 |
| H | -0.95594600 | 2.66679600 | -0.36132100 |
| H | -2.85131000 | 3.59664200 | 0.70724000 |
| H | -4.76335200 | 2.06128800 | 0.05545700 |
| H | -3.62940900 | 2.42746200 | -1.27350300 |
| H | -3.44072500 | -0.02916400 | -2.53381300 |
| H | -5.68518900 | -2.97373200 | 0.83763200 |
| H | -4.42865900 | -2.56376200 | 2.02457600 |
| H | -5.89485400 | -1.59018200 | 1.93120500 |
| H | -4.92539700 | -2.10272600 | -1.66048700 |

SCF energy: -1076.612243 hartree

SCF energy in acetonitrile: -1076.636613 hartree

zero-point correction: + 0.294643 hartree

free energy correction: + 0.241702 hartree

**TS2/3-Au(0)**

| | | | |
|---|---|---|---|
| C | 4.08126300 | -0.45082800 | 1.89265100 |
| H | 5.17104600 | -0.42478100 | 1.97313800 |
| H | 3.65252500 | 0.31576200 | 2.54040100 |
| H | 3.71670100 | -1.42253000 | 2.22991200 |
| C | 4.36766800 | 1.40780900 | -0.27047100 |
| H | 5.44385300 | 1.35390900 | -0.08611600 |

| | | | |
|---|---|---|---|
| H | 4.19216700 | 1.62790600 | -1.32487500 |
| H | 3.94112500 | 2.21938000 | 0.32155000 |
| C | 4.47708100 | -1.41468200 | -0.77884800 |
| H | 4.30523400 | -1.26585200 | -1.84622600 |
| H | 5.54820600 | -1.34653200 | -0.57192800 |
| H | 4.12120500 | -2.41155700 | -0.51316700 |
| P | 3.53538800 | -0.16297900 | 0.16891100 |
| Au | 1.24477900 | -0.19517600 | -0.15044000 |
| C | -0.77183100 | -0.25594800 | -0.42577900 |
| C | -1.67777800 | 0.68288300 | -0.07500700 |
| C | -1.42197900 | 2.03730900 | 0.56007800 |
| N | -2.55288300 | 2.88304300 | 0.12990700 |
| C | -3.69546100 | 1.95749600 | 0.14920600 |
| C | -3.12859700 | 0.58864900 | -0.29899600 |
| C | -3.66280000 | -0.17457100 | -1.40404200 |
| C | -4.72766300 | -1.00226600 | -1.09307500 |
| C | -4.85832800 | -1.14191000 | 0.29895900 |
| O | -4.09041200 | -0.39871700 | 1.02304500 |
| C | -5.73714000 | -2.13860000 | 0.99105700 |
| H | -1.19281100 | -1.15097500 | -0.88915600 |
| H | -1.44146600 | 1.97085500 | 1.65507600 |
| H | -0.46598800 | 2.47062900 | 0.26358800 |
| H | -2.38052000 | 3.15435900 | -0.83621700 |
| H | -4.06452900 | 1.87973400 | 1.17417400 |
| H | -4.50498300 | 2.30831500 | -0.49033800 |
| H | -3.13964500 | -0.20048600 | -2.35294300 |
| H | -6.29845000 | -2.73668200 | 0.27142000 |
| H | -5.12696900 | -2.80194000 | 1.61139900 |
| H | -6.44296200 | -1.63203800 | 1.65652300 |
| H | -5.27524100 | -1.60750100 | -1.80325700 |

SCF energy: -1076.594125 hartree

SCF energy in acetonitrile: -1076.618049 hartree

zero-point correction: + 0.293729 hartree

free energy correction: + 0.241186 hartree

imaginary frequency: -487.47 *i* $cm^{-1}$

**IM3-Au(0)**

| | | | |
|---|---|---|---|
| C | 4.74689100 | -1.54012300 | -0.34787200 |
| H | 5.82154100 | -1.35779000 | -0.26571000 |
| H | 4.46748600 | -2.35573900 | 0.32121100 |
| H | 4.50876300 | -1.84100200 | -1.36946300 |
| C | 4.44012800 | 0.41320300 | 1.73156100 |
| H | 5.52870900 | 0.51059700 | 1.71320600 |

| | | | |
|---|---|---|---|
| H | 3.99798300 | 1.36000900 | 2.04624100 |
| H | 4.15762900 | -0.35116400 | 2.45738900 |
| C | 4.49216500 | 1.23904200 | -1.01476700 |
| H | 4.06135600 | 2.20945600 | -0.76220100 |
| H | 5.57957400 | 1.29009200 | -0.91637700 |
| H | 4.23358900 | 1.01094800 | -2.05015000 |
| P | 3.78573900 | -0.04308300 | 0.08421400 |
| Au | 1.48884800 | -0.28459100 | -0.03205800 |
| C | -0.52880300 | -0.53074700 | -0.12990700 |
| C | -1.48517600 | 0.44665600 | -0.08118000 |
| C | -1.20389100 | 1.93873800 | 0.03856600 |
| N | -2.43517900 | 2.61955700 | -0.38683700 |
| C | -3.52002100 | 1.69077500 | -0.00950800 |
| C | -2.91666700 | 0.30301200 | -0.10657400 |
| C | -3.56191800 | -0.93330300 | -0.25885000 |
| C | -4.88820700 | -1.31650400 | -0.21330300 |
| C | -6.06992100 | -0.56839400 | 0.20497200 |
| O | -6.04132000 | 0.54855000 | 0.71459400 |
| C | -7.39757000 | -1.28522300 | 0.00542900 |
| H | -0.89618900 | -1.55546800 | -0.21928800 |
| H | -0.99525100 | 2.19566900 | 1.08545900 |
| H | -0.34686000 | 2.25713400 | -0.55714400 |
| H | -2.41977000 | 2.67270900 | -1.40261000 |
| H | -3.83986900 | 1.89594300 | 1.01721400 |
| H | -4.39593600 | 1.83129600 | -0.63977800 |
| H | -2.88024100 | -1.75151800 | -0.48603600 |
| H | -7.41017200 | -2.22762700 | 0.56226400 |
| H | -8.21052100 | -0.64848300 | 0.35045300 |
| H | -7.54703200 | -1.53384500 | -1.04998800 |
| H | -5.08515100 | -2.35034300 | -0.48564000 |

SCF energy: -1076.629735 hartree

SCF energy in acetonitrile: -1076.655376 hartree

zero-point correction: + 0.294341 hartree

free energy correction: + 0.239344 hartree

imaginary frequency: -844.57 *i* $cm^{-1}$

**TS3/4-Au(0)**

| | | | |
|---|---|---|---|
| C | -3.85818300 | -1.67475000 | 0.49353500 |
| H | -4.94198000 | -1.61830800 | 0.62376600 |
| H | -3.62697500 | -2.36876700 | -0.31630800 |
| H | -3.40364400 | -2.05736700 | 1.40893000 |
| C | -4.13526900 | 0.52062300 | -1.33388100 |
| H | -5.20661700 | 0.48060200 | -1.12046100 |

| | | | |
|---|---|---|---|
| H | -3.85645100 | 1.54393500 | -1.59097100 |
| H | -3.91375100 | -0.11777000 | -2.19079400 |
| C | -3.76514000 | 1.02363100 | 1.46774200 |
| H | -3.47658800 | 2.05918900 | 1.27999600 |
| H | -4.85255600 | 0.96090400 | 1.55927500 |
| H | -3.30409000 | 0.70852100 | 2.40527800 |
| P | -3.14954500 | -0.03278400 | 0.10576900 |
| Au | -0.86017400 | -0.00265400 | -0.19370100 |
| C | 1.17163000 | 0.05428100 | -0.45152000 |
| C | 2.07069600 | -0.96393400 | -0.05592800 |
| C | 1.72923100 | -2.32171100 | 0.52876200 |
| N | 2.93128100 | -3.15269900 | 0.30179100 |
| C | 4.05890600 | -2.19914600 | 0.24097500 |
| C | 3.45089900 | -0.86188900 | -0.14549800 |
| C | 4.19912500 | 0.28821400 | -0.44016000 |
| C | 3.81576200 | 1.63127100 | -0.37217500 |
| C | 2.67580000 | 2.20823200 | 0.23270400 |
| O | 1.66322800 | 1.57145800 | 0.69088800 |
| C | 2.62692100 | 3.71088000 | 0.41196600 |
| H | 1.53351600 | 0.64515100 | -1.29178700 |
| H | 1.53848300 | -2.24137400 | 1.60896300 |
| H | 0.84977700 | -2.78552500 | 0.07663100 |
| H | 2.83575800 | -3.56560800 | -0.62176700 |
| H | 4.52891300 | -2.12956800 | 1.23096600 |
| H | 4.82713400 | -2.54917300 | -0.45496700 |
| H | 5.24337000 | 0.12261800 | -0.70303700 |
| H | 1.76756800 | 4.11577400 | -0.13199100 |
| H | 2.48277900 | 3.95323600 | 1.46865100 |
| H | 3.53591500 | 4.19869900 | 0.05693800 |
| H | 4.56928300 | 2.34925000 | -0.68026700 |

SCF energy: -1076.606278 hartree

SCF energy in acetonitrile: -1076.631390 hartree

zero-point correction: + 0.294624 hartree

free energy correction: + 0.242375 hartree

imaginary frequency: -346.51 *i* $cm^{-1}$

**IM4-Au(0)**

| | | | |
|---|---|---|---|
| C | -4.13106600 | 1.06711300 | -0.90977600 |
| H | -5.19925800 | 0.93260200 | -0.71999600 |
| H | -3.85159400 | 2.09780000 | -0.68465900 |
| H | -3.92597700 | 0.88200300 | -1.96556300 |
| C | -3.71832400 | 0.26792500 | 1.81254000 |
| H | -4.80584600 | 0.18080400 | 1.87886500 |

| | | | |
|---|---|---|---|
| H | -3.25593100 | -0.43787100 | 2.50466600 |
| H | -3.41799600 | 1.27566600 | 2.10451500 |
| C | -3.84243100 | -1.71252700 | -0.26179100 |
| H | -3.37902600 | -2.46449000 | 0.37914000 |
| H | -4.92414900 | -1.72009300 | -0.10436200 |
| H | -3.62732900 | -1.97150500 | -1.29997200 |
| P | -3.12597100 | -0.07050200 | 0.11419000 |
| Au | -0.83456500 | 0.09352000 | -0.15889000 |
| C | 1.24169000 | 0.28888500 | -0.39585600 |
| C | 2.05938500 | -0.91068500 | -0.07742800 |
| C | 1.50995600 | -2.29536900 | 0.16751300 |
| N | 2.67241000 | -3.20667400 | 0.11474100 |
| C | 3.86191800 | -2.35869700 | 0.34222800 |
| C | 3.42656100 | -0.93950500 | 0.02015500 |
| C | 4.31654900 | 0.13939300 | -0.13528700 |
| C | 3.98088200 | 1.51018500 | -0.16762500 |
| C | 2.78298200 | 2.11411400 | 0.13300900 |
| O | 1.62715200 | 1.46835500 | 0.42078800 |
| C | 2.63496200 | 3.59786300 | 0.26705100 |
| H | 1.43379400 | 0.58589500 | -1.43584900 |
| H | 1.02856200 | -2.34802000 | 1.15750800 |
| H | 0.75138000 | -2.59827300 | -0.56193700 |
| H | 2.73140300 | -3.56651700 | -0.83233500 |
| H | 4.17360100 | -2.43122500 | 1.39277500 |
| H | 4.70293000 | -2.70396000 | -0.26631100 |
| H | 5.37514000 | -0.09495300 | -0.21081600 |
| H | 3.58871900 | 4.10672300 | 0.12268900 |
| H | 1.91175300 | 3.98238700 | -0.46113500 |
| H | 2.25000200 | 3.84996700 | 1.26119300 |
| H | 4.79759200 | 2.20025000 | -0.35687200 |

SCF energy: -1076.618999 hartree

SCF energy in acetonitrile: -1076.643101 hartree

zero-point correction: + 0.295729 hartree

free energy correction: + 0.243492 hartree

**TS1/5-Au(0)**

| | | | |
|---|---|---|---|
| C | 3.78439000 | 1.47390600 | 0.63842500 |
| H | 4.83579900 | 1.36131500 | 0.91617300 |
| H | 3.71101400 | 2.11165600 | -0.24420700 |
| H | 3.24652300 | 1.95952900 | 1.45464400 |
| C | 4.14709600 | -0.86966600 | -0.96226700 |
| H | 5.18050000 | -0.86869200 | -0.60540200 |
| H | 3.83988600 | -1.89384500 | -1.18030200 |

| | | | |
|---|---|---|---|
| H | 4.08360500 | -0.29260100 | -1.88642400 |
| C | 3.39047500 | -1.11542700 | 1.79076600 |
| H | 3.06857600 | -2.14846700 | 1.64907400 |
| H | 4.45990700 | -1.09676700 | 2.01726100 |
| H | 2.83599600 | -0.69981000 | 2.63404400 |
| P | 3.01103500 | -0.14946400 | 0.28078500 |
| Au | 0.79606300 | -0.13751600 | -0.34013800 |
| C | -1.16447000 | -0.20066200 | -0.96969400 |
| C | -2.19589500 | -0.87521700 | -0.30309400 |
| C | -3.22643000 | -1.82514800 | -0.84220200 |
| N | -4.47436400 | -1.52072900 | -0.11441000 |
| C | -4.12824600 | -0.87141200 | 1.15578000 |
| C | -2.90565100 | -0.05672100 | 0.81480000 |
| C | -1.93458600 | 0.49128400 | 1.80256400 |
| C | -1.33530500 | 1.52776700 | 1.17751800 |
| C | -2.00199100 | 1.70392300 | -0.10513800 |
| O | -3.24578500 | 1.13191900 | 0.03158100 |
| C | -1.91280300 | 2.88356300 | -1.00880800 |
| H | -1.24516400 | -0.24507200 | -2.06331400 |
| H | -3.37666900 | -1.69778000 | -1.92292600 |
| H | -2.89543700 | -2.86714800 | -0.68758700 |
| H | -5.03751100 | -2.35060900 | 0.03165800 |
| H | -4.95323600 | -0.24898900 | 1.50995800 |
| H | -3.85199400 | -1.57557500 | 1.95865100 |
| H | -1.63280500 | -0.00134400 | 2.71563600 |
| H | -0.86801200 | 3.15950100 | -1.16437800 |
| H | -2.36241100 | 2.65842700 | -1.97697600 |
| H | -2.43852600 | 3.74984100 | -0.58453300 |
| H | -0.46721900 | 2.08478400 | 1.50436600 |

SCF energy: -1076.5502800 hartree
SCF energy in acetonitrile: -1076.573499 hartree
zero-point correction: + 0.293350 hartree
free energy correction: + 0.243038 hartree
imaginary frequency: -477.12 *i* $cm^{-1}$

**IM5-Au(0)**

| | | | |
|---|---|---|---|
| C | 3.91305100 | 1.23608700 | 0.82083100 |
| H | 4.96414700 | 1.02497800 | 1.03466000 |
| H | 3.84884500 | 2.00854900 | 0.05260100 |
| H | 3.42990900 | 1.61393200 | 1.72357500 |
| C | 4.07933200 | -0.84853200 | -1.13959200 |
| H | 5.12106600 | -0.96803300 | -0.83032300 |
| H | 3.69781400 | -1.80520700 | -1.50048800 |

| | | | |
|---|---|---|---|
| H | 4.02628700 | -0.13081000 | -1.96001700 |
| C | 3.38720200 | -1.48063100 | 1.56905900 |
| H | 2.98481200 | -2.45329000 | 1.28075900 |
| H | 4.46134400 | -1.57332400 | 1.74978400 |
| H | 2.89176300 | -1.16797200 | 2.48988700 |
| P | 3.03358800 | -0.26368400 | 0.24595000 |
| Au | 0.79844200 | 0.03571400 | -0.27638700 |
| C | -1.23210400 | 0.24398900 | -0.75371100 |
| C | -2.07326500 | -0.82152400 | -0.15975700 |
| C | -2.64084300 | -2.09503100 | -0.69062500 |
| N | -4.09438900 | -1.95000400 | -0.44126900 |
| C | -4.28601100 | -1.08941000 | 0.74090900 |
| C | -3.13519300 | -0.11273400 | 0.66068900 |
| C | -2.44211900 | 0.51887400 | 1.85540900 |
| C | -1.71258900 | 1.51145200 | 1.34323700 |
| C | -1.97851400 | 1.50611100 | -0.16143500 |
| O | -3.36137100 | 1.05112200 | -0.18204200 |
| C | -1.82477000 | 2.79982000 | -0.91910600 |
| H | -1.31907400 | 0.26237600 | -1.84753200 |
| H | -2.45609000 | -2.23024100 | -1.76298200 |
| H | -2.21043400 | -2.97448800 | -0.17521700 |
| H | -4.54881500 | -2.84947100 | -0.32450300 |
| H | -5.25758900 | -0.59203800 | 0.70034800 |
| H | -4.21440500 | -1.63554200 | 1.69603400 |
| H | -2.44053500 | 0.12630000 | 2.86378700 |
| H | -0.77890100 | 3.11703000 | -0.91046800 |
| H | -2.13722300 | 2.66835000 | -1.95758100 |
| H | -2.43438700 | 3.58572100 | -0.46745200 |
| H | -0.98263600 | 2.13728900 | 1.84021900 |

SCF energy: -1076.581921 hartree
SCF energy in acetonitrile: -1076.605739 hartree
zero-point correction: + 0.295972 hartree
free energy correction: + 0.245987 hartree

**TS5/6-Au(0)**

| | | | |
|---|---|---|---|
| C | 3.91145000 | 1.14410800 | 0.82813900 |
| H | 4.95010000 | 0.88590900 | 1.05094600 |
| H | 3.88889300 | 1.91835800 | 0.05931800 |
| H | 3.43777100 | 1.54352200 | 1.72651400 |
| C | 3.99778600 | -0.94422700 | -1.13466300 |
| H | 5.03118100 | -1.10998300 | -0.81895100 |
| H | 3.57663300 | -1.88293400 | -1.49867300 |
| H | 3.98184600 | -0.22434600 | -1.95470900 |

| | | | |
|---|---|---|---|
| C | 3.26137700 | -1.54909600 | 1.56829800 |
| H | 2.81970700 | -2.50304300 | 1.27502200 |
| H | 4.32940000 | -1.68814600 | 1.75560800 |
| H | 2.77381100 | -1.21680900 | 2.48639500 |
| P | 2.97189800 | -0.31541900 | 0.24577300 |
| Au | 0.75396600 | 0.07801100 | -0.28695700 |
| C | -1.25995700 | 0.40745600 | -0.79171000 |
| C | -2.13093600 | -0.69246600 | -0.35237200 |
| C | -2.63434500 | -1.91507700 | -1.04115500 |
| N | -3.92503700 | -2.18962300 | -0.37708100 |
| C | -4.00385400 | -1.43606900 | 0.89018100 |
| C | -2.93010200 | -0.39923800 | 0.76988900 |
| C | -2.31202600 | 0.38034700 | 1.86347200 |
| C | -1.69499500 | 1.47051100 | 1.40186200 |
| C | -1.99362600 | 1.60026600 | -0.09200500 |
| O | -3.37781200 | 1.26305300 | -0.20202200 |
| C | -1.73563800 | 2.96333200 | -0.70185200 |
| H | -1.30581500 | 0.53031800 | -1.87842900 |
| H | -2.78245700 | -1.74775800 | -2.11559200 |
| H | -1.91615600 | -2.74776100 | -0.94338000 |
| H | -4.06847600 | -3.18017200 | -0.22922000 |
| H | -4.99115500 | -0.97799900 | 1.01105000 |
| H | -3.82068200 | -2.06230600 | 1.77941100 |
| H | -2.30371600 | 0.01236100 | 2.88284100 |
| H | -0.67277600 | 3.21778700 | -0.64223300 |
| H | -2.03629000 | 2.96449200 | -1.75212800 |
| H | -2.31175300 | 3.73004500 | -0.17804100 |
| H | -1.07493500 | 2.15075000 | 1.97447000 |

SCF energy: -1076.558482 hartree

SCF energy in acetonitrile: -1076.585912 hartree

zero-point correction: + 0.294075 hartree

free energy correction: + 0.243679 hartree

imaginary frequency: -406.49 *i* $cm^{-1}$

**IM6-Au(0)**

| | | | |
|---|---|---|---|
| C | 3.75918200 | 1.03220400 | 0.89852700 |
| H | 4.77936900 | 0.71794900 | 1.13349700 |
| H | 3.78847900 | 1.83004700 | 0.15472300 |
| H | 3.28456300 | 1.42320800 | 1.79998400 |
| C | 3.78160200 | -0.99068900 | -1.13975400 |
| H | 4.80179000 | -1.21361900 | -0.81687700 |
| H | 3.32401200 | -1.89615900 | -1.54151900 |
| H | 3.80909200 | -0.24140500 | -1.93254200 |

| | | | |
|---|---|---|---|
| C | 2.97513100 | -1.65441400 | 1.53597600 |
| H | 2.50314000 | -2.57888000 | 1.19946200 |
| H | 4.03229200 | -1.84187100 | 1.74215300 |
| H | 2.47903900 | -1.33216100 | 2.45289800 |
| P | 2.77326700 | -0.36611400 | 0.25254100 |
| Au | 0.60669800 | 0.16208100 | -0.28333800 |
| C | -1.42276900 | 0.58479900 | -0.79828000 |
| C | -2.11116200 | -0.64728600 | -0.42416400 |
| C | -2.39182600 | -1.85141200 | -1.29121800 |
| N | -2.88606600 | -2.89103000 | -0.36027400 |
| C | -3.33580500 | -2.18248900 | 0.86272700 |
| C | -2.66215300 | -0.83456500 | 0.79905100 |
| C | -2.62775500 | 0.21935500 | 1.78154300 |
| C | -2.22301600 | 1.45684500 | 1.43691400 |
| C | -1.92568700 | 1.85999300 | -0.00540700 |
| O | -3.04604400 | 2.12166300 | -0.74214100 |
| C | -0.94521600 | 3.03497200 | -0.08359100 |
| H | -1.43978800 | 0.80034300 | -1.86928100 |
| H | -3.16823500 | -1.60429800 | -2.02906300 |
| H | -1.52392500 | -2.21562100 | -1.84945500 |
| H | -2.09398000 | -3.47051100 | -0.10255500 |
| H | -4.42932100 | -2.07536400 | 0.84990700 |
| H | -3.08498200 | -2.76681100 | 1.75476400 |
| H | -2.92421000 | 0.00985100 | 2.80625000 |
| H | -0.05467800 | 2.85596000 | 0.52740600 |
| H | -0.64273400 | 3.19919300 | -1.12001000 |
| H | -1.44094400 | 3.94109500 | 0.27813600 |
| H | -2.17948600 | 2.24642900 | 2.18280000 |

SCF energy: -1076.593021 hartree

SCF energy in acetonitrile: -1076.624962 hartree

zero-point correction: + 0.295629 hartree

free energy correction: + 0.244990 hartree

**TS6/7-Au(0)**

| | | | |
|---|---|---|---|
| C | 3.71243000 | -0.68230300 | -1.08542000 |
| H | 4.76825400 | -0.52456500 | -0.85104500 |
| H | 3.50596800 | -1.75315900 | -1.11750000 |
| H | 3.49237100 | -0.26018800 | -2.06702000 |
| C | 3.25132800 | -0.57963200 | 1.75208600 |
| H | 4.32609200 | -0.41255300 | 1.86369700 |
| H | 2.72395200 | -0.10174000 | 2.57919800 |
| H | 3.04524100 | -1.65038700 | 1.78694100 |
| C | 3.23038700 | 1.83968700 | 0.21236400 |

| | | | |
|---|---|---|---|
| H | 2.70193000 | 2.37955800 | 0.99976000 |
| H | 4.30623700 | 1.88306500 | 0.40127400 |
| H | 3.00723100 | 2.32170000 | -0.74043400 |
| P | 2.64487400 | 0.10825900 | 0.16875600 |
| Au | 0.42573500 | -0.11294400 | -0.23564700 |
| C | -1.71269600 | 0.71208300 | -0.93357100 |
| C | -1.73442300 | -0.63313400 | -0.48060800 |
| C | -1.99881900 | -1.92106300 | -1.25144200 |
| N | -1.80689200 | -3.00440100 | -0.26703300 |
| C | -2.19016400 | -2.41461700 | 1.03548900 |
| C | -1.95656600 | -0.93032300 | 0.89948900 |
| C | -2.15687400 | 0.11065700 | 1.83411700 |
| C | -2.19323600 | 1.41501700 | 1.42315600 |
| C | -2.18115900 | 1.83033600 | -0.03524900 |
| O | -3.43189100 | 1.74945900 | -0.60555700 |
| C | -1.50245300 | 3.18114300 | -0.25298200 |
| H | -1.65181500 | 0.94736600 | -1.98826800 |
| H | -3.04503700 | -1.91720000 | -1.58257700 |
| H | -1.36989800 | -2.07850400 | -2.12830000 |
| H | -0.80983300 | -3.20311300 | -0.22750700 |
| H | -3.25833700 | -2.60727700 | 1.20937000 |
| H | -1.64130900 | -2.89256000 | 1.85149100 |
| H | -2.30452100 | -0.13275500 | 2.88299400 |
| H | -0.47671000 | 3.18994200 | 0.13289700 |
| H | -1.48747200 | 3.41578600 | -1.32001300 |
| H | -2.07626800 | 3.96021000 | 0.25758600 |
| H | -2.36537200 | 2.20309900 | 2.15135500 |

SCF energy: -1076.584191 hartree

SCF energy in acetonitrile: -1076.622118 hartree

zero-point correction: + 0.294359 hartree

free energy correction: + 0.244151 hartree

imaginary frequency: -154.20 *i* $cm^{-1}$

**IM7-Au(0)**

| | | | |
|---|---|---|---|
| C | 3.56016000 | 1.34653500 | -1.19592400 |
| H | 4.60583400 | 1.57357500 | -0.97246900 |
| H | 3.50409900 | 0.77675900 | -2.12499800 |
| H | 3.00965100 | 2.27849200 | -1.33519400 |
| C | 3.92037500 | -1.04273100 | 0.34741200 |
| H | 4.95168800 | -0.71066000 | 0.49231500 |
| H | 3.60950000 | -1.63917200 | 1.20681700 |
| H | 3.86647500 | -1.67206100 | -0.54257400 |
| C | 3.12951900 | 1.39582000 | 1.63996100 |

| | | | |
|---|---|---|---|
| H | 2.79745900 | 0.85712800 | 2.52904000 |
| H | 4.19516000 | 1.62294400 | 1.73025500 |
| H | 2.56579200 | 2.32826100 | 1.57844000 |
| P | 2.78748100 | 0.38233900 | 0.15376500 |
| Au | 0.56032700 | -0.13478000 | -0.19965900 |
| C | -2.18115100 | 0.67253900 | -0.95101100 |
| C | -1.51788200 | -0.57772700 | -0.45915700 |
| C | -1.70515000 | -1.89174900 | -1.24466800 |
| N | -1.35134100 | -2.96390500 | -0.29275100 |
| C | -1.81425200 | -2.47303300 | 1.02475000 |
| C | -1.91441000 | -0.96955000 | 0.90474600 |
| C | -2.43987200 | -0.06902900 | 1.82541000 |
| C | -2.77451300 | 1.21974300 | 1.44973100 |
| C | -2.77707300 | 1.61110500 | 0.02598000 |
| O | -3.61747900 | 0.76549500 | -0.83402700 |
| C | -2.87704300 | 3.08198100 | -0.28982700 |
| H | -1.80976100 | 1.08914100 | -1.88727700 |
| H | -2.76217200 | -2.00492000 | -1.51867800 |
| H | -1.10619700 | -1.98026400 | -2.15205700 |
| H | -0.33497100 | -3.00921200 | -0.26208100 |
| H | -2.80574200 | -2.89416200 | 1.23640300 |
| H | -1.14440800 | -2.81986000 | 1.81859300 |
| H | -2.60996700 | -0.38578600 | 2.85161700 |
| H | -2.01944700 | 3.62443800 | 0.11904400 |
| H | -2.91190100 | 3.23830100 | -1.36921000 |
| H | -3.78554900 | 3.50566700 | 0.14877300 |
| H | -3.14666000 | 1.93385100 | 2.17683200 |

SCF energy: -1076.611889 hartree

SCF energy in acetonitrile: -1076.637542 hartree

zero-point correction: + 0.296383 hartree

free energy correction: + 0.246127 hartree

**TS1/8-Au(0)**

| | | | |
|---|---|---|---|
| C | 4.70063000 | 0.87415500 | -0.26152000 |
| H | 5.73199100 | 0.51311300 | -0.29278100 |
| H | 4.47085800 | 1.39380100 | -1.19327600 |
| H | 4.59096700 | 1.58463800 | 0.55957700 |
| C | 3.96484800 | -1.65766100 | -1.38329600 |
| H | 5.03069900 | -1.90057200 | -1.36639600 |
| H | 3.38398100 | -2.57608000 | -1.28211900 |
| H | 3.71386200 | -1.20115900 | -2.34228500 |
| C | 4.16108300 | -1.35059400 | 1.46173500 |
| H | 3.58638200 | -2.26182900 | 1.63603400 |

| | | | |
|---|---|---|---|
| H | 5.21870600 | -1.60501700 | 1.35226200 |
| H | 4.03395000 | -0.69867500 | 2.32768500 |
| P | 3.51881600 | -0.50530700 | -0.03085200 |
| Au | 1.30759600 | 0.15126500 | 0.05385700 |
| C | -1.56745900 | -0.27795400 | -0.06101200 |
| C | -0.69077100 | 0.67687900 | 0.12510000 |
| C | -1.10631800 | 2.11022600 | 0.36219700 |
| N | -2.54418100 | 2.25978800 | 0.58303400 |
| C | -3.38300100 | 1.85706600 | -0.54155600 |
| C | -3.76338900 | 0.40601700 | -0.54396000 |
| C | -4.03956300 | -0.43554400 | -1.60465900 |
| C | -4.79548800 | -1.51891600 | -1.08322800 |
| C | -5.00323000 | -1.25725300 | 0.24085000 |
| O | -4.42644600 | -0.06211900 | 0.56928600 |
| C | -5.69823700 | -1.98182300 | 1.33354300 |
| H | -1.51771000 | -1.33797900 | -0.27214900 |
| H | -0.59495700 | 2.49721400 | 1.24892600 |
| H | -0.75073300 | 2.71356200 | -0.49554200 |
| H | -2.74382300 | 3.22656500 | 0.81242800 |
| H | -4.30598300 | 2.44699100 | -0.49104400 |
| H | -2.91952000 | 2.06522500 | -1.51983300 |
| H | -3.67847600 | -0.31158000 | -2.61366900 |
| H | -5.00701900 | -2.24262900 | 2.14131900 |
| H | -6.49723100 | -1.37313600 | 1.76934700 |
| H | -6.13807500 | -2.90111300 | 0.94481200 |
| H | -5.14402200 | -2.39079800 | -1.61593200 |

SCF energy: -1076.565888 hartree

SCF energy in acetonitrile: -1076.591905 hartree

zero-point correction: + 0.293039 hartree

free energy correction: + 0.240567 hartree

imaginary frequency: -261.28 *i* $cm^{-1}$

**IM8-Au(0)**

| | | | |
|---|---|---|---|
| C | 3.80252100 | -2.05155800 | -0.91064000 |
| H | 4.86305000 | -2.31192400 | -0.86068600 |
| H | 3.21067600 | -2.86863500 | -0.49439000 |
| H | 3.51134200 | -1.91874600 | -1.95394700 |
| C | 4.15536800 | -0.86419000 | 1.67299800 |
| H | 5.19950800 | -1.17968700 | 1.60055100 |
| H | 4.09066500 | 0.03279600 | 2.29125800 |
| H | 3.57246500 | -1.65096500 | 2.15489300 |
| C | 4.64141300 | 0.68241100 | -0.69036300 |
| H | 4.58880100 | 1.61880300 | -0.13224400 |

| | | | |
|---|---|---|---|
| H | 5.66334300 | 0.29608100 | -0.65233200 |
| H | 4.37139000 | 0.88924400 | -1.72732700 |
| P | 3.45038600 | -0.51394600 | 0.01966200 |
| Au | 1.23972800 | 0.16037900 | 0.00558800 |
| C | -1.71192900 | -0.14148400 | -0.28904600 |
| C | -0.73382600 | 0.73180800 | -0.00159900 |
| C | -1.08538400 | 2.16612900 | 0.31446900 |
| N | -2.49673300 | 2.31708400 | 0.66137000 |
| C | -3.35910800 | 1.74217200 | -0.35823700 |
| C | -3.17708700 | 0.22067000 | -0.40337800 |
| C | -3.85827300 | -0.40847700 | -1.58797900 |
| C | -4.84050200 | -1.26891100 | -1.12809500 |
| C | -4.85107500 | -1.23216300 | 0.25601700 |
| O | -3.90471600 | -0.38079700 | 0.74142100 |
| C | -5.68600500 | -1.93081800 | 1.26175600 |
| H | -1.49347700 | -1.18512900 | -0.49744000 |
| H | -0.48893800 | 2.51389400 | 1.16288000 |
| H | -0.79015000 | 2.79010100 | -0.55363700 |
| H | -2.72157500 | 3.29707000 | 0.79968900 |
| H | -4.40229000 | 1.96529800 | -0.12621200 |
| H | -3.14466700 | 2.12672300 | -1.37299500 |
| H | -3.57567200 | -0.20895500 | -2.61066600 |
| H | -5.06786200 | -2.53191900 | 1.93857900 |
| H | -6.23822400 | -1.21603000 | 1.88301300 |
| H | -6.40241300 | -2.58836300 | 0.76736600 |
| H | -5.50207200 | -1.87711500 | -1.72913000 |

SCF energy: -1076.615932 hartree

SCF energy in acetonitrile: -1076.641273 hartree

zero-point correction: + 0.295506 hartree

free energy correction: + 0.243794 hartree

**TS8/9-Au(0)**

| | | | |
|---|---|---|---|
| C | 4.22104700 | -0.56037000 | 1.61119100 |
| H | 5.24109600 | -0.94593900 | 1.53372200 |
| H | 4.24991400 | 0.46237000 | 1.99103200 |
| H | 3.65723700 | -1.16948300 | 2.31974900 |
| C | 4.53463800 | 0.32852300 | -1.09724400 |
| H | 5.54044100 | -0.09691300 | -1.04784800 |
| H | 4.17471700 | 0.28646300 | -2.12664900 |
| H | 4.57061100 | 1.37584100 | -0.79248500 |
| C | 3.56406100 | -2.31632200 | -0.56069800 |
| H | 3.17263600 | -2.41970000 | -1.57414000 |
| H | 4.61225400 | -2.62565700 | -0.54454100 |

| | | | |
|---|---|---|---|
| H | 2.98461500 | -2.96834600 | 0.09511900 |
| P | 3.37345900 | -0.58061200 | -0.01172600 |
| Au | 1.19833900 | 0.19898800 | 0.00050500 |
| C | -1.76991500 | 0.04568100 | -0.31829900 |
| C | -0.74253900 | 0.85729000 | 0.02517900 |
| C | -1.03885700 | 2.29241600 | 0.38537000 |
| N | -2.42938400 | 2.47054600 | 0.79309900 |
| C | -3.37347000 | 1.97609600 | -0.19048900 |
| C | -3.13976700 | 0.51650700 | -0.48219700 |
| C | -3.96073000 | -0.09528100 | -1.50351000 |
| C | -4.55222000 | -1.29857200 | -1.14542600 |
| C | -4.53381300 | -1.48491500 | 0.24875500 |
| O | -3.89782000 | -0.61929700 | 0.95682000 |
| C | -5.28130400 | -2.57088300 | 0.96589500 |
| H | -1.60168100 | -0.99015000 | -0.59461400 |
| H | -0.40269800 | 2.60816500 | 1.21700400 |
| H | -0.75707400 | 2.92694400 | -0.48040300 |
| H | -2.61921400 | 3.44465200 | 1.00325200 |
| H | -4.38811700 | 2.11034000 | 0.19003300 |
| H | -3.32117100 | 2.50259500 | -1.16820000 |
| H | -4.22828700 | 0.46003200 | -2.39734300 |
| H | -4.58740600 | -3.19849000 | 1.53372200 |
| H | -5.97664800 | -2.12767100 | 1.68474900 |
| H | -5.83688300 | -3.20022500 | 0.26842200 |
| H | -5.12949900 | -1.92617300 | -1.81202100 |

SCF energy: -1076.592379 hartree

SCF energy in acetonitrile: -1076.619773 hartree

zero-point correction: + 0.293412 hartree

free energy correction: + 0.240822 hartree

imaginary frequency: -455.84 *i* $cm^{-1}$

**IM9-Au(0)**

| | | | |
|---|---|---|---|
| C | -1.84214000 | -0.48422000 | -0.04500600 |
| C | -0.69036600 | -1.23957500 | -0.02583100 |
| C | -0.80631200 | -2.73829100 | 0.00386800 |
| N | -2.11174400 | -3.19367300 | -0.47289900 |
| C | -3.20684000 | -2.55161400 | 0.24327200 |
| C | -3.13572800 | -1.05181900 | 0.07145000 |
| C | -4.36245800 | -0.36225400 | 0.11610900 |
| C | -4.76033100 | 0.96814300 | 0.06665800 |
| C | -4.03935600 | 2.22865000 | -0.03519300 |
| O | -2.81703500 | 2.36596400 | -0.09377500 |
| C | -4.93214100 | 3.46445400 | -0.06329000 |

| | | | |
|---|---|---|---|
| H | -1.79020900 | 0.59466900 | -0.11121400 |
| H | -0.03713100 | -3.18940300 | -0.62949800 |
| H | -0.58786000 | -3.07022100 | 1.04075800 |
| H | -2.18231000 | -4.20203400 | -0.37748600 |
| H | -4.15314000 | -2.93117600 | -0.15175600 |
| H | -3.19613400 | -2.77814500 | 1.32990100 |
| H | -5.21403000 | -1.03682000 | 0.20907400 |
| H | -5.53737400 | 3.52406600 | 0.84677300 |
| H | -4.31281500 | 4.35610700 | -0.14656800 |
| H | -5.62561000 | 3.42062200 | -0.90893900 |
| H | -5.83811600 | 1.10311100 | 0.11672200 |
| Au | 1.14088900 | -0.32881100 | 0.00308800 |
| P | 3.16578400 | 0.78777900 | 0.01455900 |
| C | 3.58174300 | 1.62813900 | -1.55741100 |
| H | 4.53602400 | 2.15641300 | -1.48468300 |
| H | 3.63692100 | 0.88980300 | -2.35915700 |
| H | 2.79215400 | 2.33970200 | -1.80466700 |
| C | 4.64813300 | -0.23297600 | 0.34951800 |
| H | 5.55795200 | 0.37271100 | 0.33525000 |
| H | 4.54699500 | -0.70851900 | 1.32658600 |
| H | 4.72534600 | -1.01760200 | -0.40509700 |
| C | 3.29074900 | 2.13103900 | 1.25110200 |
| H | 4.25750500 | 2.63758900 | 1.19039400 |
| H | 2.49127200 | 2.85350800 | 1.07855700 |
| H | 3.16230800 | 1.71495700 | 2.25174900 |

SCF energy: -1076.631255 hartree

SCF energy in acetonitrile: -1076.658113 hartree

zero-point correction: + 0.295048 hartree

free energy correction: + 0.240591 hartree

**TS9/10-Au(0)**

| | | | |
|---|---|---|---|
| C | -2.08087700 | -0.16501300 | 0.44773800 |
| C | -1.00330000 | -1.00365600 | -0.02142800 |
| C | -1.40396400 | -2.32177400 | -0.64278500 |
| N | -2.63001600 | -2.92255700 | -0.09673200 |
| C | -3.74642100 | -1.98512900 | -0.22983100 |
| C | -3.45688600 | -0.60769700 | 0.32074600 |
| C | -4.40506100 | 0.33169600 | 0.59712000 |
| C | -4.07369700 | 1.71946400 | 0.63586100 |
| C | -2.97857200 | 2.17064200 | -0.09198900 |
| O | -1.99511700 | 1.42223700 | -0.48570600 |
| C | -2.92582500 | 3.58648000 | -0.60676600 |
| H | -1.89050500 | 0.41689100 | 1.34954100 |

| | | | |
|---|---|---|---|
| H | -1.56491100 | -2.18292000 | -1.72480200 |
| H | -0.59362800 | -3.04885400 | -0.54937700 |
| H | -2.47491700 | -3.10027200 | 0.89441300 |
| H | -3.97482500 | -1.92583000 | -1.30337700 |
| H | -4.63277000 | -2.40721600 | 0.25442700 |
| H | -5.45882800 | 0.05575100 | 0.62348700 |
| H | -3.01299400 | 3.57976000 | -1.69747900 |
| H | -3.73555500 | 4.18778700 | -0.19152400 |
| H | -1.96625800 | 4.04740200 | -0.35853400 |
| H | -4.83295200 | 2.44531500 | 0.89910300 |
| Au | 0.92860700 | -0.35598500 | 0.01777000 |
| P | 3.11005900 | 0.40863000 | 0.05292000 |
| C | 4.28410900 | -0.50177700 | -1.01653300 |
| H | 3.94087100 | -0.45557700 | -2.05142200 |
| H | 5.29001800 | -0.07908500 | -0.95029700 |
| H | 4.31267500 | -1.54986500 | -0.71374300 |
| C | 3.92771400 | 0.37830700 | 1.69081400 |
| H | 4.95055800 | 0.75992800 | 1.63384600 |
| H | 3.35395400 | 0.98720400 | 2.39158000 |
| H | 3.94505100 | -0.64619200 | 2.06648800 |
| C | 3.31133600 | 2.14608100 | -0.48538500 |
| H | 2.71591300 | 2.79447200 | 0.15962000 |
| H | 4.35838900 | 2.45737400 | -0.44626100 |
| H | 2.93962000 | 2.25153300 | -1.50592800 |

SCF energy: -1076.589875 hartree

SCF energy in acetonitrile: -1076.614087 hartree

zero-point correction: + 0.295031 hartree

free energy correction: + 0.242714 hartree

imaginary frequency: -448.85 *i* $cm^{-1}$

**IM10-Au(0)**

| | | | |
|---|---|---|---|
| C | 2.21008700 | -0.05875200 | -0.47684000 |
| C | 1.05590600 | -0.99497700 | -0.33703200 |
| C | 1.43764000 | -2.45464700 | -0.45159300 |
| N | 2.86311200 | -2.77403300 | -0.21654900 |
| C | 3.42536400 | -1.89240100 | 0.81555200 |
| C | 3.39452400 | -0.45528700 | 0.38647600 |
| C | 4.31884400 | 0.48894800 | 0.61488900 |
| C | 4.06571400 | 1.85279100 | 0.19081400 |
| C | 2.80356400 | 2.21582100 | -0.12219200 |
| O | 1.79346700 | 1.30356100 | -0.17556400 |
| C | 2.31731600 | 3.61132100 | -0.32822700 |

| | | | |
|---|---|---|---|
| H | 2.54904900 | -0.02653400 | -1.53558700 |
| H | 0.84257200 | -3.03989700 | 0.26090200 |
| H | 1.17818700 | -2.84941100 | -1.44474800 |
| H | 3.38558800 | -2.63324200 | -1.07736400 |
| H | 2.82107700 | -2.04037800 | 1.71998500 |
| H | 4.44533800 | -2.20685900 | 1.05345200 |
| H | 5.22113800 | 0.26936100 | 1.17973800 |
| H | 1.54052000 | 3.84654700 | 0.40710100 |
| H | 3.13462200 | 4.32403100 | -0.21543400 |
| H | 1.87121600 | 3.73013600 | -1.32023300 |
| H | 4.83785200 | 2.60903000 | 0.24745600 |
| Au | -0.85997200 | -0.36280200 | -0.10230700 |
| P | -3.02881600 | 0.34833200 | 0.17601100 |
| C | -3.54989900 | 0.67347700 | 1.90258200 |
| H | -2.89519800 | 1.42966500 | 2.33916300 |
| H | -4.58597600 | 1.01976300 | 1.95030900 |
| H | -3.44751800 | -0.24179800 | 2.48821600 |
| C | -4.32190100 | -0.79835600 | -0.43017200 |
| H | -5.32302600 | -0.39062500 | -0.26727000 |
| H | -4.17386600 | -0.97860000 | -1.49619000 |
| H | -4.23204000 | -1.75269000 | 0.09159800 |
| C | -3.43579700 | 1.91857800 | -0.67447700 |
| H | -3.26570600 | 1.80289900 | -1.74616400 |
| H | -4.47568700 | 2.20809500 | -0.50161900 |
| H | -2.77579700 | 2.70753200 | -0.30958000 |

SCF energy: -1076.601829 hartree

SCF energy in acetonitrile: -1076.624346 hartree

zero-point correction: + 0.296597 hartree

free energy correction: + 0.244200 hartree

**TS10/11-Au(0)**

| | | | |
|---|---|---|---|
| C | 2.18835000 | -0.06173300 | -0.04699200 |
| C | 1.03302200 | -0.98135400 | -0.04238500 |
| C | 1.45703300 | -2.44125500 | 0.03580500 |
| N | 2.82829300 | -2.75473700 | -0.39658500 |
| C | 3.81776000 | -1.92235000 | 0.29407000 |
| C | 3.55681900 | -0.43824800 | 0.17482400 |
| C | 4.52636900 | 0.52695700 | 0.17581200 |
| C | 4.14299700 | 1.89949700 | 0.00232900 |
| C | 2.83917800 | 2.23982900 | -0.04896200 |
| O | 1.84010000 | 1.29319200 | 0.09910900 |
| C | 2.27051200 | 3.61018400 | -0.15784900 |
| H | 1.78423200 | -0.47263500 | -1.15853200 |

| | | | |
|---|---|---|---|
| H | 1.38060400 | -2.75573300 | 1.08641400 |
| H | 0.77328700 | -3.07837800 | -0.52892600 |
| H | 2.90649600 | -2.60274400 | -1.39950800 |
| H | 3.80356700 | -2.21520500 | 1.35156600 |
| H | 4.81188000 | -2.16690400 | -0.08992800 |
| H | 5.57268000 | 0.26121900 | 0.27739700 |
| H | 1.64715400 | 3.83649800 | 0.71471300 |
| H | 3.07035400 | 4.34863300 | -0.21882000 |
| H | 1.63255000 | 3.70326100 | -1.04327900 |
| H | 4.88844200 | 2.68050800 | -0.08101100 |
| Au | -0.89508300 | -0.34504800 | -0.01695600 |
| P | -3.07847400 | 0.32382200 | 0.03106600 |
| C | -4.28785100 | -1.03028400 | 0.27520800 |
| H | -4.07339000 | -1.54121500 | 1.21509300 |
| H | -5.31138200 | -0.64679800 | 0.29658700 |
| H | -4.19108900 | -1.75315700 | -0.53659400 |
| C | -3.71966100 | 1.17164900 | -1.46441900 |
| H | -4.76792500 | 1.45909300 | -1.34292500 |
| H | -3.12058900 | 2.06357600 | -1.65603200 |
| H | -3.62311100 | 0.50715700 | -2.32457200 |
| C | -3.50459100 | 1.50581700 | 1.36488200 |
| H | -2.88802800 | 2.40075300 | 1.26336900 |
| H | -4.56026800 | 1.78789600 | 1.32577100 |
| H | -3.28529000 | 1.05097500 | 2.33204300 |

SCF energy: -1076.558104 hartree

SCF energy in acetonitrile: -1076.580062 hartree

zero-point correction: + 0.292432 hartree

free energy correction: + 0.241725 hartree

imaginary frequency: -1657.65 *i* $cm^{-1}$

**IM11-Au(0)**

| | | | |
|---|---|---|---|
| C | 2.13817400 | -0.07708100 | -0.22129300 |
| C | 1.10865400 | -1.02228700 | -0.70628900 |
| C | 1.40456700 | -2.43862200 | -0.17825800 |
| N | 2.83203100 | -2.79291800 | -0.15901600 |
| C | 3.56192800 | -1.87631900 | 0.71414500 |
| C | 3.26411600 | -0.40706700 | 0.47645300 |
| C | 4.15212500 | 0.60323700 | 0.92587600 |
| C | 3.84357900 | 1.94057400 | 0.59881400 |
| C | 2.74047600 | 2.24162100 | -0.13804300 |
| O | 1.87476900 | 1.25026800 | -0.56409700 |
| C | 2.29166300 | 3.58846200 | -0.58114900 |
| H | 1.12249700 | -1.02667300 | -1.80749900 |

| | | | |
|---|---|---|---|
| H | 1.05296500 | -2.54367400 | 0.85259100 |
| H | 0.86809000 | -3.17854400 | -0.77739600 |
| H | 3.20104300 | -2.69901300 | -1.10321400 |
| H | 3.33111800 | -2.14178600 | 1.75422800 |
| H | 4.63425700 | -2.04962600 | 0.58016400 |
| H | 5.05059600 | 0.35122700 | 1.47550900 |
| H | 1.29567300 | 3.82336600 | -0.18705700 |
| H | 2.99132200 | 4.35091000 | -0.23663000 |
| H | 2.22509700 | 3.64226900 | -1.67388200 |
| H | 4.48473400 | 2.75644200 | 0.91312200 |
| Au | -0.84366000 | -0.36648000 | -0.22431900 |
| P | -2.97320700 | 0.35115000 | 0.30798500 |
| C | -3.57954000 | -0.16565900 | 1.95632900 |
| H | -2.89843400 | 0.20675800 | 2.72347300 |
| H | -4.58580200 | 0.21528600 | 2.15013200 |
| H | -3.58950600 | -1.25557100 | 2.01164800 |
| C | -4.30716500 | -0.20300100 | -0.81768000 |
| H | -5.28080600 | 0.17957300 | -0.50036400 |
| H | -4.09477700 | 0.14717700 | -1.82934800 |
| H | -4.33621400 | -1.29384900 | -0.83475700 |
| C | -3.18551100 | 2.16973000 | 0.33745600 |
| H | -2.94596400 | 2.57592100 | -0.64681800 |
| H | -4.20801300 | 2.44908100 | 0.60501500 |
| H | -2.49142300 | 2.60216600 | 1.06021400 |

SCF energy: -1076.641933 hartree

SCF energy in acetonitrile: -1076.664033 hartree

zero-point correction: + 0.296616 hartree

free energy correction: + 0.244922 hartree