Supporting Information for

Ag-Catalyzed Azide Alkyne Cycloaddition:A DFT Approach

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Contents

Benchmark Study

Firstly, we investigated optimized silver catalyst structures of the Complex_1 and Complex_2 (Figure S1) by using different functionals (B3LYP, BPW91, M06L, wb97xd) and basis sets (6-31+G*, 6-311+G* with Lanl2dz, SDD, MWB as effective core potential). Then, critical distances in these complexes are compared to the ones in the X-ray crystal structures shown in Figure S1.

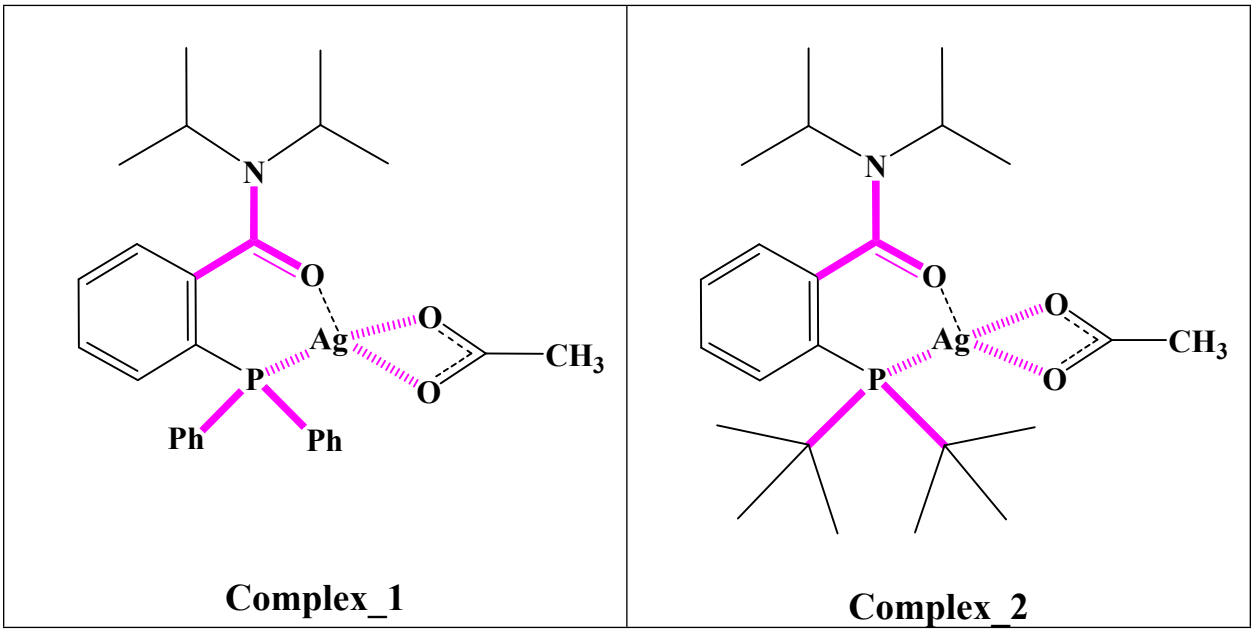

Figure S1. Critical distances in the X-ray crystal structures of Complex_1 and Complex_2 [23]

For each method, percent mean relative errors have been calculated using the formula below.

$$\% \text{ mean relative error} = \frac{100}{n}\sum_{i=1}^{n}\left|\frac{e_i - m_i}{m_i}\right|$$

Formula S1. Percent mean relative error. (the estimated value denoted by *e*, was compared with the measured value, which is denoted by m and number of observations are denoted by n.)

Percent mean errors of the benchmark study is given in Table S1. The combination of wb97xd functional with 6-31+G* where MWB basis set was used for Ag, is found to have lowest % error among the full set. Although the chosen methodology is not significantly successful than the

other methods, we employed it because it is also highlighted in the literature for transition metals and dispersion corrections.

		Lanl2dz	SDD	MWB
b3lyp	6-31+G*	1.51 (1.73)	1.41 (1.44)	1.41 (1.44)
	6-311+G*	1.52 (1.53)	1.33 (1.70)	1.33 (1.70)
bpw91	6-31+G*	1.31 (1.89)	1.25 (1.77)	1.25 (1.77)
	6-311+G*	1.35 (1.78)	1.16 (1.79)	1.16 (1.79)
M06L	6-31+G*	1.78 (1.40)	1.24 (0.98)	0.87 (0.91)
	6-311+G*	1.64 (1.25)	1.20 (0.74)	1.20 (0.74)
wb97xd	6-31+G*	0.80 (1.01)	0.53 (0.87)	0.43 (0.94)
	6-311+G*	0.71 (1.13)	0.53 (0.94)	0.53 (0.94)

Table S1. Critical bond length deviations in Complex_1 and Complex_2 (in parenthesis) structures.

Uncatalyzed Reaction

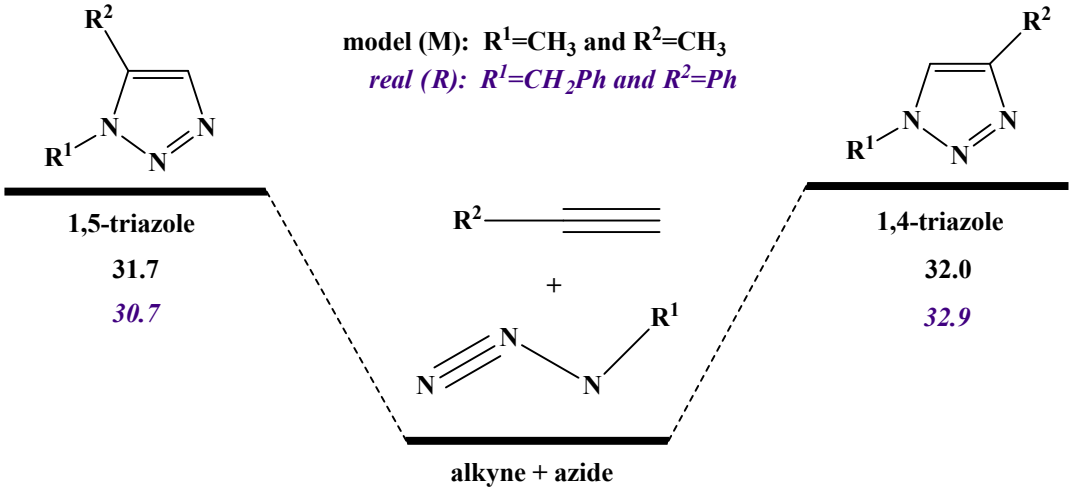

Figure S2. Uncatalyzed reaction barriers for model and real systems (with respect to azide-alkyne complex, kcal/mol)

CARTESIAN COORDINATES OF THE STRUCTURES

Ag_1_A_M

C	1.67511600	-0.00533600	0.00120500
C	2.89819300	-0.00160000	0.00138200
Ag	-0.35209600	-0.00228600	-0.00069800
P	-2.73914300	0.00446200	0.00072600
H	-3.42414400	-0.71678300	-0.99289400
H	-3.41815100	-0.49516200	1.12561100
H	-3.41702900	1.22960800	-0.12585400
C	4.36287600	0.00621600	0.00014800
H	4.75372600	0.66502400	-0.78447000
H	4.75836800	0.36039900	0.95961900
H	4.76577200	-0.99823200	-0.17650000

Zero-point correction=	0.074808
(Hartree/Particle)	
Thermal correction to Energy=	0.083735
Thermal correction to Enthalpy=	0.084679
Thermal correction to Gibbs Free Energy=	0.039435
Sum of electronic and zero-point Energies=	-606.081919
Sum of electronic and thermal Energies=	-606.072993
Sum of electronic and thermal Enthalpies=	-606.072048
Sum of electronic and thermal Free Energies=	-606.117293

Ag_1_TS_{AD}_M

C	-1.22811400	-1.22537900	-0.00361800
C	-2.45411500	-0.92521500	0.00292300
N	-2.64467600	0.89292900	-0.00221900
N	-1.71657100	1.63863600	-0.00604000
N	-0.44191600	1.57246500	-0.01910200
C	0.21179200	2.88058900	0.01407100
H	1.28145000	2.71275400	-0.13463800
H	-0.14882900	3.54053300	-0.78403600
Ag	0.67738900	-0.48002300	-0.00508200
P	3.06605000	-0.41335600	0.00721800
H	3.77601500	-1.11528300	-0.98351100
H	3.75016900	0.81311900	-0.09804700
H	3.74486900	-0.91711300	1.13117000
C	-3.86313800	-1.38166700	0.01364100
H	-4.38850700	-1.00730700	-0.87097300
H	-3.91181400	-2.47356200	0.02291000
H	-4.37932000	-0.99270900	0.89734500

H	0.07155000	3.38281900	0.97981400

Zero-point correction=	0.126878
(Hartree/Particle)	
Thermal correction to Energy=	0.140211
Thermal correction to Enthalpy=	0.141156
Thermal correction to Gibbs Free Energy=	0.084956
Sum of electronic and zero-point Energies=	-810.030085
Sum of electronic and thermal Energies=	-810.016752
Sum of electronic and thermal Enthalpies=	-810.015807
Sum of electronic and thermal Free Energies=	-810.072007

Ag_1_D_M

C	1.11010200	0.02415100	0.00173300
C	2.01384100	1.08060700	-0.00099200
N	3.28722200	0.59671400	-0.00505000
N	3.24306200	-0.70143500	-0.00571100
N	1.94658000	-1.05411600	-0.00143500
C	1.60726300	-2.45885300	-0.00074700
H	1.02751800	-2.71259300	-0.89361300
H	2.54128700	-3.02337500	-0.00062100
Ag	-0.96386000	0.00126300	0.00538400
P	-3.36478600	0.02564000	-0.00731800
H	-4.02476500	1.00405700	-0.77070200
H	-4.04790300	-1.10753100	-0.48126800
H	-4.05575700	0.19888500	1.20438900
C	1.75363700	2.55400500	-0.00103500
H	2.17060500	3.02967800	-0.89580900
H	0.67699400	2.75533700	0.02260900
H	2.21032100	3.03552200	0.87079800
H	1.02779500	-2.71156300	0.89255900

Zero-point correction=	0.133195 (Hartree/Particle)
Thermal correction to Energy=	0.145438
Thermal correction to Enthalpy=	0.146382
Thermal correction to Gibbs Free Energy=	0.091523
Sum of electronic and zero-point Energies=	-810.161859
Sum of electronic and thermal Energies=	-810.149616
Sum of electronic and thermal Enthalpies=	-810.148672
Sum of electronic and thermal Free Energies=	-810.203531

Ag_1_A_R

C	-0.00326400	-0.01993000	-0.00212800
C	-1.22787000	-0.01478800	-0.00164600
Ag	2.02764400	-0.01019000	-0.00093000
P	4.41556000	0.02147600	0.00239600

C	-2.66176400	-0.00511500	-0.00073200
C	-3.38798300	-1.20731600	-0.00011900
C	-3.36924200	1.20823000	-0.00023200
C	-4.77955400	-1.19362700	0.00111400
H	-2.84703200	-2.14890700	-0.00056400
C	-4.76076000	1.21651100	0.00098800
H	-2.81356700	2.14122800	-0.00076100
C	-5.47211400	0.01688600	0.00170500
H	-5.32575900	-2.13320500	0.00164800
H	-5.29224900	2.16445700	0.00141700
H	-6.55867000	0.02545400	0.00277300
H	5.11118600	-0.88452100	-0.81620500
H	5.07235900	1.20265400	-0.38321500
H	5.09638200	-0.21548000	1.20897200

Zero-point correction=	0.129146 (Hartree/Particle)
Thermal correction to Energy=	0.140829
Thermal correction to Enthalpy=	0.141773
Thermal correction to Gibbs Free Energy=	0.086879
Sum of electronic and zero-point Energies=	-797.704743
Sum of electronic and thermal Energies=	-797.693061
Sum of electronic and thermal Enthalpies=	-797.692116
Sum of electronic and thermal Free Energies=	-797.747010

Ag_1_TS_{AD}_R

C	1.46951200	0.91291700	-0.03358400
C	2.42871500	0.08922700	-0.04231700
N	1.77398100	-1.61274000	-0.35366600
N	0.61877700	-1.81415800	-0.54533800
N	-0.46836500	-1.15026900	-0.59286000
C	-1.65601600	-1.93703000	-0.93553000
H	-1.88294500	-1.81990900	-2.00393900
H	-1.46210800	-3.00221100	-0.75870800
Ag	-0.54512900	1.19413100	-0.27281600
P	-2.75118300	2.11335200	-0.43312900
C	3.86988700	-0.06731400	0.12276300
C	4.55985800	0.82757100	0.95453500
C	4.58853200	-1.06827300	-0.54062400
C	5.93712900	0.72093900	1.11710200
H	4.00301900	1.60197700	1.47355700
C	5.96760500	-1.17000500	-0.37527000
H	4.06247900	-1.76469800	-1.18368200
C	6.64721300	-0.27932800	0.45307200
H	6.45734600	1.41925200	1.76701600
H	6.51274700	-1.95100300	-0.89840300
H	7.72251700	-0.36472000	0.58279200
C	-2.85171300	-1.49755900	-0.11822600

C	-4.09813000	-1.31414000	-0.72059000
C	-2.73258400	-1.28984300	1.26058500
C	-5.21061700	-0.94357500	0.03691600
H	-4.20389600	-1.46750100	-1.79265800
C	-3.83811400	-0.91429100	2.01856500
H	-1.76207100	-1.41389800	1.73358700
C	-5.08272300	-0.74101500	1.40925300
H	-6.17416300	-0.81006100	-0.44715400
H	-3.72928800	-0.75817200	3.08822600
H	-5.94610400	-0.45204100	2.00206900
H	-2.99381800	3.48874100	-0.26068300
H	-3.45936300	1.93239600	-1.63450400
H	-3.71759300	1.60789500	0.45492500

Zero-point correction=	0.263869
(Hartree/Particle)	
Thermal correction to Energy=	0.283886
Thermal correction to Enthalpy=	0.284831
Thermal correction to Gibbs Free Energy=	0.211976
Sum of electronic and zero-point Energies=	-1232.553352
Sum of electronic and thermal Energies=	-1232.533335
Sum of electronic and thermal Enthalpies=	-1232.532390
Sum of electronic and thermal Free Energies=	-1232.605245

Ag_1_D_R

C	-0.59125000	0.82272200	-0.37935000
C	-1.91216500	1.17169500	-0.10928500
N	-2.03537600	2.53375300	-0.08722200
N	-0.87990400	3.06565000	-0.31897200
N	-0.00826400	2.05010400	-0.49136500
C	1.36310600	2.37282100	-0.84309300
H	1.51175700	2.20729500	-1.91625200
H	1.47629300	3.44436500	-0.65244300
Ag	0.52724700	-0.94014600	-0.43253600
P	2.00215800	-2.82303000	-0.36643200
C	-3.08763100	0.31680500	0.12912700
C	-2.96376700	-1.02764700	0.50112300
C	-4.37710600	0.84901300	-0.01095800
C	-4.08832600	-1.82197600	0.71001400
H	-1.97431700	-1.45487600	0.64616200
C	-5.50168700	0.05796400	0.20492000
H	-4.48489600	1.89266300	-0.28914700
C	-5.36523600	-1.28325000	0.56201100
H	-3.96552800	-2.86292300	0.99870000
H	-6.49127800	0.49245700	0.08958100
H	-6.24427500	-1.89975900	0.72889300
C	2.37812500	1.57412500	-0.05461300
C	3.44260900	0.94535400	-0.70365700

C	2.26320800	1.44810600	1.33422900
C	4.37792200	0.20015200	0.01745900
H	3.54127900	1.03610600	-1.78322600
C	3.18827700	0.69906100	2.05454000
H	1.42676500	1.92028000	1.84299000
C	4.24934900	0.07102800	1.39834100
H	5.20743800	-0.27390200	-0.50103300
H	3.08241700	0.60480400	3.13156300
H	4.97524800	-0.50666200	1.96430000
H	2.84408400	-3.04873100	-1.46882800
H	2.97488700	-2.80883900	0.64676800
H	1.51937700	-4.13235500	-0.19430200

Zero-point correction=	0.270195 (Hartree/Particle)
Thermal correction to Energy=	0.289136
Thermal correction to Enthalpy=	0.290081
Thermal correction to Gibbs Free Energy=	0.219192
Sum of electronic and zero-point Energies=	-1232.687491
Sum of electronic and thermal Energies=	-1232.668549
Sum of electronic and thermal Enthalpies=	-1232.667605
Sum of electronic and thermal Free Energies=	-1232.738494

Methyl azide

C	-1.53252400	-0.28958400	-0.00000300
H	-1.53386800	-0.92464500	-0.89401200
H	-2.43312100	0.32368000	-0.00105700
N	-0.39537600	0.63965800	0.00000000
N	0.71227700	0.10306000	-0.00001700
N	1.78268300	-0.27678200	0.00001300
H	-1.53495900	-0.92308300	0.89511800

Zero-point correction=	0.051094 (Hartree/Particle)
Thermal correction to Energy=	0.055514
Thermal correction to Enthalpy=	0.056458
Thermal correction to Gibbs Free Energy=	0.024616
Sum of electronic and zero-point Energies=	-203.972257
Sum of electronic and thermal Energies=	-203.967838
Sum of electronic and thermal Enthalpies=	-203.966894
Sum of electronic and thermal Free Energies=	-203.998736

Benzyl azide

H	-3.61865000	0.80872000	-0.75751300

C	-2.65476800	0.45674100	-0.40110700
C	-1.89751500	1.24718500	0.45883300
C	-2.17141400	-0.78779900	-0.80641700
C	-0.66037000	0.79328200	0.91470600
H	-2.26816800	2.21744700	0.77672900
C	-0.93679000	-1.23795000	-0.35006300
H	-2.75991600	-1.40838100	-1.47608600
C	-0.17080700	-0.45181100	0.51629100
H	-0.07164400	1.41417600	1.58656400
H	-0.55665600	-2.20480500	-0.67168800
C	1.18822600	-0.92479300	0.97331800
H	1.49450100	-0.39602200	1.88515500
H	1.17879500	-1.99335400	1.19394200
N	2.23882600	-0.77379600	-0.06325200
N	2.37917200	0.37733000	-0.48055200
N	2.58519600	1.39547900	-0.93769100

Zero-point correction=	0.134152
(Hartree/Particle)	
Thermal correction to Energy=	0.142477
Thermal correction to Enthalpy=	0.143421
Thermal correction to Gibbs Free Energy=	0.099247
Sum of electronic and zero-point Energies=	-434.870079
Sum of electronic and thermal Energies=	-434.861755
Sum of electronic and thermal Enthalpies=	-434.860810
Sum of electronic and thermal Free Energies=	-434.904984

μ^2-η_1-η_2 coordination of the silver (I) acetylide (lamellar structure)

Ag	-0.95056600	1.36285500	-0.12793100
P	-3.17981400	2.28338400	-0.33607400
C	1.13828000	1.35686400	-0.01673400
C	2.35992200	1.23622200	0.07043800
C	3.77999700	1.07343800	0.18029200
C	4.38791600	0.92315900	1.43850200
C	4.58582200	0.99988600	-0.96873700
C	5.75595000	0.68980900	1.54057900
H	3.77024000	0.98236300	2.32985000
C	5.95405600	0.76636000	-0.86110000
H	4.12227300	1.12468200	-1.94322600
C	6.54447600	0.60475500	0.39209900
H	6.21009700	0.57337900	2.52089200
H	6.56212200	0.71212700	-1.76022100
H	7.61202200	0.42186700	0.47502600
Ag	0.95080600	-1.36097900	-0.12801500
P	3.17977800	-2.28304800	-0.33489500
C	-1.13809900	-1.35574600	-0.01731700
C	-2.35977700	-1.23558700	0.07000700

C	-3.77995800	-1.07390300	0.18025400
C	-4.38739100	-0.92230000	1.43854800
C	-4.58658000	-1.00346000	-0.96841100
C	-5.75573100	-0.69094000	1.54104800
H	-3.76909900	-0.97900900	2.32964100
C	-5.95511700	-0.77195400	-0.86035800
H	-4.12337800	-1.12904000	-1.94296600
C	-6.54508500	-0.60922000	0.39290900
H	-6.20947300	-0.57353200	2.52143400
H	-6.56380900	-0.72025100	-1.75920900
H	-7.61289000	-0.42800800	0.47615600
H	-4.18908300	1.86536200	0.54972900
H	-3.37863400	3.67361200	-0.24358200
H	-3.86941400	2.06247500	-1.54131700
H	4.19004400	-1.86359900	0.54914700
H	3.37706600	-3.67321400	-0.23832100
H	3.86908800	-2.06674800	-1.54114400

Zero-point correction=	0.258996 (Hartree/Particle)
Thermal correction to Energy=	0.283959
Thermal correction to Enthalpy=	0.284903
Thermal correction to Gibbs Free Energy=	0.197686
Sum of electronic and zero-point Energies=	-1595.448195
Sum of electronic and thermal Energies=	-1595.423233
Sum of electronic and thermal Enthalpies=	-1595.422288
Sum of electronic and thermal Free Energies=	-1595.509506

Ag_2_A_M

C	1.02672600	-1.46589300	-0.00464600
C	1.90574500	-2.32514600	0.00725400
C	2.89924900	-3.39584500	0.02145900
H	2.40833300	-4.36037100	-0.14919400
H	3.64517100	-3.25566200	-0.76807100
H	3.41737500	-3.44670000	0.98480200
C	-2.91698500	-0.15107400	-0.00434400
C	-4.05838800	0.29169000	0.00579500
C	-5.43052600	0.80677100	0.02081700
H	-5.66559300	1.28509700	0.97944600
H	-5.58648100	1.55200200	-0.76886000
H	-6.15930800	0.00218700	-0.13498700
Ag	-1.00730600	-0.85785200	-0.00976700
Ag	1.37433300	0.63418000	-0.00043100
P	1.66677400	3.00944300	0.00306900
H	2.94312100	3.59679700	0.00271400
H	1.09635600	3.71565600	1.07411800
H	1.09422900	3.71888700	-1.06469700

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 Zero-point correction=                           0.123268
(Hartree/Particle)
 Thermal correction to Energy=                    0.139035
 Thermal correction to Enthalpy=                  0.139979
 Thermal correction to Gibbs Free Energy=         0.074429
 Sum of electronic and zero-point Energies=           -869.088733
 Sum of electronic and thermal Energies=              -869.072966
 Sum of electronic and thermal Enthalpies=            -869.072021
 Sum of electronic and thermal Free Energies=         -869.137572
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Ag_2_TS_{AC}_M_ 1

C	-0.85980700	1.29697100	-0.00033800
C	-1.81587900	2.12252400	0.00416500
C	-2.16745900	3.56525400	0.01266600
H	-1.26011600	4.17359000	0.01451300
H	-2.76584200	3.81236300	-0.86964200
H	-2.76270200	3.80254400	0.89978700
C	3.23861400	0.52832300	-0.00156400
C	4.41516100	0.18825700	0.00038600
C	5.83511100	-0.17572900	0.00278600
H	6.09713900	-0.76129100	0.89228000
H	6.09758000	-0.77210900	-0.87936900
H	6.46896000	0.71901400	-0.00248500
N	-3.46686400	1.37604600	-0.00098100
N	-3.63314500	0.20308000	-0.00549300
N	-2.96385900	-0.87664400	-0.01923600
C	-3.76614800	-2.10239200	0.01004300
H	-4.50990600	-2.11350600	-0.79356900
H	-3.08146500	-2.93985800	-0.13475900
H	-4.27250600	-2.22609700	0.97412900
Ag	1.25583000	1.01869800	-0.00266500
Ag	-0.75537800	-0.85070400	-0.00154000
P	0.89308400	-2.65419700	0.00555300
H	0.62983700	-4.03872400	0.00727400
H	1.80181500	-2.59579600	1.07359500
H	1.80922200	-2.59954300	-1.05629400

```
 Zero-point correction=                           0.175127 (Hartree/Particle)
 Thermal correction to Energy=                    0.195476
 Thermal correction to Enthalpy=                  0.196420
 Thermal correction to Gibbs Free Energy=         0.120244
 Sum of electronic and zero-point Energies=          -1073.045097
 Sum of electronic and thermal Energies=             -1073.024749
 Sum of electronic and thermal Enthalpies=           -1073.023804
 Sum of electronic and thermal Free Energies=        -1073.099980
```

Ag_2_TS_{AC}_M_2

C	1.23438200	-1.08904900	0.00383700
C	2.40135600	-1.57410300	0.01081900
C	3.19645700	-2.82916900	0.02222300
H	2.53562500	-3.69961100	0.02123400
H	3.84814900	-2.87047500	-0.85610400
H	3.83457700	-2.86271600	0.91086700
C	-1.45954400	1.85946600	0.00094400
C	-2.61860700	2.26310900	0.01165400
C	-3.97630400	2.81826800	0.02825600
H	-4.19321800	3.30734000	0.98540900
H	-4.10915700	3.56520600	-0.76339700
H	-4.73965000	2.04279300	-0.12390300
N	3.73479000	-0.35112400	0.00627600
N	3.48696800	0.80785000	-0.00131500
N	2.49527900	1.58929600	-0.00833000
C	2.79948400	3.02262500	-0.01590400
H	3.36534700	3.30328800	-0.91115200
H	1.84485100	3.54979400	-0.02089800
H	3.36170000	3.31361800	0.87831900
Ag	-0.87065000	-1.49893700	-0.00262500
Ag	0.39399100	0.90569100	-0.00238300
P	-3.27170000	-1.29708100	-0.01250200
H	-3.78825700	-0.56495100	1.06628500
H	-4.19207700	-2.36246900	-0.03511200
H	-3.77200000	-0.53206200	-1.07605100

Zero-point correction=	0.175562
(Hartree/Particle)	
Thermal correction to Energy=	0.195734
Thermal correction to Enthalpy=	0.196678
Thermal correction to Gibbs Free Energy=	0.121268
Sum of electronic and zero-point Energies=	-1073.037508
Sum of electronic and thermal Energies=	-1073.017336
Sum of electronic and thermal Enthalpies=	-1073.016392
Sum of electronic and thermal Free Energies=	-1073.091802

Ag_2_TS_{AD}_M_3

C	0.95378600	1.52948100	-0.00477700
C	1.52290800	2.61928600	0.00086000
C	2.12359100	3.95294100	0.00784700
H	3.19685900	3.89971000	-0.20395400

H	1.66333800	4.58936500	-0.75589000
H	1.99470600	4.43765100	0.98158100
C	-1.88076500	-1.49427400	-0.00717900
C	-3.08386700	-1.87822000	-0.00035300
C	-4.03439100	-3.01516300	0.00624900
H	-4.66293100	-2.97890600	0.90232100
H	-4.69648600	-2.96190700	-0.86428800
H	-3.49675800	-3.96691000	-0.01275000
N	-4.20651000	-0.44488400	0.00744900
N	-3.79686200	0.67543300	0.00747800
N	-2.66860500	1.26552300	0.00322500
C	-2.74716400	2.72461700	0.00598800
H	-3.26160400	3.10372300	0.89792600
H	-1.72018000	3.09691800	0.01025300
H	-3.25557700	3.10735200	-0.88791800
Ag	2.09461700	-0.28184100	0.00002800
Ag	-0.64549700	0.12206800	-0.00786000
P	3.47934800	-2.23430400	0.00599900
H	3.49148100	-3.01408300	1.17440800
H	4.86497100	-2.15634100	-0.21776100
H	3.16255300	-3.23718400	-0.92467600

Zero-point correction=	0.174752 (Hartree/Particle)
Thermal correction to Energy=	0.195316
Thermal correction to Enthalpy=	0.196260
Thermal correction to Gibbs Free Energy=	0.118387
Sum of electronic and zero-point Energies=	-1073.038287
Sum of electronic and thermal Energies=	-1073.017722
Sum of electronic and thermal Enthalpies=	-1073.016778
Sum of electronic and thermal Free Energies=	-1073.094652

Ag_2_C_M

C	0.88359900	1.20134800	0.01528700
C	1.91924000	1.99767400	0.00715700
C	1.79438800	3.50099500	0.03663000
H	0.75266500	3.82862500	0.07029100
H	2.32188900	3.88155600	0.91676600
H	2.27486100	3.91321300	-0.85606400
C	-3.20423500	0.52920900	-0.01085800
C	-4.39267800	0.23484400	-0.02635000
C	-5.82341500	-0.08105200	-0.04625400
H	-5.99464700	-1.15093400	-0.21470800
H	-6.30195500	0.18684300	0.90286500
H	-6.33648800	0.46624600	-0.84568700
N	3.31535100	1.60663600	-0.03050600
N	3.66504000	0.40748400	-0.04702800
N	2.90927500	-0.63059500	-0.05071100
C	3.64776600	-1.89783700	-0.03319400

H	3.50309800	-2.40666700	0.92661400
H	3.28297100	-2.54810100	-0.83488000
H	4.71457300	-1.71123400	-0.18106700
Ag	0.76325900	-0.88485800	0.01299400
Ag	-1.21818500	0.98653000	0.00518700
P	-0.75419100	-2.80209600	0.02685200
H	-1.59695500	-2.87917900	1.14656100
H	-1.73026300	-2.76985700	-0.98064400
H	-0.37101400	-4.15345800	-0.06410100

```
 Zero-point correction=                           0.176801
(Hartree/Particle)
 Thermal correction to Energy=                    0.196996
 Thermal correction to Enthalpy=                  0.197940
 Thermal correction to Gibbs Free Energy=         0.121619
 Sum of electronic and zero-point Energies=          -1073.051265
 Sum of electronic and thermal Energies=             -1073.031070
 Sum of electronic and thermal Enthalpies=           -1073.030126
 Sum of electronic and thermal Free Energies=        -1073.106447
```

Ag_2_TS_{CD}_M

C	0.86188100	-1.18024400	-0.09892400
C	1.86107000	-2.02210100	-0.21521200
C	1.63609800	-3.46282700	-0.60767200
H	0.58065200	-3.68575500	-0.78010200
H	2.20357800	-3.67196600	-1.51956400
H	2.01666800	-4.10797600	0.19018100
C	-3.21600900	-0.52975600	0.20991800
C	-4.41154200	-0.27247600	0.26860200
C	-5.84787900	0.00684800	0.34498000
H	-6.03876100	1.07564400	0.49873300
H	-6.35967200	-0.29327900	-0.57687300
H	-6.31219500	-0.53543000	1.17692000
N	3.24844900	-1.74918100	0.01651000
N	3.60511800	-0.59023200	0.34669900
N	2.82337700	0.41587700	0.50112300
C	3.51872200	1.63655200	0.92645600
H	3.51183700	2.38387600	0.12417700
H	3.01375700	2.05527700	1.80272300
H	4.55488200	1.40426500	1.18654100
Ag	0.78484900	0.91938200	-0.19392000
Ag	-1.22506800	-0.93710100	0.08957400
P	-0.52051600	2.94871300	-0.44580200
H	-1.23782700	3.08183500	-1.64530300
H	-1.58477900	3.05117400	0.46371000
H	-0.00279700	4.25323100	-0.34904400

```
 Zero-point correction=                           0.176987 (Hartree/Particle)
 Thermal correction to Energy=                    0.196164
 Thermal correction to Enthalpy=                  0.197109
 Thermal correction to Gibbs Free Energy=         0.124820
 Sum of electronic and zero-point Energies=          -1073.050531
 Sum of electronic and thermal Energies=             -1073.031353
 Sum of electronic and thermal Enthalpies=           -1073.030409
 Sum of electronic and thermal Free Energies=        -1073.102697
```

Ag_2_D_M

```
C                 -1.13132900   -0.90730800    0.01510100
C                 -1.82596600   -1.46330900    1.09760000
C                 -1.64271500   -1.22040700    2.56124000
H                 -0.84191200   -0.49599900    2.73963600
H                 -2.56643200   -0.84418000    3.01332000
H                 -1.37987000   -2.15119700    3.07366600
C                  3.07863500   -0.57246800    0.02633200
C                  4.29558300   -0.44136200    0.02595400
C                  5.75469800   -0.30506100    0.02579300
H                  6.06291400    0.69315000   -0.30808400
H                  6.16971200   -0.46302500    1.02837000
H                  6.21989200   -1.03716900   -0.64503300
N                 -2.75381100   -2.34455300    0.64661900
N                 -2.69393400   -2.38071600   -0.65597900
N                 -1.74868800   -1.53650400   -1.04737600
C                 -1.45955600   -1.40598100   -2.46289100
H                 -1.65868200   -0.38416500   -2.79795000
H                 -0.41319200   -1.65310300   -2.65678400
H                 -2.11055500   -2.09932600   -2.99645100
Ag                -0.85435200    1.24639600   -0.02888600
Ag                 1.05548500   -0.76240600    0.02521000
P                 -0.62562800    3.63520100   -0.03457900
H                 -0.06364400    4.22531400    1.10916000
H                  0.21542000    4.19137200   -1.01181400
H                 -1.74354300    4.47054000   -0.19417700
```

```
 Zero-point correction=                           0.181511
(Hartree/Particle)
 Thermal correction to Energy=                    0.200647
 Thermal correction to Enthalpy=                  0.201591
 Thermal correction to Gibbs Free Energy=         0.128849
 Sum of electronic and zero-point Energies=          -1073.165585
 Sum of electronic and thermal Energies=             -1073.146449
 Sum of electronic and thermal Enthalpies=           -1073.145505
 Sum of electronic and thermal Free Energies=        -1073.218247
```

Ag_2_A_R

C	1.74465500	-0.25862800	-0.04990400
C	2.89186300	-0.70479700	-0.02750700
C	-2.38239500	-0.73819900	-0.08085900
C	-3.60557200	-0.81529200	-0.05369100
Ag	-0.35065800	-0.57498400	-0.08200000
Ag	1.18054300	1.79244200	0.00164100
P	0.47384100	4.08046600	0.07653900
H	1.39908200	5.12959800	-0.05427700
H	-0.18853600	4.50849500	1.23811800
H	-0.46727600	4.48497100	-0.88327900
C	4.21146500	-1.25948000	0.00443300
C	4.84003600	-1.51837000	1.23264400
C	4.88694500	-1.55495500	-1.19009400
C	6.11997400	-2.06122700	1.26232800
H	4.31290300	-1.29511800	2.15516700
C	6.16646400	-2.09873200	-1.15304900
H	4.39617200	-1.36007400	-2.13867100
C	6.78499900	-2.35186800	0.07116000
H	6.59899000	-2.26054900	2.21644400
H	6.68135400	-2.32778000	-2.08150100
H	7.78312900	-2.77963000	0.09726900
C	-5.03445000	-0.92018900	-0.00596600
C	-5.80312400	-0.87435600	-1.18132600
C	-5.69904200	-1.07584700	1.22235300
C	-7.18985300	-0.98090800	-1.12718400
H	-5.29730800	-0.75711500	-2.13515700
C	-7.08561800	-1.18208200	1.27163700
H	-5.11152900	-1.11534500	2.13490600
C	-7.83807600	-1.13540000	0.09803300
H	-7.76707400	-0.94585300	-2.04763200
H	-7.58124800	-1.30513200	2.23113700
H	-8.92051500	-1.22200300	0.13823300

Zero-point correction=	0.231699
(Hartree/Particle)	
Thermal correction to Energy=	0.253104
Thermal correction to Enthalpy=	0.254048
Thermal correction to Gibbs Free Energy=	0.171944
Sum of electronic and zero-point Energies=	-1252.334682
Sum of electronic and thermal Energies=	-1252.313277
Sum of electronic and thermal Enthalpies=	-1252.312333
Sum of electronic and thermal Free Energies=	-1252.394437

Ag_2_TS_{AC}_R

C	-1.57633300	-1.00224600	-0.10145800

C	-2.75124900	-1.45785100	0.00530300
C	2.53889200	-1.64396700	-0.05519300
C	3.76282500	-1.57357400	-0.02243900
N	-4.04488600	-0.16053200	0.09000200
N	-3.77816400	0.98718700	0.00543900
N	-2.77742100	1.75885900	-0.11540800
C	-3.09932800	3.19266900	-0.23236000
H	-3.39543300	3.42398600	-1.26302200
H	-3.94896700	3.42465200	0.42037600
Ag	0.50003500	-1.48839800	-0.08575500
Ag	-0.71905300	0.95418800	-0.35276000
P	1.42158000	2.10204600	-0.63113400
H	1.54591700	3.48723600	-0.84326400
H	2.26331800	1.62560000	-1.64924400
H	2.29737900	1.95318300	0.45593100
C	-3.49276100	-2.71334600	0.11893500
C	-2.87147600	-3.79944900	0.75311700
C	-4.77686500	-2.87393100	-0.41048300
C	-3.52526900	-5.02227300	0.85276300
H	-1.87792400	-3.67261900	1.17275400
C	-5.42495500	-4.10257400	-0.31174000
H	-5.26320800	-2.03741900	-0.90007400
C	-4.80441000	-5.17858300	0.31939500
H	-3.03432200	-5.85492200	1.34831000
H	-6.41928100	-4.21857000	-0.73365700
H	-5.31396200	-6.13477600	0.39661500
C	5.19387300	-1.50028300	0.03501200
C	5.85204100	-1.35927600	1.26834200
C	5.96839600	-1.56174200	-1.13552000
C	7.23986800	-1.27708900	1.32668800
H	5.25974200	-1.31836600	2.17780000
C	7.35633900	-1.47890100	-1.07211500
H	5.46739100	-1.67869000	-2.09196600
C	7.99843800	-1.33493400	0.15755000
H	7.73187200	-1.16869700	2.28966900
H	7.93939100	-1.52927500	-1.98799000
H	9.08200200	-1.27013400	0.20520500
C	-1.90439700	4.02901600	0.15707400
C	-1.38034400	4.97579200	-0.72320700
C	-1.30748800	3.86722200	1.41261600
C	-0.28488900	5.75907000	-0.35637400
H	-1.83234600	5.10641300	-1.70375800
C	-0.20650500	4.63723500	1.77701800
H	-1.70491100	3.12698100	2.10306600
C	0.30574100	5.58911400	0.89310200
H	0.10701000	6.49739800	-1.05030400
H	0.24843200	4.50101900	2.75407100
H	1.16048300	6.19500000	1.18031500

Zero-point correction=	0.366159 (Hartree/Particle)
Thermal correction to Energy=	0.396192
Thermal correction to Enthalpy=	0.397136
Thermal correction to Gibbs Free Energy=	0.296750
Sum of electronic and zero-point Energies=	-1687.190423
Sum of electronic and thermal Energies=	-1687.160390
Sum of electronic and thermal Enthalpies=	-1687.159446
Sum of electronic and thermal Free Energies=	-1687.259832

Ag_2_C_R

C	-2.08588400	-0.78268500	-0.10050100
C	-3.29287000	-1.28939800	-0.03563800
C	1.99025200	-1.54845200	-0.03436600
C	3.20568600	-1.69977100	0.01298700
N	-4.53196100	-0.53678300	0.00430900
N	-4.54084600	0.70957100	-0.02858200
N	-3.52207100	1.49690700	-0.05129900
C	-3.89070500	2.91615400	-0.18173300
H	-3.78355700	3.22279300	-1.23009200
H	-4.94890200	3.01723300	0.08230600
Ag	-0.02499900	-1.23768500	-0.08286600
Ag	-1.36434300	1.14721200	-0.15123000
P	0.36839900	2.86274600	-0.15071300
H	0.35032000	3.78234500	0.91145900
H	0.48006200	3.76354200	-1.22336600
H	1.69983700	2.42071100	-0.07692900
C	-3.52233600	-2.75940700	-0.05063700
C	-2.67750800	-3.62908800	0.64811800
C	-4.58891200	-3.27923300	-0.78981200
C	-2.88803500	-5.00434000	0.59308200
H	-1.87237200	-3.22795700	1.25785100
C	-4.79757500	-4.65432000	-0.83851400
H	-5.24975400	-2.60045200	-1.31936700
C	-3.94628800	-5.52013000	-0.15218900
H	-2.22868800	-5.67048300	1.14167500
H	-5.62763600	-5.05129200	-1.41594600
H	-4.11114200	-6.59299800	-0.19447200
C	4.62616900	-1.88484200	0.07520700
C	5.27144200	-2.05545600	1.31127500
C	5.40177400	-1.89999000	-1.09597700
C	6.64999800	-2.23454000	1.37203700
H	4.67678300	-2.04820700	2.22002600
C	6.78029000	-2.07915900	-1.03000700
H	4.90845500	-1.77240900	-2.05496100
C	7.41051000	-2.24688900	0.20281800
H	7.13299000	-2.36740200	2.33646300
H	7.36486600	-2.09024400	-1.94620600
H	8.48653200	-2.38901000	0.25264300

C	-3.04513400	3.81226100	0.69499100
C	-2.51028300	4.99700800	0.18341100
C	-2.79948100	3.48348700	2.03275400
C	-1.75233800	5.84553000	0.99146400
H	-2.69158000	5.26169200	-0.85631100
C	-2.03342900	4.32191600	2.83846900
H	-3.20661000	2.56085100	2.43838500
C	-1.50874200	5.50781500	2.32093500
H	-1.34827700	6.76596000	0.57906000
H	-1.85091300	4.05437700	3.87536000
H	-0.91535300	6.16324300	2.95191700

Zero-point correction=	0.368489
(Hartree/Particle)	
Thermal correction to Energy=	0.398033
Thermal correction to Enthalpy=	0.398977
Thermal correction to Gibbs Free Energy=	0.300094
Sum of electronic and zero-point Energies=	-1687.197469
Sum of electronic and thermal Energies=	-1687.167925
Sum of electronic and thermal Enthalpies=	-1687.166981
Sum of electronic and thermal Free Energies=	-1687.265864

Ag_2_TS_{CD}_R

C	-1.52444800	0.33442400	-1.06015600
C	-2.55056600	1.29013400	-1.09645300
C	2.63497900	0.57785500	-0.53238400
C	3.84732300	0.58374600	-0.35257900
N	-3.49526400	0.91888800	-2.00510600
N	-3.13347200	-0.20529300	-2.54796400
N	-1.97491400	-0.56561700	-1.99979500
C	-1.35817800	-1.82437000	-2.40210000
H	-1.98485100	-2.21575900	-3.20726000
H	-0.36345200	-1.61792900	-2.80681300
Ag	-1.26587800	-0.53642300	0.95849900
Ag	0.61704300	0.52487800	-0.78537300
P	-1.13530400	-1.58707300	3.10661200
C	5.26546000	0.60796300	-0.14242600
C	6.14507700	0.06976100	-1.09650300
C	5.80645100	1.17364000	1.02433300
C	7.52071100	0.09750200	-0.88785200
H	5.73456300	-0.36605500	-2.00254900
C	7.18250100	1.19886800	1.22872200
H	5.13181900	1.59435800	1.76424300
C	8.04636700	0.66109200	0.27472700

H	8.18701100	-0.32055500	-1.63806000
H	7.58353700	1.64303700	2.13602600
H	9.12081800	0.68382200	0.43475100
C	-2.71175400	2.52377800	-0.30448900
C	-3.98675900	3.08166200	-0.14644100
C	-1.62011400	3.15383800	0.30584600
C	-4.16438100	4.23478000	0.61229800
H	-4.83427700	2.60298800	-0.62719800
C	-1.80033500	4.30353700	1.06952900
H	-0.61691300	2.75833200	0.16828400
C	-3.07350600	4.84831400	1.22733800
H	-5.15927000	4.65727400	0.72318500
H	-0.93943800	4.78120000	1.52861800
H	-3.21294700	5.75109100	1.81533800
C	-1.27466100	-2.80097200	-1.24893600
C	-0.03961300	-3.18417300	-0.72167800
C	-2.44961900	-3.30077100	-0.67444600
C	0.02336000	-4.06244800	0.36187100
H	0.87732500	-2.78280900	-1.14657200
C	-2.38818600	-4.17488000	0.40725800
H	-3.41231800	-2.99615200	-1.07917100
C	-1.14950200	-4.55987000	0.92632800
H	0.99077700	-4.35526000	0.75984600
H	-3.30538500	-4.56677000	0.83825500
H	-1.10131100	-5.25646200	1.75931200
H	-1.18655200	-0.80653000	4.27400200
H	-2.08306300	-2.56624700	3.44423600
H	0.04059800	-2.30921400	3.36465800

Zero-point correction=	0.372500
(Hartree/Particle)	
Thermal correction to Energy=	0.401421
Thermal correction to Enthalpy=	0.402366
Thermal correction to Gibbs Free Energy=	0.304844
Sum of electronic and zero-point Energies=	-1687.321504
Sum of electronic and thermal Energies=	-1687.292582
Sum of electronic and thermal Enthalpies=	-1687.291638
Sum of electronic and thermal Free Energies=	-1687.389159

Ag_2_D_R

C	-1.52444800	0.33442400	-1.06015600
C	-2.55056600	1.29013400	-1.09645300
C	2.63497900	0.57785500	-0.53238400
C	3.84732300	0.58374600	-0.35257900
N	-3.49526400	0.91888800	-2.00510600
N	-3.13347200	-0.20529300	-2.54796400

N	-1.97491400	-0.56561700	-1.99979500
C	-1.35817800	-1.82437000	-2.40210000
H	-1.98485100	-2.21575900	-3.20726000
H	-0.36345200	-1.61792900	-2.80681300
Ag	-1.26587800	-0.53642300	0.95849900
Ag	0.61704300	0.52487800	-0.78537300
P	-1.13530400	-1.58707300	3.10661200
C	5.26546000	0.60796300	-0.14242600
C	6.14507700	0.06976100	-1.09650300
C	5.80645100	1.17364000	1.02433300
C	7.52071100	0.09750200	-0.88785200
H	5.73456300	-0.36605500	-2.00254900
C	7.18250100	1.19886800	1.22872200
H	5.13181900	1.59435800	1.76424300
C	8.04636700	0.66109200	0.27472700
H	8.18701100	-0.32055500	-1.63806000
H	7.58353700	1.64303700	2.13602600
H	9.12081800	0.68382200	0.43475100
C	-2.71175400	2.52377800	-0.30448900
C	-3.98675900	3.08166200	-0.14644100
C	-1.62011400	3.15383800	0.30584600
C	-4.16438100	4.23478000	0.61229800
H	-4.83427700	2.60298800	-0.62719800
C	-1.80033500	4.30353700	1.06952900
H	-0.61691300	2.75833200	0.16828400
C	-3.07350600	4.84831400	1.22733800
H	-5.15927000	4.65727400	0.72318500
H	-0.93943800	4.78120000	1.52861800
H	-3.21294700	5.75109100	1.81533800
C	-1.27466100	-2.80097200	-1.24893600
C	-0.03961300	-3.18417300	-0.72167800
C	-2.44961900	-3.30077100	-0.67444600
C	0.02336000	-4.06244800	0.36187100
H	0.87732500	-2.78280900	-1.14657200
C	-2.38818600	-4.17488000	0.40725800
H	-3.41231800	-2.99615200	-1.07917100
C	-1.14950200	-4.55987000	0.92632800
H	0.99077700	-4.35526000	0.75984600
H	-3.30538500	-4.56677000	0.83825500
H	-1.10131100	-5.25646200	1.75931200
H	-1.18655200	-0.80653000	4.27400200
H	-2.08306300	-2.56624700	3.44423600
H	0.04059800	-2.30921400	3.36465800

```
 Zero-point correction=                           0.372500
(Hartree/Particle)
 Thermal correction to Energy=                    0.401421
 Thermal correction to Enthalpy=                  0.402366
 Thermal correction to Gibbs Free Energy=         0.304844
 Sum of electronic and zero-point Energies=          -1687.321504
 Sum of electronic and thermal Energies=             -1687.292582
 Sum of electronic and thermal Enthalpies=           -1687.291638
 Sum of electronic and thermal Free Energies=        -1687.389159
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Ag_2_A_RL

C	-2.43450500	-2.29080700	0.10969900
C	-3.56954200	-1.79888700	0.04157500
C	1.63000800	-2.76125000	0.22370100
C	2.81068400	-2.43112100	0.17410800
Ag	-0.41202800	-2.82654400	0.19084400
Ag	-1.59297100	-0.22477600	0.01190500
P	0.10724100	1.46168500	-0.06196800
C	-4.94495600	-1.37639300	-0.03009900
C	-5.66883300	-1.11695200	1.14297200
C	-5.57256200	-1.21569800	-1.27412100
C	-6.99621400	-0.70626100	1.06960100
H	-5.18218000	-1.24549900	2.10509300
C	-6.89997500	-0.80444900	-1.34083200
H	-5.01183900	-1.42028000	-2.18126900
C	-7.61399500	-0.54770900	-0.17060100
H	-7.54974400	-0.51101700	1.98360700
H	-7.37882300	-0.68503400	-2.30843500
H	-8.65064600	-0.22769800	-0.22548800
C	4.16966700	-1.98857100	0.08113500
C	4.68305200	-1.05804100	1.00017400
C	5.00397500	-2.42681700	-0.96054500
C	5.97858500	-0.56762600	0.87018300
H	4.04591900	-0.70988800	1.80732600
C	6.29937200	-1.93448500	-1.08777200
H	4.61564500	-3.14651400	-1.67510100
C	6.79299600	-0.99914800	-0.17719300
H	6.35364400	0.15555200	1.59011900
H	6.92935700	-2.28351900	-1.90207700
H	7.80457500	-0.61558700	-0.27946400
C	1.43157300	0.96227000	-1.20891800
C	2.78000600	1.20451500	-0.93049500
C	1.07793800	0.29746400	-2.38742500
C	3.76173900	0.79057500	-1.82570600
H	3.07080800	1.68806300	-0.00221200
C	2.06081200	-0.10798700	-3.28408500
H	0.03387200	0.07591800	-2.59783400

C	3.40330300	0.13626800	-3.00123500
H	4.80935300	0.94306300	-1.58355800
H	1.77957500	-0.63723700	-4.18955500
H	4.17407900	-0.20623300	-3.68534200
C	0.92940400	1.62474900	1.56207500
C	1.11319900	2.85648600	2.19466400
C	1.37810500	0.44966700	2.18014300
C	1.74083100	2.91329800	3.43902000
H	0.77080800	3.77344800	1.72350100
C	2.00667600	0.51448800	3.41922700
H	1.26517100	-0.51477700	1.68670000
C	2.18719300	1.74499200	4.05166800
H	1.88089700	3.87395800	3.92625600
H	2.35463500	-0.40135600	3.88864700
H	2.67529300	1.79210900	5.02099500
C	-0.36527600	3.15982400	-0.53386800
C	0.47053400	3.97493100	-1.30281300
C	-1.59044300	3.66134600	-0.07997600
C	0.08637200	5.27946000	-1.60678400
H	1.41770000	3.59022900	-1.67065300
C	-1.96648100	4.96892900	-0.37450300
H	-2.25155000	3.02819300	0.50825000
C	-1.12791100	5.77894400	-1.13961800
H	0.73759700	5.90518100	-2.21011900
H	-2.91633000	5.35246700	-0.01355200
H	-1.42349300	6.79718000	-1.37565000

Zero-point correction=	0.482889
(Hartree/Particle)	
Thermal correction to Energy=	0.517971
Thermal correction to Enthalpy=	0.518915
Thermal correction to Gibbs Free Energy=	0.407661
Sum of electronic and zero-point Energies=	-1945.054856
Sum of electronic and thermal Energies=	-1945.019774
Sum of electronic and thermal Enthalpies=	-1945.018830
Sum of electronic and thermal Free Energies=	-1945.130084

Ag_2_TS_{AD}_RL

C	2.80659200	-0.75420300	0.05437900
C	4.06869600	-0.68805000	0.01175400
C	-0.52858500	-3.11918800	-0.72813400
C	-1.69770000	-3.47279100	-0.83240500
N	4.68811500	1.01707400	-0.21092200
N	3.95510000	1.94344000	-0.17958500
N	2.72526300	2.22198000	-0.06035700
C	2.40848100	3.65341200	-0.02323200

H	2.12091700	3.91760600	1.00323400
H	3.30870100	4.22782500	-0.26777700
Ag	1.18376900	-2.07139400	-0.33478800
Ag	1.18866700	0.62341800	0.37599900
P	-1.21154800	0.90548900	0.74468800
C	5.27353700	-1.51554700	0.04215600
C	5.19344600	-2.82919700	-0.44465100
C	6.48637400	-1.05378200	0.56249500
C	6.30740400	-3.66029700	-0.41116900
H	4.25521600	-3.18801000	-0.85750200
C	7.59737000	-1.89309400	0.59897200
H	6.55746500	-0.04004300	0.94057500
C	7.51389400	-3.19553700	0.11188500
H	6.23178600	-4.67245300	-0.79816500
H	8.53215200	-1.52396500	1.01141400
H	8.38366700	-3.84591900	0.13816400
C	-3.08882800	-3.80840400	-0.88960500
C	-4.00064500	-2.94017300	-1.51336300
C	-3.58355600	-4.96770000	-0.27122000
C	-5.36433400	-3.21404700	-1.50161900
H	-3.62593700	-2.03786400	-1.98767600
C	-4.94885600	-5.23829600	-0.26152900
H	-2.88442300	-5.64285200	0.21338600
C	-5.84688400	-4.36180300	-0.87161800
H	-6.05455500	-2.52677700	-1.98447800
H	-5.31518700	-6.13863400	0.22505600
H	-6.91251000	-4.57425600	-0.86126500
C	1.27950400	4.04376300	-0.95593800
C	0.72828900	5.32402800	-0.82630100
C	0.74959400	3.17760800	-1.91174400
C	-0.34625400	5.71931500	-1.61643500
H	1.13153000	6.00922000	-0.08261300
C	-0.34026800	3.56507800	-2.69265500
H	1.17829500	2.18905100	-2.04590200
C	-0.89474700	4.83198300	-2.54446900
H	-0.76752700	6.71399500	-1.49810100
H	-0.76286700	2.86296900	-3.40576900
H	-1.74955900	5.12750500	-3.14591200
C	-1.96993800	-0.54753400	1.54316600
C	-3.28956400	-0.92018900	1.27206900
C	-1.20430400	-1.31469300	2.42547600
C	-3.83367600	-2.05104800	1.87190400
H	-3.88704300	-0.34850700	0.56765700
C	-1.75384900	-2.43916400	3.03412000
H	-0.16600700	-1.05324200	2.61816800
C	-3.06657900	-2.81033200	2.75236200
H	-4.84410300	-2.36049200	1.62062600
H	-1.14568300	-3.04135600	3.70243100
H	-3.48687500	-3.70613300	3.20013800
C	-2.10327700	1.06781300	-0.84789700
C	-3.12694100	1.99426700	-1.05882100
C	-1.73244500	0.20576900	-1.88714000

C	-3.76202200	2.06801100	-2.29757100
H	-3.43046400	2.66816300	-0.26360700
C	-2.37415100	0.27561300	-3.11993100
H	-0.96565000	-0.54860500	-1.72973200
C	-3.38664100	1.21177400	-3.33015100
H	-4.55283000	2.79684500	-2.45165500
H	-2.08365000	-0.40931500	-3.91142500
H	-3.88358000	1.26975900	-4.29456100
C	-1.75640900	2.33540800	1.74588500
C	-2.39433500	2.18507100	2.97951900
C	-1.47167900	3.62136500	1.27165000
C	-2.74080600	3.31063600	3.72803400
H	-2.62354500	1.19365600	3.35957900
C	-1.82809800	4.74127800	2.01391600
H	-0.98650000	3.74983100	0.30918800
C	-2.46112700	4.58773900	3.24814400
H	-3.23457400	3.18438600	4.68724600
H	-1.61070400	5.73200600	1.62434000
H	-2.73669900	5.46149300	3.83198400

Zero-point correction=	0.617904
(Hartree/Particle)	
Thermal correction to Energy=	0.661434
Thermal correction to Enthalpy=	0.662379
Thermal correction to Gibbs Free Energy=	0.534149
Sum of electronic and zero-point Energies=	-2379.910368
Sum of electronic and thermal Energies=	-2379.866837
Sum of electronic and thermal Enthalpies=	-2379.865893
Sum of electronic and thermal Free Energies=	-2379.994123

Ag_2_D_RL

C	3.00374300	-0.12817900	-0.20592800
C	3.87051400	0.40770500	0.75892900
C	-0.33651300	-2.41250500	1.12830000
C	-1.49450000	-2.57737400	1.49838400
N	5.16200600	0.25720800	0.35596800
N	5.16904400	-0.33566200	-0.80154800
N	3.90425000	-0.56648400	-1.14819500
C	3.63696300	-1.14941800	-2.45970700
H	3.26466800	-0.36179900	-3.12380000
H	4.61005100	-1.47537000	-2.83656500
Ag	1.42497700	-1.60360700	0.45546000
Ag	1.13622500	0.86714800	-0.70963100
P	-1.13970900	1.60472900	-0.84634000
C	3.55765400	1.11136600	2.01873800
C	2.36600700	0.89252400	2.72182400

C	4.47414900	2.04201400	2.52584200
C	2.09256100	1.59522200	3.89192000
H	1.64826700	0.15322200	2.37408600
C	4.20013800	2.74174000	3.69750000
H	5.40393200	2.20869700	1.99092700
C	3.00634600	2.52482300	4.38459200
H	1.16821000	1.39569200	4.42688000
H	4.92311500	3.45995100	4.07447800
H	2.79586600	3.06690800	5.30243200
C	-2.85019700	-2.70164500	1.94308500
C	-3.91151000	-2.69913500	1.02257900
C	-3.15499300	-2.77472200	3.31249800
C	-5.23251100	-2.75208500	1.45720900
H	-3.68856600	-2.63806500	-0.03832500
C	-4.47686000	-2.83042800	3.74378100
H	-2.34103900	-2.77515800	4.03114400
C	-5.52294500	-2.81545000	2.82027600
H	-6.03852400	-2.74511700	0.72791100
H	-4.69198000	-2.88732300	4.80773900
H	-6.55417000	-2.86040300	3.15975800
C	2.65434000	-2.29369200	-2.40268200
C	1.42404200	-2.20686800	-3.05306300
C	2.96099000	-3.44752300	-1.67162300
C	0.50998400	-3.25765700	-2.97879100
H	1.16929500	-1.30832900	-3.61155000
C	2.04375900	-4.49050300	-1.58628000
H	3.91675600	-3.51725500	-1.15672600
C	0.81479000	-4.39630000	-2.24032600
H	-0.44513800	-3.17211800	-3.48752300
H	2.28243000	-5.37319100	-1.00068200
H	0.09361900	-5.20406100	-2.16061900
C	-1.88508900	1.41511300	0.80932500
C	-3.09019600	0.74202400	1.01855600
C	-1.18850500	1.94504000	1.90272000
C	-3.59609300	0.59817500	2.30853000
H	-3.62700600	0.29917600	0.18532000
C	-1.70679000	1.81650400	3.18641800
H	-0.23399800	2.44775100	1.75821200
C	-2.90866700	1.13838700	3.39086900
H	-4.51369000	0.03818800	2.46439200
H	-1.16411600	2.23432500	4.02922000
H	-3.30038400	1.01481800	4.39640700
C	-2.13509000	0.53881200	-1.94694400
C	-3.00006700	1.05657300	-2.91489700
C	-2.01776400	-0.84880300	-1.78990400
C	-3.74680900	0.19420300	-3.71696100
H	-3.09859800	2.13027800	-3.04653500
C	-2.77747800	-1.70192800	-2.58371300
H	-1.36200500	-1.27073600	-1.02959600
C	-3.64054900	-1.18470700	-3.54951700
H	-4.41719900	0.60308400	-4.46741600
H	-2.69254800	-2.77558400	-2.43908900

H	-4.23019600	-1.85460100	-4.16900200
C	-1.50833600	3.31611100	-1.35389200
C	-2.63465700	3.99499700	-0.87656800
C	-0.65399100	3.95010300	-2.26136300
C	-2.90396400	5.29048500	-1.31007100
H	-3.29624900	3.51405400	-0.16094500
C	-0.92853300	5.24371500	-2.69877700
H	0.23241000	3.43386200	-2.62368000
C	-2.05363400	5.91428700	-2.22249500
H	-3.77724300	5.81368600	-0.93176200
H	-0.25891400	5.73011400	-3.40186900
H	-2.26346000	6.92651700	-2.55588400

Zero-point correction=	0.623515 (Hartree/Particle)
Thermal correction to Energy=	0.666315
Thermal correction to Enthalpy=	0.667259
Thermal correction to Gibbs Free Energy=	0.538742
Sum of electronic and zero-point Energies=	-2380.039345
Sum of electronic and thermal Energies=	-2379.996545
Sum of electronic and thermal Enthalpies=	-2379.995601
Sum of electronic and thermal Free Energies=	-2380.124118

Ag_1_A_RL

Ag	0.87003000	0.00578500	0.00291500
P	-1.52470300	0.00065400	0.00132900
C	-2.27282200	1.65991300	-0.17202400
C	-3.42672300	2.04209600	0.51868100
H	-3.89984300	1.35528500	1.21493100
C	-3.97127700	3.30991500	0.32215800
H	-4.86508600	3.60134200	0.86617900
C	-3.37040100	4.20034700	-0.56528200
H	-3.79546700	5.18863800	-0.71496300
C	-2.21673100	3.82574400	-1.25314700
H	-1.73846300	4.51972100	-1.93784900
C	-1.66596100	2.56342800	-1.05247800
C	-2.26314500	-0.98064800	-1.35315400
C	-1.64555500	-2.18837300	-1.69911500
H	-0.73433300	-2.49813200	-1.19198700
C	-2.18775000	-2.99411100	-2.69608400
H	-1.70069500	-3.92867100	-2.95790600
C	-3.34373200	-2.59298000	-3.36472600
H	-3.76204500	-3.21717000	-4.14908200
C	-3.95561400	-1.38572800	-3.03339400
H	-4.85134900	-1.06596400	-3.55799100
C	-3.41952900	-0.58086900	-2.02976100
H	-3.90118100	0.36058000	-1.78052000
C	-2.26847000	-0.68387600	1.52465800

C	-3.42943200	-1.46297300	1.51132400
H	-3.91044300	-1.71122600	0.56928900
C	-3.97094700	-1.93093000	2.70714400
H	-4.87029100	-2.53972300	2.68833100
C	-3.35974700	-1.62237900	3.92081800
H	-3.78221700	-1.99052300	4.85131100
C	-2.19919600	-0.84975100	3.93930900
H	-1.71272000	-0.61565700	4.88150100
C	-1.65162200	-0.38787000	2.74592400
H	-0.73695500	0.20078000	2.76482600
H	-0.75691100	2.28198700	-1.57964800
C	4.13112100	0.00490900	0.00273100
C	2.90576000	0.00622800	0.00288500
C	5.56462400	0.00328600	0.00179300
C	6.28124900	-1.20499700	-0.00917000
C	6.28406200	1.20990000	0.01144000
C	7.67281100	-1.20410500	-0.01042900
H	5.73117100	-2.14131200	-0.01659200
C	7.67562300	1.20576400	0.01013900
H	5.73616400	2.14748200	0.02000100
C	8.37670000	0.00001500	-0.00083800
H	8.21085100	-2.14846300	-0.01898700
H	8.21587500	2.14886500	0.01770200
H	9.46328400	-0.00125300	-0.00189500

Zero-point correction=	0.380065
(Hartree/Particle)	
Thermal correction to Energy=	0.405639
Thermal correction to Enthalpy=	0.406583
Thermal correction to Gibbs Free Energy=	0.316169
Sum of electronic and zero-point Energies=	-1490.416793
Sum of electronic and thermal Energies=	-1490.391219
Sum of electronic and thermal Enthalpies=	-1490.390275
Sum of electronic and thermal Free Energies=	-1490.480689

Ag_1_TS_{AD}_RL

C	2.83648900	0.70201200	-0.18748000
C	3.97191300	0.14721900	-0.22946800
N	3.77409400	-1.61385300	-0.73674300
N	2.70708800	-2.07206700	-0.98815500
N	1.49139400	-1.69251200	-1.02849600
C	0.54560500	-2.71988900	-1.45284000
H	-0.07960800	-2.28205100	-2.24259200
H	1.08064400	-3.56706800	-1.89787800
Ag	0.80403000	0.47926800	-0.35711700

P	-1.53932400	0.91577600	-0.07138500
C	5.40133700	0.34198400	-0.01107600
C	5.82071000	1.29740400	0.92719200
C	6.36834400	-0.37641700	-0.72335900
C	7.17484100	1.52814800	1.14461800
H	5.07202400	1.85215800	1.48489700
C	7.72319100	-0.14084300	-0.50294600
H	6.05368300	-1.11842300	-1.44831000
C	8.13321100	0.80929200	0.43008500
H	7.48278500	2.26984000	1.87656800
H	8.46195300	-0.70440800	-1.06639500
H	9.19119700	0.98847400	0.60050800
C	-0.37661700	-3.21915800	-0.35460600
C	-1.34794500	-4.17214400	-0.68250000
C	-0.33351400	-2.72922500	0.94959700
C	-2.27085100	-4.60647800	0.26277500
H	-1.39092000	-4.56381500	-1.69739800
C	-1.26674500	-3.15227100	1.89804300
H	0.42634800	-2.00377200	1.22385500
C	-2.24147200	-4.08545500	1.55846200
H	-3.01857700	-5.34632900	-0.01081100
H	-1.23411500	-2.73804500	2.90181600
H	-2.96949700	-4.41037300	2.29633700
C	-2.00008600	2.68518500	-0.18382300
C	-3.32489800	3.10606700	-0.01053700
C	-1.00802700	3.63433000	-0.44017800
C	-3.64948800	4.45492700	-0.09522400
H	-4.10728800	2.37751600	0.18431700
C	-1.33455100	4.98835500	-0.52527300
H	0.02409700	3.31715800	-0.57105200
C	-2.65304500	5.39866500	-0.35289200
H	-4.67948500	4.77204400	0.04062800
H	-0.55576300	5.71826900	-0.72536700
H	-2.90752400	6.45263700	-0.41970100
C	-2.11248600	0.41044200	1.59455400
C	-3.43700500	0.06414300	1.88001500
C	-1.16899700	0.40454600	2.62769600
C	-3.80790200	-0.28740800	3.17521300
H	-4.18234700	0.04763400	1.08999400
C	-1.54260700	0.06383400	3.92512200
H	-0.13222300	0.66012300	2.41853000
C	-2.86271000	-0.28667600	4.19987900
H	-4.83814000	-0.56194600	3.38303800
H	-0.79876800	0.06353000	4.71641700
H	-3.15420500	-0.56093800	5.20985700
C	-2.66556100	0.09258800	-1.25677200
C	-3.04996800	0.75007200	-2.43135000
C	-3.04073900	-1.24178400	-1.06624000
C	-3.80420500	0.08489700	-3.39490800
H	-2.76434300	1.78519600	-2.59792700
C	-3.79623100	-1.90263500	-2.03117100
H	-2.74691600	-1.77374500	-0.16652800

C	-4.17982700	-1.24262700	-3.19675900
H	-4.09696700	0.60625800	-4.30171300
H	-4.07680800	-2.93884400	-1.86621900
H	-4.76781300	-1.76088100	-3.94894800

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 Zero-point correction=                           0.515371
(Hartree/Particle)
 Thermal correction to Energy=                    0.549359
 Thermal correction to Enthalpy=                  0.550303
 Thermal correction to Gibbs Free Energy=         0.443503
 Sum of electronic and zero-point Energies=          -1925.261374
 Sum of electronic and thermal Energies=             -1925.227386
 Sum of electronic and thermal Enthalpies=           -1925.226442
 Sum of electronic and thermal Free Energies=        -1925.333242
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Ag_I_D_RL

C	2.57884500	-1.27881700	-0.37265800
C	3.83120900	-0.70111200	-0.17948900
N	4.80214200	-1.66135000	-0.22481000
N	4.24054300	-2.81159600	-0.42208800
N	2.91046200	-2.59161700	-0.50646300
C	2.05084500	-3.72002400	-0.83428400
H	1.90643000	-3.75929100	-1.92015000
H	2.60461600	-4.61664800	-0.54014700
Ag	0.65528100	-0.46989500	-0.33990100
P	-1.42791600	0.67800500	-0.12111700
C	4.16844400	0.71613500	0.03638000
C	3.28558600	1.58649800	0.69076200
C	5.39362400	1.22927500	-0.41205500
C	3.60102800	2.93144400	0.86891800
H	2.34970800	1.19927400	1.08684700
C	5.71381100	2.57172600	-0.22705000
H	6.09001500	0.56021800	-0.90960100
C	4.81797600	3.43233200	0.40837800
H	2.90089500	3.58173200	1.38812600
H	6.66855700	2.94991100	-0.58494400
H	5.07067500	4.47959500	0.55328800
C	0.71081600	-3.65139000	-0.13909700
C	-0.47314100	-3.64626800	-0.87786200
C	0.63570500	-3.56008800	1.25532200
C	-1.71183700	-3.53570800	-0.24228800
H	-0.42522000	-3.71476900	-1.96288900
C	-0.59622900	-3.44379200	1.88980200
H	1.55441800	-3.54676600	1.83643700
C	-1.77541700	-3.42516500	1.14267100

H	-2.62559600	-3.52241800	-0.83120700
H	-0.64060600	-3.35487900	2.97166700
H	-2.73471700	-3.30886900	1.63940000
C	-1.18044200	2.43905700	0.29745400
C	-2.08245600	3.15885400	1.08919800
C	-0.04208000	3.07929700	-0.20609100
C	-1.85256200	4.50561300	1.36051900
H	-2.95872400	2.66682900	1.50354600
C	0.18184600	4.42717700	0.06174000
H	0.68421900	2.52434600	-0.79586400
C	-0.72372100	5.14132200	0.84389900
H	-2.55341900	5.05815600	1.97976800
H	1.07216800	4.90938600	-0.33089800
H	-0.54551600	6.19092500	1.05961900
C	-2.48663100	0.02970800	1.22120300
C	-3.83081100	-0.30023200	1.03911900
C	-1.89194800	-0.16848100	2.47301500
C	-4.57257000	-0.82071500	2.10017400
H	-4.30322000	-0.15949000	0.07106700
C	-2.63622800	-0.67466600	3.53254700
H	-0.83883300	0.06266600	2.61747100
C	-3.97895400	-1.00547600	3.34632500
H	-5.61729900	-1.07731900	1.94962600
H	-2.16588800	-0.82211800	4.50030500
H	-4.55876100	-1.40927300	4.17144500
C	-2.48868000	0.67148800	-1.60779900
C	-3.31796100	1.74519400	-1.94564200
C	-2.47119600	-0.46815900	-2.42010300
C	-4.12830700	1.67350700	-3.07673200
H	-3.32594700	2.64292800	-1.33337900
C	-3.28830000	-0.54097200	-3.54511000
H	-1.81206700	-1.29687600	-2.17207600
C	-4.11799600	0.53012700	-3.87393400
H	-4.76483800	2.51409000	-3.33714400
H	-3.26793500	-1.42859800	-4.17096100
H	-4.74820400	0.47803100	-4.75711600

Zero-point correction=	0.521109
(Hartree/Particle)	
Thermal correction to Energy=	0.554005
Thermal correction to Enthalpy=	0.554949
Thermal correction to Gibbs Free Energy=	0.451236
Sum of electronic and zero-point Energies=	-1925.402964
Sum of electronic and thermal Energies=	-1925.370068
Sum of electronic and thermal Enthalpies=	-1925.369124
Sum of electronic and thermal Free Energies=	-1925.472837