

Electronic Supplementary Information

for

**Is Silver a Mere Terminal Oxidant in Palladium Catalyzed C-H Bond Activation
Reactions?**

Bangaru Bhaskararao,^a Sukriti Singh,^a Megha Anand,^b Pritha Verma,^a Prafull Prakash,^a Athira
C,^a Santanu Malakar,^a Henry F. Schaefer,^b and Raghavan B. Sunoj*,^a

^a*Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai 400076,
India*

and

^b*Center for Computational Quantum Chemistry, University of Georgia, Athens, GA 30602, USA*

corresponding author: sunoj@chem.iitb.ac.in

Table of Contents

PART-B	
Details	Page No.
Section 1: Single point energies relevant to reactions 1 to 4	S3
Section 2: Cartesian coordinates of the optimized geometries	S4

Single Point Energies Relevant to Reactions 1 to 4

The Gibbs free energies employed in our discussion are obtained by adding the thermal and entropic corrections, as obtained through fully optimization of the stationary points, to the single point energies at the SMD_(Solvent)/M06/6-31G**,LANL2TZ(f) (Pd,Ag), LANL2DZ(d,p) (I, Br)// SMD_(solvent)/M06/6-31G**/LANL2DZ(Pd,Ag,Br,I) level of theory (provided below)

Reaction 1	total energy
[Pd(OAc) ₂] ₃	-1750.641544
AcOH	-228.9715094
2phenylpyridine	-478.986785
phosphonate-methyl	-647.307926
t-Amyl alcohol	-272.8048692
Quinol	-382.457278
Benzoquinone	-381.2202732
[Ag(OAc) (t-Amyl alcohol)] ₂	-1294.072892
1CH1(Pd)	-1899.209218
1CH1(Pd-Ag)	-2920.806055
1RE1(Pd)	-1633.134211
1RE1(Pd-Ag)	-2691.792451

Reaction 2	total energy
[Pd(OAc) ₂] ₃	-1750.62543
AcOH	-228.967223
HI	-11.9561347
Amide	-515.081692
Phenyl Iodide	-242.821513
Ag(OAc).2AcOH	-832.167194
2CH1(Pd)	-1098.58250
2CH1(Pd-Ag)	-1701.81414
2RE1(Pd)	-1341.43519
2RE1(Pd-Ag)	-1944.67705

Reaction 3	total energy
[Pd(OAc) ₂] ₃	-1750.6347652
[AgOAc] ₂	-748.4158446
Phenyl Amide	-479.238288
Alkyl Silane	-734.0620219
[Ag(OTf)] ₂	-2214.0799004
3CH1(Pd)	-1795.5761904
3CH1(Pd-Ag)	-2902.6518323
3RE1(Pd)	-2529.6736345
3RE1(Pd-Ag)	-2903.9214189

Reaction 4	total energy
[Pd(OAc) ₂] ₃	-1750.644996
AcOH	-228.972702
DMF	-248.355269
DPA	-539.0412031
ISATIN	-512.7566217
{[Ag(OAc)(DMF)] ₂ }	-1245.172218
4CH1(Pd)	-1945.431937
4CH1(Pd–Ag)	-2548.672903
4RE1(Pd)	-2174.462948
4RE1(Pd–Ag)	-2548.705966

I. Cartesian coordinates of the Optimized Geometries Obtained at the SMD_(solvent)/M06/6-31G**/LANL2DZ(Pd,Ag,Br,I) Level of Theory

Descriptor '-PRC' represents the optimized geometries from the end point of intrinsic reaction coordinate computations in the 'reverse' direction from the transition state.

The coordinates of various intermediates and transition states of the monometallic and heterobimetallic pathways are provided in the same order as shown in the energy profile (Figure 3)

Reaction 1

NaOAc(3-tamyl-OH)

Number of imaginary frequencies : 0

The smallest frequency is : 21.9875 cm(-1)

Electronic energy : =-1209.2077004
 Zero-point correction= 0.549237
 Thermal correction to Energy= 0.582471
 Thermal correction to Enthalpy= 0.583415
 Thermal correction to Gibbs Free Energy= 0.483543
 Sum of electronic and zero-point Energies= -1208.658464
 Sum of electronic and thermal Energies= -1208.625229
 Sum of electronic and thermal Enthalpies= -1208.624285
 Sum of electronic and thermal Free Energies= -1208.724157

Cartesian Coordinates

```

11  0.032932  0.089543  0.042443
 8  1.465574  1.743853 -0.846085
 8  1.402026 -1.626137 -0.627723
 1  1.922647 -1.662422 -1.440607
 1  0.782484  2.266901 -0.365888
 6  2.712238  1.927662 -0.164437
 6  2.634201  1.295020  1.222091
 1  3.538713  1.506344  1.806562
 1  1.774258  1.694910  1.776983
 1  2.538300  0.201381  1.145301
 6  3.776155  1.206824 -0.989583
 1  4.719844  1.238109 -0.424358
 1  3.481213  0.146097 -1.037537
 6  2.987302  3.419360 -0.036405
 1  2.935718  3.915308 -1.012222
 1  2.235746  3.883569  0.616199
 1  3.977671  3.605850  0.398626
 6  3.987559  1.752354 -2.390472

```

1	4.670508	1.113584	-2.962245
1	3.039389	1.806005	-2.937720
1	4.422643	2.758930	-2.375751
6	1.542119	-2.882499	0.069219
6	0.968708	-3.986738	-0.801835
1	1.495372	-4.027905	-1.764796
1	1.076077	-4.969316	-0.327988
1	-0.096313	-3.807882	-0.996841
6	3.018452	-3.109485	0.348135
1	3.192472	-4.069210	0.848006
1	3.587861	-3.122811	-0.591607
1	3.419994	-2.308133	0.981782
6	0.733237	-2.686123	1.350238
1	1.156608	-1.820235	1.884901
1	-0.295358	-2.418376	1.058910
6	0.696970	-3.882304	2.284956
1	1.700677	-4.175462	2.615781
1	0.114613	-3.645913	3.181962
1	0.227676	-4.754598	1.814688
8	-2.155150	-0.939790	0.044647
1	-2.133513	-0.318078	0.802249
6	-3.095249	-0.443488	-0.921244
6	-3.393879	-1.613333	-1.839473
1	-2.458819	-2.005424	-2.259237
1	-3.888886	-2.422828	-1.288791
1	-4.038070	-1.313617	-2.673975
6	-4.339275	0.022413	-0.160997
1	-4.020704	0.806026	0.546714
1	-4.681296	-0.825846	0.450270
6	-2.448542	0.693992	-1.704624
1	-1.546913	0.330669	-2.220244
1	-3.115449	1.092026	-2.478662
1	-2.165623	1.525508	-1.041751
6	-5.484703	0.542690	-1.011536
1	-5.848495	-0.216199	-1.715206
1	-6.332789	0.831663	-0.380802
1	-5.197588	1.427793	-1.591949
8	-1.238998	0.907269	1.832010
6	-1.246459	2.146107	1.568722
8	-0.587522	2.692007	0.644859
6	-2.137983	3.044641	2.400676
1	-1.598735	3.952579	2.689655
1	-2.992362	3.362772	1.790051
1	-2.514368	2.533091	3.290426

Quinol

Number of imaginary frequencies : 0
The smallest frequency is : 152.7801 cm(-1)

Electronic energy : =-382.4572536
Zero-point correction= 0.108930
Thermal correction to Energy= 0.115662
Thermal correction to Enthalpy= 0.116607
Thermal correction to Gibbs Free Energy= 0.078431
Sum of electronic and zero-point Energies= -382.348323
Sum of electronic and thermal Energies= -382.341591
Sum of electronic and thermal Enthalpies= -382.340647
Sum of electronic and thermal Free Energies= -382.378822

Cartesian Coordinates

6	1.207931	0.689142	0.000000
1	2.158767	1.217099	0.000000
6	1.207931	-0.704143	0.000000
6	-0.007072	-1.388981	0.000000
6	-1.207931	-0.689142	0.000000
6	-1.207931	0.704143	0.000000

6	0.007072	1.388981	0.000000
8	2.410738	-1.338560	0.000000
1	-0.015302	-2.478911	0.000000
1	-2.158766	-1.217098	0.000000
8	-2.410738	1.338560	0.000000
1	0.015302	2.478911	0.000000
1	2.263999	-2.292920	0.000000
1	-2.263998	2.292920	0.000000

Benzoquinone

Number of imaginary frequencies : 0
The smallest frequency is : 89.9644 cm(-1)

Electronic energy : =-381.2202732
Zero-point correction= 0.085172
Thermal correction to Energy= 0.091456
Thermal correction to Enthalpy= 0.092400
Thermal correction to Gibbs Free Energy= 0.054559
Sum of electronic and zero-point Energies= -381.135101
Sum of electronic and thermal Energies= -381.128817
Sum of electronic and thermal Enthalpies= -381.127873
Sum of electronic and thermal Free Energies= -381.165714

Cartesian Coordinates

6	1.232253	-0.000175	0.741481
6	-0.078446	-0.000360	1.428026
6	-1.225383	-0.000203	0.738414
6	-1.232253	0.000175	-0.741481
6	0.078446	0.000360	-1.428026
6	1.225383	0.000203	-0.738414
8	-2.278348	0.000329	-1.371997
8	2.278348	-0.000329	1.371997
1	-0.049090	-0.000632	2.515630
1	-2.199356	-0.000336	1.223268
1	2.199356	0.000336	-1.223268
1	0.049090	0.000632	-2.515630

acetic acid

Number of imaginary frequencies : 0
The smallest frequency is : 67.3148 cm(-1)

Electronic energy : =-228.9715094
Zero-point correction= 0.061960
Thermal correction to Energy= 0.066504
Thermal correction to Enthalpy= 0.067448
Thermal correction to Gibbs Free Energy= 0.034745
Sum of electronic and zero-point Energies= -228.909549
Sum of electronic and thermal Energies= -228.905005
Sum of electronic and thermal Enthalpies= -228.904061
Sum of electronic and thermal Free Energies= -228.936764

Cartesian Coordinates

6	-0.090929	0.121158	-0.000009
8	-0.650807	1.193064	0.000001
6	1.385466	-0.100928	-0.000003
8	-0.764133	-1.042871	-0.000002
1	-1.709095	-0.816163	0.000023
1	1.677338	-0.681661	0.881179
1	1.677296	-0.682268	-0.880794
1	1.906763	0.857176	-0.000327

Coordinates for monometallic pathway

First P-H-activation-PRC

Number of imaginary frequencies : 1
The smallest frequency is : -42.8908 cm(-1)

Electronic energy : =-2167.2458095
Zero-point correction= 0.593891
Thermal correction to Energy= 0.636606
Thermal correction to Enthalpy= 0.637551
Thermal correction to Gibbs Free Energy= 0.520361
Sum of electronic and zero-point Energies= -2166.651918
Sum of electronic and thermal Energies= -2166.609203
Sum of electronic and thermal Enthalpies= -2166.608259
Sum of electronic and thermal Free Energies= -2166.725448

Cartesian Coordinates

```
46 -0.840868 -1.175561 0.245793
15 -3.060903 0.736208 0.990544
8 -4.469274 0.040737 0.483709
6 -4.489683 -1.375256 0.409434
8 0.289861 -0.317477 1.855961
6 0.030039 0.110861 2.991482
8 -1.168864 0.324916 3.446554
8 -2.014464 0.482473 -0.175001
6 1.125622 0.459163 3.934824
8 -3.518014 2.291261 0.793465
6 -4.138467 2.710093 -0.420073
1 2.034117 -0.098570 3.693400
1 1.331184 1.533311 3.834636
1 0.824706 0.272363 4.968595
1 -1.873510 0.290056 2.724330
1 -5.535381 -1.692298 0.352682
1 -3.949080 -1.737027 -0.474884
1 -4.040925 -1.838109 1.304077
1 -5.182535 2.380100 -0.455989
1 -4.108164 3.803564 -0.441631
1 -3.611718 2.322874 -1.301383
8 0.215244 -2.866862 0.625529
8 1.603898 -2.440534 -1.093395
6 1.193752 -3.149739 -0.167835
6 1.835647 -4.480485 0.140630
1 2.136350 -4.518650 1.193226
1 1.109944 -5.285435 -0.018163
1 2.706288 -4.644290 -0.498847
6 4.727115 -0.236656 -0.726941
6 3.949845 -0.096866 0.582029
6 4.727599 0.982408 -1.633878
1 5.296555 0.778870 -2.548074
1 3.711610 1.266892 -1.939395
1 5.180416 1.860617 -1.157081
1 4.300642 -1.094690 -1.269224
1 5.761033 -0.513617 -0.473994
8 2.610530 0.267617 0.223282
6 3.926038 -1.436505 1.301455
6 4.518420 0.988451 1.484810
1 3.948191 1.037424 2.423246
1 5.567273 0.788172 1.738086
1 4.455915 1.973544 1.007686
1 3.275517 -1.391561 2.188151
1 3.544210 -2.215507 0.630881
1 4.930223 -1.722824 1.637435
11 1.286496 -0.202945 -1.657732
8 -0.653505 -0.838233 -2.783683
6 -1.502364 -1.676445 -2.476165
8 -1.749306 -2.114844 -1.280864
6 -2.413093 -2.287880 -3.511563
```

1	-2.619596	-3.338729	-3.291483
1	-3.369221	-1.750817	-3.493585
1	-1.975909	-2.188074	-4.507929
1	2.014470	0.058004	0.961685
6	1.837444	3.498726	-0.956311
6	0.435603	3.055549	-0.547047
6	2.028566	3.758154	-2.440809
1	3.082790	3.956286	-2.669583
1	1.712841	2.895113	-3.040625
1	1.453159	4.626549	-2.784594
1	2.525595	2.709293	-0.618690
1	2.087000	4.403643	-0.382018
8	0.184060	1.820058	-1.223007
6	0.395527	2.835563	0.960930
6	-0.629798	4.066502	-0.948243
1	-1.606823	3.759269	-0.551319
1	-0.403402	5.061904	-0.544256
1	-0.711859	4.142219	-2.038481
1	-0.579652	2.424746	1.257904
1	1.185604	2.135982	1.264003
1	0.540325	3.782107	1.497453
1	-0.694381	1.485644	-0.946615

First P-H-activation-TS

Number of imaginary frequencies : 1
The smallest frequency is : -795.0809 cm(-1)

Electronic energy : =-2167.2409683
Zero-point correction= 0.589413
Thermal correction to Energy= 0.632468
Thermal correction to Enthalpy= 0.633412
Thermal correction to Gibbs Free Energy= 0.515887
Sum of electronic and zero-point Energies= -2166.651556
Sum of electronic and thermal Energies= -2166.608500
Sum of electronic and thermal Enthalpies= -2166.607556
Sum of electronic and thermal Free Energies= -2166.725081

Cartesian Coordinates

46	-0.818799	-1.195840	0.220922
15	-3.013318	0.754772	0.919160
8	-4.431795	0.021593	0.620838
6	-4.416378	-1.390268	0.408317
8	0.225954	-0.283452	1.804993
6	-0.165310	0.183354	2.914787
8	-1.371926	0.343498	3.264073
8	-2.041777	0.450964	-0.259526
6	0.893637	0.620756	3.879440
8	-3.475474	2.293899	0.814964
6	-4.192961	2.745983	-0.338553
1	1.849544	0.128526	3.677233
1	1.026089	1.705502	3.773737
1	0.576453	0.425108	4.907136
1	-2.190908	0.460089	2.324798
1	-5.456813	-1.718895	0.351882
1	-3.894696	-1.641979	-0.522459
1	-3.928648	-1.915090	1.243049
1	-5.228147	2.391139	-0.308242
1	-4.183046	3.838315	-0.314875
1	-3.716965	2.400951	-1.264486
8	0.237426	-2.861930	0.665646
8	1.672731	-2.471730	-1.024448
6	1.241693	-3.156515	-0.090765
6	1.883881	-4.471836	0.277809
1	2.148973	-4.476673	1.340523
1	1.170829	-5.287765	0.117904
1	2.776971	-4.645363	-0.327219
6	4.734173	-0.162037	-0.495696

6	3.855774	-0.029611	0.749258
6	4.778570	1.050742	-1.409783
1	5.432186	0.860305	-2.268558
1	3.784585	1.299946	-1.805453
1	5.159221	1.945778	-0.902016
1	4.367447	-1.032075	-1.063440
1	5.751187	-0.417309	-0.163451
8	2.545241	0.313935	0.286402
6	3.802153	-1.367569	1.472360
6	4.335111	1.069615	1.686817
1	3.692725	1.110827	2.578107
1	5.365256	0.891660	2.020740
1	4.289320	2.051180	1.200051
1	3.063792	-1.343099	2.287483
1	3.515392	-2.162236	0.773285
1	4.777298	-1.619253	1.907547
11	1.376023	-0.251343	-1.633790
8	-0.537821	-0.905047	-2.784637
6	-1.370705	-1.771255	-2.507807
8	-1.679130	-2.178486	-1.316952
6	-2.139473	-2.496339	-3.584439
1	-1.802358	-3.537795	-3.632021
1	-3.208736	-2.510621	-3.350707
1	-1.975771	-2.022654	-4.554965
1	1.895737	0.133457	0.990436
6	1.825709	3.499544	-1.061254
6	0.418639	3.049276	-0.677174
6	2.062545	3.691060	-2.549292
1	3.119618	3.901895	-2.752062
1	1.785854	2.792594	-3.115494
1	1.480375	4.527751	-2.954829
1	2.516873	2.741004	-0.663265
1	2.038569	4.435609	-0.523328
8	0.207615	1.786663	-1.317769
6	0.342036	2.884825	0.835942
6	-0.650748	4.026086	-1.146287
1	-1.636242	3.710326	-0.776282
1	-0.459744	5.036839	-0.763094
1	-0.696420	4.069516	-2.240255
1	-0.633463	2.471853	1.129320
1	1.134420	2.210662	1.185191
1	0.459168	3.853710	1.338394
1	-0.676075	1.454000	-1.069198

First P-H-activation-product

Number of imaginary frequencies : 0
The smallest frequency is : 37.5992 cm(-1)

Electronic energy : =-2167.2636079
Zero-point correction= 0.594529
Thermal correction to Energy= 0.637567
Thermal correction to Enthalpy= 0.638512
Thermal correction to Gibbs Free Energy= 0.521446
Sum of electronic and zero-point Energies= -2166.669079
Sum of electronic and thermal Energies= -2166.626041
Sum of electronic and thermal Enthalpies= -2166.625096
Sum of electronic and thermal Free Energies= -2166.742162

Cartesian Coordinates

46	-0.829374	-1.186539	0.214947
15	-3.009558	1.124377	0.925187
8	-4.089317	0.004878	1.197495
6	-3.843630	-1.397986	1.408356
8	0.328045	-0.667847	1.830654
6	-0.265583	-0.142582	2.854607
8	-1.484933	0.013557	2.972957
8	-1.773418	0.700596	0.163813

6	0.671299	0.301886	3.950011
8	-3.806820	2.203470	0.067428
6	-4.028426	1.901090	-1.320032
1	1.696702	-0.042153	3.783639
1	0.664228	1.397484	3.996695
1	0.309720	-0.068278	4.914367
1	-2.792390	1.842789	2.090265
1	-4.770319	-1.805658	1.817659
1	-3.618402	-1.879661	0.451830
1	-3.025358	-1.539287	2.119630
1	-4.479891	0.908260	-1.436553
1	-4.718367	2.655693	-1.700653
1	-3.085687	1.946245	-1.876679
8	0.057477	-3.005147	0.218756
8	1.414087	-2.386651	-1.471477
6	0.978548	-3.212261	-0.661984
6	1.502054	-4.628330	-0.651777
1	1.494080	-5.051521	0.356282
1	0.853021	-5.249179	-1.280578
1	2.512856	-4.658173	-1.067466
6	4.640587	-0.512629	-0.608506
6	3.847859	-0.392534	0.693574
6	4.697573	0.744209	-1.461536
1	5.240628	0.552800	-2.394037
1	3.695329	1.104146	-1.734120
1	5.206751	1.572021	-0.952413
1	4.187692	-1.329020	-1.191671
1	5.660933	-0.838062	-0.357701
8	2.539338	0.056419	0.333572
6	3.742010	-1.757148	1.356660
6	4.464709	0.614453	1.655441
1	3.872120	0.665524	2.579431
1	5.489603	0.330301	1.927250
1	4.487377	1.620598	1.220545
1	3.126363	-1.701249	2.265686
1	3.276691	-2.475861	0.670354
1	4.730980	-2.137296	1.641427
11	1.283353	-0.076457	-1.628516
8	-0.765412	-0.323529	-2.693649
6	-1.697204	-1.114389	-2.504052
8	-1.964668	-1.716438	-1.394289
6	-2.625610	-1.470510	-3.639389
1	-2.101163	-2.152563	-4.318528
1	-3.538860	-1.958960	-3.291401
1	-2.874262	-0.569336	-4.208276
1	1.901865	-0.199634	1.029283
6	2.155820	3.555406	-0.595801
6	0.722863	3.160028	-0.246739
6	2.398270	3.937370	-2.045611
1	3.466276	4.108344	-2.227418
1	2.066685	3.146893	-2.729886
1	1.870552	4.857873	-2.324371
1	2.795258	2.701994	-0.324954
1	2.444534	4.387131	0.063883
8	0.397248	2.037336	-1.075407
6	0.657780	2.756766	1.221227
6	-0.271806	4.278262	-0.527965
1	-1.285911	3.970662	-0.232199
1	-0.020553	5.184670	0.037979
1	-0.296898	4.528882	-1.594697
1	-0.359361	2.447800	1.496204
1	1.336094	1.915888	1.411939
1	0.942025	3.597063	1.867890
1	-0.478945	1.709212	-0.808062

Second P-H-activation-PRC

Number of imaginary frequencies : 0

The smallest frequencies are : 18.7624 26.8212 30.9262 cm(-1)

Electronic energy : HF=-1878.1830974
 Zero-point correction= 0.308527 (Hartree/Particle)
 Thermal correction to Energy= 0.337725
 Thermal correction to Enthalpy= 0.338669
 Thermal correction to Gibbs Free Energy= 0.244719
 Sum of electronic and zero-point Energies= -1877.874570
 Sum of electronic and thermal Energies= -1877.845373
 Sum of electronic and thermal Enthalpies= -1877.844429
 Sum of electronic and thermal Free Energies= -1877.938378

 Cartesian Coordinates

46	0.484820	0.471943	-0.240928
15	-2.766569	0.479349	-0.141827
8	-2.916786	0.037932	1.372341
6	-1.807295	-0.329902	2.204563
8	0.235565	2.569390	-0.598532
6	-0.617782	3.096785	0.191755
8	-1.333073	2.469702	0.998515
8	-1.486599	0.047172	-0.825572
6	-0.776622	4.595974	0.086516
8	-4.008260	-0.228706	-0.848871
6	-3.986325	-1.652704	-0.998081
1	0.079632	5.066813	-0.402783
1	-1.675358	4.813224	-0.503839
1	-0.927790	5.028348	1.080109
1	-3.164641	1.796600	-0.280638
1	-2.201273	-0.411126	3.219879
1	-1.406121	-1.299238	1.890480
1	-1.030819	0.442071	2.170456
1	-3.558365	-2.141876	-0.114139
1	-5.021594	-1.978836	-1.116555
1	-3.412154	-1.926881	-1.889020
8	2.449414	0.963855	0.338023
8	3.803332	-0.220840	-1.024821
6	3.541176	0.763575	-0.224089
6	4.672570	1.705761	-0.004879
1	4.438033	2.412641	0.791579
1	5.586893	1.151751	0.225253
1	4.847775	2.257694	-0.935687
1	3.088578	-0.951034	-1.009014
15	0.917241	-1.713801	0.020177
8	-0.333574	-2.691109	-0.292239
8	1.082018	-1.966753	1.603121
8	2.128093	-2.133160	-0.788664
6	-0.644599	-2.937205	-1.664174
1	-1.509417	-3.605528	-1.679636
1	-0.896932	-2.002870	-2.181479
1	0.194656	-3.424212	-2.172613
6	1.390303	-3.295242	2.046251
1	1.734811	-3.214992	3.079465
1	0.497563	-3.928630	2.006408
1	2.185119	-3.738634	1.435634

 Second P-H-activation-TS

Number of imaginary frequencies : 1
 The smallest frequencies are : -1154.3642 21.3680 22.8577 cm(-1)

Electronic energy : HF=-1878.1668197
 Zero-point correction= 0.303298 (Hartree/Particle)
 Thermal correction to Energy= 0.332963
 Thermal correction to Enthalpy= 0.333907
 Thermal correction to Gibbs Free Energy= 0.237309
 Sum of electronic and zero-point Energies= -1877.863522
 Sum of electronic and thermal Energies= -1877.833857
 Sum of electronic and thermal Enthalpies= -1877.832912
 Sum of electronic and thermal Free Energies= -1877.929511

Cartesian Coordinates

```

-----
46  0.390514  0.384995 -0.211478
15  -2.590143  0.180929  0.204667
 8  -3.039537 -0.977265  1.249465
 6  -2.010685 -1.581328  2.034540
 8  -0.164318  2.491792 -0.491368
 6  -0.852363  3.218763  0.273100
 8  -1.699443  2.805612  1.123375
 8  -1.470452 -0.382497 -0.706952
 6  -0.689730  4.710612  0.162243
 8  -3.937277  0.331822 -0.653634
 6  -4.401688 -0.773706 -1.435435
 1  0.150694  4.977709 -0.481785
 1  -1.611020  5.141169 -0.246114
 1  -0.549552  5.140961  1.159109
 1  -2.168403  1.583590  0.808472
 1  -2.502092 -2.152900  2.825620
 1  -1.399072 -2.252990  1.421088
 1  -1.362361 -0.825719  2.501331
 1  -4.683997 -1.613199 -0.791032
 1  -5.279584 -0.428297 -1.985361
 1  -3.634018 -1.097830 -2.147133
 8  2.248315  1.191266  0.395285
 8  3.809666  0.329014 -0.984505
 6  3.369302  1.210237 -0.140861
 6  4.330658  2.303192  0.169627
 1  3.906310  2.998486  0.894339
 1  5.262679  1.875755  0.552382
 1  4.573553  2.835589 -0.756502
 1  3.219579 -0.499443 -1.030891
15  1.170298 -1.700818 -0.093395
 8  0.106143 -2.835480 -0.504742
 8  1.348968 -2.019172  1.470821
 8  2.437978 -1.832122 -0.907712
 6  -0.221375 -2.973042 -1.889939
 1  -1.038916 -3.694929 -1.950197
 1  -0.559276 -2.017680 -2.307400
 1  0.639548 -3.346743 -2.454475
 6  1.754076 -3.339746  1.860439
 1  2.111828 -3.270970  2.889767
 1  0.903492 -4.028145  1.812598
 1  2.565128 -3.709489  1.222547
-----

```

Second P-H-activation-product

```

-----
Number of imaginary frequencies : 0
The smallest frequencies are : 23.6045  30.7525  40.1899 cm(-1)
-----

```

```

Electronic energy : HF=-1878.1783329
Zero-point correction= 0.309302 (Hartree/Particle)
Thermal correction to Energy= 0.338727
Thermal correction to Enthalpy= 0.339671
Thermal correction to Gibbs Free Energy= 0.246491
Sum of electronic and zero-point Energies= -1877.869031
Sum of electronic and thermal Energies= -1877.839606
Sum of electronic and thermal Enthalpies= -1877.838662
Sum of electronic and thermal Free Energies= -1877.931841
-----

```

Cartesian Coordinates

```

-----
46  0.400210  0.381610 -0.259774
15  -2.547008  0.447606  0.260277
 8  -2.871076 -0.883750  1.195748
 6  -2.018608 -1.112084  2.299006
 8  -1.506962 -0.040553 -0.834928
 8  -3.952136  0.458992 -0.575269
 6  -4.261305 -0.624264 -1.444195
 1  -2.608628 -1.551694  3.110809
 1  -1.205696 -1.802694  2.039584
-----

```

1	-1.568799	-0.177629	2.675081
1	-4.166782	-1.589834	-0.932167
1	-5.299008	-0.496863	-1.766536
1	-3.612656	-0.620708	-2.328565
8	2.393196	0.866461	0.293735
8	3.750408	-0.360073	-1.029908
6	3.501561	0.609081	-0.201395
6	4.690413	1.437638	0.140030
1	4.416502	2.248230	0.815704
1	5.454767	0.804563	0.602249
1	5.121351	1.846289	-0.779909
1	2.979617	-1.007899	-1.148661
15	0.823343	-1.791177	-0.130635
8	-0.443874	-2.766182	-0.211304
8	1.283406	-2.020994	1.392853
8	1.879138	-2.148142	-1.151769
6	-1.046379	-3.009826	-1.487500
1	-1.950956	-3.592019	-1.297662
1	-1.315488	-2.063989	-1.968210
1	-0.368536	-3.586153	-2.126423
6	1.555882	-3.362737	1.825283
1	2.118720	-3.286127	2.757710
1	0.620494	-3.903433	2.004234
1	2.158702	-3.901307	1.084910
8	0.191436	2.641768	-0.467102
8	-1.344378	3.316111	1.034114
6	-0.346454	3.520611	0.202266
6	0.069859	4.949884	0.131796
1	0.985558	5.053872	-0.451302
1	-0.731440	5.533044	-0.335286
1	0.213739	5.347995	1.140913
1	-1.699234	2.386928	0.947397

P-H-activation-product (after 2 successive P-H activations)

Number of imaginary frequencies : 0
The smallest frequency is : 5.9646 cm(-1)

Electronic energy : =-1878.2328773
Zero-point correction= 0.311143
Thermal correction to Energy= 0.340146
Thermal correction to Enthalpy= 0.341090
Thermal correction to Gibbs Free Energy= 0.247897
Sum of electronic and zero-point Energies= -1877.921734
Sum of electronic and thermal Energies= -1877.892731
Sum of electronic and thermal Enthalpies= -1877.891787
Sum of electronic and thermal Free Energies= -1877.984981

Cartesian Coordinates

46	0.362020	-0.093422	0.051681
15	0.047394	2.137811	-0.200848
8	-0.137089	2.849983	1.230996
6	-1.209130	2.434551	2.076855
8	-1.282622	2.643904	-0.954137
6	-1.455025	2.262874	-2.314080
8	1.274006	2.682154	-0.888398
1	-1.222946	1.199522	-2.471632
1	-2.503856	2.431572	-2.569673
1	-0.814352	2.867667	-2.966039
1	-2.177946	2.598532	1.593040
1	-1.110682	1.373760	2.344753
1	-1.147643	3.037285	2.985597
15	-1.821195	-0.663691	0.024407
8	-2.054702	-1.813606	-0.931293
8	-2.221691	-1.083533	1.548431
8	-2.893863	0.511593	-0.191627
6	-4.273439	0.144982	-0.290799
6	-1.666237	-2.269322	2.107131

1	-4.823238	1.054976	-0.541804
1	-4.426629	-0.600311	-1.078575
1	-4.639685	-0.249142	0.663784
1	-2.203395	-2.466649	3.038158
1	-1.796373	-3.126697	1.435168
1	-0.600448	-2.139001	2.333933
8	2.544486	0.091988	0.524312
8	0.984145	-2.266712	0.158354
6	3.581354	0.685716	0.216097
6	0.858881	-3.262438	-0.560611
6	4.919949	0.201076	0.663309
1	4.836532	-0.775755	1.141160
1	5.601700	0.149654	-0.191186
1	5.343498	0.921230	1.372103
6	1.889980	-4.340462	-0.590733
1	1.418966	-5.315978	-0.435939
1	2.354342	-4.359845	-1.583045
1	2.655644	-4.163725	0.165618
8	3.626735	1.773503	-0.499100
8	-0.149854	-3.480423	-1.357962
1	-0.872522	-2.778424	-1.237883
1	2.688735	2.114264	-0.687865

C-H activation-PRC

Number of imaginary frequencies : 0
The smallest frequency is : 23.5922 cm(-1)

Electronic energy : =-1899.2466799
Zero-point correction= 0.353780
Thermal correction to Energy= 0.382163
Thermal correction to Enthalpy= 0.383107
Thermal correction to Gibbs Free Energy= 0.293606
Sum of electronic and zero-point Energies= -1898.892900
Sum of electronic and thermal Energies= -1898.864517
Sum of electronic and thermal Enthalpies= -1898.863573
Sum of electronic and thermal Free Energies= -1898.953074

Cartesian Coordinates

7	1.846084	-1.097838	-0.617070
6	2.963397	-0.403655	-0.315965
6	4.224490	-0.991773	-0.388900
6	4.329207	-2.313123	-0.802666
6	3.174089	-3.016921	-1.123360
6	1.949585	-2.373708	-1.010875
6	2.764999	0.993536	0.110813
6	1.830579	1.801531	-0.556194
6	1.545168	3.084377	-0.092841
6	2.213359	3.580847	1.022035
6	3.165792	2.796059	1.668305
6	3.439024	1.507260	1.220351
46	-0.092057	0.042593	-0.457425
15	-1.775359	1.552455	-0.671801
8	-2.165221	2.304861	0.705590
6	-2.737010	1.567727	1.781469
8	-3.240104	1.013199	-1.112315
6	-3.305901	0.219683	-2.286763
8	-1.190699	2.520722	-1.653733
1	0.794258	3.673313	-0.613396
1	1.993152	4.581027	1.387224
1	3.688090	3.183520	2.540104
1	4.154559	0.882371	1.752116
1	5.106019	-0.404582	-0.145714
1	5.304588	-2.787439	-0.877733
1	3.213034	-4.052317	-1.447984
1	1.005232	-2.884224	-1.196981
1	1.401930	1.474982	-1.512470
1	-2.558209	-0.587287	-2.272283

1	-4.300269	-0.232254	-2.324581
1	-3.151123	0.832087	-3.183801
1	-3.717168	1.162932	1.504999
1	-2.081439	0.743973	2.095607
1	-2.854656	2.263983	2.615729
15	-1.331876	-1.649292	0.402286
8	-0.980195	-2.972561	-0.204967
8	-1.047512	-1.631073	2.017151
8	-2.917775	-1.356736	0.437399
6	-3.750580	-2.194428	1.237041
6	0.260109	-1.973704	2.454752
1	-4.768834	-2.100705	0.850696
1	-3.443952	-3.245837	1.178223
1	-3.728106	-1.868801	2.283911
1	0.213433	-2.131131	3.535615
1	0.613387	-2.895265	1.975569
1	0.970808	-1.159759	2.248721

C-H-activation-TS

Number of imaginary frequencies : 1
 The smallest frequency is : -1559.4937 cm(-1)

Electronic energy : =-1899.1965442
 Zero-point correction= 0.349017
 Thermal correction to Energy= 0.376803
 Thermal correction to Enthalpy= 0.377747
 Thermal correction to Gibbs Free Energy= 0.290451
 Sum of electronic and zero-point Energies= -1898.847527
 Sum of electronic and thermal Energies= -1898.819742
 Sum of electronic and thermal Enthalpies= -1898.818797
 Sum of electronic and thermal Free Energies= -1898.906093

 Cartesian Coordinates

7	-1.613471	1.379403	-0.279092
6	-2.806491	0.750780	-0.378668
6	-3.931568	1.441166	-0.831667
6	-3.821242	2.781174	-1.172195
6	-2.588563	3.413668	-1.056180
6	-1.503867	2.672805	-0.612781
6	-2.851598	-0.658883	0.057779
6	-1.724106	-1.508959	-0.087884
6	-1.802707	-2.766996	0.533596
6	-2.936730	-3.200986	1.214957
6	-4.042311	-2.364407	1.306096
6	-3.992360	-1.095823	0.739262
46	0.041015	-0.013906	-0.067314
15	1.344542	-1.730289	-0.735109
8	1.885912	-2.815361	0.320491
6	2.777835	-2.367459	1.344304
8	2.669986	-1.500619	-1.618208
6	2.597842	-0.555829	-2.683270
8	0.247172	-2.404500	-1.601481
1	-0.956533	-3.447246	0.439552
1	-2.956951	-4.189287	1.669649
1	-4.936204	-2.685727	1.836075
1	-4.836733	-0.420322	0.867600
1	-4.878373	0.917932	-0.932875
1	-4.690451	3.325547	-1.533234
1	-2.459680	4.460262	-1.314799
1	-0.504300	3.100555	-0.518350
1	-0.766799	-1.833246	-1.068981
1	2.085880	0.365506	-2.371143
1	3.623229	-0.307823	-2.966190
1	2.071707	-0.984805	-3.543613
1	3.752053	-2.096640	0.923105
1	2.360720	-1.503102	1.877853
1	2.899619	-3.197365	2.043619

15	1.698358	1.476289	0.445845
8	1.602722	2.832837	-0.185537
8	1.665175	1.574054	2.084867
8	3.163039	0.800278	0.282266
6	4.299521	1.626694	0.536465
6	0.565083	2.264180	2.662015
1	5.185574	1.004297	0.388803
1	4.333847	2.473907	-0.157708
1	4.292370	2.002042	1.566765
1	0.755547	2.343829	3.735563
1	0.459978	3.272892	2.242493
1	-0.374872	1.712374	2.514728

C-H-activation-product

Number of imaginary frequencies : 0
 The smallest frequency is : 29.5452 cm(-1)

Electronic energy : =-1899.2283581
 Zero-point correction= 0.354996
 Thermal correction to Energy= 0.382665
 Thermal correction to Enthalpy= 0.383609
 Thermal correction to Gibbs Free Energy= 0.297203
 Sum of electronic and zero-point Energies= -1898.873362
 Sum of electronic and thermal Energies= -1898.845693
 Sum of electronic and thermal Enthalpies= -1898.844749
 Sum of electronic and thermal Free Energies= -1898.931155

 Cartesian Coordinates

7	-1.544206	1.466394	-0.258000
6	-2.809569	0.974004	-0.265608
6	-3.883811	1.817350	-0.551257
6	-3.656214	3.157347	-0.824643
6	-2.354520	3.641372	-0.818168
6	-1.322688	2.759033	-0.535692
6	-2.937877	-0.454569	0.048375
6	-1.747691	-1.216098	0.149400
6	-1.873588	-2.541692	0.581104
6	-3.118996	-3.119492	0.839827
6	-4.278404	-2.371192	0.682893
6	-4.184195	-1.037800	0.303691
46	-0.023679	-0.054617	-0.112402
15	1.260596	-1.868298	-0.490117
8	1.718317	-2.713519	0.796145
6	2.066122	-1.964769	1.969460
8	2.641449	-1.764547	-1.293715
6	2.641994	-1.084783	-2.548737
8	0.498425	-2.968172	-1.392916
1	-0.991725	-3.159357	0.755198
1	-3.175131	-4.154848	1.170881
1	-5.252703	-2.813489	0.877241
1	-5.096519	-0.448358	0.231128
1	-4.894969	1.422828	-0.573876
1	-4.491857	3.815452	-1.050043
1	-2.130627	4.681829	-1.032920
1	-0.277569	3.076533	-0.529348
1	-0.464010	-2.876799	-1.297802
1	2.008709	-0.187078	-2.523387
1	3.670837	-0.781177	-2.751967
1	2.289749	-1.755345	-3.340444
1	2.946669	-1.338927	1.787439
1	1.226907	-1.329862	2.285648
1	2.284831	-2.694415	2.751286
15	1.816890	1.452146	0.187454
8	1.753347	2.849461	-0.371082
8	1.963271	1.514674	1.842121
8	3.270142	0.758674	-0.092673

6	4.430619	1.554522	0.115951
6	0.900734	2.132871	2.540234
1	5.295092	0.951590	-0.176792
1	4.404182	2.464828	-0.494744
1	4.533741	1.836842	1.171082
1	1.179395	2.187363	3.597080
1	0.712413	3.152335	2.175524
1	-0.032100	1.550775	2.461262

reductive-elimination-PRC

Electronic energy : -1633.1290729
 Zero-point correction= 0.337087
 Thermal correction to Energy= 0.363836
 Thermal correction to Enthalpy= 0.364780
 Thermal correction to Gibbs Free Energy= 0.278930
 Sum of electronic and zero-point Energies= -1632.791985
 Sum of electronic and thermal Energies= -1632.765237
 Sum of electronic and thermal Enthalpies= -1632.764293
 Sum of electronic and thermal Free Energies= -1632.850143

 Cartesian Coordinates

6	-2.177914	-2.492003	1.886282
6	-1.697174	-1.523447	0.997131
6	-0.316638	-1.238961	0.969940
6	0.542842	-1.904241	1.837228
6	0.045695	-2.857849	2.726760
6	-1.311784	-3.160979	2.741531
6	-2.599681	-0.738300	0.146460
6	-3.907999	-1.111893	-0.161822
6	-4.676585	-0.293487	-0.976833
6	-4.129345	0.883493	-1.475057
6	-2.820502	1.193736	-1.134644
7	-2.081486	0.411543	-0.342801
46	0.181392	0.405800	-0.120639
15	1.621573	-1.013741	-1.208871
8	2.208756	-0.263529	-2.362129
8	0.728889	-2.289209	-1.653033
6	1.267908	-3.112370	-2.692004
8	2.754646	-1.778561	-0.327462
6	3.901808	-1.026132	0.062142
1	2.234881	-3.536575	-2.395616
1	0.556424	-3.925461	-2.853093
1	1.388905	-2.545452	-3.621430
1	4.458322	-0.675722	-0.815126
1	3.629274	-0.162540	0.685506
1	4.536916	-1.695346	0.648394
1	1.610657	-1.696753	1.816140
1	0.727703	-3.369309	3.403273
1	-1.700146	-3.906928	3.430905
1	-3.245138	-2.704139	1.930935
1	-4.310413	-2.046818	0.217517
1	-5.695411	-0.578153	-1.228130
1	-4.697397	1.550302	-2.116442
1	-2.347712	2.110150	-1.487846
6	1.760464	2.034868	-0.220392
6	0.625919	2.560289	-0.815593
6	-0.355328	3.328693	-0.032702
6	2.017249	2.224063	1.230557
8	3.064319	1.870957	1.756479
8	-1.308492	3.896512	-0.555534
6	0.950509	2.881146	2.016867
6	-0.143067	3.393851	1.432852
1	-0.916223	3.906227	2.002247
1	1.123265	2.951571	3.088997
1	2.588243	1.667944	-0.823521
1	0.517447	2.583282	-1.899400

reductive-elimination-TS

Number of imaginary frequencies : 1
The smallest frequency is : -81.1109 cm(-1)

Electronic energy : -1633.1243536
Zero-point correction= 0.337300
Thermal correction to Energy= 0.362971
Thermal correction to Enthalpy= 0.363915
Thermal correction to Gibbs Free Energy= 0.281319
Sum of electronic and zero-point Energies= -1632.787054
Sum of electronic and thermal Energies= -1632.761383
Sum of electronic and thermal Enthalpies= -1632.760439
Sum of electronic and thermal Free Energies= -1632.843034

Cartesian Coordinates

6	-2.286206	-0.313985	2.713790
6	-1.725059	-0.041332	1.463680
6	-0.553665	-0.726306	1.080369
6	0.039819	-1.638381	1.944749
6	-0.526465	-1.887098	3.195581
6	-1.694773	-1.234524	3.572197
6	-2.273275	0.997381	0.578964
6	-3.590502	1.454548	0.628840
6	-3.990861	2.457894	-0.242108
6	-3.077696	2.983691	-1.150506
6	-1.787623	2.473149	-1.152183
7	-1.399319	1.513212	-0.309538
46	0.539972	0.349239	-0.332101
15	-0.342476	-1.626405	-1.174883
8	-0.016092	-1.353683	-2.609868
8	-1.915598	-1.894446	-0.942243
6	-2.594068	-2.627255	-1.969342
8	0.283237	-3.024860	-0.658304
6	1.639081	-3.325256	-0.997207
1	-2.124238	-3.604412	-2.133680
1	-3.617112	-2.777958	-1.617666
1	-2.607472	-2.065771	-2.908758
1	1.804241	-3.229446	-2.076206
1	2.339955	-2.674423	-0.456354
1	1.814035	-4.361224	-0.696609
1	0.937795	-2.173217	1.642580
1	-0.053628	-2.598396	3.869213
1	-2.141282	-1.428769	4.544445
1	-3.174086	0.227456	3.035926
1	-4.296271	1.016286	1.329115
1	-5.014354	2.823600	-0.216527
1	-3.354581	3.770798	-1.845087
1	-1.030554	2.843759	-1.842073
6	2.678446	0.218139	-0.819720
6	2.240286	1.516077	-1.122329
6	2.361397	2.609580	-0.143490
6	3.277172	-0.091127	0.493167
8	3.747887	-1.191810	0.763948
8	2.063459	3.769276	-0.405969
6	3.295916	1.004516	1.492786
6	2.874188	2.243942	1.201576
1	2.912828	3.051818	1.930411
1	3.696719	0.744774	2.471018
1	2.834092	-0.517557	-1.607839
1	2.027732	1.813564	-2.148661

reductive-elimination-product

Number of imaginary frequencies : 0
The smallest frequency is : 34.2191 cm(-1)

Electronic energy : =-1633.1675694
 Zero-point correction= 0.339463
 Thermal correction to Energy= 0.365505
 Thermal correction to Enthalpy= 0.366449
 Thermal correction to Gibbs Free Energy= 0.282598
 Sum of electronic and zero-point Energies= -1632.828106
 Sum of electronic and thermal Energies= -1632.802064
 Sum of electronic and thermal Enthalpies= -1632.801120
 Sum of electronic and thermal Free Energies= -1632.884971

 Cartesian Coordinates

6	-0.905613	0.927276	2.756787
6	-1.185264	0.384401	1.502060
6	-0.845182	-0.961003	1.250392
6	-0.241844	-1.717133	2.260460
6	0.051034	-1.152936	3.497018
6	-0.281175	0.172333	3.745034
6	-1.852788	1.277186	0.516533
6	-3.130289	1.768804	0.781565
6	-3.716630	2.652298	-0.114978
6	-3.007623	3.026298	-1.249376
6	-1.739452	2.496577	-1.441501
7	-1.170069	1.641849	-0.582864
46	0.738526	0.624574	-1.118444
15	-1.210308	-1.786648	-0.309135
8	-0.844601	-1.057613	-1.563400
8	-2.762849	-2.121588	-0.156295
6	-3.427152	-2.777436	-1.246126
8	-0.537212	-3.238297	-0.220512
6	0.827043	-3.379219	-0.648948
1	-2.974993	-3.756224	-1.439069
1	-4.467313	-2.911667	-0.944510
1	-3.385226	-2.162386	-2.150949
1	0.959974	-2.997550	-1.666083
1	1.509470	-2.847789	0.024729
1	1.054176	-4.446729	-0.623294
1	-0.004233	-2.762368	2.078922
1	0.530179	-1.754001	4.265660
1	-0.060047	0.624071	4.709089
1	-1.171008	1.965193	2.949281
1	-3.649802	1.450421	1.681843
1	-4.713318	3.044249	0.071440
1	-3.422008	3.718022	-1.976772
1	-1.144109	2.764417	-2.312343
6	2.849280	0.372165	-1.421111
6	2.561218	1.652360	-0.883078
6	2.584476	1.882831	0.571213
6	3.226053	-0.741590	-0.547574
8	3.576171	-1.842549	-0.970903
8	2.391674	2.983885	1.078917
6	3.166765	-0.497311	0.918525
6	2.862966	0.702158	1.431800
1	2.821389	0.881871	2.505717
1	3.399709	-1.354907	1.549922
1	3.114961	0.253879	-2.471329
1	2.614705	2.548796	-1.501400

Coordinates for heterobimetallic pathway

 First P-H-activation-PRC (Pd-Ag)

Number of imaginary frequencies : 0
 The smallest frequency is : 19.9875 cm(-1)

Electronic energy : =-2541.4627848

Zero-point correction= 0.643915
 Thermal correction to Energy= 0.695924
 Thermal correction to Enthalpy= 0.696869
 Thermal correction to Gibbs Free Energy= 0.555984
 Sum of electronic and zero-point Energies= -2540.818869
 Sum of electronic and thermal Energies= -2540.766860
 Sum of electronic and thermal Enthalpies= -2540.765916
 Sum of electronic and thermal Free Energies= -2540.906801

.....
 Cartesian Coordinates

46	-0.191758	1.680998	-0.494470
15	2.345389	2.380058	0.964186
8	3.756256	2.319609	0.095249
6	3.614370	2.539556	-1.297137
8	-1.147443	2.360360	1.271783
6	-1.079971	3.496681	1.757446
8	-0.101302	4.338789	1.540720
8	1.549786	1.105866	0.440610
6	-2.128550	4.010768	2.674820
8	2.965724	1.944956	2.406803
6	3.759100	0.769715	2.545474
1	-1.720654	4.050536	3.691047
1	-2.398894	5.032458	2.391446
1	-3.006939	3.365229	2.656897
1	0.688672	3.880752	1.136690
1	4.616014	2.642669	-1.725179
1	3.093601	1.706286	-1.789341
1	3.050602	3.463090	-1.507977
1	3.848596	0.563054	3.615725
1	3.299967	-0.103861	2.064056
1	4.759976	0.929619	2.125806
8	-1.846101	2.398272	-1.446662
8	-2.532551	0.415976	-2.285979
6	-2.611967	1.649533	-2.152063
6	-3.736663	2.378830	-2.841246
1	-3.581285	3.459347	-2.859875
1	-3.853938	1.996198	-3.859094
1	-4.665463	2.161937	-2.299255
47	-1.531661	-1.026958	-0.756690
8	0.616629	1.147551	-2.276997
6	0.941766	-0.076155	-2.474749
6	1.671426	-0.323574	-3.768117
1	2.747981	-0.377114	-3.559693
1	1.364237	-1.285112	-4.188600
1	1.501754	0.478627	-4.489627
8	0.722270	-1.026854	-1.695520
6	-4.345927	-1.332408	1.706860
6	-4.435063	-2.259982	0.489989
6	-3.568673	-0.036982	1.542450
1	-3.629855	0.561897	2.458837
1	-2.496570	-0.214406	1.367791
1	-3.948600	0.585072	0.720475
1	-3.912875	-1.910023	2.539096
1	-5.378497	-1.103532	2.010026
8	-3.132811	-2.645667	0.024124
6	-5.186368	-3.523729	0.885505
6	-5.112922	-1.590016	-0.691369
1	-5.212555	-2.301600	-1.520212
1	-6.116081	-1.241997	-0.415814
1	-4.528508	-0.735411	-1.055444
1	-5.239151	-4.215952	0.037056
1	-4.676537	-4.034411	1.713615
1	-6.209519	-3.292236	1.207835
1	-2.507224	-2.793985	0.765104
11	1.402586	-1.215043	0.593299
8	0.665772	-1.539974	2.757994
6	-0.384871	-2.124389	2.425943
8	-0.740715	-2.338409	1.214542
6	-1.318022	-2.606255	3.518026

1	-1.907299	-1.753686	3.880352
1	-2.008478	-3.379049	3.162769
1	-0.745295	-2.985893	4.369539
6	4.597283	-3.587188	-0.892420
6	4.525452	-2.290621	-0.082659
6	3.352730	-3.921859	-1.696177
1	3.458654	-4.896464	-2.185502
1	2.463309	-3.968857	-1.055736
1	3.156747	-3.182575	-2.482845
1	4.813972	-4.407040	-0.188447
1	5.471586	-3.522461	-1.557138
8	3.418220	-2.356338	0.836542
6	5.809638	-2.093722	0.705429
6	4.235021	-1.081975	-0.951978
1	4.194451	-0.167769	-0.344007
1	5.013379	-0.956252	-1.715341
1	3.271967	-1.198942	-1.464827
1	5.747888	-1.191316	1.326061
1	6.001590	-2.952738	1.362925
1	6.669063	-1.990977	0.031848
1	3.573253	-3.077870	1.460090

First P-H-activation-TS (Pd-Ag)

Number of imaginary frequencies : 1
The smallest frequency is : -1156.7642 cm(-1)

Electronic energy : =-2541.454446
Zero-point correction= 0.640114
Thermal correction to Energy= 0.691351
Thermal correction to Enthalpy= 0.692295
Thermal correction to Gibbs Free Energy= 0.552943
Sum of electronic and zero-point Energies= -2540.814332
Sum of electronic and thermal Energies= -2540.763095
Sum of electronic and thermal Enthalpies= -2540.762151
Sum of electronic and thermal Free Energies= -2540.901503

Cartesian Coordinates

46	-0.138729	1.767112	-0.382398
15	2.340103	1.994578	1.289855
8	3.706241	2.237376	0.441477
6	3.551886	2.607851	-0.929537
8	-1.062940	2.318426	1.383272
6	-0.752794	3.353968	2.043761
8	0.343954	3.983503	1.952788
8	1.532949	0.883768	0.553402
6	-1.769738	3.873214	3.012122
8	2.942070	1.426340	2.660362
6	3.813516	0.289350	2.678824
1	-1.301664	4.038851	3.987048
1	-2.128557	4.843987	2.651320
1	-2.617245	3.191838	3.106825
1	1.320670	3.227962	1.608304
1	4.551808	2.790639	-1.330080
1	3.062068	1.811807	-1.503841
1	2.955991	3.526783	-1.026312
1	3.784548	-0.117667	3.692133
1	3.487827	-0.487014	1.975601
1	4.837450	0.599478	2.441684
8	-1.608272	2.794307	-1.326339
8	-2.752161	0.975597	-2.028954
6	-2.541888	2.198868	-1.974412
6	-3.427884	3.134192	-2.757269
1	-3.500569	4.113610	-2.278455
1	-2.987188	3.275609	-3.751049
1	-4.421063	2.696415	-2.882211
47	-1.745228	-0.726379	-0.806949

8	0.666899	1.321365	-2.201519
6	0.845003	0.087964	-2.498092
6	1.587488	-0.134529	-3.788827
1	2.654886	0.063111	-3.624710
1	1.466361	-1.164971	-4.130975
1	1.241621	0.562616	-4.557187
8	0.476279	-0.884754	-1.806376
6	-4.305828	-1.635327	1.754815
6	-4.453606	-2.319821	0.389843
6	-3.498650	-0.348821	1.796413
1	-3.549176	0.104811	2.793446
1	-2.433212	-0.536794	1.599796
1	-3.858073	0.403641	1.081866
1	-3.857613	-2.362592	2.450399
1	-5.321952	-1.449094	2.132874
8	-3.177096	-2.544788	-0.227147
6	-5.127841	-3.671148	0.581004
6	-5.243454	-1.472361	-0.590862
1	-5.340235	-1.999250	-1.548190
1	-6.250918	-1.271986	-0.206172
1	-4.747393	-0.513699	-0.787763
1	-5.247494	-4.178530	-0.383606
1	-4.523751	-4.314514	1.234694
1	-6.119224	-3.557796	1.037979
1	-2.492636	-2.814661	0.428567
11	1.250844	-1.428147	0.386682
8	0.777040	-2.279714	2.501737
6	-0.354341	-2.660081	2.137213
8	-0.809214	-2.514690	0.949551
6	-1.269216	-3.311205	3.153092
1	-1.849233	-2.526549	3.657133
1	-1.975366	-4.003480	2.681162
1	-0.690816	-3.835383	3.919067
6	4.517268	-3.432742	-1.361325
6	4.499508	-2.245187	-0.396323
6	3.304461	-3.550092	-2.266763
1	3.340790	-4.477503	-2.848885
1	2.372106	-3.561940	-1.687924
1	3.247900	-2.719845	-2.981762
1	4.620606	-4.347847	-0.756346
1	5.434027	-3.365708	-1.965761
8	3.373189	-2.362439	0.492314
6	5.778076	-2.224305	0.424099
6	4.285801	-0.920165	-1.103979
1	4.355074	-0.087448	-0.391591
1	5.032962	-0.772126	-1.893826
1	3.288104	-0.889271	-1.561557
1	5.748753	-1.418340	1.167318
1	5.918964	-3.177040	0.952818
1	6.652072	-2.067438	-0.219406
1	3.487075	-3.141167	1.053833

First P-H-activation-product (Pd-Ag)

Number of imaginary frequencies : 0
The smallest frequency is : 24.1020 cm(-1)

Electronic energy : =-2541.4708114
Zero-point correction= 0.645597
Thermal correction to Energy= 0.696594
Thermal correction to Enthalpy= 0.697539
Thermal correction to Gibbs Free Energy= 0.559563
Sum of electronic and zero-point Energies= -2540.825215
Sum of electronic and thermal Energies= -2540.774217
Sum of electronic and thermal Enthalpies= -2540.773273
Sum of electronic and thermal Free Energies= -2540.911248

Cartesian Coordinates

46	-0.254938	1.671379	-0.418796
15	2.319349	2.008199	1.337747
8	3.605143	2.478922	0.522515
6	3.432055	2.802784	-0.870438
8	-1.155360	2.020381	1.358620
6	-1.082712	3.243903	1.788195
8	-0.365335	4.122644	1.310002
8	1.527392	0.976459	0.557541
6	-1.986180	3.495986	2.970655
8	2.903338	1.501089	2.708854
6	3.840101	0.404782	2.743949
1	-1.774643	4.472412	3.413059
1	-3.030062	3.470088	2.637370
1	-1.864567	2.710443	3.723493
1	1.557710	3.122244	1.687344
1	4.396708	3.166728	-1.227143
1	3.131558	1.914433	-1.437123
1	2.677057	3.589116	-0.995206
1	3.822449	0.016075	3.762825
1	3.551359	-0.394394	2.050398
1	4.841031	0.778381	2.505521
8	-1.846210	2.525785	-1.343992
8	-2.615655	0.622293	-2.292536
6	-2.610099	1.854120	-2.124921
6	-3.570677	2.703150	-2.919579
1	-3.712192	3.688587	-2.470551
1	-3.158816	2.837139	-3.926566
1	-4.530124	2.187810	-3.016055
47	-1.626128	-0.914827	-0.849645
8	0.589820	1.284325	-2.257922
6	0.872803	0.072394	-2.539925
6	1.581822	-0.127219	-3.853568
1	2.665711	-0.104800	-3.677107
1	1.327850	-1.102265	-4.277491
1	1.340688	0.669701	-4.561083
8	0.636095	-0.919876	-1.809993
6	-4.277368	-1.453668	1.757566
6	-4.324903	-2.352128	0.516232
6	-3.534015	-0.134547	1.629076
1	-3.626248	0.453176	2.550717
1	-2.455832	-0.277660	1.472539
1	-3.912632	0.493092	0.810903
1	-3.832261	-2.037476	2.579435
1	-5.319583	-1.266392	2.056454
8	-3.007650	-2.637509	0.019589
6	-4.982303	-3.675433	0.883098
6	-5.067429	-1.697192	-0.633967
1	-5.100097	-2.375612	-1.495410
1	-6.098356	-1.458259	-0.345428
1	-4.571962	-0.772916	-0.956048
1	-5.020195	-4.337911	0.010282
1	-4.414818	-4.183043	1.674665
1	-6.006579	-3.521122	1.245627
1	-2.350360	-2.747691	0.744958
11	1.355055	-1.367797	0.404395
8	0.928272	-1.756467	2.667580
6	-0.217989	-2.169542	2.398660
8	-0.668196	-2.306097	1.206984
6	-1.163529	-2.517507	3.528222
1	-1.825745	-1.660336	3.709124
1	-1.794350	-3.375616	3.269056
1	-0.617494	-2.724170	4.452638
6	4.621969	-3.276936	-1.344764
6	4.572042	-2.086658	-0.384808
6	3.368198	-3.507298	-2.168912
1	3.458872	-4.424016	-2.761951
1	2.480901	-3.614579	-1.532780
1	3.178928	-2.684263	-2.869085
1	4.843115	-4.175047	-0.745818

1	5.488381	-3.137627	-2.008104
8	3.499387	-2.266879	0.560581
6	5.885520	-1.978040	0.371156
6	4.245801	-0.780857	-1.086312
1	4.301934	0.055045	-0.375655
1	4.954479	-0.589014	-1.901500
1	3.232779	-0.806271	-1.510046
1	5.847082	-1.162165	1.103019
1	6.108061	-2.911142	0.906393
1	6.715922	-1.782292	-0.317717
1	3.686685	-3.043302	1.105161

Second P-H-activation-PRC (Pd-Ag)

Number of imaginary frequencies : 0
The smallest frequencies are : 21.4545 29.1673 29.3059 cm(-1)

Electronic energy : HF=-2916.0161917
Zero-point correction= 0.578442 (Hartree/Particle)
Thermal correction to Energy= 0.631975
Thermal correction to Enthalpy= 0.632919
Thermal correction to Gibbs Free Energy= 0.485821
Sum of electronic and zero-point Energies= -2915.437750
Sum of electronic and thermal Energies= -2915.384217
Sum of electronic and thermal Enthalpies= -2915.383273
Sum of electronic and thermal Free Energies= -2915.530371

Cartesian Coordinates

46	0.296633	1.127158	0.423945
15	-2.607024	2.309815	-0.196015
8	-3.508893	2.508153	1.106219
6	-2.895330	2.234998	2.378875
8	0.773335	2.092786	-1.327227
6	0.822610	3.386502	-1.232733
8	0.481983	4.038327	-0.245612
8	-1.873044	0.994796	-0.170104
6	1.376358	4.054638	-2.468359
8	-3.625897	2.511065	-1.384591
6	-4.735085	1.605308	-1.541393
1	0.958766	5.058947	-2.578677
1	2.462843	4.153348	-2.349722
1	1.187477	3.464807	-3.370152
1	-1.757812	3.408626	-0.322350
1	-3.642313	2.462781	3.140886
1	-2.593907	1.183556	2.448226
1	-2.015904	2.874450	2.529651
1	-5.125316	1.766078	-2.547606
1	-4.413752	0.561077	-1.438456
1	-5.509266	1.843973	-0.804597
47	1.570124	-1.545286	-0.412371
8	-0.125336	0.166409	2.227263
6	-0.483907	-1.058440	2.146938
6	-0.892033	-1.688887	3.453817
1	-1.975513	-1.563030	3.582062
1	-0.677504	-2.760907	3.442035
1	-0.395152	-1.211320	4.301787
8	-0.549737	-1.726514	1.092006
11	-1.829975	-1.243325	-0.879357
8	-1.409825	-0.587885	-3.153589
6	-0.233680	-0.941564	-2.945939
8	0.077543	-1.836965	-2.076978
6	0.888783	-0.270759	-3.703292
1	1.088249	0.689151	-3.205982
1	1.804038	-0.872387	-3.697270
1	0.587351	-0.055916	-4.733210
6	-4.624452	-3.523515	0.625407
6	-4.806490	-2.035641	0.315918
6	-3.187211	-4.015255	0.647039

1	-3.148027	-5.079025	0.906284
1	-2.711822	-3.910790	-0.337367
1	-2.565183	-3.477602	1.373149
1	-5.194895	-4.095498	-0.124080
1	-5.110486	-3.725081	1.591238
8	-4.117586	-1.707964	-0.909910
6	-6.281832	-1.714059	0.151542
6	-4.182032	-1.141891	1.372960
1	-4.348995	-0.083490	1.131340
1	-4.628436	-1.345404	2.353969
1	-3.099397	-1.303829	1.452443
1	-6.424360	-0.654375	-0.092669
1	-6.726210	-2.316556	-0.652046
1	-6.832586	-1.931563	1.074666
1	-4.501070	-2.232235	-1.626678
15	2.429670	1.104055	1.060077
8	3.425511	1.962440	0.117081
6	3.837026	1.395676	-1.126535
8	2.953040	-0.324548	1.190863
8	2.533579	1.932924	2.427223
6	3.805617	2.023602	3.082286
1	4.543427	2.096868	-1.577475
1	4.343237	0.433637	-0.974858
1	2.977576	1.267510	-1.796206
1	3.625229	2.482676	4.056321
1	4.243222	1.029509	3.228113
1	4.493144	2.650881	2.505152
8	5.086634	-1.743208	0.529751
6	4.725987	-2.723138	-0.276470
8	3.572301	-2.922124	-0.637928
6	5.876796	-3.571003	-0.706314
1	6.361642	-4.008421	0.172599
1	5.538999	-4.362393	-1.376494
1	6.623798	-2.948658	-1.210262
1	4.292409	-1.202642	0.799992

Second P-H-activation-TS (Pd-Ag)

Number of imaginary frequencies : 1
 The smallest frequencies are : -645.7178 18.7028 21.5089 cm(-1)

Electronic energy : HF=-2915.9959669
 Zero-point correction= 0.575164 (Hartree/Particle)
 Thermal correction to Energy= 0.628000
 Thermal correction to Enthalpy= 0.628944
 Thermal correction to Gibbs Free Energy= 0.483373
 Sum of electronic and zero-point Energies= -2915.420803
 Sum of electronic and thermal Energies= -2915.367967
 Sum of electronic and thermal Enthalpies= -2915.367023
 Sum of electronic and thermal Free Energies= -2915.512594

 Cartesian Coordinates

46	0.265373	1.105235	0.472499
15	-2.428925	2.417801	-0.111273
8	-3.459863	2.541966	1.157006
6	-2.913595	2.220101	2.431532
8	0.808996	2.212754	-1.227827
6	0.672195	3.465110	-1.318659
8	-0.173469	4.158287	-0.668307
8	-1.862878	0.980257	-0.076561
6	1.592976	4.185381	-2.250989
8	-3.476659	2.586849	-1.326307
6	-4.550454	1.658581	-1.484461
1	1.096649	5.047677	-2.702164
1	2.447033	4.551362	-1.667221
1	1.971445	3.508993	-3.022150
1	-1.150766	3.508319	-0.317213
1	-3.670901	2.458742	3.182789
1	-2.653049	1.155316	2.498147

1	-2.010880	2.812745	2.644577
1	-4.966139	1.814850	-2.483226
1	-4.204521	0.619172	-1.404283
1	-5.330666	1.847401	-0.737089
47	1.585741	-1.576279	-0.428171
8	-0.121073	0.108648	2.232419
6	-0.485124	-1.116449	2.116445
6	-0.923814	-1.758920	3.406517
1	-2.004271	-1.603908	3.526194
1	-0.737061	-2.835420	3.375849
1	-0.423578	-1.310036	4.268075
8	-0.522567	-1.761219	1.050175
11	-1.831998	-1.141129	-0.930900
8	-1.318305	-0.471851	-3.208525
6	-0.164079	-0.867605	-2.965156
8	0.089344	-1.780128	-2.095930
6	1.005132	-0.229551	-3.682799
1	1.209494	0.735324	-3.197610
1	1.906429	-0.850144	-3.633263
1	0.750356	-0.022793	-4.726873
6	-4.881751	-3.562782	0.497752
6	-4.848889	-2.065196	0.186043
6	-3.527885	-4.208686	0.732533
1	-3.632837	-5.290954	0.866994
1	-2.854350	-4.047897	-0.118754
1	-3.033675	-3.816226	1.629594
1	-5.391178	-4.064991	-0.340764
1	-5.529221	-3.710844	1.374639
8	-4.057994	-1.837273	-0.998696
6	-6.259615	-1.555760	-0.056974
6	-4.164609	-1.260231	1.275608
1	-4.176958	-0.189525	1.031999
1	-4.672203	-1.407361	2.237069
1	-3.116983	-1.567956	1.392209
1	-6.248741	-0.491895	-0.322407
1	-6.740593	-2.110695	-0.874003
1	-6.878173	-1.680097	0.840112
1	-4.466217	-2.309850	-1.736491
15	2.407178	1.046307	1.124740
8	3.385961	1.930421	0.184985
6	3.819206	1.364134	-1.051934
8	2.935400	-0.380935	1.224168
8	2.517150	1.851909	2.504852
6	3.763155	1.825072	3.215932
1	4.419958	2.123747	-1.557921
1	4.440887	0.476412	-0.880121
1	2.964709	1.102493	-1.689210
1	3.630167	2.447111	4.103000
1	4.011949	0.803399	3.522348
1	4.571882	2.236841	2.601994
8	5.101497	-1.762600	0.558152
6	4.782177	-2.663866	-0.351333
8	3.651045	-2.813561	-0.797499
6	5.949684	-3.485057	-0.786734
1	6.402172	-3.975495	0.081214
1	5.639106	-4.232421	-1.517801
1	6.713520	-2.832944	-1.223426
1	4.297496	-1.237251	0.825355

Second P-H-activation-product (Pd-Ag)

Number of imaginary frequencies : 0

The smallest frequencies are : 23.6908 25.5248 30.6946 cm(-1)

Electronic energy : HF=-2916.0009792

Zero-point correction= 0.579338 (Hartree/Particle)

Thermal correction to Energy= 0.632602

Thermal correction to Enthalpy= 0.633546

Thermal correction to Gibbs Free Energy= 0.487629

Sum of electronic and zero-point Energies= -2915.421641

Sum of electronic and thermal Energies= -2915.368378
 Sum of electronic and thermal Enthalpies= -2915.367433
 Sum of electronic and thermal Free Energies= -2915.513350

 Cartesian Coordinates

46	0.237553	1.127342	0.442720
15	-2.410842	2.513423	-0.021431
8	-3.545227	2.440598	1.196874
6	-3.019504	2.137453	2.474006
8	0.828089	2.136996	-1.344332
6	0.867311	3.365412	-1.504188
8	0.155758	4.219738	-0.818961
8	-1.856970	1.046629	-0.097532
6	1.773689	3.979634	-2.508075
8	-3.459501	2.696664	-1.265282
6	-4.479287	1.731882	-1.491866
1	1.244848	4.742982	-3.085037
1	2.592789	4.477026	-1.974243
1	2.187435	3.215307	-3.168365
1	-0.588206	3.761767	-0.323089
1	-3.808967	2.303438	3.213777
1	-2.677566	1.094377	2.538768
1	-2.165590	2.787182	2.730308
1	-4.898270	1.923830	-2.484432
1	-4.086812	0.705628	-1.471802
1	-5.277691	1.828194	-0.744729
47	1.551628	-1.612211	-0.344748
8	-0.175716	0.197505	2.227252
6	-0.554985	-1.026458	2.131979
6	-1.037492	-1.626651	3.426375
1	-2.122104	-1.471885	3.500431
1	-0.847880	-2.703124	3.436279
1	-0.570139	-1.148893	4.290754
8	-0.572567	-1.698041	1.082997
11	-1.851786	-1.064627	-0.960275
8	-1.205831	-0.511446	-3.247018
6	-0.091583	-0.977195	-2.948406
8	0.072644	-1.859341	-2.028458
6	1.141338	-0.465186	-3.662639
1	1.405115	0.508006	-3.225671
1	1.992800	-1.145651	-3.551848
1	0.931267	-0.298862	-4.723779
6	-4.916938	-3.522126	0.444450
6	-4.867135	-2.032399	0.098143
6	-3.572361	-4.166098	0.733282
1	-3.683451	-5.245348	0.886173
1	-2.873682	-4.021578	-0.100371
1	-3.103289	-3.755760	1.636062
1	-5.403815	-4.042545	-0.396518
1	-5.590340	-3.646925	1.305341
8	-4.043910	-1.839115	-1.070310
6	-6.266495	-1.518993	-0.195855
6	-4.207082	-1.207872	1.187990
1	-4.201308	-0.141277	0.925838
1	-4.741738	-1.332546	2.138223
1	-3.166475	-1.523835	1.339250
1	-6.236388	-0.463761	-0.492759
1	-6.731623	-2.093425	-1.008652
1	-6.909331	-1.610338	0.688083
1	-4.432892	-2.331992	-1.804896
15	2.375102	1.044731	1.132512
8	3.373895	1.875635	0.158381
6	3.873059	1.216433	-1.004431
8	2.886817	-0.381797	1.301053
8	2.484180	1.911630	2.475699
6	3.720029	1.890024	3.204552
1	4.388356	1.969551	-1.605435
1	4.589305	0.432352	-0.730739
1	3.062661	0.776491	-1.602818

1	3.598791	2.574462	4.046123
1	3.928829	0.883176	3.581499
1	4.550359	2.231707	2.576379
8	5.049824	-1.804409	0.709750
6	4.770318	-2.649099	-0.265089
8	3.666788	-2.747951	-0.787746
6	5.943139	-3.481966	-0.662362
1	6.243930	-4.110834	0.182588
1	5.692346	-4.111745	-1.516776
1	6.794629	-2.838079	-0.904258
1	4.243547	-1.269415	0.949062

Third P-H-activation-PRC (Pd-Ag)

Number of imaginary frequencies : 0
 The smallest frequencies are : 27.5040 34.4699 40.0990 cm(-1)

Electronic energy : HF=-2899.7283894
 Zero-point correction= 0.465173 (Hartree/Particle)
 Thermal correction to Energy= 0.510218
 Thermal correction to Enthalpy= 0.511162
 Thermal correction to Gibbs Free Energy= 0.385249
 Sum of electronic and zero-point Energies= -2899.263216
 Sum of electronic and thermal Energies= -2899.218171
 Sum of electronic and thermal Enthalpies= -2899.217227
 Sum of electronic and thermal Free Energies= -2899.343140

 Cartesian Coordinates

46	1.337762	0.094194	-0.554516
15	-0.763674	-2.167572	-0.924384
8	-1.128710	-3.526129	-1.669447
6	-0.119846	-4.546852	-1.742572
15	2.785739	-1.183550	0.603093
8	2.744110	-2.730878	0.145899
6	3.169577	-3.102893	-1.166577
47	-1.798242	0.909492	0.846643
8	0.498434	-1.572424	-1.526834
8	4.162152	-0.629723	-0.139404
6	5.409593	-0.918690	0.519074
8	2.847273	-1.057111	2.077543
15	-0.858758	2.238365	-0.936017
8	0.202395	1.531375	-1.789393
8	-2.065634	-1.288301	-1.116984
6	-2.364814	-0.680133	-2.388964
8	-1.960996	2.723932	-2.045753
6	-3.115796	3.371384	-1.538938
8	-0.247198	3.692640	-0.450497
6	-0.363158	4.033311	0.922906
1	0.036893	5.044844	1.043420
1	-1.409882	4.037650	1.260491
1	0.211937	3.347003	1.560932
1	-3.833880	3.460057	-2.358663
1	-3.583513	2.788807	-0.727843
1	-2.881801	4.377649	-1.164811
1	-0.612393	-5.448009	-2.111026
1	0.671830	-4.249448	-2.437450
1	0.303177	-4.751196	-0.750936
1	-3.246069	-0.056062	-2.221435
1	-1.525657	-0.056999	-2.716748
1	-2.589951	-1.453800	-3.130374
1	2.864049	-4.141694	-1.314750
1	2.701789	-2.478738	-1.935675
1	4.260142	-3.037202	-1.252943
1	6.205589	-0.636278	-0.173377
1	5.497718	-0.344447	1.446573
1	5.489229	-1.988183	0.745230
8	-1.821526	-0.513791	2.567042
6	-0.676708	-1.080097	2.823780
8	-0.350299	-2.191548	2.399427

1	-0.716182	-2.368488	0.469181
6	0.238842	-0.282602	3.720220
1	1.176908	-0.812159	3.890847
1	0.462442	0.684323	3.250062
1	-0.268982	-0.068602	4.667739
8	-4.145727	0.026853	0.561144
8	2.130952	1.827037	0.386682
6	3.041355	2.511594	-0.104368
8	4.029993	2.010433	-0.797545
6	-4.288664	-1.192298	0.598250
8	-3.595362	-1.994119	1.374730
6	3.053076	3.984680	0.062108
1	3.977958	4.428873	-0.307602
1	2.191767	4.381180	-0.490281
1	2.906376	4.231440	1.117960
6	-5.275377	-1.921430	-0.258207
1	-4.730586	-2.577100	-0.948164
1	-5.914866	-2.562329	0.357025
1	-5.886058	-1.217600	-0.826673
1	4.017934	1.020033	-0.742889
1	-2.892522	-1.463068	1.884151

Third P-H-activation-TS (Pd-Ag)

Number of imaginary frequencies : 1
The smallest frequencies are : -1080.9015 23.8940 30.7028 cm(-1)

Electronic energy : HF=-2899.7204788
Zero-point correction= 0.461131 (Hartree/Particle)
Thermal correction to Energy= 0.506317
Thermal correction to Enthalpy= 0.507262
Thermal correction to Gibbs Free Energy= 0.380758
Sum of electronic and zero-point Energies= -2899.259348
Sum of electronic and thermal Energies= -2899.214161
Sum of electronic and thermal Enthalpies= -2899.213217
Sum of electronic and thermal Free Energies= -2899.339721

Cartesian Coordinates

46	1.300251	0.233760	-0.627660
15	-0.790521	-1.953513	-1.155023
8	-1.210602	-3.141312	-2.175418
6	-0.244950	-4.170027	-2.388466
15	2.553811	-1.225635	0.519606
8	2.504486	-2.724433	-0.076912
6	3.006030	-2.977485	-1.391156
47	-1.488690	0.750621	0.934407
8	0.430207	-1.252826	-1.797965
8	4.043835	-0.696901	0.020326
6	5.180111	-1.169713	0.765576
8	2.417857	-1.231039	1.998128
15	-0.770257	2.412711	-0.693118
8	0.275761	1.897056	-1.690819
8	-2.104983	-1.023330	-1.245658
6	-2.387208	-0.274328	-2.435277
8	-1.975466	2.965333	-1.653837
6	-3.134025	3.448708	-0.992955
8	-0.224593	3.831258	-0.048695
6	-0.227297	3.960724	1.364939
1	0.161793	4.956184	1.600816
1	-1.241774	3.880724	1.782408
1	0.414613	3.207942	1.843474
1	-3.888186	3.653605	-1.757834
1	-3.540960	2.701660	-0.292775
1	-2.927596	4.379733	-0.446838
1	-0.755137	-4.996747	-2.888140
1	0.571715	-3.811747	-3.025851
1	0.165740	-4.537566	-1.436668
1	-3.224786	0.387101	-2.195729
1	-1.520867	0.331177	-2.724778

1	-2.668667	-0.949920	-3.250750
1	2.671898	-3.980215	-1.669587
1	2.613959	-2.255770	-2.116379
1	4.101826	-2.952126	-1.399366
1	6.071534	-0.868179	0.211033
1	5.194622	-0.728048	1.766782
1	5.160220	-2.262335	0.850745
8	-1.478688	-0.963001	2.438829
6	-0.696087	-1.959332	2.559309
8	-0.442563	-2.781572	1.634502
1	-0.677340	-2.392692	0.378655
6	-0.033790	-2.195520	3.881400
1	-0.016487	-3.264190	4.113854
1	1.005933	-1.862510	3.777633
1	-0.521676	-1.635267	4.681923
8	-3.981655	0.289719	0.799452
8	2.178653	1.826868	0.506739
6	3.120040	2.495252	0.055271
8	4.122281	1.970405	-0.602343
6	-4.317371	-0.874172	0.623374
8	-3.722104	-1.897108	1.213570
6	3.162828	3.966196	0.235522
1	4.063177	4.404932	-0.196271
1	2.263231	4.381492	-0.235787
1	3.107020	4.198799	1.304064
6	-5.430895	-1.293724	-0.277182
1	-5.011126	-1.859627	-1.117336
1	-6.120123	-1.960676	0.249888
1	-5.965539	-0.420604	-0.654601
1	4.070602	0.981480	-0.550912
1	-2.939929	-1.554609	1.720269

Third P-H-activation-product (Pd-Ag)

Number of imaginary frequencies : 0

The smallest frequencies are : 27.0514 33.7208 40.2143 cm(-1)

Electronic energy : HF=-2899.7318553
 Zero-point correction= 0.465450 (Hartree/Particle)
 Thermal correction to Energy= 0.511363
 Thermal correction to Enthalpy= 0.512307
 Thermal correction to Gibbs Free Energy= 0.384003
 Sum of electronic and zero-point Energies= -2899.266405
 Sum of electronic and thermal Energies= -2899.220492
 Sum of electronic and thermal Enthalpies= -2899.219548
 Sum of electronic and thermal Free Energies= -2899.347853

Cartesian Coordinates

46	1.292270	0.255711	-0.658688
15	-0.778889	-1.954147	-1.178671
8	-1.259081	-2.932007	-2.425285
6	-0.323103	-3.919476	-2.816921
15	2.476597	-1.291790	0.439695
8	2.490092	-2.748723	-0.260076
6	2.972334	-2.873951	-1.599235
47	-1.550511	0.748610	0.824491
8	0.379643	-1.128155	-1.866354
8	4.002439	-0.735740	0.096185
6	5.085564	-1.315154	0.842096
8	2.239686	-1.424752	1.902208
15	-0.724395	2.494077	-0.675037
8	0.336929	1.999527	-1.663333
8	-2.117844	-0.981486	-1.173704
6	-2.461511	-0.211212	-2.326331
8	-1.886738	3.133892	-1.638387
6	-3.024942	3.660927	-0.980706
8	-0.161150	3.864625	0.057678
6	-0.220815	3.929999	1.473126
1	0.184101	4.902157	1.771756

1	-1.253713	3.860287	1.845566
1	0.380317	3.138411	1.942272
1	-3.791224	3.847322	-1.738290
1	-3.433042	2.950681	-0.241951
1	-2.794073	4.606624	-0.471079
1	-0.854006	-4.674100	-3.405289
1	0.477607	-3.490901	-3.434171
1	0.131358	-4.421562	-1.947238
1	-3.265773	0.470313	-2.027702
1	-1.603969	0.374528	-2.678416
1	-2.818096	-0.863444	-3.131934
1	2.755616	-3.896384	-1.918997
1	2.462312	-2.171086	-2.267986
1	4.055900	-2.711171	-1.640029
1	6.012216	-0.926335	0.414198
1	5.018323	-1.037348	1.898677
1	5.076590	-2.407559	0.751252
8	-1.248712	-1.044787	2.420231
6	-0.570132	-2.045666	2.689012
8	-0.362465	-3.015416	1.834370
1	-0.599197	-2.725759	0.906594
6	0.057661	-2.267078	4.015720
1	-0.039718	-3.312597	4.320791
1	1.125393	-2.050411	3.892483
1	-0.372532	-1.600756	4.764692
8	-3.949045	0.178691	0.981246
8	2.163094	1.789030	0.575572
6	3.137130	2.457078	0.202316
8	4.166348	1.939400	-0.419258
6	-4.274397	-0.980479	0.762834
8	-3.640874	-2.015674	1.297145
6	3.195998	3.919433	0.442701
1	4.118150	4.359811	0.061452
1	2.320202	4.369327	-0.040853
1	3.107478	4.109588	1.517547
6	-5.405958	-1.384430	-0.117033
1	-4.997108	-1.889424	-1.000278
1	-6.056017	-2.100638	0.394642
1	-5.977025	-0.508511	-0.428118
1	4.094293	0.950121	-0.404558
1	-2.859977	-1.667997	1.782356

P-H-activation-product (Pd-Ag) (after 3 successive P-H activations)

Number of imaginary frequencies : 0
The smallest frequency is : 21.6202 cm(-1)

Electronic energy : =-2899.7866359
Zero-point correction= 0.469535
Thermal correction to Energy= 0.514048
Thermal correction to Enthalpy= 0.514992
Thermal correction to Gibbs Free Energy= 0.389058
Sum of electronic and zero-point Energies= -2899.317101
Sum of electronic and thermal Energies= -2899.272588
Sum of electronic and thermal Enthalpies= -2899.271643
Sum of electronic and thermal Free Energies= -2899.397577

Cartesian Coordinates

46	-1.382548	0.383234	0.249840
15	-0.519501	-1.115892	1.719852
8	-0.900099	-0.639874	3.222231
6	-0.082157	0.320399	3.895674
15	-2.522469	-1.276619	-0.826049
8	-3.698803	-1.957013	0.065754
6	-4.469611	-1.114465	0.906042
47	2.116017	0.213827	0.024408
8	0.968767	-1.323573	1.572505

8	-3.434322	-0.387632	-1.893275
6	-4.284369	-1.107017	-2.796592
8	-1.834065	-2.377185	-1.586260
15	1.026681	2.261679	0.777109
8	-0.401704	2.010115	1.297511
8	-1.339017	-2.501201	1.664850
6	-0.814413	-3.615824	2.390276
8	1.735131	3.014316	2.046341
6	3.106684	3.339371	1.903025
8	1.027739	3.518441	-0.285016
6	1.115348	3.221891	-1.668506
1	1.397085	4.143094	-2.187497
1	1.888520	2.461701	-1.869766
1	0.156534	2.861302	-2.060756
1	3.464971	3.701848	2.870358
1	3.703315	2.456947	1.618934
1	3.257669	4.123840	1.150142
1	-0.345533	0.268362	4.955459
1	0.981218	0.079281	3.777013
1	-0.270992	1.326633	3.508183
1	-1.515436	-4.440674	2.245992
1	0.170296	-3.904340	2.006366
1	-0.741843	-3.385019	3.459708
1	-5.076282	-1.756785	1.549075
1	-3.830590	-0.484176	1.543617
1	-5.139547	-0.467282	0.321163
1	-4.815901	-0.362605	-3.394759
1	-3.685871	-1.745197	-3.453503
1	-5.009245	-1.720514	-2.248850
8	1.492408	-1.793594	-1.546602
6	1.426767	-2.868529	-0.930650
8	0.315820	-3.518452	-0.753747
1	-0.491697	-3.019210	-1.115427
6	2.619033	-3.531781	-0.324368
1	2.437536	-4.594685	-0.152229
1	3.500626	-3.399425	-0.957334
1	2.813917	-3.050505	0.641800
8	4.322325	-0.488505	-0.520615
8	-1.848520	2.089100	-1.150931
6	-2.884371	2.722031	-1.343052
8	-4.072984	2.158158	-1.388547
6	4.702484	-0.772437	-1.653034
8	3.901953	-1.241318	-2.589412
6	-2.894397	4.190897	-1.578400
1	-3.018721	4.377787	-2.651362
1	-3.740845	4.655223	-1.064660
1	-1.954742	4.632101	-1.241211
6	6.113406	-0.618749	-2.107585
1	6.488124	-1.572973	-2.491230
1	6.151587	0.098488	-2.934766
1	6.742598	-0.269223	-1.288224
1	-3.937997	1.175664	-1.424722
1	2.991547	-1.394787	-2.210295

C-H-activation-PRC (Pd-Ag)

Number of imaginary frequencies : 0

The smallest frequency is : 13.8823 cm(-1)

Electronic energy :	=-2920.8203201
Zero-point correction=	0.509739
Thermal correction to Energy=	0.554490
Thermal correction to Enthalpy=	0.555435
Thermal correction to Gibbs Free Energy=	0.429089
Sum of electronic and zero-point Energies=	-2920.310581
Sum of electronic and thermal Energies=	-2920.265830
Sum of electronic and thermal Enthalpies=	-2920.264886
Sum of electronic and thermal Free Energies=	-2920.391232

Cartesian Coordinates

6	3.220844	-1.223369	1.202638
6	3.757955	-0.742282	0.001293
6	4.903005	0.059792	0.034443
6	5.495905	0.389243	1.248891
6	4.957956	-0.090291	2.440594
6	3.825387	-0.900783	2.413837
6	3.121463	-1.064746	-1.291189
6	3.884682	-1.443746	-2.398102
6	3.254971	-1.720684	-3.601965
6	1.870371	-1.618501	-3.680710
6	1.177920	-1.232849	-2.544202
7	1.782751	-0.964976	-1.380834
46	0.523428	-0.080250	0.212136
15	-0.914849	0.900532	1.741355
8	-1.072866	-0.123501	2.992262
6	0.087075	-0.667412	3.613501
15	0.722219	1.991400	-0.699595
8	1.360171	3.114026	0.293507
6	2.501873	2.758110	1.058376
47	-2.480487	-0.603307	-0.515273
8	-2.292012	1.209065	1.211740
8	1.884782	1.847330	-1.836745
6	2.209672	3.019037	-2.583121
8	-0.526464	2.591955	-1.288847
15	-1.364102	-2.530631	0.484955
8	0.103113	-2.199540	0.806577
8	-0.261283	2.190950	2.485830
6	-0.848591	3.477389	2.312110
8	-2.021062	-3.073512	1.875847
6	-3.425478	-2.935972	2.015065
8	-1.413253	-3.953022	-0.339798
6	-1.011222	-3.903926	-1.694836
1	2.345397	-1.872537	1.180332
1	3.413625	-1.293040	3.341692
1	5.425798	0.161493	3.389787
1	6.379009	1.024128	1.264351
1	5.312642	0.449900	-0.896461
1	4.962838	-1.535614	-2.296224
1	3.838438	-2.018488	-4.469682
1	1.333654	-1.823215	-4.602067
1	0.094658	-1.109026	-2.559718
1	-1.228845	-4.877215	-2.143378
1	-1.568511	-3.133632	-2.254891
1	0.065659	-3.704241	-1.791575
1	-3.703956	-3.371524	2.978306
1	-3.725973	-1.877385	2.011205
1	-3.970757	-3.467528	1.222202
1	-0.234715	-1.102955	4.563479
1	0.517950	-1.455599	2.984197
1	0.835750	0.108900	3.821924
1	-0.136032	4.207202	2.706777
1	-1.033245	3.701232	1.255424
1	-1.789710	3.555270	2.868501
1	2.712753	3.590660	1.735637
1	2.312627	1.856864	1.659494
1	3.376893	2.588920	0.415548
1	2.949034	2.727162	-3.333478
1	1.324789	3.424455	-3.087522
1	2.640490	3.794313	-1.936810
8	-3.655801	0.877642	-1.752467
6	-3.946261	2.051920	-1.506884
8	-3.092757	2.975494	-1.170028
1	-2.143613	2.649286	-1.121010
6	-5.355279	2.543324	-1.573542
1	-5.399983	3.546859	-2.004503
1	-5.975378	1.850871	-2.145277
1	-5.748405	2.606096	-0.551790

C-H-activation-TS (Pd-Ag)

Number of imaginary frequencies : 1
The smallest frequency is : -1527.0759 cm(-1)

Electronic energy : =-2920.7851846
Zero-point correction= 0.502991
Thermal correction to Energy= 0.547576
Thermal correction to Enthalpy= 0.548520
Thermal correction to Gibbs Free Energy= 0.423178
Sum of electronic and zero-point Energies= -2920.282194
Sum of electronic and thermal Energies= -2920.237609
Sum of electronic and thermal Enthalpies= -2920.236665
Sum of electronic and thermal Free Energies= -2920.362007

Cartesian Coordinates

6	2.025940	-0.227583	-1.645933
6	3.357753	-0.462770	-1.223868
6	4.258743	-1.142854	-2.047554
6	3.854267	-1.569847	-3.308107
6	2.559293	-1.318904	-3.760375
6	1.658891	-0.665158	-2.927635
6	3.756922	0.048352	0.099744
6	5.077163	0.366117	0.421160
6	5.373927	0.869124	1.678993
6	4.344558	1.047536	2.594196
6	3.053458	0.712401	2.212247
7	2.760928	0.228565	0.999097
46	0.833514	-0.575126	0.219684
15	-0.794655	-1.812442	-0.830107
8	-0.095021	-2.817697	-1.908688
6	0.945896	-3.672684	-1.460458
15	-0.558656	-0.590181	2.077083
8	-0.617430	-1.943499	2.982252
6	0.557267	-2.740491	3.012280
47	-1.857633	1.146069	-0.469074
8	-1.897344	-1.082363	-1.553143
8	0.155875	0.475966	3.094566
6	-0.587132	0.944387	4.219266
8	-1.991168	-0.127798	1.859867
15	-0.095242	2.756669	-0.955820
8	1.335153	2.246200	-1.241502
8	-1.377610	-2.867195	0.268039
6	-2.425267	-3.739036	-0.159049
8	-0.405084	3.780287	-2.186648
6	-1.690156	4.379550	-2.211214
8	0.017132	3.869084	0.251834
6	0.105255	3.329891	1.559653
1	1.524772	0.985428	-1.334013
1	0.646656	-0.466036	-3.280457
1	2.258185	-1.639322	-4.755512
1	4.559299	-2.098566	-3.946279
1	5.270911	-1.357903	-1.708868
1	5.859533	0.241184	-0.321945
1	6.397914	1.127081	1.937448
1	4.528003	1.443578	3.588409
1	2.210278	0.826059	2.888855
1	0.041063	4.159259	2.270031
1	-0.720636	2.627604	1.760776
1	1.056256	2.799906	1.714804
1	-1.839360	4.803195	-3.208059
1	-2.485562	3.639455	-2.023161
1	-1.771343	5.180698	-1.465852
1	1.375351	-4.155524	-2.342342
1	1.740410	-3.109308	-0.947198
1	0.564626	-4.445429	-0.779576
1	-2.690992	-4.362143	0.698336

1	-3.306161	-3.168251	-0.473334
1	-2.093879	-4.382924	-0.983843
1	0.375764	-3.563739	3.708013
1	0.776569	-3.157392	2.019166
1	1.428421	-2.168501	3.363879
1	0.037774	1.681921	4.731137
1	-1.523958	1.417253	3.904339
1	-0.813727	0.122781	4.910213
8	-4.169226	0.705971	-0.387780
6	-4.624433	-0.401352	-0.112653
8	-4.161460	-1.176466	0.840688
1	-3.327615	-0.791818	1.247439
6	-5.763925	-1.007241	-0.863391
1	-6.362131	-1.664271	-0.227339
1	-6.385828	-0.228103	-1.308526
1	-5.342708	-1.612837	-1.676211

C-H-activation- product (Pd-Ag)

Number of imaginary frequencies : 0
The smallest frequency is : 25.7117 cm(-1)

Electronic energy : =-2920.809267
Zero-point correction= 0.511105
Thermal correction to Energy= 0.555384
Thermal correction to Enthalpy= 0.556329
Thermal correction to Gibbs Free Energy= 0.432496
Sum of electronic and zero-point Energies= -2920.298161
Sum of electronic and thermal Energies= -2920.253883
Sum of electronic and thermal Enthalpies= -2920.252938
Sum of electronic and thermal Free Energies= -2920.376771

Cartesian Coordinates

6	1.960550	0.049106	-1.689508
6	3.308686	0.248597	-1.296468
6	4.175729	1.026933	-2.073560
6	3.725651	1.629584	-3.240162
6	2.402776	1.458169	-3.634685
6	1.536734	0.675967	-2.868744
6	3.739024	-0.321010	-0.013513
6	5.070504	-0.408743	0.396834
6	5.375499	-0.957514	1.632555
6	4.345034	-1.415354	2.444700
6	3.043614	-1.309342	1.978988
7	2.743479	-0.774818	0.787155
46	0.812493	-0.897283	-0.232177
15	-0.942811	-1.239847	-1.660579
8	-0.476405	-1.650922	-3.173259
6	0.415302	-2.744583	-3.318345
15	-0.669191	-1.499688	1.560367
8	-1.157860	-3.055548	1.729425
6	-0.163947	-4.040434	1.516801
47	-1.553233	1.292465	0.074283
8	-1.942106	-0.113980	-1.829486
8	0.142988	-1.265900	2.979254
6	-0.581631	-1.386480	4.197661
8	-1.956463	-0.667999	1.642727
15	0.161835	2.954389	0.563430
8	1.631403	2.726524	-0.053240
8	-1.657667	-2.618655	-1.158055
6	-2.865467	-3.002887	-1.812410
8	-0.066651	4.496012	0.146277
6	-1.311412	5.080776	0.527860
8	0.449793	3.139728	2.148861
6	0.472272	1.938843	2.923401
1	1.646278	1.969441	-0.670518
1	0.509050	0.559726	-3.208351
1	2.036301	1.939608	-4.539534

1	4.401299	2.244632	-3.829999
1	5.202320	1.194705	-1.752954
1	5.864980	-0.063513	-0.258270
1	6.410921	-1.030127	1.956052
1	4.536650	-1.851322	3.420495
1	2.195908	-1.639635	2.574428
1	0.562657	2.232323	3.971948
1	-0.455876	1.365327	2.788518
1	1.328881	1.307641	2.651574
1	-1.420494	6.006793	-0.040279
1	-2.155661	4.416635	0.288505
1	-1.323933	5.308994	1.599702
1	0.923739	-2.634905	-4.280694
1	1.175925	-2.758393	-2.522367
1	-0.127413	-3.698972	-3.304404
1	-3.189521	-3.944201	-1.361112
1	-3.645573	-2.246810	-1.665348
1	-2.703333	-3.156873	-2.887545
1	-0.664856	-5.008589	1.426466
1	0.398698	-3.851929	0.588619
1	0.544756	-4.086977	2.357676
1	0.066734	-1.028430	5.003120
1	-1.496410	-0.781650	4.176194
1	-0.852291	-2.432472	4.393149
8	-3.952670	1.356144	0.092381
6	-4.572001	0.315599	-0.113942
8	-4.246888	-0.852936	0.390535
1	-3.381775	-0.801873	0.902558
6	-5.773523	0.256384	-0.999020
1	-6.510991	-0.457268	-0.622724
1	-6.216594	1.247678	-1.111366
1	-5.445113	-0.090889	-1.987052

reductive-elimination-PRC (Pd-Ag)

Electronic energy: -2691.8038354
 Zero-point correction= 0.445523
 Thermal correction to Energy= 0.484732
 Thermal correction to Enthalpy= 0.485676
 Thermal correction to Gibbs Free Energy= 0.370306
 Sum of electronic and zero-point Energies= -2691.358313
 Sum of electronic and thermal Energies= -2691.319104
 Sum of electronic and thermal Enthalpies= -2691.318160
 Sum of electronic and thermal Free Energies= -2691.433529

 Cartesian Coordinates

6	-4.341191	-0.065441	-2.545733
6	-3.495028	-0.290038	-1.451674
6	-2.543829	0.681819	-1.062176
6	-2.458953	1.844147	-1.833251
6	-3.297087	2.061169	-2.926283
6	-4.249981	1.109880	-3.277545
6	-3.533475	-1.547940	-0.698181
7	-2.516062	-1.734569	0.178942
6	-2.479594	-2.843023	0.930161
6	-3.438452	-3.839618	0.839950
6	-4.480133	-3.669952	-0.064449
6	-4.528360	-2.518934	-0.834465
46	-1.287700	0.039501	0.456740
47	1.763941	0.955721	-0.786867
15	3.448452	-0.700284	-1.283234
8	3.075254	-1.909716	-2.270565
6	3.967403	-3.023224	-2.411453
15	0.471490	-0.897576	1.818808
8	0.181924	-0.902411	3.420787
6	1.241804	-1.275902	4.294253
15	-0.508974	2.152337	0.811285

8	0.552241	2.681741	-0.166293
8	0.517426	-2.551955	1.618230
6	0.845697	-3.009662	0.320324
8	1.898566	-0.409401	1.534052
8	-1.719480	3.240331	0.862849
6	-1.606349	4.551017	0.321608
8	0.058187	2.219932	2.336928
6	0.459213	3.490741	2.838782
8	3.849466	-1.351878	0.122229
8	4.887550	-0.264577	-1.891895
6	5.555249	0.795543	-1.212211
1	-1.716470	2.603879	-1.597872
1	-3.201364	2.977835	-3.506259
1	-4.907965	1.274693	-4.127816
1	-5.066232	-0.819681	-2.847189
1	-5.348573	-2.363209	-1.528563
1	-5.255944	-4.425233	-0.164739
1	-3.363482	-4.721837	1.468165
1	-1.635876	-2.929300	1.611615
1	-0.413869	4.083451	3.139377
1	1.047189	4.051002	2.100322
1	1.083589	3.312164	3.718129
1	-1.540863	5.285081	1.134398
1	-2.506384	4.758321	-0.267656
1	-0.724593	4.649932	-0.320609
1	0.826853	-1.328000	5.304561
1	1.654243	-2.257776	4.030267
1	2.046609	-0.531690	4.275185
1	0.467010	-4.031818	0.210999
1	0.383684	-2.391514	-0.467950
1	1.932754	-3.020141	0.161115
1	3.150262	-1.091602	0.802143
1	6.363806	1.142446	-1.859133
1	4.872718	1.638203	-1.020134
1	5.973167	0.449579	-0.259946
1	3.397789	-3.828128	-2.880820
1	4.814508	-2.755808	-3.051072
1	4.333618	-3.362024	-1.435820

reductive-elimination-TS (Pd-Ag)

Number of imaginary frequencies : 1
The smallest frequency is : -88.9079 cm(-1)

Electronic energy : -2691.7729306
Zero-point correction= 0.442930
Thermal correction to Energy= 0.482256
Thermal correction to Enthalpy= 0.483200
Thermal correction to Gibbs Free Energy= 0.367175
Sum of electronic and zero-point Energies= -2691.330000
Sum of electronic and thermal Energies= -2691.290675
Sum of electronic and thermal Enthalpies= -2691.289731
Sum of electronic and thermal Free Energies= -2691.405755

Cartesian Coordinates

6	4.155117	-1.685450	-1.975598
6	3.384891	-0.882675	-1.132524
6	2.047492	-1.252089	-0.863968
6	1.519347	-2.405594	-1.445488
6	2.295548	-3.186220	-2.303292
6	3.613936	-2.828994	-2.559442
6	3.927881	0.363975	-0.561665
7	3.045195	1.369603	-0.414944
6	3.449796	2.518728	0.128178
6	4.761247	2.737459	0.532840
6	5.680174	1.705475	0.374603
6	5.261805	0.500031	-0.173477
46	0.785304	0.400005	-0.506224

47	-1.606989	-0.914475	0.168655
15	-4.014034	-0.585697	-0.083796
8	-4.602811	-0.797524	-1.567305
6	-5.923190	-0.342008	-1.882921
15	-0.830178	2.112860	-0.141808
8	0.031453	3.422871	0.337623
6	-0.678120	4.620846	0.630390
15	1.194587	-1.093928	1.218006
8	0.105506	-2.146963	1.314009
8	-1.293709	2.700055	-1.630821
6	-2.211455	1.898302	-2.339966
8	-2.090518	2.021576	0.722050
8	2.597463	-1.678427	1.803292
6	3.045785	-2.987649	1.479919
8	1.042336	0.086581	2.329847
6	1.161802	-0.255065	3.714015
8	-4.368145	0.912247	0.332566
8	-5.089819	-1.463522	0.765017
6	-4.884083	-1.500968	2.173357
1	0.506129	-2.717587	-1.196804
1	1.870280	-4.078462	-2.757546
1	4.226029	-3.436305	-3.222228
1	5.177221	-1.390611	-2.209553
1	5.950458	-0.335042	-0.277797
1	6.713716	1.833504	0.687605
1	5.050475	3.692211	0.962540
1	2.682909	3.286288	0.235177
1	2.213057	-0.342470	4.006434
1	0.640362	-1.192279	3.943169
1	0.693110	0.556265	4.276716
1	3.586507	-3.367442	2.351905
1	3.731531	-2.962062	0.623356
1	2.209902	-3.662536	1.264043
1	0.058869	5.370975	0.931186
1	-1.220119	4.988299	-0.250124
1	-1.391161	4.470164	1.449446
1	-2.260441	2.263481	-3.370557
1	-1.894336	0.839631	-2.369454
1	-3.220006	1.944928	-1.902361
1	-3.508775	1.432477	0.488978
1	-5.516303	-2.294978	2.577102
1	-3.834806	-1.729794	2.417801
1	-5.159706	-0.547228	2.638804
1	-6.085397	-0.549913	-2.942638
1	-6.673590	-0.876310	-1.290464
1	-6.015297	0.735408	-1.706634

reductive-elimination-product (Pd-Ag)

Number of imaginary frequencies : 0

The smallest frequency is : 17.0481 cm(-1)

Electronic energy : =-2691.8116924
 Zero-point correction= 0.446062
 Thermal correction to Energy= 0.485631
 Thermal correction to Enthalpy= 0.486575
 Thermal correction to Gibbs Free Energy= 0.370268
 Sum of electronic and zero-point Energies= -2691.365631
 Sum of electronic and thermal Energies= -2691.326062
 Sum of electronic and thermal Enthalpies= -2691.325117
 Sum of electronic and thermal Free Energies= -2691.441424

 Cartesian Coordinates

6	2.002807	-0.234696	-2.842101
6	2.326110	-0.499074	-1.511026
6	1.667743	-1.541774	-0.836560
6	0.678905	-2.274698	-1.514298
6	0.353821	-1.988125	-2.835064

6	1.023822	-0.969253	-3.502511
6	3.300983	0.405514	-0.847838
7	2.787947	1.420037	-0.129454
6	3.635291	2.264622	0.478010
6	5.014098	2.139922	0.395034
6	5.541644	1.100420	-0.361878
6	4.672040	0.224667	-0.998371
46	0.623419	1.824147	0.090057
47	-0.824843	-0.456340	0.430851
15	-3.123645	-1.382681	0.118374
8	-3.502238	-1.839747	-1.384846
6	-4.873872	-2.013935	-1.750627
15	-1.550982	2.473624	0.212638
8	-1.490956	4.044595	0.686833
6	-2.718343	4.749259	0.819631
15	1.953731	-2.049015	0.875871
8	0.659760	-2.254418	1.591489
8	-2.117893	2.751558	-1.329697
6	-2.484596	1.612537	-2.071874
8	-2.688088	1.796939	0.986573
8	2.905693	-3.337713	0.807152
6	2.381508	-4.568976	0.304715
8	2.970106	-1.035050	1.557630
6	2.537673	-0.222081	2.659477
8	-4.172984	-0.239797	0.503359
8	-3.690226	-2.678992	0.933633
6	-3.505536	-2.640102	2.344084
1	0.144624	-3.069880	-0.995235
1	-0.424227	-2.559164	-3.335429
1	0.778426	-0.736192	-4.535744
1	2.511902	0.581337	-3.352139
1	5.039433	-0.605908	-1.595738
1	6.617107	0.972191	-0.455039
1	5.654592	2.849150	0.910694
1	3.175384	3.066966	1.053135
1	2.220097	-0.844307	3.501556
1	1.719623	0.445387	2.355212
1	3.403656	0.374668	2.953512
1	3.108488	-5.346082	0.548651
1	2.257116	-4.526502	-0.784532
1	1.423527	-4.810406	0.779108
1	-2.497313	5.708391	1.297388
1	-3.175369	4.936933	-0.160376
1	-3.429649	4.193256	1.442040
1	-2.622975	1.914009	-3.115402
1	-1.701104	0.831538	-2.042801
1	-3.425256	1.171405	-1.707980
1	-3.664998	0.619568	0.691127
1	-3.694341	-3.644759	2.729844
1	-2.474441	-2.353956	2.604444
1	-4.201620	-1.936151	2.816419
1	-4.885836	-2.362813	-2.785648
1	-5.361340	-2.760057	-1.113527
1	-5.417290	-1.064922	-1.683058

Reaction 2

Coordinates for monometallic pathway

N-H-activation-TS

Number of imaginary frequencies : 1
 Electronic energy : =-1098.5861105
 Zero-point correction= 0.259619
 Thermal correction to Energy= 0.280992
 Thermal correction to Enthalpy= 0.281937

Thermal correction to Gibbs Free Energy= 0.207622
 Sum of electronic and zero-point Energies= -1098.326491
 Sum of electronic and thermal Energies= -1098.305118
 Sum of electronic and thermal Enthalpies= -1098.304174
 Sum of electronic and thermal Free Energies= -1098.378488

 Cartesian Coordinates

6	-3.536217	-1.859756	-1.790243
6	-3.965688	-1.366823	-0.560465
6	-3.045901	-1.137212	0.452766
6	-1.687607	-1.391208	0.238447
6	-1.257902	-1.882551	-0.999790
6	-2.185575	-2.120775	-2.006247
1	-4.257491	-2.041561	-2.583901
1	-5.019904	-1.159981	-0.392252
1	-3.362585	-0.749091	1.418233
1	-0.208057	-2.102669	-1.184281
1	-1.851031	-2.512965	-2.963636
6	-0.772327	-1.110531	1.369161
8	-1.128395	-1.050936	2.527958
7	0.583038	-0.848439	1.002368
1	1.221786	-1.455219	0.184304
8	1.401363	-0.634377	2.116993
46	0.600032	0.947174	-0.040025
8	2.118055	-1.830444	-0.670383
8	2.307008	0.378935	-1.038135
8	0.239884	2.880227	-0.797869
8	-1.064859	1.954645	0.683528
6	2.678147	-0.824084	-1.198391
6	-0.786749	2.968228	-0.047778
6	3.874829	-1.061041	-2.060882
1	4.139807	-0.168921	-2.630927
1	4.718499	-1.343131	-1.420879
1	3.677560	-1.901370	-2.732891
6	-1.610594	4.195302	0.004445
1	-1.237031	4.836773	0.811319
1	-1.533866	4.743896	-0.937796
1	-2.651810	3.944319	0.223928
6	1.894859	-1.873452	2.623157
1	1.077054	-2.514116	2.974652
1	2.491116	-2.401976	1.868160
1	2.533107	-1.605922	3.468724

C-H-activation-PRC

Number of imaginary frequencies : 0
 Electronic energy : =-1098.5932112
 Zero-point correction= 0.264042
 Thermal correction to Energy= 0.286079
 Thermal correction to Enthalpy= 0.287023
 Thermal correction to Gibbs Free Energy= 0.211123
 Sum of electronic and zero-point Energies= -1098.329169
 Sum of electronic and thermal Energies= -1098.307132
 Sum of electronic and thermal Enthalpies= -1098.306188
 Sum of electronic and thermal Free Energies= -1098.382088

 Cartesian Coordinates

6	-1.658652	-1.200307	0.930900
6	-1.046938	-1.910552	-0.145480
6	-1.743651	-2.076516	-1.361762
6	-2.994644	-1.522481	-1.508512
6	-3.599058	-0.809706	-0.452542
6	-2.953625	-0.665865	0.754077
6	0.347844	-2.441178	-0.029860
7	1.033172	-1.543291	0.759579
46	0.023404	0.139284	0.159848
8	1.604388	1.570253	-0.205246
6	2.697677	1.471296	-0.769772

6	3.468841	2.668007	-1.191936
8	0.783951	-3.414043	-0.626549
8	2.400737	-1.645438	0.557040
6	3.093479	-1.194596	1.720128
8	-1.225342	1.635958	-0.530825
6	-1.691793	2.375865	0.422730
8	-1.388519	2.254334	1.614791
6	-2.706597	3.390605	-0.035049
8	3.288421	0.335071	-1.053019
1	2.836999	-0.150622	1.945932
1	2.849264	-1.830835	2.577174
1	4.157200	-1.273754	1.481779
1	-1.265558	-2.630054	-2.166469
1	-3.525524	-1.633584	-2.450914
1	-4.592096	-0.388982	-0.591454
1	-3.427016	-0.144640	1.582136
1	-1.235350	-1.251080	1.932923
1	-2.833469	4.176409	0.713876
1	-2.424543	3.825482	-0.998234
1	-3.669114	2.881660	-0.173478
1	2.902140	3.576938	-0.988240
1	4.422641	2.691246	-0.654008
1	3.697751	2.594185	-2.260045
1	2.811496	-0.442919	-0.668097

C-H-activation-1-TS

Number of imaginary frequencies : 1
 Electronic energy : =-1098.5705762
 Zero-point correction= 0.258874
 Thermal correction to Energy= 0.280040
 Thermal correction to Enthalpy= 0.280984
 Thermal correction to Gibbs Free Energy= 0.208549
 Sum of electronic and zero-point Energies= -1098.311702
 Sum of electronic and thermal Energies= -1098.290536
 Sum of electronic and thermal Enthalpies= -1098.289592
 Sum of electronic and thermal Free Energies= -1098.362027

Cartesian Coordinates

6	-1.782957	0.057837	-0.125744
6	-2.060310	-1.317918	0.026194
6	-3.285940	-1.842052	-0.350562
6	-4.238503	-1.012095	-0.939454
6	-3.956152	0.331403	-1.170676
6	-2.733500	0.863629	-0.774984
6	-0.961021	-2.246498	0.418657
7	0.223983	-1.633349	0.191789
46	0.312056	0.341333	-0.161619
8	2.443628	0.680116	-0.320857
6	3.413330	0.017087	-0.700602
6	4.727131	0.651285	-0.982592
8	-1.125229	-3.400431	0.813839
8	1.355445	-2.405703	0.411225
6	1.815758	-2.275342	1.759432
8	0.199436	2.439513	-0.202222
6	-0.522593	2.877054	0.750069
8	-1.245728	2.145211	1.483028
6	-0.544524	4.358915	0.970079
8	3.404145	-1.279814	-0.879986
1	2.015982	-1.222132	1.999545
1	1.072086	-2.684171	2.452011
1	2.740762	-2.855630	1.819545
1	-3.467398	-2.906936	-0.218015
1	-5.198344	-1.423005	-1.244171
1	-4.694336	0.970058	-1.649657
1	-2.537404	1.926101	-0.908521
1	-1.363650	0.854481	0.810089
1	-0.736206	4.586938	2.021079
1	0.389650	4.817787	0.639022

1	-1.364338	4.781808	0.377327
1	4.649789	1.736689	-0.912607
1	5.464962	0.281755	-0.262053
1	5.071894	0.356674	-1.978877
1	2.556201	-1.699264	-0.571891

C-H-activation-product

Number of imaginary frequencies : 0
 Electronic energy : =-1098.6150989
 Zero-point correction= 0.264391
 Thermal correction to Energy= 0.286380
 Thermal correction to Enthalpy= 0.287324
 Thermal correction to Gibbs Free Energy= 0.211754
 Sum of electronic and zero-point Energies= -1098.350708
 Sum of electronic and thermal Energies= -1098.328719
 Sum of electronic and thermal Enthalpies= -1098.327775
 Sum of electronic and thermal Free Energies= -1098.403345

Cartesian Coordinates

6	-1.753963	0.216374	-0.287000
6	-2.353867	-1.033338	-0.110414
6	-3.736410	-1.170935	-0.138915
6	-4.530033	-0.047498	-0.353287
6	-3.933948	1.197567	-0.534376
6	-2.542452	1.340475	-0.499415
6	-1.451149	-2.192613	0.112863
7	-0.171602	-1.757118	-0.017843
46	0.236758	0.199660	-0.217479
8	2.487494	0.253484	-0.113703
6	3.373913	-0.531596	-0.449833
6	4.794039	-0.115944	-0.603365
8	-1.810922	-3.342167	0.374265
8	0.824070	-2.703231	0.207335
6	1.152799	-2.780415	1.595157
8	0.505558	2.334265	-0.458352
6	0.429877	3.111225	0.495207
8	0.099365	2.726842	1.712073
6	0.694558	4.565061	0.376935
8	3.174474	-1.803936	-0.709066
1	1.464225	-1.794820	1.970597
1	0.294792	-3.147909	2.168635
1	1.983039	-3.488560	1.672404
1	-4.170929	-2.159482	0.006669
1	-5.613307	-0.141147	-0.380921
1	-4.554779	2.074719	-0.709188
1	-2.098370	2.323231	-0.651314
1	-0.061358	1.759541	1.718142
1	1.521474	4.837632	1.040993
1	0.940464	4.822030	-0.653753
1	-0.186106	5.125032	0.708182
1	4.911431	0.941403	-0.362795
1	5.430281	-0.726430	0.045622
1	5.114336	-0.301514	-1.634158
1	2.234661	-2.080489	-0.531936

oxidative-addition-TS

Number of imaginary frequencies : 1
 Electronic energy : =-1341.4078598
 Zero-point correction= 0.355097
 Thermal correction to Energy= 0.384041
 Thermal correction to Enthalpy= 0.384985
 Thermal correction to Gibbs Free Energy= 0.293246
 Sum of electronic and zero-point Energies= -1341.052763
 Sum of electronic and thermal Energies= -1341.023819
 Sum of electronic and thermal Enthalpies= -1341.022875
 Sum of electronic and thermal Free Energies= -1341.114613

Cartesian Coordinates

```

-----
 6  -2.178007  1.221538 -1.440041
 8  -2.788893  1.659614 -2.413677
 7  -1.057083  0.437896 -1.498418
 8  -0.447441  0.407361 -2.733705
 6  -0.747666 -0.797525 -3.421442
 1  -0.452274 -1.677925 -2.834542
 1  -1.817777 -0.845403 -3.664664
 1  -0.167612 -0.770267 -4.348651
 6  -2.560227  1.432295 -0.023860
 6  -3.744408  2.063320  0.343418
 6  -4.015845  2.266857  1.693001
 6  -3.101115  1.852607  2.658389
 6  -1.903157  1.227519  2.294000
 6  -1.656325  1.016524  0.947000
 1  -4.430388  2.394610 -0.435381
 1  -4.938651  2.756457  1.995800
 1  -3.316096  2.016103  3.713132
 1  -1.193231  0.919812  3.059244
46  -0.002758  0.085806  0.218683
 6  2.364067  1.761519  0.992507
 6  1.738883  1.356236 -0.175676
 6  1.684386  2.122736 -1.327426
 6  2.212797  3.411735 -1.261912
 6  2.807587  3.879859 -0.093656
 6  2.883544  3.057091  1.024413
 1  2.430755  1.110935  1.858337
 1  1.232307  1.742711 -2.239943
 1  2.160969  4.044293 -2.145693
 1  3.225062  4.883333 -0.060243
 1  3.359890  3.408585  1.937570
53  2.257810 -1.172175 -0.763726
 8  0.740988 -0.399197  2.260793
 6  0.683438 -1.510936  2.794767
 8  -0.089960 -2.483973  2.383545
 6  1.509170 -1.861222  3.979503
 1  2.117175 -2.741901  3.746344
 1  2.152855 -1.026417  4.258710
 1  0.855864 -2.130531  4.815915
 1  -0.720720 -2.208651  1.661304
 8  -2.026444 -2.098787  0.587015
 6  -2.073924 -2.620773 -0.520286
 8  -1.076372 -3.345108 -1.013350
 1  -0.341536 -3.364049 -0.373561
 6  -3.252296 -2.520419 -1.419379
 1  -4.085536 -3.061089 -0.956470
 1  -3.554111 -1.470474 -1.497609
 1  -3.054884 -2.940266 -2.407489
-----

```

C-C-reductive-elimination-PRC

```

-----
Number of imaginary frequencies : 0
Electronic energy :      =-1341.4333068
Zero-point correction=      0.355609
Thermal correction to Energy=    0.385156
Thermal correction to Enthalpy=   0.386100
Thermal correction to Gibbs Free Energy=  0.293517
Sum of electronic and zero-point Energies= -1341.077698
Sum of electronic and thermal Energies= -1341.048151
Sum of electronic and thermal Enthalpies= -1341.047207
Sum of electronic and thermal Free Energies= -1341.139790
-----

```

Cartesian Coordinates

```

-----
 6  2.425799  0.655286  1.579535
 8  3.187250  1.368516  2.221029
 7  1.049374  0.638622  1.748289
 8  0.597537  1.844402  2.229551
 6  -0.226664  1.690929  3.376393
-----

```

1	-1.162973	1.169705	3.139064
1	0.310031	1.160441	4.172576
1	-0.460327	2.707679	3.704586
6	2.840660	-0.308145	0.543129
6	4.175002	-0.680513	0.377585
6	4.525940	-1.505061	-0.681113
6	3.551553	-1.934881	-1.580763
6	2.215294	-1.555488	-1.437267
6	1.880686	-0.748767	-0.362565
1	4.916084	-0.298876	1.077880
1	5.561394	-1.807126	-0.818399
1	3.828939	-2.575170	-2.415865
1	1.476689	-1.888016	-2.161867
46	0.072456	0.072947	-0.000311
53	-1.195660	-0.286551	-2.446445
6	-0.381703	-1.757380	0.779482
6	-0.476231	-2.897716	-0.012907
6	-0.694411	-1.801360	2.134804
6	-0.919808	-4.088958	0.561902
1	-0.226423	-2.877941	-1.069466
6	-1.144548	-2.999359	2.691408
1	-0.589117	-0.926944	2.767304
6	-1.258286	-4.142226	1.909756
1	-0.996817	-4.978374	-0.060333
1	-1.397560	-3.028538	3.749460
1	-1.604656	-5.074843	2.349449
6	0.429905	3.251063	-0.694533
8	0.851760	2.103570	-0.815680
8	-0.714179	3.558562	-0.115508
1	-1.172561	2.751182	0.213374
6	1.173890	4.439899	-1.188656
8	-1.866266	1.206418	0.721325
6	-3.001531	0.765346	0.912277
8	-3.378833	-0.420699	0.490062
1	-2.656875	-0.822693	-0.038939
6	-4.053678	1.503280	1.652004
1	-3.686461	2.480759	1.967572
1	-4.352726	0.916293	2.527558
1	-4.940216	1.614784	1.019666
1	0.519755	5.058949	-1.810455
1	2.053912	4.129605	-1.753011
1	1.481876	5.048570	-0.331323

C-C-reductive-elimination-TS

Number of imaginary frequencies : 1
 Electronic energy : =-1341.420413
 Zero-point correction= 0.355293
 Thermal correction to Energy= 0.384431
 Thermal correction to Enthalpy= 0.385375
 Thermal correction to Gibbs Free Energy= 0.293475
 Sum of electronic and zero-point Energies= -1341.065120
 Sum of electronic and thermal Energies= -1341.035982
 Sum of electronic and thermal Enthalpies= -1341.035038
 Sum of electronic and thermal Free Energies= -1341.126938

Cartesian Coordinates

6	0.404339	2.570369	1.099810
8	0.042881	3.669126	1.504751
7	-0.060029	1.359064	1.573911
8	-1.238232	1.471976	2.266156
6	-1.206925	0.659035	3.437706
1	-0.906020	-0.367380	3.194651
1	-0.511373	1.085046	4.169905
1	-2.223996	0.664769	3.837503
6	1.432759	2.344348	0.058792
6	2.141454	3.427296	-0.460101
6	2.989663	3.243931	-1.541098
6	3.103824	1.981907	-2.125983

6	2.398878	0.894304	-1.623447
6	1.582994	1.065460	-0.506452
1	1.985024	4.409284	-0.017424
1	3.548746	4.083742	-1.946044
1	3.755940	1.837629	-2.984498
1	2.512154	-0.081973	-2.085871
46	-0.092336	-0.009349	0.026394
53	-0.449243	-1.593615	-2.228323
6	1.831873	-0.636837	0.682212
6	2.399147	-1.721380	0.006599
6	2.239687	-0.341780	1.983915
6	3.341698	-2.519643	0.648026
1	2.116440	-1.957134	-1.014864
6	3.194167	-1.143216	2.607095
1	1.824530	0.508317	2.515168
6	3.743441	-2.237140	1.949403
1	3.765153	-3.366854	0.112560
1	3.502543	-0.899745	3.621873
1	4.483944	-2.861645	2.443627
6	-2.978297	1.756798	-0.652791
8	-1.845685	1.397047	-0.947387
8	-3.404208	1.882628	0.593944
1	-2.666508	1.686802	1.218766
6	-4.023091	2.096185	-1.658049
8	-1.962764	-1.004835	0.941267
6	-1.959914	-2.136178	1.419089
8	-1.002089	-3.019426	1.195504
1	-0.369401	-2.666981	0.536437
6	-3.023328	-2.643683	2.323082
1	-3.733933	-1.849070	2.554748
1	-2.569915	-3.030477	3.241851
1	-3.542729	-3.478404	1.840187
1	-4.863666	1.401773	-1.550523
1	-3.614709	2.025840	-2.666916
1	-4.408118	3.103902	-1.472252

C-C-reductive-elimination-product

Number of imaginary frequencies : 0

Electronic energy : =-1341.4806285

Zero-point correction= 0.357831

Thermal correction to Energy= 0.387141

Thermal correction to Enthalpy= 0.388085

Thermal correction to Gibbs Free Energy= 0.295700

Sum of electronic and zero-point Energies= -1341.122797

Sum of electronic and thermal Energies= -1341.093488

Sum of electronic and thermal Enthalpies= -1341.092544

Sum of electronic and thermal Free Energies= -1341.184928

 Cartesian Coordinates

6	0.914396	-1.193279	2.005357
8	0.832287	-1.746714	3.090920
7	0.573397	-1.694244	0.768176
8	-0.245921	-2.790749	0.878752
6	-0.105660	-3.624412	-0.266837
1	-0.154458	-3.038802	-1.193102
1	0.852708	-4.155910	-0.230435
1	-0.934963	-4.336529	-0.228759
6	1.275836	0.252841	1.802757
6	0.785871	1.152616	2.784472
6	1.071749	2.493949	2.714026
6	1.858124	2.987133	1.658508
6	2.355978	2.136712	0.697206
6	2.106641	0.744464	0.737637
1	0.176428	0.746630	3.588222
1	0.684970	3.174263	3.468016
1	2.089131	4.048309	1.607554
1	3.001663	2.520851	-0.089458
46	-0.180152	0.091512	0.031554

53	-1.025773	2.487781	-0.957397
6	2.900389	-0.125023	-0.164620
6	2.979410	0.170743	-1.531110
6	3.613064	-1.219011	0.335681
6	3.734468	-0.627651	-2.381282
1	2.427126	1.021367	-1.930924
6	4.373296	-2.011753	-0.516806
1	3.587245	-1.442746	1.400997
6	4.431304	-1.723453	-1.876789
1	3.777049	-0.394160	-3.442860
1	4.926688	-2.856613	-0.113032
1	5.024779	-2.346796	-2.541888
6	-3.119916	-1.124175	1.574984
8	-2.245323	-0.475883	2.122016
8	-2.968643	-2.412549	1.259552
1	-2.031086	-2.647308	1.438824
6	-4.435563	-0.575676	1.141985
8	-1.827939	-0.882481	-0.957617
6	-1.887406	-1.197053	-2.146376
8	-1.033766	-0.774712	-3.054157
1	-0.415943	-0.126707	-2.656823
6	-2.946583	-2.099230	-2.657544
1	-3.431620	-2.602571	-1.817744
1	-2.523473	-2.825613	-3.357304
1	-3.687470	-1.504115	-3.203654
1	-4.308816	-0.188176	0.122215
1	-4.727987	0.256613	1.785656
1	-5.210701	-1.345954	1.124636

C-H-activation-2-TS-PRC

Number of imaginary frequencies : 0
 Electronic energy : =-1112.4389915
 Zero-point correction= 0.288693
 Thermal correction to Energy= 0.312569
 Thermal correction to Enthalpy= 0.313513
 Thermal correction to Gibbs Free Energy= 0.232978
 Sum of electronic and zero-point Energies= -1112.150298
 Sum of electronic and thermal Energies= -1112.126423
 Sum of electronic and thermal Enthalpies= -1112.125479
 Sum of electronic and thermal Free Energies= -1112.206014

Cartesian Coordinates

6	-2.150346	1.202093	0.911229
8	-3.029830	1.516403	1.703839
7	-0.804885	1.280293	1.182611
8	-0.533528	1.372678	2.549449
6	-0.140459	2.695716	2.892723
1	0.788401	2.981860	2.379899
1	-0.938983	3.410592	2.655762
1	0.032357	2.685561	3.972165
6	-2.444372	0.819274	-0.504978
6	-2.949901	1.797393	-1.358761
6	-3.290244	1.475496	-2.667574
6	-3.151581	0.164563	-3.114379
6	-2.671464	-0.820140	-2.257873
6	-2.301645	-0.507763	-0.947379
1	-3.077879	2.812102	-0.983787
1	-3.671467	2.244137	-3.335646
1	-3.420189	-0.093837	-4.136145
1	-2.567646	-1.846613	-2.606001
46	0.668916	0.042212	0.425396
6	-1.825412	-1.564312	-0.024929
6	-0.615264	-1.489444	0.665018
6	-2.625284	-2.690926	0.214902
6	-0.209834	-2.447499	1.581316
1	0.240864	-0.066258	-1.024538
6	-2.237996	-3.669966	1.120648

1	-3.578506	-2.771407	-0.305738
6	-1.039728	-3.543763	1.815235
1	0.743569	-2.361032	2.098742
1	-2.880565	-4.529857	1.293775
1	-0.732271	-4.302941	2.530816
8	2.076990	1.876067	0.160273
6	1.698345	2.931424	-0.349349
8	0.430834	3.291400	-0.407030
1	-0.115695	2.631318	0.093997
6	2.627747	3.921340	-0.951085
1	2.367877	4.068891	-2.004811
1	2.508461	4.887928	-0.450811
1	3.658388	3.575415	-0.866679
53	2.526722	-1.477791	-0.780346

C-H-activation-2-TS

Number of imaginary frequencies : 1
 Electronic energy : =-1112.4361011
 Zero-point correction= 0.287887
 Thermal correction to Energy= 0.311340
 Thermal correction to Enthalpy= 0.312284
 Thermal correction to Gibbs Free Energy= 0.232275
 Sum of electronic and zero-point Energies= -1112.148214
 Sum of electronic and thermal Energies= -1112.124762
 Sum of electronic and thermal Enthalpies= -1112.123817
 Sum of electronic and thermal Free Energies= -1112.203826

Cartesian Coordinates

6	-2.064950	1.384954	0.865048
8	-2.853091	1.803694	1.706288
7	-0.702279	1.397668	1.017141
8	-0.317332	1.574088	2.352656
6	-0.016728	2.935232	2.633656
1	0.884526	3.272948	2.105047
1	-0.865875	3.582593	2.383071
1	0.166931	2.978439	3.710661
6	-2.518237	0.921226	-0.481918
6	-3.071474	1.855112	-1.355901
6	-3.589160	1.448870	-2.580227
6	-3.584358	0.098402	-2.917161
6	-3.059171	-0.839555	-2.035503
6	-2.510522	-0.442616	-0.813554
1	-3.099307	2.903792	-1.063331
1	-4.005730	2.183153	-3.265647
1	-3.993979	-0.228602	-3.870148
1	-3.061416	-1.897014	-2.295282
46	0.677957	0.033893	0.285282
6	-1.991427	-1.452698	0.137407
6	-0.694436	-1.426521	0.657470
6	-2.829182	-2.497594	0.554384
6	-0.237273	-2.376806	1.563424
1	0.087665	-0.715804	-0.914602
6	-2.394368	-3.450546	1.464608
1	-3.845341	-2.534895	0.164789
6	-1.104092	-3.384282	1.979861
1	0.780337	-2.342671	1.944423
1	-3.066860	-4.245937	1.776865
1	-0.756054	-4.123446	2.697705
8	2.223428	1.689589	0.181810
6	1.995420	2.772348	-0.363120
8	0.780223	3.210354	-0.619554
1	0.115788	2.600634	-0.203728
6	3.071455	3.718162	-0.752378
1	2.835522	4.189351	-1.710583
1	3.124812	4.512805	0.001153
1	4.031691	3.202869	-0.798708
53	2.515517	-1.631791	-0.777563

C-N-reductive-elimination-PRC

Number of imaginary frequencies : 0
Electronic energy : =-1329.4849952
Zero-point correction= 0.345148
Thermal correction to Energy= 0.371671
Thermal correction to Enthalpy= 0.372615
Thermal correction to Gibbs Free Energy= 0.287791
Sum of electronic and zero-point Energies= -1329.139848
Sum of electronic and thermal Energies= -1329.113324
Sum of electronic and thermal Enthalpies= -1329.112380
Sum of electronic and thermal Free Energies= -1329.197204

Cartesian Coordinates

6	-0.873209	-2.067724	-0.526380
8	-0.825493	-3.259406	-0.858642
7	-0.234020	-1.080007	-1.192880
8	0.608119	-1.569276	-2.208726
6	-0.079461	-1.649078	-3.449174
1	-0.882454	-2.394650	-3.405734
1	-0.490970	-0.666173	-3.712702
1	0.663584	-1.951348	-4.192455
6	-1.648237	-1.642565	0.689622
6	-1.749445	-2.640144	1.665640
6	-2.435937	-2.439181	2.853413
6	-3.064191	-1.219246	3.072910
6	-2.994978	-0.228639	2.103420
6	-2.291777	-0.401668	0.901186
1	-1.273605	-3.596713	1.464028
1	-2.482589	-3.230331	3.598263
1	-3.608383	-1.034389	3.996704
1	-3.483624	0.727324	2.283583
46	0.602640	0.552768	-0.361136
6	-2.326275	0.745800	-0.044300
6	-1.186016	1.337040	-0.605763
6	-3.566198	1.347416	-0.313982
6	-1.278618	2.475585	-1.400610
6	-3.669053	2.480187	-1.112090
1	-4.467569	0.899792	0.103508
6	-2.522453	3.053328	-1.651181
1	-0.377904	2.922097	-1.820722
1	-4.646649	2.914085	-1.311175
1	-2.589935	3.945698	-2.270766
8	2.645260	-0.522140	-0.027238
6	2.991288	-1.706266	0.064940
8	2.483170	-2.664057	-0.663770
6	4.046804	-2.162004	1.006732
1	4.303303	-1.368830	1.711328
1	3.708391	-3.054780	1.540940
1	4.937843	-2.444212	0.434729
1	1.819172	-2.330935	-1.328482
8	1.364937	2.397676	0.472627
6	2.392815	2.593863	1.126923
8	3.313452	1.685388	1.347508
1	3.101623	0.827899	0.893021
6	2.693044	3.911258	1.744818
1	2.763790	3.791405	2.831217
1	3.666016	4.270755	1.394816
1	1.912469	4.632761	1.501516

C-N-reductive-elimination-TS

Number of imaginary frequencies : 1
Electronic energy : =-1329.4592319
Zero-point correction= 0.343655
Thermal correction to Energy= 0.370071
Thermal correction to Enthalpy= 0.371015

Thermal correction to Gibbs Free Energy=	0.285241
Sum of electronic and zero-point Energies=	-1329.115577
Sum of electronic and thermal Energies=	-1329.089161
Sum of electronic and thermal Enthalpies=	-1329.088217
Sum of electronic and thermal Free Energies=	-1329.173991

Cartesian Coordinates

```

6   -0.947205 -1.906353  0.000585
8   -0.751536 -3.122852 -0.090452
7   -0.565837 -1.023160 -0.979041
8    0.028407 -1.598791 -2.104350
6   -0.946070 -2.194246 -2.966307
1   -1.427695 -3.049964 -2.481357
1   -1.695126 -1.448787 -3.256420
1   -0.392787 -2.527152 -3.847975
6   -1.647565 -1.286894  1.156164
6   -1.720630 -2.072567  2.312750
6   -2.389941 -1.630585  3.440674
6   -3.020546 -0.386253  3.417170
6   -2.976519  0.393464  2.273365
6   -2.293507 -0.025652  1.121193
1   -1.236345 -3.046153  2.300465
1   -2.421735 -2.248024  4.335333
1   -3.543392 -0.020771  4.298542
1   -3.457164  1.369666  2.273427
46    0.670765  0.483629 -0.359764
6   -2.307261  0.804814 -0.085712
6   -1.232128  0.763380 -0.997605
6   -3.405631  1.611656 -0.414577
6   -1.314369  1.395499 -2.246137
6   -3.462009  2.307518 -1.614153
1   -4.251776  1.653537  0.269888
6   -2.417940  2.187232 -2.534504
1   -0.502642  1.286863 -2.963928
1   -4.332987  2.914344 -1.849720
1   -2.466071  2.712383 -3.486825
8    2.785830 -0.600937  0.007285
6    3.039871 -1.798531 -0.122914
8    2.332022 -2.616068 -0.869175
6    4.189006 -2.469925  0.540973
1    4.689760 -1.786658  1.227812
1    3.836084 -3.357321  1.075784
1    4.896147 -2.812685 -0.222190
1    1.567566 -2.185076 -1.325149
8    1.565093  2.435166  0.269523
6    2.580901  2.643401  0.929789
8    3.436308  1.705995  1.283955
1    3.198506  0.828479  0.894866
6    2.973255  3.999771  1.397271
1    3.201465  3.975308  2.467246
1    3.887312  4.305558  0.876039
1    2.177292  4.717156  1.194139

```

C-N-reductive-elimination-product

```

Number of imaginary frequencies : 0
Electronic energy :      =-1329.5320793
Zero-point correction=      0.347926
Thermal correction to Energy=    0.373712
Thermal correction to Enthalpy=   0.374656
Thermal correction to Gibbs Free Energy=  0.290868
Sum of electronic and zero-point Energies= -1329.184154
Sum of electronic and thermal Energies= -1329.158368
Sum of electronic and thermal Enthalpies= -1329.157423
Sum of electronic and thermal Free Energies= -1329.241211

```

Cartesian Coordinates

```

6   -2.277324 -1.183599 -0.352589

```

8	-2.447828	-2.410991	-0.396230
7	-1.432877	-0.561926	-1.240412
8	-0.747681	-1.390647	-2.093905
6	-1.497556	-1.598338	-3.294100
1	-2.436382	-2.123382	-3.083881
1	-1.700810	-0.643480	-3.795330
1	-0.860330	-2.221344	-3.926141
6	-2.950856	-0.288483	0.576984
6	-3.951330	-0.827786	1.397264
6	-4.625602	-0.022608	2.291649
6	-4.295062	1.335999	2.375033
6	-3.300226	1.874852	1.582452
6	-2.594744	1.076110	0.663493
1	-4.181780	-1.886393	1.303515
1	-5.406835	-0.436317	2.924168
1	-4.826385	1.978770	3.073631
1	-3.070283	2.933283	1.672005
46	1.856572	0.918367	-0.687771
6	-1.518048	1.585473	-0.165081
6	-0.938532	0.732992	-1.114655
6	-0.983846	2.891897	-0.038777
6	0.126798	1.151109	-1.959488
6	0.084191	3.307818	-0.795495
1	-1.410397	3.573372	0.692777
6	0.659408	2.447804	-1.769891
1	0.366559	0.567730	-2.845297
1	0.478838	4.313954	-0.674563
1	1.343245	2.860637	-2.509235
8	0.421899	-1.645220	0.814080
6	0.821247	-2.708484	0.344146
8	0.028848	-3.561073	-0.274472
6	2.244197	-3.151718	0.401710
1	2.620846	-3.047119	1.424245
1	2.361176	-4.182041	0.060799
1	2.840867	-2.491385	-0.240375
1	-0.892226	-3.191196	-0.342889
8	3.538721	0.296187	0.606223
6	3.440267	-0.028496	1.789088
8	2.338056	-0.496344	2.333567
1	1.627958	-0.678203	1.657361
6	4.580814	0.048985	2.742322
1	4.277098	0.584226	3.647360
1	4.864508	-0.964771	3.046689
1	5.433270	0.545781	2.277009

Coordinates for heterobimetallic pathway

N-H-activation-TS (Pd-Ag)

Number of imaginary frequencies : 1
 Electronic energy : =-1701.8070266
 Zero-point correction= 0.375257
 Thermal correction to Energy= 0.409405
 Thermal correction to Enthalpy= 0.410349
 Thermal correction to Gibbs Free Energy= 0.308043
 Sum of electronic and zero-point Energies= -1701.431769
 Sum of electronic and thermal Energies= -1701.397621
 Sum of electronic and thermal Enthalpies= -1701.396677
 Sum of electronic and thermal Free Energies= -1701.498984

Cartesian Coordinates

6	-0.373974	-3.312053	2.543949
1	-1.034673	-3.577839	3.373036
1	0.659446	-3.562568	2.814797
1	-0.673554	-3.859985	1.642793
8	-0.539832	-1.905247	2.376023
7	0.251960	-1.415673	1.322097

6	1.610015	-1.238986	1.749405
8	1.904793	-1.280152	2.926296
6	2.594277	-0.963770	0.677225
6	3.706880	-0.192293	1.026431
1	3.812810	0.137678	2.057949
6	4.639343	0.164811	0.062307
1	5.495104	0.777491	0.336805
6	4.474252	-0.256596	-1.255936
1	5.201569	0.028273	-2.012725
6	3.389167	-1.057189	-1.601560
1	3.272550	-1.416430	-2.622092
6	2.447583	-1.412259	-0.638924
1	1.627085	-2.069030	-0.913989
46	-0.651355	0.445319	0.949566
8	0.988274	1.511768	1.514386
6	1.636231	2.182135	0.623154
6	2.622903	3.165332	1.190416
1	3.480105	3.263487	0.518856
1	2.129174	4.142238	1.256596
1	2.948588	2.880136	2.193689
8	1.492552	2.098221	-0.608271
47	0.351502	0.407435	-1.742957
8	-0.425723	-1.595434	-2.457466
6	-0.790893	-2.600375	-1.803590
8	-0.552786	-2.824510	-0.570425
1	-0.042029	-2.023079	0.317259
6	-1.601168	-3.649358	-2.513898
1	-2.662476	-3.389878	-2.415038
1	-1.452344	-4.634418	-2.064020
1	-1.359379	-3.672505	-3.579499
8	-2.367538	-0.682449	0.426436
8	-1.627310	2.243761	0.663847
6	-1.874509	2.618648	-0.561464
8	-1.557846	1.989560	-1.574180
6	-2.656654	3.898381	-0.643893
1	-3.690967	3.698330	-0.337038
1	-2.249303	4.645648	0.043083
1	-2.657859	4.281275	-1.666490
6	-3.545982	-0.340482	0.596734
8	-3.914147	0.830361	1.052982
6	-4.666764	-1.254616	0.271365
1	-3.133534	1.429833	1.166571
1	-4.294659	-2.267572	0.113662
1	-5.409236	-1.234156	1.074321
1	-5.156147	-0.896334	-0.641615

N-H-activation-product (Pd-Ag)

Number of imaginary frequencies : 0
 Electronic energy : =-1701.8186088
 Zero-point correction= 0.381815
 Thermal correction to Energy= 0.415904
 Thermal correction to Enthalpy= 0.416848
 Thermal correction to Gibbs Free Energy= 0.315298
 Sum of electronic and zero-point Energies= -1701.436793
 Sum of electronic and thermal Energies= -1701.402705
 Sum of electronic and thermal Enthalpies= -1701.401761
 Sum of electronic and thermal Free Energies= -1701.503311

Cartesian Coordinates

6	1.526343	-2.808484	-2.534816
1	1.999138	-2.965062	-3.509138
1	0.896917	-3.677470	-2.296030
1	2.306289	-2.693446	-1.767946
8	0.741349	-1.636468	-2.672360
7	-0.007069	-1.406103	-1.502887
6	-1.347824	-1.685318	-1.747589
8	-1.780687	-2.136831	-2.800457
6	-2.254676	-1.441789	-0.586433

6	-3.480472	-0.822045	-0.827836
1	-3.741698	-0.554041	-1.850478
6	-4.339277	-0.526997	0.225930
1	-5.283641	-0.024538	0.028228
6	-3.993379	-0.868024	1.530148
1	-4.664360	-0.634935	2.353430
6	-2.794577	-1.538414	1.777312
1	-2.545165	-1.869980	2.783922
6	-1.925245	-1.826657	0.718958
1	-1.028432	-2.411999	0.904060
46	0.502688	0.501057	-0.956231
8	-1.238713	1.270920	-1.692684
6	-2.045911	1.914375	-0.923382
6	-3.124788	2.668043	-1.654456
1	-4.071708	2.574368	-1.114436
1	-2.855660	3.730626	-1.668509
1	-3.237310	2.323648	-2.685088
8	-1.994392	1.970996	0.316589
47	-0.768077	0.369547	1.614176
8	1.014375	-1.224988	2.324465
6	1.552675	-2.261122	1.962239
8	1.434320	-2.767718	0.740601
1	0.929777	-2.169681	0.136818
6	2.425066	-3.092034	2.839386
1	3.473417	-2.877670	2.600987
1	2.255267	-4.156450	2.655366
1	2.246386	-2.847935	3.887942
8	2.402627	-0.316439	-0.428488
8	1.186658	2.435100	-0.496950
6	1.315479	2.765515	0.752455
8	0.959484	2.072996	1.715031
6	1.998087	4.088599	0.960252
1	3.030546	4.017007	0.596385
1	1.500729	4.867038	0.373265
1	2.005010	4.363456	2.016992
6	3.503131	0.222021	-0.598459
8	3.661749	1.470948	-0.959217
6	4.764389	-0.534666	-0.406452
1	2.784826	1.937396	-1.006400
1	4.543957	-1.563054	-0.113174
1	5.337864	-0.524676	-1.339458
1	5.375019	-0.043338	0.358041

C-H-activation-1-TS (Pd-Ag)

Number of imaginary frequencies : 1

Electronic energy : =-1701.7959195

Zero-point correction= 0.377567

Thermal correction to Energy= 0.410586

Thermal correction to Enthalpy= 0.411530

Thermal correction to Gibbs Free Energy= 0.313880

Sum of electronic and zero-point Energies= -1701.418352

Sum of electronic and thermal Energies= -1701.385334

Sum of electronic and thermal Enthalpies= -1701.384389

Sum of electronic and thermal Free Energies= -1701.482039

Cartesian Coordinates

6	1.838349	3.760821	-0.077909
6	2.241310	2.429583	-0.135632
6	1.588616	1.446040	0.622836
6	0.438994	1.824138	1.352819
6	0.051379	3.154983	1.425325
6	0.765172	4.127603	0.728413
46	1.433337	-0.631891	0.163500
8	3.303496	-0.786255	-0.803970
6	4.218151	-0.341558	-0.040101
8	3.992878	0.311497	1.020408
6	-0.502806	0.785017	1.860719
7	-0.140857	-0.434469	1.389534

8	-1.051058	-1.442602	1.587271
6	-0.665302	-2.291585	2.658401
8	1.038778	-2.660993	-0.246278
6	-0.005556	-3.070230	-0.833258
8	-0.814539	-2.360186	-1.494678
47	-0.820015	-0.046786	-1.486267
8	-3.089491	-0.363272	-0.376669
6	-3.400439	-1.328984	0.323718
8	-3.117962	-2.566001	-0.031214
6	-0.322233	-4.531882	-0.683739
8	-1.497523	1.024935	2.550381
6	-4.135426	-1.194115	1.608170
6	5.637798	-0.637038	-0.410963
1	-5.078683	-0.665877	1.436097
1	-4.328295	-2.163214	2.072656
1	-3.522256	-0.572852	2.273199
1	-0.793521	-4.922013	-1.589797
1	0.567956	-5.113119	-0.433347
1	-1.042133	-4.635431	0.139610
1	3.117355	2.160259	-0.723105
1	2.376623	4.514437	-0.647959
1	0.462434	5.170833	0.790440
1	-0.841657	3.405022	1.996417
1	5.728681	-0.861219	-1.475906
1	6.287340	0.197516	-0.135431
1	5.962570	-1.517042	0.156559
1	-2.486648	-2.548838	-0.794554
1	2.611137	0.703947	1.006846
1	-1.441011	-3.062956	2.714996
1	0.307825	-2.761218	2.458340
1	-0.627564	-1.731601	3.602364
8	-1.330470	2.200254	-1.607976
6	-2.118945	2.847848	-0.919108
8	-2.973804	2.319504	-0.071494
6	-2.222618	4.331668	-1.012169
1	-2.456155	4.772274	-0.039168
1	-1.300386	4.749502	-1.420697
1	-3.049626	4.574059	-1.690565
1	-2.981870	1.325861	-0.101560

oxidative-addition-PRC (Pd-Ag)

Number of imaginary frequencies : 0

Electronic energy : =-1944.674325

Zero-point correction= 0.474385

Thermal correction to Energy= 0.515644

Thermal correction to Enthalpy= 0.516588

Thermal correction to Gibbs Free Energy= 0.397812

Sum of electronic and zero-point Energies= -1944.199940

Sum of electronic and thermal Energies= -1944.158681

Sum of electronic and thermal Enthalpies= -1944.157737

Sum of electronic and thermal Free Energies= -1944.276513

Cartesian Coordinates

6	-3.351712	3.371614	0.093915
6	-4.081504	2.507457	0.896387
6	-4.034964	1.125242	0.686105
6	-3.254598	0.635633	-0.346226
6	-2.523476	1.484378	-1.184612
6	-2.575574	2.863477	-0.952242
46	-0.235425	1.969973	0.014823
53	-3.092082	-1.470428	-0.645582
47	-0.211840	-1.038132	-0.156068
8	0.737779	-3.125919	1.109450
6	0.792629	-3.450001	2.296065
6	1.279056	-4.774856	2.769874
6	1.614997	2.361530	0.658267
6	2.567512	2.422712	-0.357944
6	3.901559	2.679386	-0.058944

6	4.277245	2.904065	1.262891
6	3.316554	2.875298	2.270694
6	1.976891	2.597916	1.978397
6	2.108635	2.171669	-1.749734
7	0.750627	2.145036	-1.769956
8	0.173428	1.797880	-2.987718
6	0.311951	0.408698	-3.255907
8	2.866370	2.010401	-2.712586
8	-1.008257	1.701610	1.982584
6	-0.757878	0.639789	2.614661
6	-1.332767	0.511716	3.995515
8	-0.031261	-0.306604	2.176314
8	0.432947	-2.644448	3.269531
1	4.627624	2.701878	-0.871142
1	1.240223	2.577672	2.779290
1	3.606383	3.068111	3.302455
1	5.316734	3.111575	1.507673
1	-0.216192	-0.194331	-2.497647
1	-0.153449	0.239312	-4.232361
1	1.365728	0.106670	-3.288032
1	-4.599386	0.453086	1.327826
1	-1.987886	1.102835	-2.050312
1	-4.694777	2.899562	1.704534
1	-2.043925	3.532219	-1.626870
1	-3.390993	4.443914	0.266772
1	-0.601856	0.900718	4.715381
1	-2.248367	1.101300	4.090888
1	-1.524345	-0.536250	4.245781
1	0.578738	-5.191222	3.500315
1	1.407221	-5.463215	1.933070
1	2.238604	-4.639706	3.281653
1	0.184906	-1.740849	2.902531
8	0.350865	-2.757717	-2.031962
8	2.147303	-0.765420	-0.616918
6	3.019188	-0.737189	0.241340
6	1.526839	-3.083161	-2.128261
8	2.765677	-0.582253	1.532859
8	2.198548	-3.656604	-1.135789
6	2.364159	-2.862642	-3.340051
1	3.068688	-2.049116	-3.123528
1	2.954127	-3.753453	-3.575512
1	1.739121	-2.581270	-4.189837
6	4.458913	-0.897406	-0.098455
1	5.117875	-0.662717	0.739653
1	4.619369	-1.935261	-0.416148
1	4.678435	-0.250918	-0.955485
1	1.807589	-0.395987	1.676545
1	1.632707	-3.653087	-0.325129

oxidative-addition-TS (Pd-Ag)

Number of imaginary frequencies : 1
 Electronic energy : =-1944.6425884
 Zero-point correction= 0.470668
 Thermal correction to Energy= 0.512371
 Thermal correction to Enthalpy= 0.513315
 Thermal correction to Gibbs Free Energy= 0.393055
 Sum of electronic and zero-point Energies= -1944.171920
 Sum of electronic and thermal Energies= -1944.130218
 Sum of electronic and thermal Enthalpies= -1944.129274
 Sum of electronic and thermal Free Energies= -1944.249533

 Cartesian Coordinates

6	-6.055723	-0.136181	0.185304
6	-5.348844	-0.378793	1.358331
6	-3.970685	-0.600117	1.326824
6	-3.351464	-0.521333	0.091587
6	-4.016859	-0.332521	-1.106844
6	-5.392545	-0.115414	-1.038740

46	-1.339638	0.342818	0.211974
53	-1.505530	-2.396519	-0.197197
47	1.218631	-1.305589	-0.026801
8	3.648184	-1.164073	0.938493
6	4.177018	-0.855338	2.007927
6	5.648875	-0.845365	2.227425
6	-0.939818	2.311504	0.527410
6	-0.609451	3.007066	-0.631472
6	-0.186533	4.330765	-0.557840
6	-0.115480	4.957185	0.682766
6	-0.468545	4.261163	1.836426
6	-0.878932	2.925823	1.770056
6	-0.710621	2.286825	-1.926952
7	-1.269484	1.066011	-1.716993
8	-1.432373	0.269961	-2.831279
6	-0.211319	-0.333261	-3.247926
8	-0.346147	2.746536	-3.012631
8	-1.189622	-0.045769	2.337589
6	-0.042823	-0.155326	2.849084
6	0.051461	-0.282147	4.340637
8	1.038080	-0.139842	2.182841
8	3.481920	-0.500106	3.063457
1	0.079384	4.851949	-1.476962
1	-1.143637	2.390970	2.680587
1	-0.421707	4.756861	2.804577
1	0.210466	5.992652	0.751523
1	0.192353	-0.986958	-2.460388
1	-0.462083	-0.938858	-4.124243
1	0.523855	0.433075	-3.520137
1	-3.409909	-0.802724	2.234097
1	-3.486149	-0.329169	-2.055328
1	-5.863559	-0.411714	2.316473
1	-5.941317	0.062830	-1.961205
1	-7.130671	0.023358	0.222550
1	0.522767	0.625729	4.736544
1	-0.932300	-0.405798	4.797714
1	0.698295	-1.125220	4.606340
1	5.899007	-1.489252	3.076830
1	6.176288	-1.185511	1.334601
1	5.969624	0.169305	2.486479
1	2.508632	-0.437394	2.820561
8	2.635643	-1.969636	-1.949399
8	1.935669	0.845469	-1.009380
6	2.402791	1.814113	-0.424668
6	3.463370	-1.162032	-2.357501
8	2.342595	1.963852	0.889919
8	4.434572	-0.679410	-1.596167
6	3.479160	-0.601773	-3.736761
1	3.230152	0.465479	-3.671910
1	4.479566	-0.678460	-4.173865
1	2.748978	-1.112430	-4.367425
6	3.108698	2.913022	-1.140618
1	3.239354	3.797902	-0.514281
1	4.092929	2.544157	-1.456225
1	2.544860	3.160350	-2.046518
1	1.823136	1.225463	1.291110
1	4.300314	-0.993139	-0.666515

oxidative-addition-product (Pd-Ag)

Number of imaginary frequencies : 0
Electronic energy : =-1944.664434
Zero-point correction= 0.472861
Thermal correction to Energy= 0.514735
Thermal correction to Enthalpy= 0.515680
Thermal correction to Gibbs Free Energy= 0.394819
Sum of electronic and zero-point Energies= -1944.191573
Sum of electronic and thermal Energies= -1944.149698
Sum of electronic and thermal Enthalpies= -1944.148754
Sum of electronic and thermal Free Energies= -1944.269615

 Cartesian Coordinates

6	-6.071777	-0.624871	-0.001043
6	-5.454188	-0.301958	1.201960
6	-4.077979	-0.071376	1.253818
6	-3.370773	-0.188046	0.072179
6	-3.941460	-0.495374	-1.149294
6	-5.319668	-0.723897	-1.166346
46	-1.341755	-0.087421	0.171108
53	-0.607945	-2.793921	-0.590090
47	1.593882	-1.095349	-0.232084
8	3.734070	-0.531391	0.936105
6	4.101094	-0.511615	2.113093
6	5.527258	-0.428965	2.526902
6	-1.536530	1.850989	0.738236
6	-1.369087	2.736177	-0.316770
6	-1.314900	4.104505	-0.062505
6	-1.438580	4.561583	1.245191
6	-1.618349	3.656823	2.288711
6	-1.672511	2.280459	2.045202
6	-1.226163	2.180817	-1.684396
7	-1.272715	0.821618	-1.636226
8	-1.293245	0.155033	-2.827444
6	0.019398	-0.050631	-3.353680
8	-1.060344	2.852800	-2.701630
8	-1.336163	-0.801107	2.177958
6	-0.192145	-0.757931	2.719523
6	-0.034106	-1.390540	4.066795
8	0.818760	-0.234717	2.165404
8	3.258861	-0.541361	3.118152
1	-1.175771	4.789849	-0.897548
1	-1.808966	1.582289	2.868439
1	-1.718323	4.018580	3.310194
1	-1.399623	5.627971	1.454306
1	0.614891	-0.707262	-2.703824
1	-0.129994	-0.541598	-4.319625
1	0.524731	0.911867	-3.499370
1	-3.594375	0.160412	2.197242
1	-3.355419	-0.582223	-2.059996
1	-6.034219	-0.226547	2.119475
1	-5.795649	-0.980355	-2.110539
1	-7.144358	-0.801760	-0.030557
1	0.593317	-0.763598	4.708358
1	-1.001137	-1.573650	4.539788
1	0.479559	-2.351294	3.936623
1	5.719748	-1.111690	3.359379
1	6.186803	-0.653637	1.687381
1	5.730851	0.587099	2.884472
1	2.313813	-0.496518	2.781069
8	3.159760	-0.875548	-2.149105
8	1.651992	1.356211	-0.682435
6	1.822138	2.330374	0.038407
6	3.732020	0.197310	-2.296482
8	1.699663	2.284824	1.357400
8	4.476178	0.754009	-1.350103
6	3.651381	1.023770	-3.531580
1	3.034702	1.904676	-3.311868
1	4.641820	1.382284	-3.827328
1	3.192799	0.453941	-4.341844
6	2.197717	3.668954	-0.496762
1	2.017841	4.464619	0.229314
1	3.263813	3.655390	-0.755329
1	1.632953	3.850535	-1.417752
1	1.390131	1.388266	1.629878
1	4.405387	0.212222	-0.526392

C-C-reductive-elimination-TS (Pd-Ag)

Number of imaginary frequencies : 1

Electronic energy : =-1715.665393
 Zero-point correction= 0.409964
 Thermal correction to Energy= 0.445094
 Thermal correction to Enthalpy= 0.446038
 Thermal correction to Gibbs Free Energy= 0.342281
 Sum of electronic and zero-point Energies= -1715.255429
 Sum of electronic and thermal Energies= -1715.220299
 Sum of electronic and thermal Enthalpies= -1715.219355
 Sum of electronic and thermal Free Energies= -1715.323112

 Cartesian Coordinates

6	-1.253379	2.742915	1.509928
6	-0.311398	1.729688	1.347929
6	0.444074	1.676501	0.181282
6	0.295546	2.608816	-0.830656
6	-0.664175	3.609419	-0.663151
6	-1.433234	3.679386	0.497905
1	-1.840662	2.768188	2.427294
1	0.902349	2.583949	-1.731689
1	-0.802024	4.344723	-1.453923
1	-2.166687	4.473934	0.614770
6	-0.084830	0.693357	2.384666
8	-0.497417	0.762335	3.544019
7	0.629248	-0.335176	1.862605
46	1.272420	-0.196430	-0.051425
8	1.166894	-1.240042	2.736440
6	0.221465	-2.237737	3.128801
1	-0.254618	-2.693455	2.252513
1	0.800621	-2.991905	3.668723
1	-0.535220	-1.801764	3.792005
6	2.692094	1.234320	0.492308
6	3.409177	1.825767	-0.540165
6	3.121169	1.288106	1.814245
6	4.611586	2.461487	-0.239619
1	3.060028	1.780590	-1.567130
6	4.329125	1.931052	2.089096
1	2.567046	0.832711	2.628617
6	5.072755	2.516516	1.071642
1	5.183200	2.918356	-1.044880
1	4.680287	1.965901	3.118157
1	6.009920	3.018956	1.299874
8	1.759974	0.002867	-2.097419
8	-0.402660	-0.032724	-2.697883
6	0.821890	0.031159	-2.961929
6	1.263506	0.110924	-4.395181
1	1.370277	-0.912960	-4.773953
1	0.508768	0.617330	-5.002652
1	2.231453	0.608833	-4.490956
47	-1.448572	-1.091741	-0.651109
53	0.760369	-2.943363	-0.577505
8	-3.030399	0.706852	-1.078801
6	-3.084620	1.667500	-1.853357
8	-2.298336	1.794277	-2.891515
6	-4.095881	2.748938	-1.707491
1	-4.987801	2.459882	-2.277099
1	-4.384046	2.857704	-0.658442
1	-3.730822	3.695589	-2.113296
1	-1.626321	1.053494	-2.931373
8	-2.598448	-1.094785	1.531824
6	-3.307337	-0.279775	2.111754
6	-3.630197	-0.356034	3.563483
1	-3.520933	-1.382638	3.918543
1	-2.915461	0.275756	4.104550
1	-4.637546	0.018539	3.762213
8	-3.845505	0.769468	1.508277
1	-3.601425	0.760580	0.546852

C-H-activation-2-PRC (Pd-Ag)

Number of imaginary frequencies : 0
 Electronic energy : =-1715.7173684
 Zero-point correction= 0.409995
 Thermal correction to Energy= 0.446431
 Thermal correction to Enthalpy= 0.447375
 Thermal correction to Gibbs Free Energy= 0.338087
 Sum of electronic and zero-point Energies= -1715.307374
 Sum of electronic and thermal Energies= -1715.270937
 Sum of electronic and thermal Enthalpies= -1715.269993
 Sum of electronic and thermal Free Energies= -1715.379282

 Cartesian Coordinates

6	4.667576	-0.615635	1.027389
6	3.550862	-1.386286	0.733919
6	2.282810	-1.029572	1.252741
6	2.161960	0.124067	2.075126
6	3.298295	0.862737	2.382227
6	4.538355	0.489541	1.866122
6	0.806758	0.605951	2.435889
6	0.318042	1.729610	1.747536
6	-0.963089	2.212534	2.016156
6	-1.764566	1.568783	2.954313
6	-1.281848	0.452696	3.632800
6	-0.003620	-0.032912	3.370904
6	1.222922	2.479710	0.827978
7	1.797285	1.760922	-0.177021
46	1.569576	-0.143689	-0.710553
8	1.439187	-2.207956	-1.333549
6	0.731001	-2.692188	-2.225261
6	0.576769	-4.157251	-2.396750
8	1.435895	3.683808	0.982079
8	2.974691	2.287450	-0.646677
6	2.799164	2.957849	-1.894748
8	0.706060	0.604027	-2.556252
6	-0.280888	1.423320	-2.514519
6	-0.502019	2.253410	-3.742177
8	-1.026044	1.572359	-1.521802
8	0.070536	-1.975586	-3.099441
53	-1.608589	-2.795087	0.783056
1	2.494888	2.257706	-2.681532
1	2.062238	3.763022	-1.782249
1	3.776373	3.384234	-2.136616
1	-1.324856	3.086945	1.475640
1	-2.770025	1.934136	3.149398
1	-1.909138	-0.051547	4.363987
1	0.369292	-0.912616	3.892645
1	1.455061	-1.744683	1.226031
1	3.206437	1.758157	2.994191
1	3.635795	-2.283169	0.124688
1	5.415432	1.085285	2.108920
1	5.638594	-0.882159	0.618824
1	0.163412	3.124600	-3.692390
1	-0.246401	1.692518	-4.644982
1	-1.534211	2.610138	-3.791558
1	1.013615	-4.454767	-3.356615
1	1.065916	-4.689594	-1.580216
1	-0.488440	-4.408234	-2.427420
1	0.260511	-1.009946	-2.979056
47	-1.436357	-0.178615	-0.023017
8	-3.613142	1.111838	0.164235
6	-4.041816	2.126370	-0.371023
8	-3.336968	2.858145	-1.219541
6	-5.414389	2.665048	-0.149943
1	-2.444915	2.439203	-1.365171
1	-5.924861	2.103912	0.634030
1	-5.365594	3.726255	0.113475
1	-5.981955	2.589002	-1.084142

C-H-activation-2-TS (Pd-Ag)

Number of imaginary frequencies : 1
Electronic energy : =-1715.6628539
Zero-point correction= 0.400224
Thermal correction to Energy= 0.437217
Thermal correction to Enthalpy= 0.438162
Thermal correction to Gibbs Free Energy= 0.325746
Sum of electronic and zero-point Energies= -1715.262630
Sum of electronic and thermal Energies= -1715.225636
Sum of electronic and thermal Enthalpies= -1715.224692
Sum of electronic and thermal Free Energies= -1715.337108

Cartesian Coordinates

6 4.690056 -1.337786 0.243660
6 3.686786 -0.379667 0.193600
6 2.335525 -0.724973 0.372525
6 2.000071 -2.081344 0.619476
6 3.029494 -3.031320 0.655753
6 4.358596 -2.668095 0.486524
6 0.602040 -2.566017 0.661683
6 -0.398069 -2.007788 1.484136
6 -1.717251 -2.483844 1.396781
6 -2.058265 -3.491927 0.500907
6 -1.063650 -4.079009 -0.275300
6 0.245012 -3.621392 -0.189388
6 -0.094174 -1.108626 2.647933
7 0.482623 0.061811 2.349433
46 1.134838 0.900411 0.640983
8 2.137820 1.952551 -1.012985
6 2.236157 3.168940 -1.208614
6 3.136442 3.723066 -2.253493
8 -0.420900 -1.473791 3.786089
8 0.877171 0.817763 3.451557
6 -0.214069 1.526779 4.027852
8 -0.081389 2.730246 0.943956
6 -1.334990 2.776070 0.720137
6 -1.971315 4.134370 0.780890
8 -2.038996 1.765760 0.484323
8 1.579352 4.081320 -0.536955
53 0.498325 -0.685484 -2.580171
1 -0.697325 2.179862 3.290185
1 -0.947925 0.835961 4.459319
1 0.222547 2.139451 4.822099
1 -2.463490 -2.068999 2.072883
1 -3.089020 -3.831038 0.431994
1 -1.308443 -4.888276 -0.959227
1 1.011113 -4.062867 -0.825043
1 1.512642 -0.635804 -1.101989
1 2.774160 -4.073855 0.839522
1 3.950446 0.658203 -0.000759
1 5.136221 -3.426774 0.540625
1 5.728482 -1.046590 0.099999
1 -1.927486 4.504349 1.811737
1 -1.402024 4.836792 0.161726
1 -3.012940 4.107048 0.451454
1 3.847976 4.414622 -1.790095
1 3.670021 2.921382 -2.765140
1 2.546114 4.300418 -2.972722
1 0.949969 3.661744 0.121331
47 -1.394648 -0.367508 -0.384032
8 -3.772118 -0.626022 -0.745921
6 -4.690225 0.187356 -0.676919
8 -4.545183 1.427550 -0.256319
6 -6.092874 -0.133539 -1.066417
1 -3.601796 1.605216 0.028880
1 -6.178990 -1.181058 -1.358091
1 -6.766795 0.082456 -0.231226
1 -6.395013 0.509202 -1.900438

C-H-activation-2-product (Pd-Ag)

Number of imaginary frequencies : 0
Electronic energy : =-1715.6750947
Zero-point correction= 0.404542
Thermal correction to Energy= 0.441382
Thermal correction to Enthalpy= 0.442326
Thermal correction to Gibbs Free Energy= 0.332003
Sum of electronic and zero-point Energies= -1715.270553
Sum of electronic and thermal Energies= -1715.233712
Sum of electronic and thermal Enthalpies= -1715.232768
Sum of electronic and thermal Free Energies= -1715.343092

Cartesian Coordinates

6 5.204504 0.232857 -0.696841
6 4.062667 0.680408 -0.034210
6 2.878351 -0.052039 -0.094944
6 2.828753 -1.257894 -0.808888
6 3.985608 -1.685142 -1.479057
6 5.163927 -0.953226 -1.422807
6 1.600805 -2.077944 -0.921072
6 0.829807 -2.446842 0.204810
6 -0.316814 -3.245480 0.031022
6 -0.725792 -3.646761 -1.241153
6 0.045399 -3.301011 -2.344497
6 1.196440 -2.537003 -2.179089
6 1.257593 -2.194141 1.629382
7 1.326089 -0.895672 1.974252
46 1.312373 0.765732 0.813285
8 1.491220 2.476847 -0.547321
6 0.922835 3.576398 -0.539882
6 1.089227 4.545845 -1.654647
8 1.437448 -3.151766 2.391452
8 1.837024 -0.694781 3.256167
6 0.778520 -0.461479 4.171427
8 -0.350639 1.905895 1.870206
6 -1.555576 1.586059 2.112542
6 -2.440120 2.644060 2.706867
8 -2.026093 0.434539 1.919648
8 0.123621 3.983596 0.410441
53 -1.232494 0.924183 -2.369879
1 0.276298 0.493695 3.961034
1 0.045314 -1.278890 4.146482
1 1.239708 -0.414274 5.162565
1 -0.857451 -3.580123 0.916174
1 -1.628304 -4.241977 -1.356153
1 -0.249732 -3.623169 -3.340458
1 1.789056 -2.260787 -3.049965
1 0.323283 1.336765 -2.197966
1 3.956453 -2.624728 -2.030029
1 4.097409 1.614921 0.525119
1 6.051485 -1.313394 -1.938403
1 6.123765 0.813157 -0.641740
1 -2.299731 2.642253 3.794479
1 -2.164099 3.637215 2.339246
1 -3.494558 2.442144 2.498595
1 1.423134 5.511504 -1.261682
1 1.804670 4.168821 -2.386947
1 0.116946 4.711247 -2.132942
1 -0.021278 3.260793 1.096474
47 -1.130319 -0.793101 0.108108
8 -3.490757 -1.345071 -0.353821
6 -4.510677 -0.897466 0.162576
8 -4.512205 -0.068050 1.187970
6 -5.883910 -1.246447 -0.300661
1 -3.580743 0.122193 1.503860
1 -5.841102 -1.884894 -1.184150
1 -6.413998 -1.764577 0.506064
1 -6.447347 -0.334009 -0.521194

C-N-reductive-elimination-PRC (Pd-Ag)

Number of imaginary frequencies : 0
Electronic energy : =-1715.7256394
Zero-point correction= 0.408512
Thermal correction to Energy= 0.445934
Thermal correction to Enthalpy= 0.446878
Thermal correction to Gibbs Free Energy= 0.333333
Sum of electronic and zero-point Energies= -1715.317127
Sum of electronic and thermal Energies= -1715.279705
Sum of electronic and thermal Enthalpies= -1715.278761
Sum of electronic and thermal Free Energies= -1715.392306

Cartesian Coordinates

6	-1.319943	3.045408	-0.556723
8	-1.741272	4.137261	-0.959612
7	-1.934250	1.862326	-0.723819
8	-3.109631	1.950509	-1.486424
6	-2.841408	1.735037	-2.868331
1	-2.088213	2.446842	-3.227022
1	-2.494720	0.706496	-3.042595
1	-3.787404	1.900785	-3.391370
6	-0.070405	2.966487	0.265365
6	-0.009365	3.818387	1.370490
6	1.129004	3.885668	2.161159
6	2.243495	3.125011	1.817880
6	2.199575	2.297712	0.702469
6	1.045300	2.187042	-0.084781
1	-0.875542	4.437951	1.595624
1	1.153831	4.541327	3.028778
1	3.152474	3.179506	2.414119
1	3.078829	1.712805	0.435511
46	-1.393188	-0.062491	-0.303899
6	1.088165	1.312453	-1.287673
6	0.164326	0.271742	-1.531861
6	2.139139	1.500712	-2.199884
6	0.297573	-0.514901	-2.686092
6	2.268775	0.710710	-3.334887
1	2.851876	2.303905	-2.013742
6	1.341955	-0.296421	-3.583009
1	-0.415271	-1.315568	-2.877744
1	3.088605	0.887415	-4.027841
1	1.428213	-0.920060	-4.470419
8	-3.109549	-0.274721	1.181341
6	-4.316261	-0.157983	0.972715
8	-4.830723	0.422513	-0.089334
6	-5.346866	-0.675185	1.913186
1	-4.875385	-1.178876	2.757730
1	-5.967338	0.154650	2.267346
1	-6.006433	-1.369925	1.382380
1	-4.143105	0.872518	-0.650529
53	-1.067467	-2.802192	0.165475
47	1.354550	-1.418854	-0.077714
8	2.043385	-0.565338	2.137008
6	1.335398	0.050027	2.932164
8	0.034832	0.200915	2.766356
6	1.840527	0.649355	4.194793
1	1.647494	-0.059646	5.009149
1	2.916890	0.819178	4.127957
1	1.309679	1.576336	4.426333
1	-0.267336	-0.237330	1.939748
8	3.590636	-1.320622	-0.777145
6	4.493512	-0.640128	-0.303605
6	5.671301	-0.178856	-1.086429
1	5.623640	0.912569	-1.183325
1	6.597644	-0.416292	-0.554364
1	5.670651	-0.634537	-2.077507
8	4.512997	-0.219513	0.951297

1 3.691033 -0.481182 1.430673

C-N-reductive-elimination-TS (Pd-Ag)

Number of imaginary frequencies : 1

Electronic energy : =-1715.7026125

Zero-point correction= 0.407830

Thermal correction to Energy= 0.444965

Thermal correction to Enthalpy= 0.445910

Thermal correction to Gibbs Free Energy= 0.333299

Sum of electronic and zero-point Energies= -1715.294783

Sum of electronic and thermal Energies= -1715.257647

Sum of electronic and thermal Enthalpies= -1715.256703

Sum of electronic and thermal Free Energies= -1715.369313

Cartesian Coordinates

6 -1.149610 2.143031 0.195385
8 -0.628999 3.221702 0.507302
7 -1.100575 1.027731 0.965976
8 -0.526808 1.158610 2.219424
6 -1.369215 1.891812 3.109288
1 -1.434217 2.943326 2.808482
1 -2.372523 1.449277 3.151380
1 -0.896397 1.821222 4.093147
6 -1.900743 1.980517 -1.084417
6 -1.438463 2.728681 -2.169423
6 -2.111144 2.719546 -3.382400
6 -3.283728 1.978661 -3.510499
6 -3.766820 1.248548 -2.433598
6 -3.088669 1.224185 -1.209280
1 -0.533880 3.319695 -2.038431
1 -1.726828 3.290983 -4.224022
1 -3.822196 1.964860 -4.455539
1 -4.676517 0.661080 -2.544379
46 -1.017108 -0.860588 0.108164
6 -3.634825 0.453414 -0.079106
6 -2.785260 -0.214038 0.809045
6 -5.008938 0.361173 0.176464
6 -3.226444 -0.833595 1.971591
6 -5.486437 -0.314004 1.294809
1 -5.706377 0.861158 -0.494436
6 -4.600658 -0.901564 2.196618
1 -2.513285 -1.267521 2.671784
1 -6.557047 -0.356518 1.480579
1 -4.975742 -1.409116 3.082957
8 2.129497 -0.380612 1.796649
6 1.474424 -0.694937 2.793386
8 0.574774 -1.656187 2.767716
6 1.659292 -0.063501 4.124204
1 1.827756 1.010052 3.996281
1 0.804385 -0.248397 4.777562
1 2.556612 -0.489018 4.588883
1 0.452993 -1.975055 1.844804
53 0.175831 -2.974775 -1.111040
47 1.645912 -0.532485 -0.781451
8 4.043819 -0.463948 -1.144128
6 4.771328 0.278906 -0.498214
6 5.926974 1.019473 -1.072050
1 5.648620 2.076475 -1.164679
1 6.791964 0.965024 -0.405210
1 6.173827 0.627914 -2.059776
8 4.591450 0.529283 0.791801
1 3.811832 0.038823 1.133226
8 1.889353 1.882951 -0.804544
6 2.072260 2.710538 0.082832
8 2.202381 2.393221 1.360371
6 2.241288 4.167943 -0.169887
1 1.687983 4.745726 0.574830
1 3.303971 4.420398 -0.071753

1	1.905075	4.419441	-1.177252
1	2.092729	1.424081	1.482265

C-N-reductive-elimination-product (Pd-Ag)

Number of imaginary frequencies : 0
 Electronic energy : =-1715.7884469
 Zero-point correction= 0.411497
 Thermal correction to Energy= 0.448037
 Thermal correction to Enthalpy= 0.448982
 Thermal correction to Gibbs Free Energy= 0.338642
 Sum of electronic and zero-point Energies= -1715.376949
 Sum of electronic and thermal Energies= -1715.340409
 Sum of electronic and thermal Enthalpies= -1715.339465
 Sum of electronic and thermal Free Energies= -1715.449804

 Cartesian Coordinates

6	-2.942671	-0.648747	1.015414
8	-3.254900	-0.230000	2.140140
7	-1.947690	-1.582408	0.849069
8	-1.231344	-1.921104	1.968872
6	-1.881283	-2.959855	2.709701
1	-2.849747	-2.621224	3.093739
1	-2.010232	-3.855868	2.090133
1	-1.206958	-3.175394	3.542775
6	-3.582226	-0.210449	-0.219746
6	-4.639979	0.704586	-0.113225
6	-5.245056	1.203690	-1.248637
6	-4.787002	0.793018	-2.506871
6	-3.740174	-0.101717	-2.623044
6	-3.107944	-0.628986	-1.482479
1	-4.960710	1.012838	0.878816
1	-6.067474	1.910101	-1.167893
1	-5.256997	1.183560	-3.406897
1	-3.407344	-0.393737	-3.615313
46	1.537317	-1.823582	-0.757041
6	-1.987272	-1.548902	-1.557786
6	-1.416588	-2.016227	-0.366756
6	-1.422819	-1.996250	-2.776362
6	-0.341955	-2.944388	-0.359873
6	-0.362888	-2.870436	-2.802774
1	-1.834887	-1.642088	-3.717085
6	0.183102	-3.378268	-1.596957
1	-0.087367	-3.455922	0.564472
1	0.039044	-3.208663	-3.754694
1	0.855222	-4.234764	-1.627006
8	-0.429885	1.031523	2.410790
6	-0.335221	0.335043	3.425445
8	-1.386816	-0.099399	4.079852
6	0.969286	-0.111438	3.976113
1	1.757239	0.601507	3.720820
1	0.915042	-0.270087	5.055860
1	1.210458	-1.073042	3.500431
1	-2.178747	-0.024688	3.479732
53	3.578268	-0.117480	-0.255358
47	0.882434	0.608174	0.443994
8	-1.061059	1.707325	-0.719843
6	-1.838151	2.540386	-0.249648
8	-2.149370	2.601435	1.025520
6	-2.472376	3.601230	-1.078364
1	-1.778342	4.451555	-1.120825
1	-2.626675	3.236402	-2.096797
1	-3.410451	3.948063	-0.638801
1	-1.628597	1.942519	1.553236
8	1.291605	3.203029	0.438821
6	1.675868	3.549286	-0.669228
8	1.081995	3.162050	-1.796965
1	0.324152	2.570793	-1.581787
6	2.870506	4.402479	-0.914947

1	3.705696	3.741402	-1.179448
1	2.706132	5.083906	-1.753743
1	3.133376	4.953552	-0.010401

Reaction 3

Coordinates for monometallic pathway

C-H-activation-PRC

Number of imaginary frequencies : 0
The smallest frequency is : 38.7478 cm(-1)

Electronic energy : =-1795.5897503
Zero-point correction= 0.267654
Thermal correction to Energy= 0.292645
Thermal correction to Enthalpy= 0.293589
Thermal correction to Gibbs Free Energy= 0.212738
Sum of electronic and zero-point Energies= -1795.322096
Sum of electronic and thermal Energies= -1795.297106
Sum of electronic and thermal Enthalpies= -1795.296161
Sum of electronic and thermal Free Energies= -1795.377012

Cartesian Coordinates

6	0.958401	-0.708744	2.061749
6	0.749012	0.425607	2.836301
6	2.003479	-0.724670	1.139551
6	2.846912	0.373724	0.996561
1	3.652357	0.342686	0.265633
6	2.628600	1.506474	1.775200
8	1.635341	-0.946719	-1.644684
46	0.343772	0.534440	-0.976259
8	1.399990	2.278521	-1.289948
6	0.421954	2.957869	-0.826365
8	-0.627238	2.309085	-0.514120
6	0.529159	4.418245	-0.612919
1	1.218367	4.860626	-1.336616
1	-0.455281	4.887840	-0.680307
1	0.927500	4.592440	0.394349
1	3.278639	2.370610	1.658519
1	0.300212	-1.572171	2.137542
1	-0.075190	0.446482	3.544730
6	1.583129	1.532961	2.693439
1	1.413235	2.420182	3.299096
7	2.232077	-1.908084	0.356124
6	2.610071	-3.127214	1.075456
1	2.705121	-2.883968	2.134650
1	1.849073	-3.907880	0.965565
1	3.575291	-3.511250	0.727962
6	2.068958	-1.916976	-0.979429
6	2.443980	-3.153942	-1.731147
1	1.808885	-3.994277	-1.426781
1	2.296069	-2.972877	-2.796326
1	3.486041	-3.437609	-1.549325
8	-3.002766	-2.257643	-0.737091
16	-2.396019	-0.939798	-0.646574
8	-2.795469	0.110036	-1.569675
8	-0.880552	-1.061402	-0.495107
6	-2.869115	-0.325697	1.020038
9	-4.185393	-0.180236	1.075065
9	-2.494996	-1.196784	1.952837
9	-2.293360	0.840069	1.276092

C-H-activation-TS

Number of imaginary frequencies : 1
The smallest frequency is : -1394.7439 cm(-1)

Electronic energy : =-1795.5641717
Zero-point correction= 0.261435
Thermal correction to Energy= 0.286375
Thermal correction to Enthalpy= 0.287320
Thermal correction to Gibbs Free Energy= 0.204719
Sum of electronic and zero-point Energies= -1795.302736
Sum of electronic and thermal Energies= -1795.277796
Sum of electronic and thermal Enthalpies= -1795.276852
Sum of electronic and thermal Free Energies= -1795.359453

Cartesian Coordinates

6	3.960078	-0.062592	1.475976
6	3.868372	0.936967	2.437581
6	2.983796	-0.171985	0.488392
6	1.934708	0.771252	0.420949
1	1.698620	1.332405	-0.695691
6	1.855979	1.753586	1.430147
8	0.884617	-1.856048	-0.197103
46	0.097540	0.059979	-0.283317
8	1.373660	2.370675	-1.640825
6	0.172046	2.648268	-1.405682
8	-0.613556	1.936161	-0.693076
6	-0.432255	3.887585	-1.995812
1	0.345646	4.599760	-2.276438
1	-0.992267	3.602713	-2.893328
1	-1.140087	4.338509	-1.296588
1	1.041442	2.474171	1.388839
1	4.772216	-0.783662	1.525931
1	4.626636	0.995163	3.214800
6	2.809355	1.842271	2.429252
1	2.737056	2.612580	3.191924
7	3.082623	-1.252392	-0.433546
6	4.409434	-1.588716	-0.953528
1	5.009161	-0.677615	-0.992492
1	4.920382	-2.332906	-0.330971
1	4.324801	-1.975838	-1.971121
6	2.032468	-2.090120	-0.630218
6	2.260134	-3.368098	-1.368148
1	3.119261	-3.923487	-0.979335
1	1.357603	-3.974510	-1.282340
1	2.439876	-3.166671	-2.430945
8	-3.570937	-2.299008	-0.336410
16	-2.638913	-1.316036	0.194534
8	-1.753745	-0.740737	-0.896311
8	-1.917371	-1.609616	1.428177
6	-3.678938	0.135384	0.619232
9	-4.268776	0.623012	-0.463320
9	-4.614515	-0.226090	1.490075
9	-2.936190	1.088572	1.170815

C-H-activation-product

Number of imaginary frequencies : 0
The smallest frequency is : 18.8092 cm(-1)

Electronic energy : =-1795.6128093
Zero-point correction= 0.268828
Thermal correction to Energy= 0.293701
Thermal correction to Enthalpy= 0.294645
Thermal correction to Gibbs Free Energy= 0.212931
Sum of electronic and zero-point Energies= -1795.343982
Sum of electronic and thermal Energies= -1795.319108
Sum of electronic and thermal Enthalpies= -1795.318164

Sum of electronic and thermal Free Energies= -1795.399879

Cartesian Coordinates

6	4.471817	0.775977	0.667270
6	4.441590	2.016979	1.286870
6	3.295324	0.180812	0.191939
6	2.082594	0.857817	0.359489
1	-1.889064	0.468209	-1.669694
6	2.059549	2.099007	0.990680
8	1.261600	-1.769892	0.051745
46	0.368735	0.058516	-0.162019
8	-2.099034	1.401370	-1.946435
6	-1.428164	2.265993	-1.236210
8	-0.485335	1.984524	-0.485571
6	-1.904592	3.666735	-1.380040
1	-2.108877	3.892509	-2.430206
1	-2.851548	3.761558	-0.835330
1	-1.178652	4.367347	-0.966639
1	1.110952	2.616725	1.109379
1	5.422042	0.257216	0.573117
1	5.368518	2.453336	1.650656
6	3.234319	2.684837	1.450391
1	3.200876	3.657353	1.935954
7	3.402780	-1.105891	-0.427742
6	4.678627	-1.457344	-1.049501
1	5.104217	-0.561222	-1.505869
1	5.393711	-1.865654	-0.325039
1	4.523688	-2.187524	-1.844217
6	2.419522	-2.027422	-0.343757
6	2.706060	-3.445464	-0.724648
1	3.647119	-3.809689	-0.302115
1	1.878570	-4.062391	-0.371096
1	2.759902	-3.544482	-1.815534
8	-3.169842	-2.638872	0.007598
16	-2.387145	-1.472133	0.380342
8	-1.579536	-0.911835	-0.780148
8	-1.626244	-1.488332	1.623127
6	-3.623036	-0.132948	0.620688
9	-4.409530	-0.025305	-0.441615
9	-4.366466	-0.384483	1.685164
9	-2.999889	1.035871	0.800525

oxidative-addition-PRC

Number of imaginary frequencies : 0
The smallest frequency is : 29.7593 cm(-1)

Electronic energy :	=-2529.6870107
Zero-point correction=	0.564045
Thermal correction to Energy=	0.607888
Thermal correction to Enthalpy=	0.608832
Thermal correction to Gibbs Free Energy=	0.488857
Sum of electronic and zero-point Energies=	-2529.122965
Sum of electronic and thermal Energies=	-2529.079123
Sum of electronic and thermal Enthalpies=	-2529.078179
Sum of electronic and thermal Free Energies=	-2529.198154

Cartesian Coordinates

6	-0.731866	1.743173	-1.962330
6	-0.593652	2.826587	-2.825086
6	0.191332	3.908204	-2.447163
6	0.814762	3.916092	-1.208170
6	0.694342	2.832516	-0.324722
6	-0.078732	1.742266	-0.736780
7	1.360765	2.924165	0.938752
6	2.562340	3.752295	1.017089
46	-0.379239	0.193302	0.448990

35	-0.753172	-2.181064	-2.235351
6	0.215712	-1.205563	-0.975975
6	1.308648	-0.854549	-0.451381
14	3.142565	-0.640187	-0.156055
6	3.386615	0.021423	1.606303
6	0.796599	2.437482	2.083507
8	-0.177705	1.674523	2.084095
6	1.397747	2.843577	3.396165
8	-0.541361	-1.484934	2.016230
6	-0.827024	-2.680577	2.010988
6	-0.072812	-3.680617	2.824458
8	-1.819765	-3.200103	1.336987
6	3.881291	-2.356926	-0.493995
6	3.743103	0.695271	-1.377576
1	-1.374277	0.908562	-2.236711
1	1.386083	4.791758	-0.910755
1	0.306581	4.764113	-3.107425
1	3.090793	3.703476	0.061978
1	2.334073	4.802218	1.240675
1	3.239235	3.370468	1.785479
1	1.538055	3.926230	3.476333
1	0.732556	2.498584	4.189123
1	2.377455	2.367207	3.536891
1	3.586506	1.642927	-0.828919
1	2.846117	0.981007	1.549751
1	4.966804	-2.265998	-0.316883
1	-1.105921	2.818013	-3.783900
1	-0.010749	-4.638643	2.301498
1	-0.613692	-3.851157	3.762409
1	0.924890	-3.302670	3.059280
1	-2.389616	-2.491276	0.921607
16	-3.540172	-0.122887	-0.141848
6	-5.197474	0.529500	0.294290
9	-5.307687	1.788109	-0.110865
9	-6.136065	-0.195377	-0.300264
9	-5.386642	0.481776	1.605350
8	-3.451637	0.013963	-1.593415
8	-2.642736	0.765620	0.643730
8	-3.589546	-1.510585	0.365698
6	4.848926	0.332036	1.920672
1	4.950192	0.754212	2.931947
1	5.470249	-0.575424	1.894618
1	5.288786	1.055972	1.222379
6	2.755285	-0.798038	2.728010
1	2.763572	-0.232423	3.672118
1	1.711966	-1.071123	2.521139
1	3.323178	-1.719418	2.915900
6	5.235060	0.564679	-1.691420
1	5.586161	1.425379	-2.277543
1	5.866314	0.501323	-0.795738
1	5.438526	-0.331076	-2.293494
6	2.931557	0.772777	-2.669209
1	3.007189	-0.155254	-3.252617
1	1.866398	0.951789	-2.481733
1	3.297310	1.587962	-3.310020
6	3.661724	-2.787322	-1.944123
1	4.094487	-2.088978	-2.670275
1	4.112228	-3.772488	-2.128739
1	2.590418	-2.880023	-2.174846
6	3.321277	-3.419153	0.450993
1	3.709651	-4.414143	0.192245
1	3.578829	-3.231701	1.499838
1	2.224112	-3.473640	0.379362

oxidative-addition-TS

Number of imaginary frequencies : 1

The smallest frequency is : -182.9316 cm(-1)

Electronic energy : =-2529.6486172
 Zero-point correction= 0.561686
 Thermal correction to Energy= 0.605834
 Thermal correction to Enthalpy= 0.606779
 Thermal correction to Gibbs Free Energy= 0.484740
 Sum of electronic and zero-point Energies= -2529.086931
 Sum of electronic and thermal Energies= -2529.042783
 Sum of electronic and thermal Enthalpies= -2529.041839
 Sum of electronic and thermal Free Energies= -2529.163878

 Cartesian Coordinates

6	-1.608445	2.397774	-1.364847
6	-1.561474	3.730928	-1.767019
6	-0.667609	4.603617	-1.160376
6	0.164256	4.159718	-0.143171
6	0.140876	2.822751	0.279268
6	-0.744414	1.967423	-0.374800
7	0.988525	2.440693	1.356894
6	2.257909	3.147027	1.513844
46	-0.844734	0.051638	0.139759
35	-0.342245	-0.844598	-2.253892
6	0.997094	-0.196798	-0.615154
6	2.206808	-0.172720	-0.380971
14	4.003162	-0.385549	-0.045661
6	4.187718	-0.611905	1.835931
6	0.575745	1.545785	2.288302
8	-0.435295	0.835655	2.134264
6	1.357939	1.411039	3.556407
8	-0.643837	-2.075895	0.967136
6	-0.931731	-3.224085	0.633917
6	-0.064423	-4.390984	0.971922
8	-1.997388	-3.556810	-0.044649
6	4.504173	-1.909486	-1.064717
6	4.912694	1.210496	-0.553971
1	-2.322232	1.712643	-1.817265
1	0.825281	4.864128	0.355499
1	-0.627686	5.646671	-1.463390
1	2.643800	3.404428	0.523594
1	2.154029	4.062441	2.109120
1	2.990374	2.494196	1.994060
1	1.554197	2.380110	4.026453
1	0.788727	0.776882	4.237822
1	2.322449	0.923459	3.361340
1	4.876418	1.843823	0.351735
1	3.993699	0.407375	2.223475
1	5.575209	-2.094911	-0.875982
1	-2.227987	4.072969	-2.554458
1	0.307597	-4.839573	0.044055
1	-0.649399	-5.158900	1.487496
1	0.776676	-4.077309	1.591663
1	-2.602047	-2.780418	-0.205602
16	-4.029571	-0.323470	-0.284289
6	-5.598357	-0.147893	0.650375
9	-5.824693	1.130878	0.915846
9	-6.602570	-0.623309	-0.072398
9	-5.531304	-0.820754	1.790173
8	-4.213467	0.457713	-1.503263
8	-3.045166	0.237737	0.687697
8	-3.902600	-1.782201	-0.469105
6	5.610380	-0.994447	2.238470
1	5.706659	-1.082927	3.329896
1	5.899621	-1.965748	1.812976
1	6.352236	-0.256515	1.907493
6	3.168994	-1.560257	2.465168
1	3.185263	-1.487727	3.562653
1	2.139792	-1.369190	2.127856
1	3.401895	-2.604412	2.219410
6	6.383959	0.973898	-0.896243
1	6.904777	1.925935	-1.070393

1	6.931143	0.445998	-0.104384
1	6.491082	0.381363	-1.814469
6	4.215269	1.968099	-1.682527
1	4.205482	1.384604	-2.613888
1	3.167840	2.201555	-1.447361
1	4.732014	2.913640	-1.901729
6	4.308807	-1.647844	-2.557870
1	4.904474	-0.803444	-2.925841
1	4.590043	-2.529502	-3.150864
1	3.255685	-1.428347	-2.785211
6	3.707667	-3.145475	-0.645023
1	3.911840	-3.988730	-1.320003
1	3.949112	-3.478935	0.371504
1	2.623585	-2.952609	-0.681045

oxidative-addition-product

Number of imaginary frequencies : 0
 The smallest frequency is : 23.5198 cm(-1)

Electronic energy : =-2529.6631483
 Zero-point correction= 0.563550
 Thermal correction to Energy= 0.607709
 Thermal correction to Enthalpy= 0.608654
 Thermal correction to Gibbs Free Energy= 0.487426
 Sum of electronic and zero-point Energies= -2529.099598
 Sum of electronic and thermal Energies= -2529.055439
 Sum of electronic and thermal Enthalpies= -2529.054495
 Sum of electronic and thermal Free Energies= -2529.175722

 Cartesian Coordinates

6	-1.704633	2.387223	-1.429210
6	-1.828996	3.739502	-1.739640
6	-1.088910	4.685767	-1.042671
6	-0.236440	4.291692	-0.023408
6	-0.083099	2.937348	0.303487
6	-0.818039	2.013702	-0.435419
7	0.778123	2.603841	1.386230
6	2.010228	3.375490	1.553255
46	-0.762771	0.076625	0.100561
35	-0.782165	-0.872354	-2.218071
6	1.147475	0.077254	-0.177070
6	2.371005	0.030382	-0.185634
14	4.171457	-0.352734	-0.090130
6	4.513491	-0.619249	1.764863
6	0.475563	1.610567	2.240525
8	-0.479883	0.816689	2.049944
6	1.308665	1.422215	3.462380
8	-0.559773	-2.019521	1.018027
6	-0.824330	-3.180838	0.709984
6	0.020969	-4.328173	1.154699
8	-1.847330	-3.551050	-0.013180
6	4.433337	-1.876701	-1.191439
6	5.175926	1.156172	-0.676019
1	-2.310991	1.651094	-1.948927
1	0.300205	5.040577	0.554693
1	-1.189799	5.742592	-1.275207
1	2.283846	3.809345	0.590008
1	1.894172	4.178517	2.290287
1	2.826200	2.716782	1.861805
1	1.527235	2.362031	3.977425
1	0.790746	0.735523	4.133682
1	2.260916	0.956826	3.167708
1	5.335929	1.756931	0.237552
1	4.374980	0.397815	2.180877
1	5.511368	-2.110619	-1.168997

1	-2.513779	4.039004	-2.528572
1	0.388837	-4.867435	0.275174
1	-0.584907	-5.032036	1.734325
1	0.861954	-3.973969	1.752860
1	-2.450053	-2.796938	-0.253579
16	-3.973992	-0.428527	-0.349904
6	-5.408726	-0.323665	0.788131
9	-5.592155	0.930317	1.173657
9	-6.494983	-0.747639	0.159735
9	-5.202860	-1.079412	1.855911
8	-4.318039	0.414871	-1.486118
8	-2.896962	0.119244	0.544630
8	-3.827956	-1.870113	-0.605896
6	5.954213	-1.042826	2.042785
1	6.136869	-1.153580	3.121224
1	6.180298	-2.014783	1.580807
1	6.685880	-0.318024	1.662941
6	3.527141	-1.546129	2.472795
1	3.627768	-1.467419	3.565251
1	2.480836	-1.332408	2.211316
1	3.717798	-2.595842	2.215273
6	6.548269	0.762316	-1.222855
1	7.153665	1.651182	-1.449317
1	7.126652	0.142876	-0.524875
1	6.454864	0.194073	-2.157836
6	4.425971	2.026294	-1.683202
1	4.212844	1.479002	-2.611641
1	3.459531	2.374602	-1.295600
1	5.018700	2.910314	-1.959572
6	4.028989	-1.571870	-2.634279
1	4.602351	-0.746860	-3.074627
1	4.178912	-2.451936	-3.275453
1	2.964667	-1.303355	-2.695665
6	3.653784	-3.089470	-0.685580
1	3.747015	-3.931240	-1.386539
1	4.002037	-3.441180	0.293662
1	2.580724	-2.858338	-0.598985

reductive-elimination-PRC

Number of imaginary frequencies : 0
The smallest frequency is : 20.2033 cm(-1)

Electronic energy : =-2529.6627457
Zero-point correction= 0.562560
Thermal correction to Energy= 0.607210
Thermal correction to Enthalpy= 0.608154
Thermal correction to Gibbs Free Energy= 0.484839
Sum of electronic and zero-point Energies= -2529.100186
Sum of electronic and thermal Energies= -2529.055536
Sum of electronic and thermal Enthalpies= -2529.054592
Sum of electronic and thermal Free Energies= -2529.177907

Cartesian Coordinates

6	-1.145490	2.259878	-1.507465
6	-1.042257	3.603007	-1.861147
6	-0.308353	4.475414	-1.068138
6	0.310003	4.017338	0.084534
6	0.224990	2.670423	0.463100
6	-0.498973	1.817318	-0.367980
7	0.868506	2.277835	1.671642
6	2.121230	2.945337	2.027483
46	-0.783131	-0.093861	0.190530
35	-0.753770	-1.113586	-2.098289
6	1.137508	-0.280842	0.049268
6	2.361680	-0.318831	0.031680
14	4.198411	-0.357988	-0.142919

6	4.946866	-1.121881	1.436774
6	0.341081	1.344094	2.481636
8	-0.636757	0.630380	2.150231
6	0.931028	1.124058	3.833645
8	-0.959180	-2.165501	1.149308
6	-1.434957	-3.274199	0.911073
6	-0.890518	-4.514972	1.537223
8	-2.455249	-3.504326	0.128328
6	4.572358	-1.386595	-1.693039
6	4.745724	1.464689	-0.238451
1	-1.728035	1.576705	-2.116791
1	0.849379	4.712651	0.723084
1	-0.228553	5.525830	-1.335001
1	2.639291	3.228550	1.107534
1	1.950861	3.837878	2.640422
1	2.769304	2.254808	2.572059
1	1.143534	2.058148	4.361341
1	0.238841	0.514852	4.416578
1	1.870282	0.564002	3.727202
1	4.536381	1.834613	0.782607
1	5.081803	-0.263321	2.120106
1	5.671024	-1.453370	-1.773866
1	-1.541363	3.953003	-2.760822
1	-0.714512	-5.273945	0.768905
1	-1.631208	-4.924460	2.232510
1	0.034490	-4.297187	2.072411
1	-2.879813	-2.676165	-0.218488
16	-4.002387	-0.107930	-0.524629
6	-5.475104	0.255943	0.510629
9	-5.494043	1.540600	0.833508
9	-6.573987	-0.035383	-0.169942
9	-5.449447	-0.468955	1.619436
8	-4.127055	0.751741	-1.692345
8	-2.913664	0.281517	0.437450
8	-4.072521	-1.560730	-0.747437
6	6.319808	-1.747319	1.187920
1	6.781329	-2.074257	2.130361
1	6.239577	-2.636717	0.548691
1	7.026129	-1.062465	0.700946
6	4.023822	-2.126925	2.123079
1	4.473991	-2.506927	3.051612
1	3.047547	-1.694357	2.373459
1	3.827293	-2.996282	1.480792
6	6.245462	1.615595	-0.484994
1	6.539450	2.674752	-0.510915
1	6.846855	1.133250	0.296188
1	6.543785	1.178997	-1.448687
6	3.942388	2.324154	-1.212243
1	4.200663	2.101417	-2.255723
1	2.858105	2.174230	-1.113082
1	4.153247	3.393557	-1.060151
6	4.023364	-0.733326	-2.960443
1	4.511427	0.221125	-3.191473
1	4.168471	-1.389430	-3.830445
1	2.943020	-0.543899	-2.876541
6	4.009580	-2.800790	-1.553610
1	4.222368	-3.396292	-2.452613
1	4.429850	-3.343009	-0.697380
1	2.917321	-2.779764	-1.430157

reductive-elimination-TS

Number of imaginary frequencies : 1
The smallest frequency is : -340.9629 cm(-1)

Electronic energy : =-2529.6525482
Zero-point correction= 0.560782
Thermal correction to Energy= 0.605390

Thermal correction to Enthalpy= 0.606334
 Thermal correction to Gibbs Free Energy= 0.481681
 Sum of electronic and zero-point Energies= -2529.091766
 Sum of electronic and thermal Energies= -2529.047158
 Sum of electronic and thermal Enthalpies= -2529.046214
 Sum of electronic and thermal Free Energies= -2529.170867

.....
 Cartesian Coordinates

6	-0.167840	1.907786	-1.716423
6	-0.041538	3.232226	-2.122009
6	0.328488	4.211650	-1.209461
6	0.583987	3.867059	0.110336
6	0.473470	2.542737	0.540056
6	0.081398	1.572788	-0.390461
7	0.841309	2.247613	1.885017
6	2.022932	2.923563	2.425673
46	-0.778344	-0.171193	0.287215
35	-0.713773	-1.495952	-1.841226
6	1.160293	-0.117580	0.089032
6	2.378063	-0.286496	0.092269
14	4.203247	-0.426732	-0.169241
6	4.978211	-1.450221	1.237521
6	0.134990	1.396585	2.650921
8	-0.781990	0.672179	2.201946
6	0.440256	1.300133	4.108966
8	-1.301632	-2.149336	1.363729
6	-2.064292	-3.108497	1.281698
6	-1.864407	-4.339171	2.106132
8	-3.108363	-3.198804	0.499836
6	4.395280	-1.252390	-1.866422
6	4.857590	1.357150	-0.042055
1	-0.469229	1.146603	-2.428093
1	0.871786	4.633224	0.826526
1	0.414581	5.249763	-1.518551
1	2.682217	3.182313	1.593797
1	1.760949	3.835122	2.975419
1	2.569171	2.249208	3.089787
1	0.589740	2.279333	4.572766
1	-0.384855	0.780219	4.598304
1	1.350568	0.704737	4.254254
1	4.707717	1.592449	1.028153
1	5.238059	-0.707153	2.012250
1	5.476571	-1.381015	-2.043599
1	-0.245996	3.488152	-3.158175
1	-1.659079	-5.186733	1.443431
1	-2.780989	-4.573990	2.655832
1	-1.032509	-4.204709	2.798235
1	-3.301916	-2.396648	-0.052375
16	-3.888989	0.114087	-0.737921
6	-5.446779	0.728072	0.010875
9	-5.298304	1.983822	0.409978
9	-6.415747	0.675014	-0.892623
9	-5.789484	-0.016237	1.052764
8	-3.623483	1.022445	-1.843210
8	-2.957941	0.230288	0.433005
8	-4.179479	-1.292098	-1.068609
6	6.271160	-2.139013	0.798040
1	6.764738	-2.629685	1.648720
1	6.074678	-2.919869	0.051181
1	6.999605	-1.446033	0.356660
6	4.018500	-2.460005	1.864305
1	4.503425	-3.001439	2.689372
1	3.114496	-1.983478	2.262624
1	3.685965	-3.213168	1.137174
6	6.352800	1.457183	-0.336194
1	6.713720	2.489028	-0.218583
1	6.955176	0.827897	0.331641
1	6.581458	1.157755	-1.369179
6	4.070440	2.380469	-0.857593

1	4.280678	2.285123	-1.930429
1	2.983578	2.272145	-0.734344
1	4.342926	3.408639	-0.575179
6	3.809621	-0.397869	-2.988840
1	4.359947	0.539076	-3.136820
1	3.830436	-0.941971	-3.943593
1	2.758177	-0.141493	-2.788141
6	3.733173	-2.630937	-1.859807
1	3.834557	-3.117342	-2.840319
1	4.167588	-3.308430	-1.113821
1	2.657282	-2.551018	-1.646933

reductive-elimination-product

Number of imaginary frequencies : 0
 The smallest frequency is : 8.1849 cm(-1)

Electronic energy : =-2529.7340182
 Zero-point correction= 0.564049
 Thermal correction to Energy= 0.608750
 Thermal correction to Enthalpy= 0.609694
 Thermal correction to Gibbs Free Energy= 0.484800
 Sum of electronic and zero-point Energies= -2529.169970
 Sum of electronic and thermal Energies= -2529.125268
 Sum of electronic and thermal Enthalpies= -2529.124324
 Sum of electronic and thermal Free Energies= -2529.249219

 Cartesian Coordinates

6	-0.344224	2.633913	-2.406054
6	-1.268056	3.599218	-2.769565
6	-1.871358	4.380676	-1.788038
6	-1.542216	4.209736	-0.447732
6	-0.603990	3.256383	-0.069384
6	0.001789	2.458961	-1.058570
7	-0.226795	3.176628	1.310082
6	0.158695	4.451927	1.926121
46	-0.350039	-0.275523	-0.083540
35	-0.031064	-1.557591	-2.197702
6	0.877561	1.405549	-0.678073
6	1.689579	0.538608	-0.285345
14	3.440503	0.011782	0.192269
6	3.522365	-0.105542	2.089706
6	-0.397623	2.068919	2.083472
8	-0.707371	0.942839	1.662352
6	-0.187815	2.217569	3.561787
8	0.172846	-2.684610	1.258550
6	-0.287925	-3.746554	0.875571
6	0.447772	-5.047559	0.939618
8	-1.484002	-3.871841	0.322616
6	3.956335	-1.591358	-0.664916
6	4.425828	1.555237	-0.348612
1	0.114120	1.985097	-3.148608
1	-2.019306	4.820167	0.315300
1	-2.611541	5.126911	-2.064092
1	0.533915	5.113789	1.143650
1	-0.685329	4.941345	2.427334
1	0.963045	4.302902	2.649894
1	-0.737822	3.063804	3.984678
1	-0.510469	1.292430	4.041713
1	0.878369	2.364882	3.777909
1	4.006678	2.351437	0.292839
1	3.652881	0.941900	2.419154
1	4.995209	-1.753292	-0.326032
1	-1.531982	3.730574	-3.814939
1	0.856706	-5.261375	-0.055749
1	-0.224325	-5.869308	1.201260
1	1.271098	-4.982138	1.653440

1	-1.874353	-2.970485	0.240664
16	-3.448800	-0.695051	-0.512880
6	-4.578330	-0.365924	0.897296
9	-4.056620	0.553971	1.697569
9	-5.739011	0.080853	0.434566
9	-4.788983	-1.472927	1.593949
8	-3.213070	0.610968	-1.112166
8	-2.234565	-1.218391	0.256555
8	-4.098291	-1.740507	-1.286615
6	4.745032	-0.903349	2.550174
1	4.848964	-0.855436	3.642999
1	4.644659	-1.964752	2.286977
1	5.689239	-0.548755	2.117796
6	2.262878	-0.661392	2.750335
1	2.363277	-0.646152	3.845812
1	1.358201	-0.099617	2.490244
1	2.064096	-1.697395	2.450908
6	5.910961	1.414076	-0.015284
1	6.467657	2.312439	-0.317453
1	6.089514	1.268272	1.057246
1	6.363392	0.564797	-0.547503
6	4.246878	1.989747	-1.801226
1	4.759964	1.308342	-2.491224
1	3.194833	2.034569	-2.110874
1	4.681139	2.986704	-1.960611
6	3.960260	-1.480978	-2.188828
1	4.717350	-0.778751	-2.557057
1	4.175515	-2.458229	-2.643386
1	2.982526	-1.158194	-2.572977
6	3.112381	-2.782541	-0.212460
1	3.475106	-3.707892	-0.683220
1	3.133620	-2.933353	0.874028
1	2.060909	-2.652725	-0.499020

Coordinates for heterobimetallic pathway

C-H-activation-PRC (Pd-Ag)

Number of imaginary frequencies : 0

The smallest frequency is : 29.7390 cm(-1)

Electronic energy : =-2902.6542667
 Zero-point correction= 0.298268
 Thermal correction to Energy= 0.333866
 Thermal correction to Enthalpy= 0.334810
 Thermal correction to Gibbs Free Energy= 0.228483
 Sum of electronic and zero-point Energies= -2902.355998
 Sum of electronic and thermal Energies= -2902.320401
 Sum of electronic and thermal Enthalpies= -2902.319456
 Sum of electronic and thermal Free Energies= -2902.425784

Cartesian Coordinates

6	-0.925788	4.338037	-0.444228
6	-0.264909	5.019146	0.577320
6	-1.166817	2.980654	-0.303893
6	-0.747764	2.278201	0.856254
1	-1.238944	1.324713	1.085054
6	-0.100498	3.009489	1.881578
8	-0.064817	1.085558	-1.911971
1	3.888268	-0.247733	3.159223
6	3.085549	0.446637	3.433405
6	2.058395	0.419019	2.337061
1	2.640022	0.093419	4.366711
1	3.520489	1.439941	3.562516
8	1.183643	-0.462254	2.337011
8	2.201478	1.350567	1.458036

46	1.003482	1.288425	-0.163909
1	0.177410	2.489877	2.794417
1	-1.246181	4.854838	-1.345626
1	-0.065644	6.081785	0.461748
6	0.153724	4.361878	1.734529
1	0.660607	4.912503	2.521186
7	-1.900154	2.286408	-1.313826
6	-3.300813	2.670363	-1.533278
1	-3.612818	3.307124	-0.703435
1	-3.419767	3.221072	-2.472990
1	-3.935909	1.777364	-1.528326
6	-1.277697	1.372076	-2.077732
6	-2.025815	0.714928	-3.181272
1	-2.378032	1.455772	-3.908175
1	-1.365913	-0.001565	-3.671549
1	-2.895842	0.183085	-2.778292
47	-0.076718	-1.305991	0.627964
8	3.178619	-1.237852	-2.932290
16	2.598627	-1.070370	-1.613652
8	1.343299	-1.774267	-1.315518
8	2.610859	0.374197	-1.150762
6	3.798883	-1.807825	-0.436523
9	3.970762	-3.089453	-0.715021
9	4.961971	-1.183229	-0.504098
9	3.319312	-1.698217	0.801127
8	-1.942740	-1.362674	-0.724742
16	-3.152679	-0.925472	0.034503
8	-4.226160	-0.413259	-0.818539
8	-2.819708	-0.134009	1.230550
6	-3.783752	-2.507449	0.714569
9	-4.107601	-3.335830	-0.264976
9	-2.835225	-3.074680	1.458924
9	-4.847909	-2.288430	1.471291

C-H-activation-TS (Pd-Ag)

Number of imaginary frequencies : 1
The smallest frequency is : -1495.8715 cm(-1)

Electronic energy : =-2902.6340408
Zero-point correction= 0.292545
Thermal correction to Energy= 0.327416
Thermal correction to Enthalpy= 0.328360
Thermal correction to Gibbs Free Energy= 0.224194
Sum of electronic and zero-point Energies= -2902.341496
Sum of electronic and thermal Energies= -2902.306625
Sum of electronic and thermal Enthalpies= -2902.305681
Sum of electronic and thermal Free Energies= -2902.409847

Cartesian Coordinates

6	3.431230	-3.081566	-0.149886
6	3.845492	-3.476594	1.116985
6	2.331685	-2.239680	-0.290833
6	1.670428	-1.735631	0.865286
1	1.765291	-0.413825	0.806079
6	2.106336	-2.181014	2.132713
8	-0.281371	-2.115894	-1.187250
1	-2.048608	0.666866	4.560043
6	-1.000994	0.880399	4.318402
6	-0.785846	0.591152	2.856317
1	-0.811497	1.936421	4.524063
1	-0.373273	0.247399	4.949636
8	-0.999154	1.492327	2.029295
8	-0.412957	-0.615599	2.614580
46	-0.341013	-1.347166	0.713298
1	1.579306	-1.809033	3.008989
1	3.947522	-3.460616	-1.027989
1	4.689191	-4.156857	1.205006

6	3.190226	-3.030282	2.263834
1	3.526145	-3.348848	3.246701
7	1.950787	-1.833262	-1.595322
6	3.007032	-1.603350	-2.589753
1	3.915282	-1.296697	-2.070586
1	3.194344	-2.501218	-3.189527
1	2.720397	-0.777223	-3.242268
6	0.648336	-1.830973	-1.975851
6	0.296680	-1.501256	-3.384955
1	0.871354	-2.082579	-4.112118
1	-0.770914	-1.681182	-3.519982
1	0.495506	-0.435582	-3.559101
47	-0.721142	1.421413	-0.216254
8	-3.684951	-1.785515	-1.634938
16	-3.062050	-0.723651	-0.864691
8	-2.173566	0.195337	-1.618693
8	-2.497206	-1.130891	0.467006
6	-4.426908	0.376948	-0.320065
9	-5.067727	0.846113	-1.380198
9	-5.275523	-0.288429	0.444667
9	-3.930709	1.400428	0.369148
8	1.330097	1.365801	-1.547474
16	2.463644	1.420188	-0.599519
8	3.754409	0.974474	-1.096438
8	2.085226	0.866133	0.760244
6	2.645530	3.205541	-0.191032
9	2.994932	3.853754	-1.288353
9	1.492205	3.688513	0.252730
9	3.573446	3.361055	0.732035

C-H-activation-product (Pd-Ag)

Number of imaginary frequencies : 0
 The smallest frequency is : 28.8563 cm(-1)

Electronic energy : =-2902.6644004
 Zero-point correction= 0.300005
 Thermal correction to Energy= 0.334671
 Thermal correction to Enthalpy= 0.335615
 Thermal correction to Gibbs Free Energy= 0.232407
 Sum of electronic and zero-point Energies= -2902.364395
 Sum of electronic and thermal Energies= -2902.329729
 Sum of electronic and thermal Enthalpies= -2902.328785
 Sum of electronic and thermal Free Energies= -2902.431993

 Cartesian Coordinates

6	2.779458	-2.844182	-0.317392
6	3.484105	-2.985831	0.869893
6	1.450029	-2.402174	-0.317285
6	0.845249	-2.094160	0.909167
1	2.175666	0.732485	1.164082
6	1.546566	-2.277513	2.098372
8	-1.336368	-2.528977	-0.722024
1	0.839452	2.179434	4.093099
6	0.742195	1.091191	4.061716
6	0.269853	0.643752	2.711091
1	1.741899	0.667567	4.225034
1	0.078606	0.739772	4.853593
8	0.802929	1.196747	1.691535
8	-0.595593	-0.266604	2.673482
46	-0.983662	-1.385698	0.947919
1	1.057670	-2.059979	3.045856
1	3.270036	-3.101818	-1.251814
1	4.516142	-3.324785	0.837523
6	2.867829	-2.713688	2.083946
1	3.408420	-2.836775	3.019576
7	0.776066	-2.292727	-1.579577

6	1.592274	-2.127786	-2.783367
1	2.459378	-1.509756	-2.544208
1	1.932194	-3.091363	-3.181972
1	1.022868	-1.601608	-3.550073
6	-0.555067	-2.483303	-1.700726
6	-1.161109	-2.649195	-3.056369
1	-0.594356	-3.331271	-3.696429
1	-2.180083	-3.017917	-2.926613
1	-1.222651	-1.674510	-3.555938
47	-0.403353	1.131414	-0.301311
8	-4.487689	-0.648958	-1.310540
16	-3.459827	0.078032	-0.586650
8	-2.301698	0.520272	-1.421219
8	-3.056148	-0.474309	0.734697
6	-4.216224	1.678690	-0.097955
9	-4.631900	2.328517	-1.174153
9	-5.239309	1.478765	0.714447
9	-3.307519	2.428333	0.527907
8	1.818240	0.839479	-1.403498
16	3.138450	0.847276	-0.777056
8	4.239879	0.154903	-1.399061
8	3.058594	0.451055	0.727758
6	3.589280	2.626967	-0.658098
9	3.636397	3.127416	-1.877104
9	2.657201	3.248559	0.047116
9	4.759197	2.756729	-0.069882

oxidative-addition-PRC (Pd-Ag)

Number of imaginary frequencies : 0
The smallest frequency is : 25.2093 cm(-1)

Electronic energy : HF=-2903.8946933
Zero-point correction= 0.615573
Thermal correction to Energy= 0.666863
Thermal correction to Enthalpy= 0.667807
Thermal correction to Gibbs Free Energy= 0.530407
Sum of electronic and zero-point Energies= -2903.279120
Sum of electronic and thermal Energies= -2903.227831
Sum of electronic and thermal Enthalpies= -2903.226886
Sum of electronic and thermal Free Energies= -2903.364286

Cartesian Coordinates

8	-4.170870	-3.154132	-1.070129
6	-4.751330	-2.359864	-0.226813
6	-6.199551	-2.634747	-0.011801
8	-4.190959	-1.424354	0.368969
1	-6.354884	-3.701792	0.171089
1	-6.743402	-2.378653	-0.928174
1	-6.587286	-2.042393	0.817458
6	-3.804436	1.778299	0.781405
6	-4.203336	2.845093	1.582640
6	-3.507507	3.127948	2.750035
6	-2.424720	2.346702	3.124240
6	-1.995627	1.274650	2.329948
6	-2.703862	1.024793	1.152067
7	-0.875867	0.515195	2.784153
6	0.132308	1.203047	3.594357
46	-2.200016	-0.571409	0.015332
35	-2.889464	0.323364	-2.224480
6	-0.569482	0.463291	-0.279780
6	0.285934	1.356599	-0.387817
14	1.268590	2.929663	-0.601425
6	-0.070922	4.282599	-0.520790
6	-0.786880	-0.809942	2.572716
8	-1.586757	-1.419823	1.814627
6	0.285128	-1.614113	3.219713

6	2.417721	3.136783	0.899881
6	2.182793	2.778619	-2.251540
1	-4.340376	1.553639	-0.135407
1	-1.912902	2.555050	4.060067
1	-3.812791	3.954247	3.386453
1	0.229302	2.230962	3.234993
1	-0.142294	1.214636	4.655519
1	1.100962	0.714624	3.481901
1	0.465952	-1.336635	4.261103
1	0.007419	-2.667732	3.156223
1	1.222352	-1.494468	2.648666
1	2.672764	3.753464	-2.419655
1	-0.379213	4.261655	0.541333
1	1.759886	3.580866	1.669608
1	-5.055789	3.448941	1.282298
47	1.172838	-0.909633	-0.506015
1	-3.171995	-2.942930	-1.147091
8	-1.718785	-2.509734	-1.007688
6	-0.799171	-3.348056	-0.657344
6	-1.165608	-4.799982	-0.823833
8	0.319405	-3.039743	-0.228779
1	-2.038255	-5.035705	-0.203664
1	-0.330779	-5.444836	-0.544807
1	-1.446001	-4.992642	-1.865272
6	2.974459	1.825226	1.448312
1	2.210591	1.045259	1.562403
1	3.742652	1.403581	0.789874
1	3.448927	1.977728	2.429091
6	3.559971	4.120205	0.636259
1	4.148596	4.286272	1.549179
1	4.253453	3.731263	-0.121900
1	3.214968	5.102283	0.289023
6	0.508244	5.663372	-0.825907
1	-0.261375	6.442538	-0.731865
1	1.330468	5.938009	-0.153210
1	0.890584	5.714601	-1.855731
6	-1.316497	4.025520	-1.363104
1	-1.743556	3.029184	-1.195857
1	-2.096847	4.764913	-1.131216
1	-1.103771	4.112635	-2.436704
6	1.216987	2.511849	-3.405274
1	1.765672	2.343700	-4.342404
1	0.606433	1.614806	-3.220832
1	0.527035	3.347301	-3.576558
6	3.266300	1.702193	-2.194550
1	3.789363	1.625717	-3.157877
1	4.022623	1.899816	-1.425940
1	2.846898	0.704587	-1.987090
8	3.223292	-1.918575	-1.054710
16	3.803806	-2.185001	0.292268
8	3.080051	-1.444807	1.350098
8	4.155225	-3.569358	0.580088
6	5.421415	-1.325226	0.176224
9	5.255437	-0.059511	-0.209609
9	6.193515	-1.931396	-0.714652
9	6.038200	-1.327002	1.351876

oxidative-addition-TS (Pd-Ag)

Number of imaginary frequencies : 1

Electronic energy : HF=-2903.8702171
Zero-point correction= 0.613809
Thermal correction to Energy= 0.665231
Thermal correction to Enthalpy= 0.666175
Thermal correction to Gibbs Free Energy= 0.527182
Sum of electronic and zero-point Energies= -2903.256408
Sum of electronic and thermal Energies= -2903.204987
Sum of electronic and thermal Enthalpies= -2903.204042
Sum of electronic and thermal Free Energies= -2903.343035

.....
 Cartesian Coordinates

8	-4.411775	-3.199985	-0.865788
6	-4.996978	-2.285426	-0.132437
6	-6.421824	-2.603671	0.181942
8	-4.445871	-1.263447	0.273640
1	-6.458924	-3.498607	0.812597
1	-6.965925	-2.836510	-0.738616
1	-6.895975	-1.770387	0.701925
6	-3.632821	1.886659	0.499675
6	-4.012982	3.031875	1.196798
6	-3.390209	3.332531	2.400464
6	-2.399418	2.500892	2.905282
6	-1.985859	1.355034	2.209752
6	-2.622614	1.080615	0.996581
7	-0.940852	0.558043	2.769954
6	-0.018650	1.208664	3.699516
46	-2.189935	-0.536873	-0.069827
35	-1.985673	0.551536	-2.530879
6	-0.695250	0.653622	-0.954454
6	0.268948	1.381822	-0.605945
14	1.349022	2.901742	-0.420094
6	0.076022	4.319301	-0.333558
6	-0.916402	-0.791108	2.613449
8	-1.717149	-1.382068	1.861574
6	0.111136	-1.607812	3.325832
6	2.305912	2.873823	1.220714
6	2.484891	2.892988	-1.938246
1	-4.120935	1.634272	-0.439834
1	-1.949641	2.734812	3.866427
1	-3.681041	4.214524	2.965265
1	0.207868	2.212956	3.331100
1	-0.443197	1.279441	4.708327
1	0.918655	0.655351	3.748063
1	0.196215	-1.366010	4.388895
1	-0.155132	-2.658964	3.204461
1	1.092717	-1.466914	2.845373
1	3.042472	3.844979	-1.900340
1	-0.359453	4.205815	0.676874
1	1.590650	3.302182	1.946648
1	-4.789722	3.676945	0.793991
47	0.981374	-0.885065	-0.512461
1	-3.440230	-2.966018	-1.010160
8	-1.912071	-2.505140	-1.047920
6	-0.999498	-3.330997	-0.661832
6	-1.383361	-4.786116	-0.721164
8	0.127760	-3.008871	-0.261044
1	-2.196963	-4.973489	-0.010154
1	-0.532733	-5.424340	-0.476530
1	-1.761185	-5.035433	-1.718513
6	2.696875	1.477431	1.690808
1	1.850153	0.778755	1.694822
1	3.461699	1.026458	1.048653
1	3.116620	1.504091	2.707454
6	3.535820	3.783910	1.188669
1	3.989755	3.857653	2.186403
1	4.307583	3.384327	0.518157
1	3.312261	4.805401	0.855994
6	0.766948	5.681026	-0.410676
1	0.035866	6.495877	-0.314533
1	1.514127	5.823236	0.380226
1	1.274629	5.819444	-1.376189
6	-1.074105	4.239527	-1.330851
1	-1.640686	3.306476	-1.232517
1	-1.781261	5.065835	-1.169179
1	-0.729045	4.310384	-2.370907
6	1.694362	2.839836	-3.243206
1	2.370441	2.808689	-4.108741
1	1.070006	1.935086	-3.290973

1	1.034982	3.706559	-3.373999
6	3.489206	1.742723	-1.874890
1	4.131473	1.740601	-2.766563
1	4.146951	1.799996	-1.000201
1	2.991726	0.760424	-1.844398
8	3.054235	-1.943090	-1.156980
16	3.513102	-2.375229	0.190539
8	2.765119	-1.670790	1.260021
8	3.745788	-3.801093	0.377986
6	5.194841	-1.646198	0.285397
9	5.157953	-0.332339	0.055568
9	5.985250	-2.202871	-0.622536
9	5.717685	-1.844828	1.489694

oxidative-addition-product (Pd-Ag)

Number of imaginary frequencies : 0
 The smallest frequency is : 17.3657 cm(-1)

Electronic energy : HF=-2903.9038332
 Zero-point correction= 0.615741
 Thermal correction to Energy= 0.667545
 Thermal correction to Enthalpy= 0.668489
 Thermal correction to Gibbs Free Energy= 0.527966
 Sum of electronic and zero-point Energies= -2903.288092
 Sum of electronic and thermal Energies= -2903.236288
 Sum of electronic and thermal Enthalpies= -2903.235344
 Sum of electronic and thermal Free Energies= -2903.375868

 Cartesian Coordinates

8	-4.065364	-3.029470	-0.969122
6	-4.504539	-2.413936	0.109972
6	-5.843574	-2.910659	0.553384
8	-3.892195	-1.526785	0.689964
1	-5.786050	-3.982837	0.768128
1	-6.572393	-2.783650	-0.253822
1	-6.174426	-2.372041	1.442351
6	-2.353921	1.031772	2.410283
6	-2.381591	1.575084	3.693421
6	-1.457281	1.146091	4.637938
6	-0.522543	0.173239	4.309240
6	-0.474136	-0.374389	3.021230
6	-1.395737	0.084715	2.072660
7	0.511470	-1.372529	2.747166
6	1.793811	-1.309398	3.450957
46	-1.471654	-0.764237	0.276226
35	-3.502700	0.721599	-2.052231
6	-1.994965	0.807447	-0.971229
6	-0.927735	1.336724	-0.543653
14	-0.065102	2.987706	-0.123265
6	-1.411479	4.108846	0.618267
6	0.216383	-2.443390	1.972441
8	-0.845919	-2.514168	1.314910
6	1.174022	-3.584026	1.909563
6	1.330851	2.822629	1.157882
6	0.587508	3.546682	-1.819544
1	-3.082481	1.353690	1.668083
1	0.165901	-0.186937	5.070102
1	-1.470528	1.553923	5.645489
1	2.000429	-0.269727	3.711642
1	1.788138	-1.913222	4.366831
1	2.592045	-1.643454	2.784421
1	1.481792	-3.923094	2.903968
1	0.696254	-4.400380	1.365398
1	2.072004	-3.273300	1.358311
1	1.128886	4.484957	-1.608230
1	-1.507190	3.745897	1.656720
1	0.842200	3.017294	2.129000

1	-3.124280	2.328963	3.944313
47	1.037476	-0.396453	-1.068013
1	-3.164124	-2.669243	-1.222582
8	-1.671563	-2.070297	-1.514587
6	-0.695396	-2.854462	-1.812144
6	-1.086694	-4.213814	-2.326851
8	0.506283	-2.568227	-1.685196
1	-1.481607	-4.801598	-1.488515
1	-0.226996	-4.734725	-2.752346
1	-1.884327	-4.131750	-3.072126
6	1.983015	1.448993	1.210119
1	1.262947	0.650071	1.422225
1	2.491090	1.214568	0.265219
1	2.763421	1.401511	1.983338
6	2.413908	3.888292	0.956096
1	3.132396	3.857840	1.786306
1	2.986899	3.703643	0.037018
1	2.022930	4.912427	0.903624
6	-0.909627	5.553561	0.666883
1	-1.645343	6.204471	1.158872
1	0.030988	5.654214	1.222931
1	-0.745755	5.960123	-0.340853
6	-2.791377	4.034279	-0.024403
1	-3.221886	3.027739	0.035335
1	-3.488343	4.715601	0.483275
1	-2.777499	4.323070	-1.083616
6	-0.519207	3.850424	-2.826662
1	-0.090323	4.170897	-3.786244
1	-1.128904	2.958991	-3.035895
1	-1.195092	4.645777	-2.490869
6	1.579643	2.550499	-2.416954
1	2.020785	2.944162	-3.343117
1	2.409347	2.295583	-1.746920
1	1.073170	1.611632	-2.699857
8	3.344044	-0.324486	-1.624834
16	4.013094	-1.268322	-0.682801
8	3.227149	-1.468411	0.552890
8	4.603805	-2.456460	-1.284835
6	5.458011	-0.279865	-0.125794
9	5.065669	0.878793	0.400999
9	6.258746	-0.024017	-1.151111
9	6.142556	-0.947160	0.796623

reductive-elimination-PRC (Pd-Ag)

Number of imaginary frequencies : 0
The smallest frequency is : 26.2158 cm(-1)

Electronic energy : =-2903.9026517
Zero-point correction= 0.615607
Thermal correction to Energy= 0.666862
Thermal correction to Enthalpy= 0.667806
Thermal correction to Gibbs Free Energy= 0.530498
Sum of electronic and zero-point Energies= -2903.287044
Sum of electronic and thermal Energies= -2903.235790
Sum of electronic and thermal Enthalpies= -2903.234846
Sum of electronic and thermal Free Energies= -2903.372154

Cartesian Coordinates

8	-4.557315	-2.356297	-1.467248
6	-4.956164	-1.825036	-0.352103
6	-6.393282	-2.057096	-0.037449
8	-4.235054	-1.168627	0.415608
1	-6.612617	-3.128539	-0.069508
1	-7.005985	-1.577465	-0.808487
1	-6.645681	-1.646712	0.940610
6	-3.442164	1.791054	1.638479
6	-3.596382	2.614081	2.751590

6	-2.707883	2.511767	3.813570
6	-1.677013	1.585424	3.776508
6	-1.494069	0.749112	2.6665474
6	-2.391140	0.891619	1.605566
7	-0.429542	-0.198284	2.714966
6	0.779541	0.136246	3.476342
46	-2.226374	-0.355416	0.022110
35	-3.104880	1.181584	-1.751061
6	-0.548733	0.591757	-0.273910
6	0.413225	1.360258	-0.419674
14	1.727592	2.672907	-0.661570
6	2.633525	2.781394	1.004481
6	-0.560496	-1.424661	2.184764
8	-1.514488	-1.725963	1.417980
6	0.436074	-2.485720	2.496372
6	2.931357	2.094584	-2.015107
6	0.722417	4.222478	-1.133404
1	-4.126340	1.871317	0.799993
1	-1.012460	1.487027	4.630497
1	-2.820773	3.146776	4.688106
1	0.915442	1.218457	3.457851
1	0.706031	-0.202715	4.516391
1	1.651869	-0.312077	2.995358
1	0.652963	-2.546510	3.567270
1	0.052829	-3.440015	2.131861
1	1.378043	-2.263351	1.972508
1	1.422683	5.073753	-1.059522
1	2.824813	1.724221	1.260329
1	3.618955	1.410416	-1.487264
1	-4.409520	3.335038	2.772982
47	1.017582	-0.967785	-0.845560
1	-3.556759	-2.216380	-1.603033
8	-2.026715	-2.001804	-1.525531
6	-1.221240	-3.005292	-1.499591
6	-1.817581	-4.322191	-1.925781
8	-0.023074	-2.961735	-1.173272
1	-2.625668	-4.598526	-1.238528
1	-1.062206	-5.109636	-1.934977
1	-2.260026	-4.225785	-2.923280
8	3.319495	-1.260785	-1.122565
16	3.945315	-1.099376	0.219655
6	4.430725	-2.820752	0.622988
8	2.949912	-0.792765	1.272468
8	5.174620	-0.317737	0.243782
9	5.029934	-2.864110	1.806777
9	3.340048	-3.585400	0.671848
9	5.253198	-3.307193	-0.293093
6	2.302613	1.313148	-3.166626
1	1.714930	0.447813	-2.828943
1	1.632635	1.938562	-3.771074
1	3.081577	0.923467	-3.836298
6	3.756819	3.260614	-2.566263
1	4.534136	2.892101	-3.249561
1	3.133411	3.959220	-3.140666
1	4.262669	3.839050	-1.783960
6	3.981352	3.494645	0.916565
1	4.446312	3.564472	1.910200
1	4.692020	2.967370	0.269450
1	3.874020	4.524252	0.542345
6	1.786815	3.401213	2.112341
1	0.775258	2.972113	2.169242
1	2.267345	3.267975	3.093145
1	1.673867	4.484728	1.964095
6	-0.465939	4.477451	-0.204605
1	-1.028372	5.361325	-0.537788
1	-1.164156	3.627569	-0.223196
1	-0.180274	4.646804	0.838586
6	0.208824	4.129206	-2.570738
1	-0.386969	5.016676	-2.827432
1	1.012625	4.052239	-3.311730

1 -0.448417 3.256064 -2.696184

reductive-elimination-TS (Pd-Ag)

Number of imaginary frequencies : 1

The smallest frequency is : -317.7310 cm(-1)

Electronic energy : =-2903.8931055
Zero-point correction= 0.613372
Thermal correction to Energy= 0.665192
Thermal correction to Enthalpy= 0.666136
Thermal correction to Gibbs Free Energy= 0.526605
Sum of electronic and zero-point Energies= -2903.279734
Sum of electronic and thermal Energies= -2903.227914
Sum of electronic and thermal Enthalpies= -2903.226969
Sum of electronic and thermal Free Energies= -2903.366501

Cartesian Coordinates

8 -5.122680 -2.055873 -0.667601
6 -5.223154 -1.324167 0.407630
6 -6.607605 -1.238132 0.955464
8 -4.274117 -0.742766 0.941818
1 -7.009912 -2.243827 1.111464
1 -7.252252 -0.743365 0.221036
1 -6.618823 -0.677398 1.890630
6 -2.490626 2.406893 1.385412
6 -2.552637 3.309089 2.440517
6 -1.875328 3.035845 3.622405
6 -1.131978 1.870928 3.744861
6 -1.040472 0.953691 2.692978
6 -1.747179 1.238059 1.515615
7 -0.196974 -0.178480 2.878262
6 1.017601 -0.009021 3.687661
46 -2.157274 -0.275774 0.184490
35 -3.039062 1.038468 -1.762772
6 -0.492568 0.740802 -0.081137
6 0.543502 1.319945 -0.434914
14 2.006058 2.445673 -0.749501
6 2.892312 2.478534 0.932722
6 -0.523664 -1.398967 2.421495
8 -1.474355 -1.598246 1.622645
6 0.239848 -2.596568 2.870680
6 3.132768 1.685904 -2.077542
6 1.213360 4.092575 -1.289880
1 -3.008986 2.619334 0.455511
1 -0.610227 1.661444 4.674697
1 -1.923252 3.728315 4.458442
1 1.345105 1.028837 3.605697
1 0.837301 -0.250340 4.741666
1 1.813120 -0.634969 3.280660
1 0.460390 -2.576423 3.941481
1 -0.341869 -3.486461 2.624801
1 1.187263 -2.630322 2.315969
1 2.015358 4.850493 -1.232044
1 2.940606 1.410943 1.209599
1 3.701173 0.917855 -1.525451
1 -3.129227 4.223339 2.327903
47 0.720146 -1.070682 -1.114740
1 -4.152157 -2.098498 -0.946443
8 -2.583303 -2.067715 -1.080894
6 -1.924949 -2.528996 -2.082861
6 -2.753662 -3.276573 -3.093887
8 -0.703289 -2.405188 -2.264290
1 -3.341547 -4.058754 -2.601695
1 -2.126784 -3.718063 -3.870494
1 -3.461408 -2.573988 -3.551263
8 3.010193 -1.723915 -1.148198
16 3.531393 -1.438807 0.215218

6	4.181080	-3.065215	0.759123
8	2.442199	-1.170630	1.182476
8	4.678121	-0.537679	0.280208
9	4.618747	-2.976939	2.010497
9	3.216851	-3.981144	0.713471
9	5.178364	-3.453723	-0.018991
6	2.432954	0.990490	-3.243583
1	1.668527	0.264425	-2.927691
1	1.931860	1.704664	-3.909240
1	3.161330	0.433243	-3.848336
6	4.130937	2.714382	-2.616703
1	4.862860	2.230340	-3.277784
1	3.630607	3.491435	-3.211263
1	4.697467	3.221293	-1.826139
6	4.321569	3.009707	0.865042
1	4.778315	3.014795	1.865219
1	4.963428	2.393234	0.225355
1	4.355846	4.045782	0.494990
6	2.102363	3.220757	2.006672
1	1.053450	2.892641	2.071898
1	2.561667	3.080094	2.997063
1	2.098306	4.303702	1.817999
6	0.050422	4.537859	-0.402799
1	-0.367949	5.486295	-0.769178
1	-0.760803	3.795748	-0.431315
1	0.326337	4.685561	0.646683
6	0.713697	4.007352	-2.733318
1	0.206202	4.938622	-3.022755
1	1.516732	3.838085	-3.459549
1	-0.020777	3.195332	-2.847257

reductive-elimination-product (Pd-Ag)

Number of imaginary frequencies : 0

The smallest frequency is : 23.1821 cm(-1)

Electronic energy : =-2903.9644329

Zero-point correction= 0.616411

Thermal correction to Energy= 0.668634

Thermal correction to Enthalpy= 0.669578

Thermal correction to Gibbs Free Energy= 0.528728

Sum of electronic and zero-point Energies= -2903.348022

Sum of electronic and thermal Energies= -2903.295799

Sum of electronic and thermal Enthalpies= -2903.294855

Sum of electronic and thermal Free Energies= -2903.435705

Cartesian Coordinates

8	-5.485631	-0.384688	-1.442783
6	-5.808207	0.089132	-0.247709
6	-7.246867	0.492993	-0.177699
8	-5.022702	0.185045	0.679782
1	-7.886366	-0.344765	-0.473435
1	-7.432245	1.305983	-0.887907
1	-7.502105	0.819725	0.831345
6	-0.784307	3.287053	1.515555
6	-2.095129	3.600476	1.888573
6	-2.962786	2.603167	2.286191
6	-2.503155	1.282635	2.406768
6	-1.163379	0.957021	2.092210
6	-0.306782	1.984041	1.582463
7	-0.593290	-0.274861	2.577353
6	0.489090	-0.208741	3.567214
46	-2.294156	0.194613	0.229288
35	-2.445229	2.139943	-1.337456
6	0.966273	1.670935	1.020303
6	2.043747	1.476533	0.457722
14	3.749317	1.466778	-0.333087

6	4.694256	0.010431	0.421654
6	-1.168431	-1.455114	2.265649
8	-2.050327	-1.530932	1.376801
6	-0.752515	-2.690754	2.977202
6	3.545717	1.204332	-2.209462
6	4.452576	3.185703	0.078376
1	-0.127805	4.057170	1.118227
1	-3.142642	0.525056	2.854678
1	-3.996828	2.824319	2.533735
1	0.798610	0.830521	3.686457
1	0.144484	-0.575561	4.540438
1	1.344265	-0.796573	3.219407
1	-0.950227	-2.610164	4.052225
1	-1.303246	-3.535460	2.560267
1	0.321366	-2.851757	2.833773
1	5.437548	3.223091	-0.417230
1	4.173746	-0.859250	-0.009707
1	3.571770	0.108459	-2.338617
1	-2.437647	4.629152	1.821240
47	0.629490	-0.276779	-0.636166
1	-4.527208	-0.622413	-1.451516
8	-2.823261	-0.988320	-1.361915
6	-1.975120	-1.310452	-2.286482
6	-2.610437	-2.030736	-3.445369
8	-0.766363	-1.069155	-2.281524
1	-3.324239	-2.779934	-3.091594
1	-1.843636	-2.499504	-4.064586
1	-3.164107	-1.301473	-4.048110
8	2.234781	-2.062818	-1.192973
16	2.288257	-2.759618	0.116330
6	0.957706	-4.016141	-0.033921
8	1.782878	-1.902679	1.216324
8	3.500402	-3.520296	0.390561
9	0.920227	-4.773761	1.060007
9	-0.227144	-3.414026	-0.160226
9	1.155343	-4.794723	-1.085243
6	2.234211	1.716453	-2.805001
1	1.351560	1.159048	-2.456196
1	2.050973	2.774892	-2.574418
1	2.244307	1.616223	-3.899151
6	4.728443	1.809269	-2.970743
1	4.689031	1.527346	-4.031646
1	4.709615	2.907069	-2.930668
1	5.704421	1.485280	-2.587175
6	6.146357	-0.052392	-0.050830
1	6.654691	-0.920468	0.391074
1	6.227679	-0.157074	-1.139827
1	6.716797	0.839974	0.246233
6	4.611931	-0.106030	1.941835
1	3.604792	0.094828	2.328856
1	4.889359	-1.119980	2.260189
1	5.302947	0.590351	2.435628
6	4.661782	3.387946	1.577083
1	5.050911	4.395049	1.784048
1	3.716861	3.288791	2.131763
1	5.370964	2.669413	2.003801
6	3.589216	4.311100	-0.488975
1	4.019561	5.293143	-0.246699
1	3.485927	4.261144	-1.579591
1	2.575638	4.289966	-0.061972

Reaction 4

Coordinates for monometallic pathway

N-H-activation-TS

Number of imaginary frequencies : 1
The smallest frequency is : -1124.2397 cm(-1)

Electronic energy : =-1096.2628368
Zero-point correction= 0.215920
Thermal correction to Energy= 0.235303
Thermal correction to Enthalpy= 0.236247
Thermal correction to Gibbs Free Energy= 0.166577
Sum of electronic and zero-point Energies= -1096.046916
Sum of electronic and thermal Energies= -1096.027534
Sum of electronic and thermal Enthalpies= -1096.026590
Sum of electronic and thermal Free Energies= -1096.096260

Cartesian Coordinates

7	0.466585	-0.964813	-0.033709
1	-0.182330	-1.732320	-0.603057
46	-1.083098	0.455095	0.069094
8	-1.162704	-2.560087	-1.071820
8	-2.503576	-0.985243	-0.185567
8	-2.274832	2.177462	0.208445
8	-0.105070	2.269467	0.363689
6	-2.284029	-2.130575	-0.709074
6	-1.225131	2.884909	0.357819
6	-3.490223	-3.007392	-0.855034
1	-3.314592	-3.773999	-1.612831
1	-3.675491	-3.502843	0.105229
1	-4.374800	-2.416272	-1.103810
6	-1.297254	4.357101	0.486234
1	-1.416435	4.792393	-0.512967
1	-2.168275	4.641662	1.082997
1	-0.381483	4.751082	0.933119
6	1.647135	-0.433479	-0.633266
6	2.740677	-0.444490	0.241763
6	1.756254	0.065333	-1.919250
6	3.981473	0.045397	-0.157999
6	3.002897	0.550822	-2.311512
1	0.899190	0.080994	-2.589141
6	4.104580	0.545169	-1.447102
1	4.823825	0.027042	0.529797
1	3.120442	0.947579	-3.317101
1	5.058502	0.933311	-1.793504
6	2.314603	-1.042200	1.496913
6	0.826021	-1.414278	1.271084
8	0.101170	-1.996625	2.031999
8	2.908243	-1.253378	2.530188

N-H-activation-product

Number of imaginary frequencies : 0
The smallest frequency is : 32.0309 cm(-1)

Electronic energy : =-1096.2709777
Zero-point correction= 0.220299
Thermal correction to Energy= 0.240286
Thermal correction to Enthalpy= 0.241230
Thermal correction to Gibbs Free Energy= 0.169725
Sum of electronic and zero-point Energies= -1096.050679
Sum of electronic and thermal Energies= -1096.030692
Sum of electronic and thermal Enthalpies= -1096.029748
Sum of electronic and thermal Free Energies= -1096.101253

 Cartesian Coordinates

7	0.634745	-0.596638	-0.005090
1	-0.103470	-1.846644	-1.019838
46	-1.197180	0.313526	0.091937
8	-0.667952	-2.619099	-1.308395
8	-2.250841	-1.466397	-0.211729
8	-2.778163	1.714902	0.274634
8	-0.680442	2.275341	0.450780
6	-1.867881	-2.479015	-0.820944
6	-1.913522	2.627531	0.459177
6	-2.775468	-3.630555	-1.039852
1	-2.747845	-3.926721	-2.092765
1	-2.415029	-4.480435	-0.449670
1	-3.793589	-3.381299	-0.740490
6	-2.295096	4.045510	0.643291
1	-2.430880	4.504067	-0.343374
1	-3.243247	4.114787	1.183036
1	-1.510493	4.590362	1.173915
6	1.741024	0.131539	-0.488735
6	2.928320	-0.161066	0.207796
6	1.753514	1.026200	-1.549473
6	4.139441	0.425489	-0.141814
6	2.971601	1.615919	-1.887995
1	0.841485	1.261204	-2.094375
6	4.155420	1.325483	-1.200671
1	5.044304	0.178177	0.410054
1	3.000155	2.320415	-2.716504
1	5.083952	1.803806	-1.500747
6	2.590047	-1.123274	1.244234
6	1.049416	-1.323395	1.099420
8	0.360396	-2.005604	1.826599
8	3.272105	-1.682347	2.074444

alkyne-insertion-1-PRC

Number of imaginary frequencies : 0
 The smallest frequency is : 19.9379 cm(-1)

Electronic energy : =-1406.3482499
 Zero-point correction= 0.348212
 Thermal correction to Energy= 0.375403
 Thermal correction to Enthalpy= 0.376347
 Thermal correction to Gibbs Free Energy= 0.288273
 Sum of electronic and zero-point Energies= -1406.000037
 Sum of electronic and thermal Energies= -1405.972847
 Sum of electronic and thermal Enthalpies= -1405.971902
 Sum of electronic and thermal Free Energies= -1406.059977

 Cartesian Coordinates

46	-0.742716	-0.821384	-0.345244
6	-1.858495	-2.990056	-0.784203
8	-0.905780	-2.588707	-1.530775
6	0.737531	1.482187	-1.666484
6	-0.361252	0.550784	1.404286
6	-1.466753	0.832012	0.910343
6	0.920023	0.453133	2.026578
6	1.879161	1.451837	1.798743
6	1.238608	-0.661541	2.816618
6	3.142114	1.332278	2.361667
1	1.621768	2.306340	1.175409
6	2.503829	-0.768871	3.376141
1	0.489063	-1.434928	2.974077
6	3.455634	0.223891	3.146370
1	3.887743	2.103263	2.182313
1	2.752641	-1.632231	3.988164

1	4.448243	0.132077	3.581218
7	0.783774	0.210968	-1.183699
6	-2.822808	1.229031	0.673209
6	-3.783501	0.986463	1.667349
6	-3.194245	1.832279	-0.537470
6	-5.102858	1.358274	1.451196
1	-3.482333	0.510814	2.598066
6	-4.518148	2.197046	-0.739766
1	-2.428613	2.001502	-1.292938
6	-5.470905	1.962065	0.250327
1	-5.848184	1.175509	2.221344
1	-4.810317	2.666459	-1.676129
1	-6.506873	2.248199	0.083641
8	-2.226856	-2.242209	0.180305
6	-2.500438	-4.306728	-1.022556
1	-2.649059	-4.464856	-2.094627
1	-1.834094	-5.097065	-0.657919
1	-3.453390	-4.375718	-0.492996
6	2.115091	-0.176814	-1.005024
6	3.024949	0.809607	-1.436833
6	2.582792	-1.370423	-0.470015
6	4.397997	0.627351	-1.333417
6	3.964005	-1.540417	-0.364018
1	1.889846	-2.137372	-0.127114
6	4.870210	-0.562614	-0.787216
1	5.078969	1.406830	-1.670540
1	4.345346	-2.465458	0.064124
1	5.938421	-0.736238	-0.687980
6	2.221671	1.926849	-1.913323
8	-0.231351	2.189793	-1.879059
8	2.538247	2.995377	-2.387471

alkyne-insertion-1-TS

Number of imaginary frequencies : 1

The smallest frequency is : -318.8559 cm(-1)

Electronic energy : =-1406.3267772
 Zero-point correction= 0.347521
 Thermal correction to Energy= 0.374179
 Thermal correction to Enthalpy= 0.375124
 Thermal correction to Gibbs Free Energy= 0.286629
 Sum of electronic and zero-point Energies= -1405.979256
 Sum of electronic and thermal Energies= -1405.952598
 Sum of electronic and thermal Enthalpies= -1405.951654
 Sum of electronic and thermal Free Energies= -1406.040148

Cartesian Coordinates

46	-1.294721	-1.028335	-0.191395
6	-3.143145	-2.721442	-0.170385
8	-1.962345	-3.137570	-0.339755
6	1.380129	-0.823766	-1.656585
6	0.232444	1.165261	-0.057305
6	-1.039343	0.953631	0.012778
6	1.496357	1.798776	0.002339
6	2.088528	2.296155	-1.176544
6	2.203875	1.847537	1.220044
6	3.368866	2.822195	-1.131516
1	1.531758	2.254422	-2.110293
6	3.487919	2.370554	1.249011
1	1.734007	1.468688	2.124655
6	4.069088	2.849310	0.076063
1	3.828634	3.209289	-2.036992
1	4.039441	2.402063	2.185045
1	5.078432	3.253229	0.102266
7	0.749519	-0.854745	-0.420542
6	-2.130876	1.914344	0.179240

6	-3.264039	1.584826	0.931497
6	-2.034109	3.185342	-0.406346
6	-4.276043	2.521116	1.109339
1	-3.344980	0.591732	1.366908
6	-3.052702	4.112377	-0.229105
1	-1.157203	3.434165	-1.002508
6	-4.173507	3.783580	0.530727
1	-5.151820	2.260730	1.699427
1	-2.971002	5.095901	-0.686267
1	-4.969774	4.511779	0.667381
8	-3.349502	-1.467586	-0.016746
6	-4.297415	-3.662316	-0.116859
1	-4.050662	-4.604834	-0.611483
1	-4.536441	-3.872557	0.932283
1	-5.181218	-3.211829	-0.577069
6	1.690834	-1.232454	0.553398
6	2.990233	-1.345451	0.027146
6	1.452534	-1.435746	1.904442
6	4.074586	-1.648550	0.844212
6	2.547068	-1.735098	2.715695
1	0.446442	-1.347047	2.310980
6	3.845053	-1.836919	2.202410
1	5.072490	-1.733124	0.418702
1	2.384795	-1.892974	3.779704
1	4.670153	-2.072488	2.869129
6	2.893998	-1.112656	-1.406479
8	0.881163	-0.576415	-2.730695
8	3.733872	-1.113949	-2.278701

alkyne-insertion-1-product

Number of imaginary frequencies : 0

The smallest frequency is : 15.9991 cm(-1)

Electronic energy : =-1406.3654446
 Zero-point correction= 0.350067
 Thermal correction to Energy= 0.376540
 Thermal correction to Enthalpy= 0.377484
 Thermal correction to Gibbs Free Energy= 0.290671
 Sum of electronic and zero-point Energies= -1406.015378
 Sum of electronic and thermal Energies= -1405.988905
 Sum of electronic and thermal Enthalpies= -1405.987960
 Sum of electronic and thermal Free Energies= -1406.074773

Cartesian Coordinates

46	-0.595398	-1.376200	-0.122328
6	-1.732289	-3.633866	0.061979
8	-0.491277	-3.664406	-0.133638
6	1.607916	-0.240228	-1.669706
6	0.126048	1.110947	-0.127431
6	-1.080618	0.538397	-0.023827
6	0.615533	2.487310	-0.027713
6	1.918251	2.820822	-0.420872
6	-0.212674	3.500195	0.480508
6	2.372949	4.131625	-0.325865
1	2.597480	2.063332	-0.807766
6	0.245731	4.806459	0.570947
1	-1.219656	3.258290	0.813175
6	1.539631	5.130330	0.166334
1	3.387102	4.369021	-0.638835
1	-0.411289	5.577187	0.967616
1	1.896835	6.154721	0.240479
7	1.099082	0.027031	-0.358527
6	-2.445795	1.013451	0.063082
6	-3.290047	0.575976	1.094572
6	-2.948830	1.893157	-0.910218
6	-4.599737	1.032429	1.165975

1	-2.904639	-0.122864	1.834396
6	-4.261570	2.338285	-0.835571
1	-2.297735	2.222602	-1.718311
6	-5.088651	1.912450	0.202778
1	-5.244262	0.696790	1.975186
1	-4.642811	3.020897	-1.591719
1	-6.116577	2.263409	0.257665
8	-2.341414	-2.507346	0.150598
6	-2.539736	-4.880983	0.214722
1	-1.939797	-5.764026	-0.015925
1	-2.904676	-4.952342	1.245508
1	-3.416551	-4.844401	-0.439419
6	2.114763	-0.326508	0.592901
6	3.186207	-0.974647	-0.030881
6	2.084783	-0.111001	1.956628
6	4.262262	-1.446830	0.716439
6	3.173921	-0.581326	2.693441
1	1.250389	0.395837	2.435544
6	4.247006	-1.245421	2.090419
1	5.088869	-1.951651	0.221698
1	3.182291	-0.427370	3.769738
1	5.072050	-1.598054	2.702987
6	2.941827	-1.006891	-1.463672
8	1.112012	0.106632	-2.705286
8	3.582733	-1.473653	-2.377305

alkyne-insertion-2-PRC

Number of imaginary frequencies : 0

The smallest frequency is : 11.0377 cm(-1)

Electronic energy : =-1945.3940335
 Zero-point correction= 0.543560
 Thermal correction to Energy= 0.582421
 Thermal correction to Enthalpy= 0.583365
 Thermal correction to Gibbs Free Energy= 0.468724
 Sum of electronic and zero-point Energies= -1944.850474
 Sum of electronic and thermal Energies= -1944.811612
 Sum of electronic and thermal Enthalpies= -1944.810668
 Sum of electronic and thermal Free Energies= -1944.925310

Cartesian Coordinates

46	-0.701185	1.598858	0.348034
6	-1.686117	3.885603	-0.117000
8	-2.402748	3.038233	0.488530
6	-0.602733	-0.778131	-2.052869
6	1.446722	-0.229389	-0.747793
6	1.129708	0.920956	-0.124059
6	2.826062	-0.667689	-1.069896
6	3.093888	-1.281743	-2.298925
6	3.873304	-0.517454	-0.152836
6	4.376806	-1.713755	-2.611324
1	2.286681	-1.409533	-3.018415
6	5.154488	-0.952405	-0.465720
1	3.672893	-0.055778	0.812695
6	5.411949	-1.551152	-1.696214
1	4.567651	-2.180020	-3.575289
1	5.955699	-0.830089	0.259661
1	6.415345	-1.893398	-1.938444
7	0.430378	-1.121733	-1.191142
6	2.049105	2.036929	0.111815
6	2.174137	2.644700	1.370667
6	2.768592	2.577708	-0.966183
6	3.029232	3.722728	1.556502
1	1.577602	2.280413	2.206336
6	3.619787	3.655643	-0.777261
1	2.642854	2.136836	-1.952650
6	3.759200	4.228124	0.484987

1	3.118648	4.176261	2.540928
1	4.171935	4.059518	-1.622673
1	4.425079	5.075624	0.629683
8	-0.501836	3.583760	-0.474417
6	-2.228728	5.239913	-0.449404
1	-2.970776	5.544504	0.292528
1	-1.419623	5.971334	-0.513223
1	-2.722714	5.192329	-1.426024
6	0.331377	-2.479284	-0.821496
6	-0.795557	-3.074873	-1.406207
6	1.160861	-3.201240	0.020822
6	-1.118134	-4.401989	-1.161680
6	0.833193	-4.538493	0.248919
1	2.020177	-2.740671	0.502259
6	-0.288281	-5.141641	-0.325328
1	-2.004167	-4.831117	-1.624705
1	1.470937	-5.123203	0.909009
1	-0.507979	-6.185108	-0.116105
6	-1.461501	-2.064551	-2.222545
8	-0.807369	0.297166	-2.562387
8	-2.460251	-2.126008	-2.899198
6	-0.986237	-0.262290	1.472921
6	-2.025734	-0.071713	0.800350
6	-3.374656	-0.089869	0.322863
6	-4.358615	-0.606461	1.182315
6	-3.730008	0.348643	-0.959921
6	-5.675115	-0.691327	0.756260
1	-4.072193	-0.930099	2.181173
6	-5.051310	0.258001	-1.373332
1	-2.968501	0.748253	-1.626289
6	-6.022793	-0.259412	-0.521614
1	-6.433770	-1.090671	1.424973
1	-5.321312	0.590431	-2.372060
1	-7.056113	-0.326312	-0.853802
6	-0.152000	-1.089921	2.303598
6	1.114687	-0.712009	2.760575
6	-0.657009	-2.351087	2.659856
6	1.860772	-1.576445	3.551112
1	1.515812	0.257825	2.480286
6	0.086765	-3.204758	3.460217
1	-1.628232	-2.657441	2.272478
6	1.349884	-2.822189	3.905896
1	2.846645	-1.271946	3.894820
1	-0.314823	-4.180544	3.723848
1	1.935782	-3.493983	4.528775

alkyne-insertion-2-TS (Gas Phase)

Number of imaginary frequencies : 1

The smallest frequency is : -282.8015 cm(-1)

Electronic energy : =-1945.3911396
 Zero-point correction= 0.543230
 Thermal correction to Energy= 0.580952
 Thermal correction to Enthalpy= 0.581896
 Thermal correction to Gibbs Free Energy= 0.472248
 Sum of electronic and zero-point Energies= -1944.847910
 Sum of electronic and thermal Energies= -1944.810188
 Sum of electronic and thermal Enthalpies= -1944.809244
 Sum of electronic and thermal Free Energies= -1944.918891

Cartesian Coordinates

6	3.690450	-3.937401	-1.422370
6	2.920858	-3.240377	-2.349396
6	1.832929	-2.484085	-1.929263
6	1.502889	-2.448211	-0.571059
6	2.275521	-3.148028	0.361056

6	3.368158	-3.888769	-0.068047
6	0.364047	-1.655473	-0.138299
6	-0.894011	-1.655970	0.114436
6	-2.255711	-1.951808	-0.212104
6	-3.283813	-1.789874	0.730768
6	-4.597065	-2.031498	0.356882
6	-4.898605	-2.429207	-0.945475
6	-3.882012	-2.588397	-1.883333
6	-2.563300	-2.348110	-1.525980
46	-0.257420	-0.376782	1.567115
8	0.080556	0.976327	3.315354
6	-1.006387	0.571130	3.829004
6	-1.437039	1.125473	5.155186
8	-1.728702	-0.283484	3.237700
6	1.150876	0.192934	0.174707
6	2.563110	0.087354	0.579005
6	3.546269	-0.053914	-0.410561
6	4.878241	-0.224440	-0.063266
6	5.250390	-0.251127	1.278212
6	4.283933	-0.098938	2.267871
6	2.946110	0.061989	1.926004
6	0.694630	1.093076	-0.734106
7	-0.639794	1.018707	-1.247587
6	-0.994747	0.383062	-2.423693
6	-2.529256	0.602862	-2.582473
6	-2.928661	1.336622	-1.385485
6	-1.776476	1.582445	-0.626603
6	-4.180467	1.730112	-0.936401
6	-4.267449	2.384594	0.288943
6	-3.109546	2.639408	1.025472
6	-1.841416	2.250689	0.583405
8	-0.268049	-0.217810	-3.182754
8	-3.167615	0.223956	-3.535010
6	1.472293	2.263459	-1.200383
6	2.126635	3.084705	-0.274675
6	2.825439	4.206295	-0.701346
6	2.879394	4.521820	-2.055853
6	2.227277	3.712582	-2.982170
6	1.520976	2.593594	-2.559920
1	2.071955	2.836065	0.784910
1	1.027506	1.951270	-3.286722
1	3.323106	4.840794	0.028177
1	2.269247	3.953728	-4.041825
1	3.426769	5.400505	-2.389213
1	3.246751	-0.046191	-1.457365
1	2.190929	0.185415	2.701579
1	5.627401	-0.345318	-0.842369
1	4.571516	-0.108455	3.316732
1	6.294064	-0.389470	1.551712
1	-0.657250	0.939956	5.900285
1	-1.550591	2.211597	5.075975
1	-2.377405	0.677473	5.481714
1	-0.952938	2.445507	1.180515
1	-5.058949	1.502860	-1.536722
1	-3.190506	3.152595	1.981455
1	-5.232553	2.699394	0.676096
1	-3.034419	-1.460552	1.738314
1	-1.762932	-2.438343	-2.259615
1	-5.393982	-1.903118	1.085316
1	-4.117131	-2.870424	-2.906255
1	-5.932241	-2.608529	-1.232206
1	1.245740	-1.893686	-2.631851
1	2.015441	-3.091978	1.416759
1	3.175532	-3.274572	-3.406061
1	3.970900	-4.430365	0.656830
1	4.547612	-4.518527	-1.754815

alkyne-insertion-2-product

Number of imaginary frequencies : 0
The smallest frequency is : 23.8176 cm(-1)

Electronic energy : =-1945.4280846
Zero-point correction= 0.546453
Thermal correction to Energy= 0.583963
Thermal correction to Enthalpy= 0.584907
Thermal correction to Gibbs Free Energy= 0.475523
Sum of electronic and zero-point Energies= -1944.881632
Sum of electronic and thermal Energies= -1944.844122
Sum of electronic and thermal Enthalpies= -1944.843178
Sum of electronic and thermal Free Energies= -1944.952562

.....
Cartesian Coordinates
.....

46	1.473053	0.915188	-0.213407
6	3.607969	2.003476	-1.025712
8	2.592393	2.675673	-0.638488
6	-0.549910	-0.243642	-2.413521
6	0.485464	-1.110926	-0.287899
6	0.330938	-0.528914	0.988780
6	1.380758	-2.251361	-0.643685
6	2.333479	-2.123139	-1.658233
6	1.207316	-3.490143	-0.017015
6	3.109212	-3.218096	-2.023017
1	2.486055	-1.154763	-2.129563
6	1.980127	-4.582026	-0.390734
1	0.479316	-3.590951	0.786945
6	2.934101	-4.446998	-1.395183
1	3.859060	-3.104701	-2.802056
1	1.838356	-5.539469	0.105140
1	3.542954	-5.300037	-1.685720
7	-0.599178	-0.974344	-1.234766
6	1.196137	-0.773185	2.173991
6	0.784283	-0.266520	3.416188
6	2.453353	-1.399510	2.106829
6	1.557432	-0.435903	4.557457
1	-0.147543	0.289328	3.484627
6	3.228369	-1.555188	3.246803
1	2.851088	-1.740372	1.156349
6	2.781187	-1.089721	4.479934
1	1.205655	-0.038487	5.506446
1	4.200086	-2.035940	3.164091
1	3.393627	-1.216988	5.369294
8	3.593495	0.743498	-0.993272
6	4.799427	2.748980	-1.542665
1	5.002868	3.618677	-0.912165
1	5.672121	2.094270	-1.588291
1	4.578172	3.117541	-2.550094
6	-1.818723	-1.684932	-1.150921
6	-2.640549	-1.391788	-2.247861
6	-2.245333	-2.553108	-0.162528
6	-3.907011	-1.944314	-2.369375
6	-3.522473	-3.101725	-0.291566
1	-1.630525	-2.779036	0.703908
6	-4.352140	-2.808745	-1.374639
1	-4.518800	-1.690322	-3.232237
1	-3.879064	-3.774642	0.485176
1	-5.339899	-3.256747	-1.436488
6	-1.917617	-0.468631	-3.115330
8	0.360644	0.444245	-2.811792
8	-2.236330	0.051911	-4.156900
6	-0.798155	0.474909	1.099453
6	-0.308369	1.548845	0.465848
6	-0.746113	2.910389	0.233921
6	-1.351392	3.640046	1.270405
6	-0.569819	3.516336	-1.018230
6	-1.796416	4.934329	1.046820
1	-1.469195	3.172777	2.246730
6	-1.024095	4.810126	-1.235424

1	-0.070701	2.959933	-1.809226
6	-1.638377	5.520097	-0.207679
1	-2.266172	5.491193	1.854378
1	-0.891178	5.269240	-2.212018
1	-1.987346	6.535611	-0.380632
6	-2.155712	0.165802	1.573980
6	-2.404441	-0.802344	2.556112
6	-3.254160	0.781062	0.955258
6	-3.706107	-1.127027	2.922426
1	-1.572044	-1.317150	3.033996
6	-4.551531	0.447207	1.314295
1	-3.075723	1.507947	0.164086
6	-4.785018	-0.504520	2.304616
1	-3.875152	-1.876431	3.692862
1	-5.387487	0.927269	0.810672
1	-5.802927	-0.763763	2.586070

C-H-activation-PRC

Number of imaginary frequencies : 0
 The smallest frequency is : 17.5117 cm(-1)

Electronic energy : =-1945.4638816
 Zero-point correction= 0.544396
 Thermal correction to Energy= 0.582744
 Thermal correction to Enthalpy= 0.583688
 Thermal correction to Gibbs Free Energy= 0.470025
 Sum of electronic and zero-point Energies= -1944.919485
 Sum of electronic and thermal Energies= -1944.881137
 Sum of electronic and thermal Enthalpies= -1944.880193
 Sum of electronic and thermal Free Energies= -1944.993856

 Cartesian Coordinates

46	1.688494	-0.326979	1.201460
8	3.341148	0.233573	2.653639
6	2.603297	-0.082337	3.634260
8	1.418337	-0.491310	3.461760
6	3.140229	0.022593	5.032266
1	2.491970	0.672620	5.629855
1	4.160310	0.413166	5.046078
1	3.123296	-0.966058	5.503952
1	-0.815953	-0.053041	2.220405
6	-1.506293	-0.885143	2.095518
6	-1.569675	-1.908853	3.044949
1	-0.911208	-1.847399	3.908231
6	-2.436766	-2.996247	2.911203
1	-2.453662	-3.770367	3.673678
6	-3.284135	-3.077029	1.810069
1	-3.984881	-3.900309	1.688412
6	-3.222434	-2.071090	0.853496
6	-2.327735	-0.998462	0.988647
6	-3.430105	-0.542401	-0.971333
6	-0.276311	0.912541	-0.545954
6	-1.620100	1.026790	-0.346350
7	-2.426094	-0.121821	-0.111484
6	-3.980712	-1.865656	-0.371708
8	-4.859559	-2.522378	-0.885784
8	-3.785892	-0.007851	-1.994854
6	0.444456	-0.360840	-0.712176
6	-2.370836	2.299085	-0.327596
6	-2.169975	3.294359	-1.292200
6	-3.341887	2.506405	0.661290
6	-2.904924	4.472691	-1.254451
1	-1.442805	3.133482	-2.085773
6	-4.071897	3.688447	0.700457
1	-3.513572	1.737005	1.413653
6	-3.856191	4.676260	-0.257146

1	-2.743290	5.231798	-2.016768
1	-4.814503	3.837217	1.481412
1	-4.432602	5.598326	-0.231571
6	0.579679	2.132078	-0.542529
6	0.658379	2.934653	0.601255
6	1.334143	2.473571	-1.668910
6	1.472798	4.061227	0.613950
1	0.073868	2.664558	1.481254
6	2.144840	3.604518	-1.656287
1	1.265736	1.858741	-2.566511
6	2.216183	4.399176	-0.515261
1	1.527817	4.677370	1.508685
1	2.717822	3.868409	-2.542464
1	2.850104	5.283045	-0.505461
6	1.842139	-0.406379	-0.686284
6	-0.199310	-1.599540	-1.245545
6	-0.040031	-2.829072	-0.600427
6	-0.925952	-1.544158	-2.440924
6	-0.612728	-3.982541	-1.130771
1	0.517320	-2.865598	0.336787
6	-1.505170	-2.694173	-2.962434
1	-1.049314	-0.588776	-2.950220
6	-1.352090	-3.916135	-2.307347
1	-0.490697	-4.931435	-0.613081
1	-2.080374	-2.636244	-3.884026
1	-1.808638	-4.814387	-2.716999
6	2.919172	-0.684074	-1.563356
6	4.204644	-0.937766	-1.037516
6	2.725477	-0.683286	-2.963573
6	5.264991	-1.187740	-1.889776
1	4.337432	-0.931545	0.043037
6	3.790501	-0.940064	-3.806481
1	1.733504	-0.482709	-3.364091
6	5.056055	-1.190515	-3.270062
1	6.255558	-1.381785	-1.487607
1	3.645369	-0.944232	-4.883310
1	5.890693	-1.389694	-3.938182

C-H-activation-TS

Number of imaginary frequencies : 1
The smallest frequency is : -876.6078 cm(-1)

Electronic energy : =-1945.4219986
Zero-point correction= 0.539180
Thermal correction to Energy= 0.576557
Thermal correction to Enthalpy= 0.577501
Thermal correction to Gibbs Free Energy= 0.468611
Sum of electronic and zero-point Energies= -1944.882819
Sum of electronic and thermal Energies= -1944.845442
Sum of electronic and thermal Enthalpies= -1944.844498
Sum of electronic and thermal Free Energies= -1944.953387

Cartesian Coordinates

46	0.835299	0.088066	1.425065
8	1.113443	1.422589	3.163402
6	0.065025	2.002259	3.530631
8	-1.103929	1.748180	3.067700
6	0.139843	3.069413	4.579007
1	-0.505279	2.803026	5.422555
1	-0.240511	4.010302	4.167082
1	1.164705	3.210414	4.926787
1	-1.084326	0.698892	2.463354
6	-1.183024	-0.677009	2.077133
6	-1.222388	-1.474443	3.240655
1	-0.732308	-1.084336	4.135994
6	-1.851192	-2.719599	3.324700

1	-1.832057	-3.281790	4.255131
6	-2.505552	-3.227146	2.208219
1	-3.013043	-4.189732	2.226803
6	-2.503707	-2.469685	1.042254
6	-1.845180	-1.229343	0.978472
6	-2.699925	-1.548580	-1.145472
6	-0.051838	0.660572	-0.945982
6	-1.404382	0.508336	-0.861452
7	-1.952813	-0.700457	-0.343509
6	-3.067587	-2.765966	-0.263115
8	-3.685943	-3.728156	-0.665769
8	-2.988701	-1.383289	-2.308104
6	0.876967	-0.466285	-0.643816
6	-2.405345	1.521556	-1.242729
6	-2.300596	2.255433	-2.431287
6	-3.506113	1.745315	-0.405483
6	-3.259923	3.205156	-2.758924
1	-1.468273	2.065724	-3.106684
6	-4.461613	2.700605	-0.732987
1	-3.603030	1.172498	0.516380
6	-4.340894	3.435240	-1.909816
1	-3.169827	3.761601	-3.689407
1	-5.303772	2.871677	-0.065967
1	-5.090857	4.179122	-2.169182
6	0.578031	1.973046	-1.243164
6	0.282014	3.102599	-0.471561
6	1.509669	2.082519	-2.280517
6	0.897107	4.319418	-0.742101
1	-0.429480	3.015129	0.349468
6	2.119918	3.302684	-2.553443
1	1.745582	1.205807	-2.883938
6	1.815174	4.423288	-1.785108
1	0.662660	5.189343	-0.132394
1	2.835418	3.378180	-3.369296
1	2.296332	5.376018	-1.994924
6	2.112236	-0.207963	-0.029168
6	0.603466	-1.841802	-1.152691
6	0.720230	-2.956538	-0.315718
6	0.262047	-2.031454	-2.496665
6	0.483367	-4.235898	-0.808343
1	0.972014	-2.807641	0.734996
6	0.036398	-3.312159	-2.988678
1	0.166696	-1.168962	-3.155566
6	0.142077	-4.417093	-2.145958
1	0.560903	-5.092280	-0.142055
1	-0.231314	-3.447014	-4.034375
1	-0.044769	-5.416721	-2.531821
6	3.477173	-0.460742	-0.295555
6	4.423688	-0.348018	0.746739
6	3.916231	-0.792406	-1.599160
6	5.764644	-0.575312	0.497034
1	4.072906	-0.078090	1.741247
6	5.258870	-1.017237	-1.839152
1	3.185689	-0.875652	-2.401395
6	6.179415	-0.909975	-0.793454
1	6.493791	-0.490706	1.298250
1	5.598530	-1.276680	-2.838361
1	7.234583	-1.087268	-0.989019

C-H-activation-product

Number of imaginary frequencies : 0

The smallest frequency is : 23.4524 cm(-1)

Electronic energy : =-1945.4281937

Zero-point correction= 0.543984

Thermal correction to Energy= 0.581832

Thermal correction to Enthalpy= 0.582776

Thermal correction to Gibbs Free Energy= 0.472425
 Sum of electronic and zero-point Energies= -1944.884209
 Sum of electronic and thermal Energies= -1944.846362
 Sum of electronic and thermal Enthalpies= -1944.845418
 Sum of electronic and thermal Free Energies= -1944.955768

 Cartesian Coordinates

46	0.809815	0.168273	1.425266
8	1.003256	1.460020	3.251011
6	-0.000936	1.984947	3.737167
8	-1.223732	1.694785	3.348330
6	0.064803	3.005344	4.816179
1	-0.444790	2.626649	5.708433
1	-0.464092	3.910024	4.499354
1	1.101726	3.243452	5.054990
1	-1.170269	0.935088	2.702425
6	-0.927271	-0.910786	1.968853
6	-1.024121	-1.652223	3.163012
1	-0.423938	-1.334309	4.019244
6	-1.828704	-2.786909	3.318903
1	-1.845307	-3.315869	4.269101
6	-2.586445	-3.241972	2.246886
1	-3.207734	-4.132661	2.316392
6	-2.538254	-2.522080	1.058388
6	-1.739668	-1.370638	0.934303
6	-2.736146	-1.623274	-1.137241
6	-0.049475	0.662927	-0.943865
6	-1.386393	0.398920	-0.903972
7	-1.879479	-0.831271	-0.388202
6	-3.189051	-2.777695	-0.213943
8	-3.928803	-3.671870	-0.567398
8	-3.062544	-1.454322	-2.290145
6	0.968275	-0.378588	-0.628653
6	-2.437080	1.351629	-1.316659
6	-2.377730	2.028571	-2.540208
6	-3.528606	1.578568	-0.469224
6	-3.374707	2.928654	-2.895484
1	-1.548866	1.833817	-3.219140
6	-4.522924	2.483326	-0.824453
1	-3.585690	1.048815	0.482176
6	-4.448099	3.162668	-2.038048
1	-3.319403	3.443312	-3.852420
1	-5.358365	2.659661	-0.150306
1	-5.228025	3.866935	-2.318969
6	0.478036	2.019325	-1.245055
6	0.090536	3.135083	-0.495231
6	1.414963	2.182693	-2.271470
6	0.619732	4.389761	-0.776453
1	-0.624424	3.009633	0.318655
6	1.936038	3.439974	-2.557917
1	1.726026	1.315133	-2.854477
6	1.540729	4.546436	-1.810310
1	0.316791	5.248809	-0.181595
1	2.655162	3.555335	-3.365939
1	1.953324	5.528842	-2.029024
6	2.181537	0.000853	-0.017000
6	0.793237	-1.765270	-1.149500
6	1.028321	-2.880027	-0.339165
6	0.424881	-1.962044	-2.485648
6	0.882532	-4.166344	-0.848476
1	1.297587	-2.727768	0.706383
6	0.287091	-3.248360	-2.994880
1	0.228325	-1.097992	-3.120592
6	0.511057	-4.354094	-2.177105
1	1.054766	-5.024468	-0.202491
1	-0.003904	-3.388181	-4.033834
1	0.392454	-5.359447	-2.575129
6	3.539144	-0.309947	-0.301667
6	4.512816	-0.167261	0.709693

6	3.946463	-0.711479	-1.594633
6	5.843745	-0.441443	0.445948
1	4.191539	0.159579	1.697420
6	5.280709	-0.968807	-1.855343
1	3.195815	-0.817621	-2.376279
6	6.226690	-0.839556	-0.835730
1	6.589873	-0.338929	1.229702
1	5.592908	-1.275658	-2.850459
1	7.273597	-1.048053	-1.044810

reductive-elimination-PRC

Number of imaginary frequencies : 0

Electronic energy : HF=-2174.4888772
 Zero-point correction= 0.609578
 Thermal correction to Energy= 0.653190
 Thermal correction to Enthalpy= 0.654135
 Thermal correction to Gibbs Free Energy= 0.529857
 Sum of electronic and zero-point Energies= -2173.879300
 Sum of electronic and thermal Energies= -2173.835687
 Sum of electronic and thermal Enthalpies= -2173.834742
 Sum of electronic and thermal Free Energies= -2173.959020

 Cartesian Coordinates

6	-4.980558	2.860931	1.639304
6	-4.047046	2.606647	2.641367
6	-2.934494	1.816636	2.370288
6	-2.750523	1.261965	1.099796
6	-3.692270	1.520133	0.100523
6	-4.800497	2.316819	0.369983
6	-1.522417	0.464390	0.835323
6	-1.586674	-0.858620	0.555872
6	-2.899829	-1.566831	0.536901
6	-3.543445	-1.848869	1.745953
6	-4.775090	-2.495918	1.757836
6	-5.377549	-2.873753	0.560917
6	-4.741472	-2.603441	-0.647435
6	-3.509846	-1.954899	-0.660220
46	0.696317	-1.373929	-1.428813
6	-0.381820	-1.723754	0.425783
6	0.697739	-1.573514	1.325644
6	1.523832	-2.635710	1.705385
6	1.448572	-3.871578	1.039370
6	0.543246	-4.003220	0.007722
6	-0.383363	-2.962363	-0.294447
6	2.275724	-2.208045	2.864010
6	1.872871	-0.726273	3.090792
7	0.947350	-0.409651	2.091018
8	2.299917	0.018018	3.939177
6	0.862448	0.877391	1.479298
6	2.125733	1.650370	1.447098
6	3.309967	1.023113	1.040925
6	4.496136	1.741693	0.955371
6	4.517983	3.095167	1.286024
6	3.349071	3.721207	1.709975
6	2.160545	3.003609	1.792462
8	3.063222	-2.800526	3.576315
8	2.719756	-0.318831	-2.238174
6	3.758360	-0.804019	-1.811452
6	5.116286	-0.292965	-2.142032
6	-0.260849	1.250013	0.830584
6	-0.248764	2.412855	-0.109238
6	-0.928950	3.610423	0.137988
6	-0.912023	4.636881	-0.801341
6	-0.227770	4.480574	-2.004357
6	0.449872	3.292161	-2.261756

6	0.438593	2.267689	-1.320534
8	3.775457	-1.876096	-1.023725
1	3.297394	-0.039532	0.789747
1	1.250418	3.491030	2.137065
1	5.407516	1.242711	0.631694
1	3.362378	4.773223	1.986051
1	5.446904	3.657314	1.222191
1	-1.464196	3.744799	1.077108
1	0.975369	1.336370	-1.517963
1	-1.437947	5.565634	-0.590131
1	0.991476	3.160459	-3.196567
1	-0.220897	5.284402	-2.737319
1	5.832519	-0.512158	-1.346924
1	5.459733	-0.798578	-3.052834
1	5.072915	0.779407	-2.342157
1	2.838909	-2.149613	-0.879134
1	2.094061	-4.694503	1.338003
1	-1.258082	-3.220485	-0.888702
1	0.463750	-4.939915	-0.538321
1	-3.072737	-1.548447	2.681393
1	-3.024901	-1.734163	-1.611181
1	-5.266495	-2.703014	2.706153
1	-5.207495	-2.892336	-1.587018
1	-6.341393	-3.377762	0.569566
1	-2.192440	1.626867	3.145844
1	-3.540701	1.108463	-0.896794
1	-4.183366	3.027756	3.635193
1	-5.524483	2.517697	-0.416873
1	-5.847768	3.483698	1.847680
8	-0.007572	-0.829723	-3.749815
6	-0.968725	-0.086538	-3.860063
8	-1.690744	0.317541	-2.813376
6	-1.453055	0.489899	-5.144208
1	-2.537672	0.379377	-5.233156
1	-1.232409	1.563856	-5.151523
1	-0.952216	0.011852	-5.986889
1	-1.250122	-0.020704	-2.001627

reductive-elimination-TS

Number of imaginary frequencies : 1

The smallest frequency is : -240.2635 cm(-1)

Electronic energy : HF=-2174.4554941
 Zero-point correction= 0.607791
 Thermal correction to Energy= 0.650947
 Thermal correction to Enthalpy= 0.651891
 Thermal correction to Gibbs Free Energy= 0.530143
 Sum of electronic and zero-point Energies= -2173.847703
 Sum of electronic and thermal Energies= -2173.804547
 Sum of electronic and thermal Enthalpies= -2173.803603
 Sum of electronic and thermal Free Energies= -2173.925351

Cartesian Coordinates

6	-3.724301	1.006096	4.218874
6	-2.448286	0.488367	4.429172
6	-1.612441	0.228004	3.349638
6	-2.040557	0.466233	2.034680
6	-3.324726	0.993676	1.838217
6	-4.157050	1.258906	2.919501
6	-1.106420	0.206543	0.913580
6	-1.432469	-0.396553	-0.270615
6	-2.785211	-0.924282	-0.564677
6	-3.337048	-1.934837	0.234297
6	-4.596545	-2.450167	-0.046439
6	-5.323420	-1.969307	-1.134290
6	-4.775516	-0.980880	-1.947045
6	-3.510453	-0.469667	-1.670355

46	-0.107721	0.087769	-1.784182
6	-0.212481	-1.762310	-0.889718
6	0.523519	-2.272825	0.183900
6	0.707426	-3.650671	0.375688
6	0.203994	-4.586565	-0.520564
6	-0.513335	-4.116496	-1.614586
6	-0.733582	-2.747007	-1.768990
6	1.401014	-3.838849	1.641436
6	1.628378	-2.410594	2.194168
7	1.088404	-1.543945	1.256945
8	2.168629	-2.112871	3.234120
6	1.325119	-0.137957	1.292621
6	2.745782	0.248950	1.436277
6	3.706675	-0.343955	0.608364
6	5.045079	0.020662	0.711042
6	5.439838	0.974643	1.646307
6	4.490220	1.558366	2.481612
6	3.151855	1.196532	2.379940
8	1.747559	-4.848049	2.215325
8	1.818975	0.327411	-3.115069
6	2.713228	-0.508455	-3.088445
6	4.079515	-0.292028	-3.632728
6	0.295849	0.708517	1.101109
6	0.494439	2.176808	0.949458
6	-0.161844	3.093068	1.780360
6	-0.013313	4.462356	1.579836
6	0.782457	4.939541	0.542730
6	1.443406	4.036633	-0.288340
6	1.304025	2.668780	-0.083902
8	2.554588	-1.713194	-2.550604
1	3.397821	-1.091998	-0.124528
1	2.412205	1.641293	3.043912
1	5.783704	-0.443548	0.060964
1	4.795518	2.292713	3.223844
1	6.487043	1.257031	1.728396
1	-0.783744	2.734936	2.598808
1	1.815413	1.965294	-0.741322
1	-0.524128	5.159502	2.240646
1	2.070632	4.398428	-1.100793
1	0.892681	6.010323	0.384805
1	4.788706	-0.246302	-2.797787
1	4.375186	-1.133609	-4.266140
1	4.122211	0.641044	-4.195457
1	1.647666	-1.757558	-2.177331
1	0.359511	-5.648794	-0.346104
1	-1.361430	-2.416189	-2.595674
1	-0.932423	-4.810817	-2.338424
1	-2.761153	-2.316687	1.077939
1	-3.073248	0.287056	-2.322568
1	-5.011689	-3.234289	0.583307
1	-5.331041	-0.609916	-2.805792
1	-6.309297	-2.373201	-1.353807
1	-0.610124	-0.164895	3.521872
1	-3.670443	1.209980	0.828651
1	-2.099954	0.288821	5.440408
1	-5.146506	1.676900	2.745985
1	-4.374841	1.219212	5.064125
8	-0.577925	2.152727	-2.748180
6	-1.305581	2.988902	-2.226110
8	-1.971556	2.768661	-1.101569
6	-1.538068	4.350003	-2.780070
1	-2.611657	4.529632	-2.896136
1	-1.158203	5.094688	-2.071329
1	-1.032724	4.463328	-3.739738
1	-1.716518	1.881284	-0.764738

reductive-elimination-product

Number of imaginary frequencies : 0

The smallest frequency is : 22.9834 cm(-1)

Electronic energy : =-2174.4681131
Zero-point correction= 0.610035
Thermal correction to Energy= 0.653248
Thermal correction to Enthalpy= 0.654192
Thermal correction to Gibbs Free Energy= 0.532549
Sum of electronic and zero-point Energies= -2173.858078
Sum of electronic and thermal Energies= -2173.814866
Sum of electronic and thermal Enthalpies= -2173.813921
Sum of electronic and thermal Free Energies= -2173.935564

.....
Cartesian Coordinates

.....
6 -3.783435 1.583899 4.020052
6 -2.586209 0.917814 4.267589
6 -1.735985 0.592004 3.216424
6 -2.076260 0.912450 1.894541
6 -3.280221 1.590852 1.659400
6 -4.124904 1.921672 2.712138
6 -1.139418 0.582344 0.792590
6 -1.486847 0.141568 -0.440635
6 -2.823340 -0.319335 -0.848581
6 -3.486512 -1.305562 -0.101104
6 -4.720948 -1.796001 -0.509988
6 -5.321603 -1.309082 -1.669046
6 -4.671880 -0.334248 -2.422755
6 -3.429635 0.147134 -2.023531
46 0.024187 -0.084839 -1.767873
6 -0.126859 -1.956797 -1.020847
6 0.154053 -2.345727 0.285934
6 -0.069598 -3.660424 0.731907
6 -0.586253 -4.637641 -0.109226
6 -0.874996 -4.283283 -1.421099
6 -0.651867 -2.970262 -1.849671
6 0.298679 -3.736376 2.137426
6 0.776588 -2.310899 2.504778
7 0.661170 -1.553005 1.355306
8 1.158877 -1.932111 3.590140
6 1.152513 -0.210683 1.317929
6 2.608185 -0.087944 1.557050
6 3.491990 -0.881049 0.816061
6 4.866182 -0.761552 0.994889
6 5.372013 0.140912 1.927335
6 4.497018 0.918814 2.682741
6 3.123599 0.804436 2.501523
8 0.263204 -4.661214 2.919991
8 1.908546 -0.295731 -3.026717
6 2.787119 -1.146740 -2.931404
6 4.166815 -0.969710 -3.453039
6 0.317691 0.815922 1.059649
6 0.782836 2.218779 0.904192
6 0.192787 3.255246 1.639285
6 0.575732 4.576268 1.431835
6 1.542800 4.886378 0.480061
6 2.132888 3.863699 -0.260350
6 1.759459 2.541385 -0.047727
8 2.600565 -2.315277 -2.337528
1 3.095361 -1.588650 0.087011
1 2.438413 1.404260 3.098946
1 5.543123 -1.377053 0.405710
1 4.887083 1.613463 3.423573
1 6.446322 0.232448 2.071093
1 -0.565570 3.026125 2.385901
1 2.206227 1.747959 -0.646335
1 0.112293 5.367734 2.016897
1 2.883989 4.095918 -1.012874
1 1.835673 5.920867 0.313751
1 4.853458 -0.893817 -2.601083
1 4.468491 -1.842401 -4.039763

1	4.234199	-0.063128	-4.054980
1	1.686834	-2.337583	-1.975920
1	-0.755187	-5.644529	0.266884
1	-0.904417	-2.718743	-2.880710
1	-1.282183	-5.014008	-2.115456
1	-3.018599	-1.691019	0.804707
1	-2.918351	0.894517	-2.630723
1	-5.216514	-2.565224	0.078826
1	-5.130442	0.048515	-3.332240
1	-6.288049	-1.692902	-1.988268
1	-0.790775	0.089002	3.420757
1	-3.549422	1.874297	0.642590
1	-2.308332	0.654752	5.286079
1	-5.050379	2.457228	2.510873
1	-4.443209	1.847605	4.843634
8	0.058339	1.959227	-2.707144
6	-0.506542	3.001376	-2.386809
8	-1.377466	3.082611	-1.396790
6	-0.279852	4.298372	-3.076939
1	-1.226665	4.678628	-3.474430
1	0.087329	5.032186	-2.350506
1	0.443550	4.179951	-3.884311
1	-1.426271	2.209152	-0.945684

Coordinates for heterobimetallic pathway

N-H-activation-TS (Pd-Ag)

Number of imaginary frequencies : 1

The smallest frequency is : -1175.4656 cm(-1)

Electronic energy : =-1699.4977192
 Zero-point correction= 0.332694
 Thermal correction to Energy= 0.364712
 Thermal correction to Enthalpy= 0.365656
 Thermal correction to Gibbs Free Energy= 0.267587
 Sum of electronic and zero-point Energies= -1699.165026
 Sum of electronic and thermal Energies= -1699.133008
 Sum of electronic and thermal Enthalpies= -1699.132063
 Sum of electronic and thermal Free Energies= -1699.230132

Cartesian Coordinates

8	-0.262257	2.668868	-0.715772
6	-0.796564	2.743679	0.424597
6	-1.558977	3.978832	0.795064
1	-1.332814	4.796602	0.107773
1	-2.629938	3.751969	0.747136
1	-1.326984	4.271571	1.822734
8	-0.750216	1.832241	1.313924
47	-1.576555	-1.280741	-1.024895
46	0.167819	0.014543	0.970700
1	0.636430	1.669064	-0.768745
6	2.966518	2.164531	0.850972
6	4.299040	2.341644	1.222181
1	4.545647	3.126910	1.932749
6	5.324669	1.538326	0.709155
1	6.349504	1.710257	1.026492
6	5.035900	0.531534	-0.201684
1	5.815471	-0.102325	-0.618103
6	3.708693	0.351637	-0.584199
6	2.691264	1.158614	-0.059619
6	1.604450	-0.191499	-1.546159
7	1.402399	0.805764	-0.563233
6	3.106143	-0.574418	-1.528303
8	3.575166	-1.472491	-2.191542
8	0.757508	-0.666817	-2.262916

8	-0.996813	-0.769862	2.456257
6	-2.242090	-0.921886	2.212438
8	-2.812683	-0.684848	1.123401
6	-3.053532	-1.473261	3.351956
1	-2.508626	-1.444169	4.297513
1	-3.990546	-0.915511	3.439016
1	-3.311488	-2.513552	3.122430
1	2.178118	2.788797	1.265157
8	1.268216	-1.709638	0.797076
8	-0.322850	-2.977896	-0.182873
6	0.805944	-2.805745	0.308526
6	1.796583	-3.937989	0.322933
1	2.345121	-3.967107	1.268212
1	1.296787	-4.892397	0.144146
1	2.527866	-3.766843	-0.476882
8	-2.665742	0.417669	-2.123848
6	-3.089133	1.437317	-1.582393
8	-3.321998	1.540376	-0.291624
1	-3.065934	0.717396	0.207648
6	-3.354429	2.692222	-2.338325
1	-4.156897	3.274917	-1.880063
1	-2.435870	3.293605	-2.316117
1	-3.587741	2.464289	-3.380104

N-H-activation-product (Pd-Ag)

Number of imaginary frequencies : 0
The smallest frequency is : 23.6357 cm(-1)

Electronic energy : =-1699.5069517
Zero-point correction= 0.336766
Thermal correction to Energy= 0.369355
Thermal correction to Enthalpy= 0.370299
Thermal correction to Gibbs Free Energy= 0.270762
Sum of electronic and zero-point Energies= -1699.170186
Sum of electronic and thermal Energies= -1699.137597
Sum of electronic and thermal Enthalpies= -1699.136652
Sum of electronic and thermal Free Energies= -1699.236190

Cartesian Coordinates

8	-0.202535	2.724144	0.132666
6	0.422421	2.656006	-1.014656
6	0.980094	3.938640	-1.510635
1	0.457444	4.791443	-1.073578
1	2.036803	3.983616	-1.222266
1	0.928430	3.969569	-2.600948
8	0.565990	1.601694	-1.651503
47	1.488025	-0.823767	1.361914
46	-0.055392	-0.345420	-1.041793
1	-0.624476	1.844668	0.334489
6	-3.151250	1.043510	-1.594543
6	-4.493125	1.281224	-1.901514
1	-4.745946	1.646535	-2.894563
6	-5.517652	1.063366	-0.975881
1	-6.548807	1.262645	-1.254769
6	-5.213743	0.590578	0.296534
1	-5.990882	0.408148	1.036101
6	-3.881319	0.349851	0.609691
6	-2.854435	0.575515	-0.323798
6	-1.728827	-0.206242	1.461156
7	-1.571778	0.302604	0.201746
6	-3.246384	-0.146613	1.821076
8	-3.704190	-0.472095	2.893477
8	-0.866089	-0.630169	2.217499
8	1.442111	-1.074946	-2.255146
6	2.633483	-0.932099	-1.823121
8	2.952712	-0.425863	-0.720630

6	3.724255	-1.440559	-2.723550
1	3.337598	-1.809558	-3.675588
1	4.447572	-0.638554	-2.903580
1	4.258055	-2.247778	-2.210145
1	-2.368926	1.212040	-2.332612
8	-0.749024	-2.231242	-0.760124
8	0.921107	-2.941217	0.591639
6	-0.091289	-3.120734	-0.102461
6	-0.692509	-4.499601	-0.198087
1	-1.168928	-4.661789	-1.167894
1	0.073403	-5.258046	-0.019545
1	-1.461440	-4.599470	0.576865
8	2.335767	1.207519	2.171890
6	2.685651	2.159937	1.480654
8	2.970202	2.068311	0.196403
1	2.890386	1.131181	-0.138827
6	2.808503	3.545369	2.015110
1	3.669663	4.058637	1.579438
1	1.910117	4.111329	1.738974
1	2.881625	3.525538	3.103537

alkyne-insertion-1-PRC (Pd-Ag)

Number of imaginary frequencies : 0

The smallest frequency is : 21.8109 cm(-1)

Electronic energy : =-2009.5852406
 Zero-point correction= 0.467627
 Thermal correction to Energy= 0.506331
 Thermal correction to Enthalpy= 0.507275
 Thermal correction to Gibbs Free Energy= 0.394437
 Sum of electronic and zero-point Energies= -2009.117614
 Sum of electronic and thermal Energies= -2009.078910
 Sum of electronic and thermal Enthalpies= -2009.077966
 Sum of electronic and thermal Free Energies= -2009.190803

Cartesian Coordinates

46	0.446440	-0.930732	0.956171
6	-2.006440	-2.411251	1.412308
8	-2.215369	-2.307900	0.177132
6	1.975653	0.372539	-1.265332
6	0.347338	1.549154	0.274352
6	-0.546134	0.806459	0.940607
6	0.340656	2.908491	-0.307090
6	-0.328994	3.141933	-1.516644
6	1.028233	3.960542	0.307850
6	-0.319112	4.408478	-2.090343
1	-0.852486	2.317855	-2.003082
6	1.036537	5.226029	-0.270562
1	1.550048	3.785524	1.247271
6	0.363332	5.451075	-1.468215
1	-0.842824	4.580720	-3.028124
1	1.567000	6.039777	0.218802
1	0.370080	6.441435	-1.918103
7	1.569843	0.722946	0.056596
6	-1.895585	1.102182	1.406045
6	-2.358150	0.560630	2.615161
6	-2.762332	1.920917	0.662843
6	-3.642228	0.835295	3.070039
1	-1.701834	-0.089601	3.188720
6	-4.043192	2.198001	1.125405
1	-2.429726	2.334285	-0.286622
6	-4.489253	1.654538	2.327191
1	-3.983802	0.403844	4.008692
1	-4.697935	2.839219	0.538399
1	-5.495293	1.866384	2.682312
8	-0.934915	-2.075205	2.006454

6	-3.099116	-2.979545	2.275517
1	-3.282071	-4.022743	1.995886
1	-2.853777	-2.926059	3.338481
1	-4.025997	-2.426979	2.082840
6	2.765871	0.909323	0.837444
6	3.904490	0.514188	0.126691
6	2.843974	1.367608	2.138857
6	5.165948	0.564216	0.716715
6	4.114108	1.424842	2.714435
1	1.956322	1.662195	2.693169
6	5.262902	1.027931	2.021306
1	6.043645	0.255195	0.153644
1	4.208666	1.785208	3.735994
1	6.231533	1.086986	2.509695
6	3.498875	0.101799	-1.206333
8	1.264454	0.324662	-2.234260
8	4.128429	-0.347675	-2.136840
8	1.801046	-2.605895	0.619145
6	1.886927	-3.154886	-0.519792
6	2.964676	-4.200470	-0.681519
1	3.811960	-3.749246	-1.212200
1	3.318506	-4.570343	0.283878
1	2.602759	-5.032220	-1.292717
8	1.194240	-2.893935	-1.537380
47	-0.657859	-1.579554	-1.602315
8	-2.333062	-0.034314	-2.164799
6	-3.497264	0.056043	-1.774765
8	-4.043504	-0.737660	-0.883081
1	-3.374924	-1.377202	-0.505612
6	-4.441214	1.066272	-2.335535
1	-5.231410	1.314559	-1.623570
1	-3.897090	1.963814	-2.639883
1	-4.910675	0.638841	-3.229860

alkyne-insertion-1-TS (Pd-Ag)

Number of imaginary frequencies : 1

The smallest frequency is : -347.7399 cm(-1)

Electronic energy : =-2009.5577898
 Zero-point correction= 0.464419
 Thermal correction to Energy= 0.503321
 Thermal correction to Enthalpy= 0.504265
 Thermal correction to Gibbs Free Energy= 0.390541
 Sum of electronic and zero-point Energies= -2009.093371
 Sum of electronic and thermal Energies= -2009.054469
 Sum of electronic and thermal Enthalpies= -2009.053525
 Sum of electronic and thermal Free Energies= -2009.167249

 Cartesian Coordinates

46	-0.100689	-1.173487	0.880932
6	-2.995094	-1.578137	0.884214
8	-3.000124	-1.158714	-0.301476
6	2.130981	-0.406323	-1.080971
6	0.623081	1.351517	0.535815
6	-0.418149	0.824623	1.093837
6	1.421176	2.337626	-0.105971
6	1.071670	2.754208	-1.406960
6	2.573346	2.853862	0.517721
6	1.865351	3.684033	-2.062005
1	0.181961	2.332613	-1.878478
6	3.359901	3.776772	-0.154173
1	2.833232	2.524510	1.522237
6	3.007323	4.187530	-1.439599
1	1.600165	4.013598	-3.063442
1	4.249333	4.181132	0.322083
1	3.629087	4.911300	-1.961563

7	1.706975	-0.392353	0.231521
6	-1.594542	1.518841	1.629852
6	-2.329134	0.981844	2.693829
6	-1.993237	2.744659	1.075816
6	-3.442185	1.654115	3.186789
1	-2.029377	0.027858	3.119866
6	-3.103174	3.413768	1.575149
1	-1.428944	3.165904	0.243655
6	-3.833547	2.868579	2.628920
1	-4.007882	1.222221	4.009630
1	-3.402472	4.363431	1.136224
1	-4.707580	3.389273	3.013518
8	-1.957029	-1.820354	1.573764
6	-4.319262	-1.823954	1.554771
1	-4.841823	-2.638492	1.041154
1	-4.204905	-2.075575	2.611555
1	-4.941185	-0.927247	1.454996
6	2.847082	-0.353169	1.063689
6	4.041668	-0.240378	0.333357
6	2.860575	-0.381004	2.449268
6	5.272376	-0.138691	0.974941
6	4.098318	-0.270431	3.083836
1	1.935125	-0.477416	3.014011
6	5.292709	-0.147622	2.364336
1	6.187703	-0.054236	0.392916
1	4.134391	-0.282525	4.170847
1	6.235934	-0.066467	2.897795
6	3.684496	-0.269280	-1.077458
8	1.447366	-0.454338	-2.085976
8	4.358875	-0.203594	-2.080166
8	0.469006	-3.186508	0.528845
6	0.204628	-3.768211	-0.572465
6	0.580480	-5.231861	-0.629776
1	0.856389	-5.518731	-1.648070
1	1.393798	-5.467064	0.061358
1	-0.293479	-5.828203	-0.340938
8	-0.346835	-3.271846	-1.579747
47	-1.052774	-1.064961	-1.796922
8	-1.843553	1.144784	-2.280567
6	-2.856855	1.733905	-1.906587
8	-3.797493	1.191315	-1.168168
1	-3.538446	0.274721	-0.866366
6	-3.151481	3.142724	-2.300535
1	-3.686489	3.669620	-1.506169
1	-2.227481	3.666343	-2.557483
1	-3.796576	3.130249	-3.187421

alkyne-insertion-1-product (Pd-Ag)

Number of imaginary frequencies : 0
 The smallest frequency is : 25.7394 cm(-1)

Electronic energy : =-2009.5770394
 Zero-point correction= 0.465612
 Thermal correction to Energy= 0.505205
 Thermal correction to Enthalpy= 0.506149
 Thermal correction to Gibbs Free Energy= 0.391764
 Sum of electronic and zero-point Energies= -2009.111428
 Sum of electronic and thermal Energies= -2009.071834
 Sum of electronic and thermal Enthalpies= -2009.070890
 Sum of electronic and thermal Free Energies= -2009.185275

 Cartesian Coordinates

46	-0.225211	0.819166	0.842194
6	-3.082369	0.283719	0.803978
8	-2.774479	-0.847302	0.359713

6	2.325514	-0.759407	0.836450
6	0.081514	0.544415	-1.532744
6	-0.791782	1.386547	-1.277946
6	1.168086	-0.210243	-2.073408
6	1.155028	-1.612271	-2.072806
6	2.263827	0.475805	-2.623808
6	2.227864	-2.316114	-2.599668
1	0.308888	-2.140452	-1.637208
6	3.332591	-0.237549	-3.149220
1	2.269616	1.564091	-2.623645
6	3.318780	-1.630798	-3.132160
1	2.215828	-3.403249	-2.590433
1	4.183312	0.296619	-3.565709
1	4.161665	-2.185958	-3.537032
7	1.778078	0.464931	0.742531
6	-1.924328	2.248357	-1.475469
6	-1.927953	3.561768	-0.990905
6	-3.037329	1.753412	-2.170203
6	-3.030075	4.375518	-1.213645
1	-1.066047	3.930088	-0.437579
6	-4.137196	2.574603	-2.383515
1	-3.030045	0.725775	-2.529932
6	-4.135004	3.884052	-1.907688
1	-3.030063	5.397069	-0.841491
1	-4.999973	2.189955	-2.922110
1	-4.997707	4.523954	-2.077364
8	-2.246996	1.167038	1.181504
6	-4.532222	0.655369	0.944705
1	-4.894926	0.298458	1.916169
1	-4.672156	1.738997	0.905153
1	-5.126387	0.167032	0.167126
6	2.761681	1.404147	0.415439
6	4.034112	0.815083	0.283844
6	2.591875	2.762634	0.197473
6	5.143775	1.560460	-0.086397
6	3.715776	3.506135	-0.174156
1	1.612800	3.227606	0.303009
6	4.977242	2.923926	-0.321832
1	6.114918	1.080898	-0.194792
1	3.600632	4.572728	-0.356328
1	5.824978	3.537007	-0.615817
6	3.857859	-0.607174	0.558803
8	1.778800	-1.842226	1.054187
8	4.651517	-1.520875	0.579635
8	-0.009502	0.788851	2.889860
6	-0.411136	-0.206800	3.595552
6	-0.288048	0.035074	5.081809
1	0.772310	0.037083	5.358177
1	-0.696852	1.013713	5.349499
1	-0.799304	-0.750114	5.642868
8	-0.844922	-1.293820	3.184999
47	-0.654595	-2.018837	0.942299
8	-1.451235	-3.583239	-0.688669
6	-2.074866	-3.323652	-1.716169
8	-2.847499	-2.267899	-1.856196
1	-2.874892	-1.733888	-1.014583
6	-1.985097	-4.160341	-2.945805
1	-1.234479	-3.710154	-3.608149
1	-1.661990	-5.172049	-2.694982
1	-2.935229	-4.180266	-3.484870

alkyne-insertion-2-PRC (Pd-Ag)

Number of imaginary frequencies : 1
The smallest frequency is : -8.1597 cm(-1)

Electronic energy : =-2548.6679906
Zero-point correction= 0.659183

Thermal correction to Energy= 0.709862
 Thermal correction to Enthalpy= 0.710806
 Thermal correction to Gibbs Free Energy= 0.572254
 Sum of electronic and zero-point Energies= -2548.008807
 Sum of electronic and thermal Energies= -2547.958129
 Sum of electronic and thermal Enthalpies= -2547.957185
 Sum of electronic and thermal Free Energies= -2548.095736

 Cartesian Coordinates

6	-3.072927	2.093629	3.792822
6	-1.963937	1.461077	4.352391
6	-1.193423	0.594055	3.588967
6	-1.532402	0.353450	2.247593
6	-2.639151	1.004220	1.688129
6	-3.409013	1.863490	2.459557
6	-0.728426	-0.570813	1.507190
6	0.085554	-1.472984	1.226302
6	0.851526	-2.680684	1.354268
6	1.602018	-3.234915	0.307761
6	2.279981	-4.432518	0.502300
6	2.230721	-5.077184	1.735039
6	1.503678	-4.518694	2.785846
6	0.818496	-3.327123	2.602688
46	-0.094281	-0.339852	-0.630755
8	-2.828706	-2.512995	-0.833239
6	-1.691925	-3.006865	-1.091031
6	-1.524213	-4.494990	-0.924139
8	-0.695023	-2.337294	-1.471828
6	0.694195	1.413427	-0.047533
6	-0.229293	2.545555	0.045961
6	-0.212141	3.307612	1.227289
6	-1.081730	4.376835	1.396537
6	-1.988631	4.705743	0.390598
6	-2.021752	3.952665	-0.781880
6	-1.156434	2.877808	-0.953540
6	2.016176	1.493305	0.189727
7	2.783443	0.314280	0.452881
6	2.971991	-0.215037	1.714808
6	3.995933	-1.376069	1.538639
6	4.312594	-1.390830	0.114471
6	3.569833	-0.368856	-0.494607
6	5.119637	-2.232710	-0.639637
6	5.178776	-2.033358	-2.016015
6	4.434355	-1.008553	-2.607414
6	3.614082	-0.158001	-1.860892
8	2.475966	0.160334	2.753663
8	4.402254	-2.057766	2.453214
6	2.803410	2.750442	0.151260
6	2.581416	3.683680	-0.869711
6	3.326321	4.854664	-0.934781
6	4.314642	5.108034	0.013741
6	4.555495	4.179205	1.022890
6	3.810422	3.006803	1.089968
1	1.826222	3.471374	-1.626043
1	4.004035	2.293246	1.888860
1	3.144395	5.566060	-1.737411
1	5.328340	4.367490	1.765047
1	4.900982	6.022695	-0.038299
1	0.490305	3.038865	2.015981
1	-1.195737	2.292663	-1.869701
1	-1.057354	4.950229	2.320921
1	-2.726475	4.204853	-1.571602
1	-2.672682	5.541016	0.522425
1	-2.423868	-5.026591	-1.246861
1	-0.649515	-4.862886	-1.466144
1	-1.380721	-4.709850	0.143412
1	3.012074	0.614545	-2.334202
1	5.677922	-3.030600	-0.153541
1	4.487912	-0.869214	-3.685043

1	5.800597	-2.673734	-2.635870
1	1.624307	-2.739240	-0.659777
1	0.242237	-2.886065	3.414161
1	2.850638	-4.864365	-0.316949
1	1.467524	-5.016798	3.751826
1	2.760609	-6.015855	1.880056
1	-0.322503	0.099210	4.013747
1	-2.883561	0.839204	0.640032
1	-1.697386	1.645464	5.390398
1	-4.269827	2.359315	2.014849
1	-3.674350	2.769418	4.396418
47	-2.884987	-0.277477	-1.625979
8	0.335174	0.318511	-2.604012
6	-0.514170	0.467245	-3.538021
8	-1.762898	0.482718	-3.425432
6	0.058804	0.641375	-4.922246
1	1.127078	0.868503	-4.894723
1	-0.085869	-0.293311	-5.476764
1	-0.479776	1.427614	-5.458864
8	-4.951611	-0.163843	-0.396073
6	-5.213791	-0.783495	0.632643
6	-6.270558	-0.352586	1.592870
1	-7.021364	-1.142127	1.701476
1	-5.821227	-0.195038	2.579868
1	-6.746070	0.567994	1.251525
8	-4.598757	-1.885021	1.007098
1	-3.917742	-2.164889	0.334398

alkyne-insertion-2-TS (Pd-Ag)

Number of imaginary frequencies : 1

The smallest frequency is : -294.0851 cm(-1)

Electronic energy : =-2548.6513574
 Zero-point correction= 0.660053
 Thermal correction to Energy= 0.709913
 Thermal correction to Enthalpy= 0.710857
 Thermal correction to Gibbs Free Energy= 0.575850
 Sum of electronic and zero-point Energies= -2547.991304
 Sum of electronic and thermal Energies= -2547.941445
 Sum of electronic and thermal Enthalpies= -2547.940500
 Sum of electronic and thermal Free Energies= -2548.075507

Cartesian Coordinates

6	1.611074	-3.158844	4.033325
6	0.667107	-2.196111	4.383285
6	0.250386	-1.250552	3.452310
6	0.800258	-1.253634	2.163652
6	1.747596	-2.223021	1.815178
6	2.146869	-3.173065	2.746722
6	0.371891	-0.233748	1.222836
6	0.442392	1.002041	0.880764
6	0.555206	2.371314	1.307994
6	0.353637	3.453029	0.438801
6	0.439379	4.755224	0.918405
6	0.728317	4.991447	2.259351
6	0.924857	3.919617	3.131187
6	0.830538	2.617733	2.665852
46	0.190578	0.139742	-0.955233
8	3.173774	1.632669	-1.309710
6	2.243380	2.233690	-1.918625
6	2.547179	3.610005	-2.453638
8	1.084466	1.775421	-2.121421
6	-1.085367	-1.154865	0.067966
6	-0.868603	-2.609499	0.122944
6	-1.402124	-3.313826	1.215345
6	-1.176170	-4.675333	1.363316

6	-0.408082	-5.360646	0.423697
6	0.126112	-4.673646	-0.663133
6	-0.094524	-3.308234	-0.810254
6	-2.316547	-0.593355	0.213947
7	-2.469754	0.799835	0.499601
6	-2.487126	1.343108	1.770051
6	-2.744961	2.866596	1.574622
6	-2.881104	3.049436	0.135066
6	-2.713196	1.796281	-0.470180
6	-3.072050	4.193657	-0.627789
6	-3.101835	4.065691	-2.013692
6	-2.944958	2.808889	-2.603029
6	-2.747960	1.649391	-1.845392
8	-2.355962	0.759798	2.823066
8	-2.821505	3.656344	2.488524
6	-3.594181	-1.317599	0.022674
6	-3.738226	-2.233283	-1.029191
6	-4.944877	-2.889117	-1.235434
6	-6.030712	-2.636460	-0.400120
6	-5.904398	-1.714297	0.635302
6	-4.699764	-1.051972	0.841226
1	-2.898046	-2.413774	-1.698302
1	-4.616543	-0.337132	1.657346
1	-5.041492	-3.591676	-2.060114
1	-6.749648	-1.505969	1.287435
1	-6.976364	-3.148668	-0.562684
1	-1.980808	-2.769410	1.960974
1	0.338956	-2.773087	-1.650052
1	-1.588683	-5.199439	2.222665
1	0.724892	-5.202792	-1.401412
1	-0.222859	-6.426041	0.541555
1	3.405147	3.562616	-3.132632
1	1.690692	4.045028	-2.973997
1	2.834389	4.260859	-1.619453
1	-2.615602	0.679973	-2.320941
1	-3.183269	5.160701	-0.141107
1	-2.974572	2.723705	-3.686965
1	-3.250259	4.940301	-2.640997
1	0.124252	3.259916	-0.607427
1	0.966721	1.775149	3.342101
1	0.276445	5.588271	0.237691
1	1.145115	4.102798	4.180291
1	0.796291	6.011584	2.630260
1	-0.515640	-0.517474	3.699115
1	2.160657	-2.232696	0.807563
1	0.242413	-2.187246	5.384548
1	2.880456	-3.925696	2.466088
1	1.926819	-3.901809	4.762126
47	2.879559	-0.776829	-1.316591
8	-0.133812	-0.828188	-2.884730
6	0.802805	-1.284659	-3.604364
8	1.990524	-1.501386	-3.249224
6	0.454931	-1.593289	-5.040989
1	-0.617460	-1.760704	-5.167979
1	0.741333	-0.734395	-5.660025
1	1.017382	-2.460388	-5.397768
8	4.266932	-0.761926	0.594125
6	4.162535	0.086006	1.478749
6	4.428076	-0.203517	2.917250
1	5.097754	0.550004	3.342451
1	3.480559	-0.147328	3.469243
1	4.854532	-1.200871	3.035517
8	3.800523	1.331812	1.260314
1	3.602769	1.479805	0.294699

alkyne-insertion-2-product (Pd-Ag)

Number of imaginary frequencies : 0

The smallest frequency is : 9.3012 cm(-1)

Electronic energy : =-2548.6963179
Zero-point correction= 0.662744
Thermal correction to Energy= 0.712782
Thermal correction to Enthalpy= 0.713727
Thermal correction to Gibbs Free Energy= 0.576544
Sum of electronic and zero-point Energies= -2548.033574
Sum of electronic and thermal Energies= -2547.983536
Sum of electronic and thermal Enthalpies= -2547.982591
Sum of electronic and thermal Free Energies= -2548.119774

.....
Cartesian Coordinates

.....
6 1.499089 -2.034596 5.077970
6 0.284227 -1.354435 5.073708
6 -0.175694 -0.741732 3.912306
6 0.585456 -0.785383 2.738427
6 1.794716 -1.494615 2.746034
6 2.251087 -2.107383 3.908013
6 0.095779 -0.183289 1.475612
6 0.719752 0.636420 0.594080
6 1.841663 1.564212 0.648731
6 1.896704 2.639429 -0.255377
6 2.924598 3.572005 -0.198235
6 3.920259 3.460697 0.768950
6 3.868506 2.414895 1.686644
6 2.844044 1.478185 1.633034
46 -0.268040 0.022017 -1.033569
8 2.871326 -0.007784 -2.406295
6 2.111244 0.916379 -2.811852
6 2.721407 1.996993 -3.664637
8 0.873106 0.994057 -2.586225
6 -1.225548 -0.593781 0.900908
6 -1.687254 -1.986526 1.133233
6 -2.832416 -2.206510 1.907290
6 -3.265826 -3.501375 2.166457
6 -2.564634 -4.589796 1.652471
6 -1.411825 -4.378189 0.900378
6 -0.966536 -3.083335 0.656600
6 -2.099732 0.394132 0.372777
7 -1.925451 1.751367 0.790358
6 -2.037927 2.133545 2.113535
6 -1.727878 3.654323 2.149690
6 -1.521210 4.030835 0.759589
6 -1.692760 2.881750 -0.027841
6 -1.211497 5.257405 0.185692
6 -1.089876 5.327930 -1.198739
6 -1.303035 4.187042 -1.974889
6 -1.614963 2.946884 -1.407969
8 -2.332219 1.432427 3.054710
8 -1.696277 4.306250 3.168912
6 -3.422713 0.125462 -0.242025
6 -3.706419 -1.054137 -0.951351
6 -4.960995 -1.268052 -1.501278
6 -5.967749 -0.314465 -1.360145
6 -5.704012 0.857950 -0.661105
6 -4.446472 1.077829 -0.110876
1 -2.930307 -1.796385 -1.097550
1 -4.268499 2.003352 0.431936
1 -5.153247 -2.187452 -2.050555
1 -6.478718 1.611532 -0.539903
1 -6.949412 -0.484142 -1.796674
1 -3.378968 -1.353521 2.307093
1 -0.066632 -2.916970 0.063847
1 -4.156260 -3.661007 2.770314
1 -0.853426 -5.223746 0.504506
1 -2.911614 -5.602402 1.845688
1 3.700812 2.277814 -3.264195
1 2.879965 1.605620 -4.676339

1	2.073322	2.875187	-3.722882
1	-1.775297	2.073467	-2.035177
1	-1.070574	6.132241	0.816610
1	-1.225326	4.258610	-3.057631
1	-0.846027	6.270868	-1.680451
1	1.114258	2.738684	-1.004199
1	2.821079	0.672185	2.361966
1	2.940982	4.393125	-0.912765
1	4.636812	2.319640	2.451730
1	4.728262	4.187597	0.812009
1	-1.122768	-0.207610	3.912033
1	2.373152	-1.579650	1.824743
1	-0.313192	-1.301175	5.981461
1	3.191459	-2.655350	3.894137
1	1.854339	-2.514033	5.987496
47	1.827725	-1.908517	-1.456235
8	-1.237591	-1.199190	-2.606552
6	-0.905859	-2.395166	-2.839330
8	0.160798	-2.972565	-2.489792
6	-1.916255	-3.246182	-3.571637
1	-1.423877	-3.919152	-4.279608
1	-2.431289	-3.871566	-2.829731
1	-2.661856	-2.634691	-4.086379
8	3.724592	-1.900469	-0.030570
6	4.571973	-1.031378	0.179480
6	5.432307	-1.054338	1.396851
1	6.343377	-0.467304	1.262787
1	4.855941	-0.614584	2.222215
1	5.671283	-2.085231	1.669078
8	4.786989	-0.006954	-0.610812
1	4.109043	0.019992	-1.344979

C-H-activation-PRC (Pd-Ag)

Number of imaginary frequencies : 1

The smallest frequency is : -9.0801 cm(-1)

Electronic energy : =-2548.6877633
 Zero-point correction= 0.661661
 Thermal correction to Energy= 0.711326
 Thermal correction to Enthalpy= 0.712270
 Thermal correction to Gibbs Free Energy= 0.576519
 Sum of electronic and zero-point Energies= -2548.026103
 Sum of electronic and thermal Energies= -2547.976438
 Sum of electronic and thermal Enthalpies= -2547.975493
 Sum of electronic and thermal Free Energies= -2548.111244

Cartesian Coordinates

8	-2.575284	0.639488	-3.309967
47	-2.756761	-0.204703	-0.857755
46	0.039390	-1.270620	-1.131800
8	-5.091534	-1.950247	1.347386
6	-5.638988	-0.859137	0.843235
8	-5.190555	-0.258166	-0.124727
6	-6.859711	-0.431528	1.589564
1	-7.565809	-1.264007	1.671321
1	-7.336830	0.415616	1.094592
1	-6.576635	-0.146843	2.610211
1	-0.288618	1.117374	-1.677355
6	0.666886	0.752475	-2.071403
6	0.761383	0.108361	-3.327304
1	-0.168575	-0.194933	-3.807979
6	1.988515	-0.074984	-3.974921
1	2.020440	-0.582581	-4.934443
6	3.154593	0.440084	-3.416455
1	4.110447	0.344044	-3.927566
6	3.087984	1.095151	-2.187077

6	1.867140	1.230029	-1.522329
6	3.312225	2.357945	-0.158757
6	0.672822	0.737380	1.223780
6	0.960039	1.941023	0.667895
7	1.998436	1.925889	-0.321664
6	4.091566	1.794263	-1.388290
8	5.278611	1.951549	-1.556864
8	3.755131	3.018943	0.745955
6	1.693707	-0.348871	1.048141
6	0.327661	3.245963	0.908070
6	-0.041730	4.061376	-0.167960
6	0.115803	3.698831	2.215472
6	-0.636924	5.296218	0.060937
1	0.108201	3.704110	-1.186231
6	-0.474877	4.935828	2.441156
1	0.428774	3.076707	3.053119
6	-0.855743	5.735412	1.365032
1	-0.932456	5.917425	-0.782029
1	-0.629260	5.283191	3.460338
1	-1.317555	6.704232	1.542566
6	-0.571611	0.405974	1.941731
6	-1.780177	1.062266	1.641765
6	-0.600119	-0.641109	2.874573
6	-2.960198	0.702562	2.282901
1	-1.799473	1.847006	0.887244
6	-1.783482	-0.995783	3.515792
1	0.315795	-1.183273	3.108356
6	-2.966992	-0.323349	3.226975
1	-3.882116	1.226731	2.034928
1	-1.777254	-1.804622	4.243459
1	-3.894478	-0.606108	3.720581
6	1.561422	-1.321840	0.137798
6	2.927123	-0.204454	1.871228
6	2.850082	0.344656	3.158867
6	4.191252	-0.525733	1.357320
6	3.999110	0.543540	3.915467
1	1.880768	0.619839	3.572909
6	5.339206	-0.320340	2.113651
1	4.278044	-0.915983	0.344966
6	5.248061	0.212366	3.396700
1	3.916746	0.966221	4.914487
1	6.311041	-0.565325	1.690610
1	6.147071	0.378646	3.985778
6	2.293700	-2.552662	-0.098294
6	2.958506	-2.788651	-1.313369
6	2.312221	-3.541058	0.900172
6	3.638605	-3.982051	-1.515893
1	2.949307	-2.018376	-2.084372
6	2.999509	-4.728476	0.692691
1	1.785767	-3.357041	1.835883
6	3.660227	-4.952166	-0.515003
1	4.159889	-4.155109	-2.454531
1	3.018674	-5.486245	1.472570
1	4.195405	-5.885318	-0.675663
8	-0.676669	-3.017822	-0.111532
6	-1.851417	-3.094324	0.344417
8	-2.800562	-2.311571	0.061731
6	-2.149072	-4.242739	1.270995
1	-1.232720	-4.639440	1.714813
1	-2.839985	-3.925277	2.059048
1	-2.638086	-5.043952	0.704802
1	-4.246505	-2.157061	0.856533
6	-2.370564	1.761258	-2.790499
6	-2.094141	2.946043	-3.689485
1	-1.027754	2.943827	-3.953081
1	-2.660083	2.876428	-4.623041
1	-2.313071	3.893302	-3.188029
8	-2.323378	1.968655	-1.535929

C-H-activation-TS (Pd-Ag)

Number of imaginary frequencies : 1
The smallest frequency is : -1620.8825 cm(-1)

Electronic energy : =-2548.6576134
Zero-point correction= 0.656742
Thermal correction to Energy= 0.706733
Thermal correction to Enthalpy= 0.707678
Thermal correction to Gibbs Free Energy= 0.570543
Sum of electronic and zero-point Energies= -2548.000872
Sum of electronic and thermal Energies= -2547.950880
Sum of electronic and thermal Enthalpies= -2547.949936
Sum of electronic and thermal Free Energies= -2548.087070

Cartesian Coordinates

8	-2.639340	1.715808	-2.223056
47	-2.756370	-0.023168	-0.827617
46	-0.138816	-1.289791	-1.190071
8	-5.496069	-1.614128	0.968052
6	-5.910618	-0.466969	0.460563
8	-5.315053	0.142641	-0.418136
6	-7.168790	0.028161	1.095510
1	-7.865663	-0.792798	1.284390
1	-7.636248	0.790660	0.470243
1	-6.916931	0.476059	2.065064
1	0.081679	1.007150	-2.086017
6	1.146561	0.201746	-2.117967
6	1.454773	-0.402882	-3.365016
1	0.635236	-0.857829	-3.923084
6	2.730893	-0.442136	-3.927746
1	2.892896	-0.936921	-4.881731
6	3.785588	0.177198	-3.265549
1	4.793256	0.184684	-3.676460
6	3.529644	0.820641	-2.059790
6	2.244378	0.828615	-1.494491
6	3.516705	2.099498	-0.048194
6	0.618530	0.652403	1.114023
6	1.131706	1.783255	0.566073
7	2.245783	1.598560	-0.307484
6	4.416864	1.591209	-1.202195
8	5.601300	1.829413	-1.291824
8	3.853961	2.779438	0.890816
6	1.491430	-0.562403	1.063302
6	0.731619	3.178257	0.810868
6	0.768339	4.134878	-0.210836
6	0.372217	3.583366	2.103985
6	0.415615	5.455319	0.048126
1	1.042916	3.827988	-1.217386
6	0.020412	4.901706	2.359433
1	0.381074	2.854391	2.912959
6	0.035774	5.842493	1.330489
1	0.436760	6.185278	-0.758878
1	-0.252901	5.200853	3.368983
1	-0.235857	6.876382	1.532079
6	-0.718111	0.517568	1.719304
6	-1.795556	1.338481	1.328275
6	-0.975842	-0.506208	2.642373
6	-3.068320	1.148681	1.863299
1	-1.629476	2.147197	0.617392
6	-2.247793	-0.692642	3.175785
1	-0.165343	-1.164605	2.952356
6	-3.299831	0.130744	2.790399
1	-3.884198	1.795799	1.545410
1	-2.413474	-1.488991	3.898225
1	-4.295432	-0.021184	3.201546
6	1.283852	-1.533397	0.165318
6	2.670378	-0.533086	1.970618

6	2.563639	0.031161	3.249502
6	3.931972	-0.962264	1.535494
6	3.677749	0.143084	4.073461
1	1.595060	0.382606	3.603731
6	5.046140	-0.845578	2.359343
1	4.045046	-1.370316	0.532550
6	4.923979	-0.293692	3.631706
1	3.571395	0.579372	5.064504
1	6.017548	-1.176410	1.997824
1	5.797045	-0.197921	4.273246
6	1.896286	-2.849098	0.027092
6	2.643709	-3.203500	-1.106333
6	1.715475	-3.794599	1.048879
6	3.215282	-4.466001	-1.201841
1	2.784627	-2.473007	-1.903049
6	2.286975	-5.056063	0.946868
1	1.118483	-3.523826	1.918973
6	3.036661	-5.395273	-0.177830
1	3.804190	-4.727263	-2.078273
1	2.144534	-5.780721	1.745502
1	3.481168	-6.384763	-0.258074
8	-1.116818	-2.998298	-0.281216
6	-2.320340	-3.022734	0.079289
8	-3.189429	-2.146242	-0.211061
6	-2.786133	-4.187999	0.908821
1	-1.977823	-4.895898	1.103335
1	-3.176633	-3.811549	1.862137
1	-3.610655	-4.699879	0.401186
1	-4.635073	-1.880561	0.534823
6	-1.669195	2.497279	-2.346251
6	-1.959034	3.955866	-2.585700
1	-1.136132	4.450093	-3.108964
1	-2.894443	4.081941	-3.137104
1	-2.078009	4.439504	-1.606704
8	-0.436758	2.189281	-2.259552

C-H-activation-product (Pd-Ag)

Number of imaginary frequencies : 0

The smallest frequency is : 21.1476 cm(-1)

Electronic energy : =-2548.6824932

Zero-point correction= 0.661492

Thermal correction to Energy= 0.712348

Thermal correction to Enthalpy= 0.713293

Thermal correction to Gibbs Free Energy= 0.573465

Sum of electronic and zero-point Energies= -2548.021001

Sum of electronic and thermal Energies= -2547.970145

Sum of electronic and thermal Enthalpies= -2547.969201

Sum of electronic and thermal Free Energies= -2548.109028

Cartesian Coordinates

8	-2.663412	2.124905	-1.426722
47	-2.465363	-0.059903	-0.562630
46	0.122483	-1.223542	-1.372970
8	-5.292029	-2.086787	0.428876
6	-5.661855	-0.825614	0.306961
8	-5.029137	0.010564	-0.326110
6	-6.924606	-0.517548	1.043255
1	-7.682041	-1.283654	0.853034
1	-7.301236	0.467056	0.761162
1	-6.717664	-0.526548	2.120543
1	-0.638005	1.346804	-2.350020
6	1.365800	0.282676	-1.984225
6	1.707650	0.113576	-3.345656
1	1.145291	-0.619053	-3.928298
6	2.739015	0.795911	-3.996245

1	2.941409	0.598927	-5.046313
6	3.515884	1.696032	-3.279357
1	4.352241	2.227494	-3.728945
6	3.188997	1.916577	-1.948337
6	2.120026	1.250753	-1.316072
6	3.011746	2.643024	0.310884
6	0.531792	0.365259	1.301253
6	0.869434	1.608626	0.881871
7	2.003827	1.737413	0.029816
6	3.839126	2.786781	-0.982419
8	4.816118	3.497678	-1.089745
8	3.199422	3.216714	1.360709
6	1.570086	-0.690937	1.094746
6	0.198464	2.884949	1.197246
6	-0.140870	3.780792	0.177764
6	-0.076390	3.228608	2.525507
6	-0.798765	4.969997	0.476023
1	0.105566	3.536873	-0.857175
6	-0.725165	4.419541	2.823564
1	0.222868	2.545373	3.319918
6	-1.098332	5.288174	1.798313
1	-1.072276	5.653212	-0.325785
1	-0.934337	4.677439	3.859437
1	-1.609727	6.219354	2.032006
6	-0.760055	-0.043784	1.898002
6	-1.930879	0.746387	1.829716
6	-0.880869	-1.316915	2.480123
6	-3.144869	0.278880	2.332542
1	-1.897791	1.749186	1.409822
6	-2.095076	-1.779587	2.976959
1	-0.008816	-1.966610	2.526928
6	-3.236249	-0.987608	2.906093
1	-4.022234	0.919183	2.269801
1	-2.145503	-2.771385	3.421066
1	-4.188616	-1.351321	3.285576
6	1.524096	-1.484632	0.015402
6	2.687687	-0.676578	2.074248
6	2.451854	-0.409203	3.430264
6	4.016083	-0.824738	1.649620
6	3.504701	-0.331312	4.335950
1	1.430481	-0.264560	3.781500
6	5.067559	-0.744093	2.554775
1	4.225124	-0.981476	0.592270
6	4.816923	-0.502480	3.903349
1	3.297168	-0.129944	5.384950
1	6.090450	-0.854723	2.200577
1	5.640400	-0.434638	4.610853
6	2.355371	-2.648496	-0.299443
6	3.204483	-2.683552	-1.416523
6	2.290916	-3.773266	0.536640
6	3.980479	-3.806587	-1.674977
1	3.262619	-1.811859	-2.068735
6	3.063670	-4.897533	0.269756
1	1.625045	-3.751216	1.399094
6	3.910580	-4.918060	-0.835840
1	4.644845	-3.815553	-2.536518
1	3.005318	-5.761746	0.928178
1	4.514042	-5.798319	-1.045903
8	-0.883535	-3.106757	-0.889777
6	-2.109556	-3.223283	-0.656161
8	-2.964543	-2.289992	-0.773123
6	-2.634724	-4.561437	-0.209140
1	-1.844513	-5.313548	-0.165957
1	-3.087034	-4.452958	0.784213
1	-3.426065	-4.896234	-0.888372
1	-4.422660	-2.227175	-0.050848
6	-1.999835	2.689719	-2.285958
6	-2.363926	4.004138	-2.881150
1	-2.710680	3.842491	-3.908543
1	-3.161067	4.473065	-2.302994

1	-1.488096	4.658105	-2.932130
8	-0.887367	2.185612	-2.800207

reductive-elimination-PRC (Pd-Ag)

Number of imaginary frequencies : 0
 The smallest frequency is : 18.8252 cm(-1)

Electronic energy : =-2548.700713
 Zero-point correction= 0.661723
 Thermal correction to Energy= 0.712372
 Thermal correction to Enthalpy= 0.713317
 Thermal correction to Gibbs Free Energy= 0.573505
 Sum of electronic and zero-point Energies= -2548.038990
 Sum of electronic and thermal Energies= -2547.988341
 Sum of electronic and thermal Enthalpies= -2547.987396
 Sum of electronic and thermal Free Energies= -2548.127208

 Cartesian Coordinates

6	-0.540981	3.752460	3.959333
6	-1.213811	2.539945	4.070933
6	-1.179451	1.619963	3.027677
6	-0.484678	1.903022	1.841562
6	0.204068	3.122447	1.749760
6	0.172789	4.035791	2.796028
6	-0.465278	0.906504	0.742247
6	-0.452165	1.173803	-0.601899
6	-0.671304	2.509631	-1.190300
6	-1.816208	3.248684	-0.850486
6	-2.055969	4.491734	-1.423643
6	-1.160203	5.026167	-2.347839
6	-0.028534	4.297955	-2.705993
6	0.205169	3.046961	-2.143203
46	-0.499547	-0.417879	-1.892220
6	-2.445194	-0.019441	-1.676995
6	-3.225656	-0.161915	-0.538279
6	-4.591700	0.177178	-0.542712
6	-5.221339	0.663975	-1.680978
6	-4.462462	0.801416	-2.836519
6	-3.103709	0.471121	-2.818451
6	-5.122441	-0.039550	0.793261
6	-3.928012	-0.567715	1.621381
7	-2.845779	-0.610482	0.763011
8	-3.938625	-0.872686	2.793904
6	-1.625946	-1.235554	1.162367
6	-1.769890	-2.652533	1.563229
6	-2.472352	-3.531138	0.730702
6	-2.598588	-4.873537	1.072148
6	-2.038812	-5.348459	2.255535
6	-1.357107	-4.473699	3.099416
6	-1.226613	-3.132789	2.758428
8	-6.233524	0.135667	1.245665
8	-0.361719	-2.211227	-3.233883
6	0.887191	-2.288971	-3.161176
6	1.616507	-3.469552	-3.723779
6	-0.472251	-0.538459	1.148770
6	0.850153	-1.145273	1.453807
6	1.712935	-0.539584	2.383950
6	2.958770	-1.093861	2.661230
6	3.372613	-2.253153	2.009916
6	2.535972	-2.850526	1.069123
6	1.288677	-2.301696	0.788470
8	1.571950	-1.372630	-2.577847
1	-2.910881	-3.158735	-0.195748
1	-0.707959	-2.443843	3.424107
1	-3.137266	-5.550056	0.412184
1	-0.935500	-4.836557	4.034330

1	-2.140252	-6.397559	2.524438
1	1.395118	0.361420	2.908360
1	0.643849	-2.770827	0.046275
1	3.607403	-0.615804	3.392354
1	2.855655	-3.748977	0.544688
1	4.342128	-2.692159	2.236606
1	0.949217	-4.103910	-4.310420
1	2.457040	-3.143320	-4.345109
1	2.029264	-4.058890	-2.895366
1	-6.276564	0.926763	-1.649234
1	-2.527026	0.618292	-3.732211
1	-4.911258	1.178844	-3.752224
1	-2.521559	2.838317	-0.128054
1	1.084842	2.474102	-2.443990
1	-2.948871	5.048430	-1.146139
1	0.673693	4.700729	-3.433034
1	-1.347294	6.001095	-2.792520
1	-1.696958	0.667056	3.135248
1	0.802131	3.338278	0.867787
1	-1.767210	2.302277	4.976932
1	0.719256	4.972749	2.705416
1	-0.561952	4.469027	4.777400
8	4.148432	-0.199233	-0.781906
6	4.563224	-1.340639	-1.037978
8	3.927927	-2.163209	-1.818238
6	5.861884	-1.851053	-0.519895
1	5.821686	-2.931708	-0.361602
1	6.636970	-1.651806	-1.269781
1	6.139178	-1.338814	0.404630
47	1.913133	0.629601	-0.562580
8	3.107820	2.400035	0.620295
6	3.936141	2.183089	1.498437
8	4.864982	1.248386	1.396678
6	4.006177	2.955351	2.770129
1	4.832892	3.673027	2.716012
1	3.071299	3.499209	2.924316
1	4.203895	2.288083	3.614371
1	4.720519	0.743642	0.555845
1	3.039217	-1.783237	-2.127176

reductive-elimination-TS (Pd-Ag)

Number of imaginary frequencies : 1

The smallest frequency is : -209.7998 cm(-1)

Electronic energy : =-2548.6912912
 Zero-point correction= 0.661877
 Thermal correction to Energy= 0.711593
 Thermal correction to Enthalpy= 0.712537
 Thermal correction to Gibbs Free Energy= 0.575944
 Sum of electronic and zero-point Energies= -2548.029414
 Sum of electronic and thermal Energies= -2547.979698
 Sum of electronic and thermal Enthalpies= -2547.978754
 Sum of electronic and thermal Free Energies= -2548.115347

Cartesian Coordinates

6	-1.292037	3.368265	4.208387
6	-1.725083	2.045774	4.229743
6	-1.550697	1.235463	3.114020
6	-0.944368	1.724792	1.944116
6	-0.487100	3.052374	1.949954
6	-0.670027	3.863342	3.064092
6	-0.850161	0.826102	0.767743
6	-0.923036	1.205525	-0.541262
6	-1.073335	2.600851	-1.003363
6	-2.250789	3.317774	-0.747587
6	-2.380381	4.636620	-1.165436

6	-1.341200	5.261097	-1.852982
6	-0.176720	4.551235	-2.134552
6	-0.049166	3.227955	-1.722560
46	-0.427379	-0.220039	-1.929702
6	-2.395516	0.182819	-1.627880
6	-3.275764	-0.384707	-0.713647
6	-4.668166	-0.281926	-0.881704
6	-5.229265	0.363283	-1.976419
6	-4.369027	0.927992	-2.909941
6	-2.987560	0.857062	-2.714966
6	-5.309152	-0.890126	0.272931
6	-4.147797	-1.383571	1.167653
7	-2.978430	-1.056852	0.498846
8	-4.243005	-1.934266	2.240221
6	-1.704427	-1.506117	0.949216
6	-1.612827	-2.960748	1.204430
6	-2.072829	-3.860452	0.236817
6	-1.971082	-5.231392	0.447289
6	-1.423552	-5.717161	1.632455
6	-0.979682	-4.826127	2.606988
6	-1.075977	-3.455652	2.396407
8	-6.480968	-1.015068	0.556739
8	0.678404	-1.609174	-3.213427
6	1.929961	-1.599511	-3.167926
6	2.682477	-2.680775	-3.896780
6	-0.684461	-0.635371	1.064856
6	0.696668	-1.088860	1.397184
6	1.362321	-0.651482	2.551272
6	2.663155	-1.067933	2.817311
6	3.331611	-1.912336	1.932211
6	2.684821	-2.352070	0.781169
6	1.376988	-1.946227	0.514844
8	2.623611	-0.746351	-2.523233
1	-2.503720	-3.477773	-0.689184
1	-0.743736	-2.757030	3.163327
1	-2.322960	-5.922773	-0.315341
1	-0.566740	-5.201049	3.541002
1	-1.349290	-6.789465	1.799436
1	0.852502	0.008358	3.251561
1	0.865442	-2.303064	-0.379128
1	3.159830	-0.727964	3.723594
1	3.193916	-3.009547	0.077615
1	4.352215	-2.227537	2.141664
1	2.044352	-3.192221	-4.620324
1	3.564729	-2.272242	-4.399296
1	3.033733	-3.417046	-3.162245
1	-6.310602	0.429157	-2.073704
1	-2.339480	1.368558	-3.425811
1	-4.760753	1.450342	-3.779096
1	-3.063946	2.831011	-0.208539
1	0.860413	2.668391	-1.950081
1	-3.297884	5.181610	-0.952769
1	0.635396	5.027641	-2.679801
1	-1.442589	6.294978	-2.175580
1	-1.896607	0.202739	3.143807
1	0.041593	3.447568	1.087838
1	-2.204707	1.639976	5.117943
1	-0.306260	4.888717	3.042294
1	-1.428895	4.005838	5.078870
8	4.581381	0.305465	-0.362617
6	5.241498	-0.703429	-0.632261
8	4.954638	-1.472986	-1.648050
6	6.440648	-1.124603	0.144229
1	6.470760	-2.212866	0.247840
1	7.340727	-0.820921	-0.403472
1	6.450978	-0.646703	1.126604
47	1.995015	0.525337	-0.607911
8	2.469447	2.188281	1.028056
6	3.217847	2.140599	2.000276
8	4.400191	1.558224	1.979546

6	2.896318	2.768709	3.313949
1	3.456550	3.706340	3.408861
1	1.826898	2.985563	3.378696
1	3.206023	2.117636	4.136926
1	4.543592	1.133324	1.091342
1	4.092890	-1.155949	-2.078202

reductive-elimination-product (Pd-Ag)

Number of imaginary frequencies : 0
The smallest frequency is : 23.9982 cm(-1)

Electronic energy : =-2548.733858
Zero-point correction= 0.664136
Thermal correction to Energy= 0.713961
Thermal correction to Enthalpy= 0.714905
Thermal correction to Gibbs Free Energy= 0.578137
Sum of electronic and zero-point Energies= -2548.069722
Sum of electronic and thermal Energies= -2548.019898
Sum of electronic and thermal Enthalpies= -2548.018953
Sum of electronic and thermal Free Energies= -2548.155721

Cartesian Coordinates

6	-0.856104	5.034518	3.128988
6	-1.683478	3.978128	3.502961
6	-1.758215	2.839058	2.709664
6	-1.014548	2.739345	1.525504
6	-0.181148	3.801798	1.162490
6	-0.105857	4.940264	1.959621
6	-1.149915	1.492189	0.732794
6	-1.463185	1.483318	-0.582583
6	-1.538968	2.733725	-1.388607
6	-2.714867	3.487893	-1.403671
6	-2.793201	4.652994	-2.160886
6	-1.702137	5.065919	-2.921486
6	-0.532040	4.310574	-2.922873
6	-0.449607	3.148890	-2.160289
46	-0.635316	-1.334720	-1.768551
6	-1.984063	0.274296	-1.277723
6	-2.926520	-0.547585	-0.603070
6	-3.968745	-1.202273	-1.258915
6	-4.037157	-1.220135	-2.664544
6	-3.034337	-0.597572	-3.373244
6	-2.015740	0.142259	-2.704076
6	-4.882636	-1.684144	-0.244717
6	-4.223811	-1.314871	1.111949
7	-3.029888	-0.657071	0.803383
8	-4.642372	-1.573568	2.213384
6	-1.843066	-0.743877	1.593936
6	-1.653101	-2.006178	2.340640
6	-1.875342	-3.235706	1.707415
6	-1.638197	-4.426385	2.382629
6	-1.186976	-4.404185	3.700915
6	-0.977239	-3.185533	4.341050
6	-1.211432	-1.992419	3.666300
8	-5.953027	-2.251819	-0.333552
8	0.523495	-3.164472	-1.732729
6	1.771789	-3.193776	-1.844091
6	2.456036	-4.535696	-1.805227
6	-0.913030	0.226742	1.485420
6	0.498999	0.018567	1.922306
6	1.198784	0.922038	2.731227
6	2.545485	0.719779	3.025039
6	3.229247	-0.380017	2.515298
6	2.548241	-1.294901	1.716019
6	1.198022	-1.097572	1.421667
8	2.513516	-2.168344	-1.971615

1	-2.213741	-3.255072	0.670086
1	-1.053577	-1.037566	4.166049
1	-1.802686	-5.375695	1.877466
1	-0.636583	-3.163415	5.373769
1	-1.003346	-5.336987	4.229500
1	0.689259	1.784537	3.154805
1	0.662493	-1.838461	0.826966
1	3.063870	1.433159	3.662847
1	3.059522	-2.169547	1.313378
1	4.282368	-0.526623	2.747492
1	1.735409	-5.354075	-1.856107
1	3.175320	-4.622689	-2.626146
1	3.020146	-4.618433	-0.867974
1	-4.862965	-1.722056	-3.163498
1	-1.408313	0.822711	-3.299699
1	-3.040254	-0.603379	-4.460265
1	-3.565637	3.160675	-0.806210
1	0.472313	2.565085	-2.140649
1	-3.709041	5.240220	-2.156511
1	0.323047	4.629590	-3.515193
1	-1.763022	5.976892	-3.512852
1	-2.398003	2.007747	3.005476
1	0.435712	3.712549	0.270441
1	-2.271557	4.039993	4.416105
1	0.551754	5.757728	1.668998
1	-0.792660	5.925846	3.749248
8	4.493937	-0.217226	-0.762913
6	5.207266	-1.206309	-0.568320
8	4.928190	-2.373793	-1.083424
6	6.447051	-1.178504	0.256036
1	6.391624	-1.951987	1.029202
1	7.311366	-1.414407	-0.374083
1	6.589554	-0.199081	0.717223
47	1.846923	-0.099420	-0.971787
8	2.403660	2.134033	-0.263036
6	3.333413	2.646164	0.357004
8	4.505509	2.076730	0.525687
6	3.231119	3.995978	0.986458
1	2.771347	4.695185	0.281966
1	2.574005	3.930409	1.861736
1	4.206991	4.369516	1.302445
1	4.523833	1.190261	0.068433
1	4.021822	-2.316397	-1.539235

(II) Cartesian coordinates of optimized geometries employed in the energy stacking diagram for the transition states (Section 5 in Electronic Supplementary Information)

Stacking of Transition States for Reactions 1 to 4. Stacking of transition states generated through conformational and configurational sampling and the corresponding relative free energies with respect to the lowest energy transition state obtained at the SMD_(solvent)/M06/6-31G**/LANL2DZ(Pd,Ag,Br,I) level of theory. The nomenclature used is as follows. The C-H activation transition states via a cyclometallation deprotonation (CMD) are given a generic representation using subscript “_{CH}”. The numerical prefix pertains to the reaction. The numerical suffix is assigned on the basis of the position of a given transition state with respect to the lowest

energy transition state. The monometallic and heterobimetallic transition states are respectively designated by using “Pd” or “Pd-Ag” in parentheses. Similar notations are followed for the reductive elimination (denoted as “_{RE}” instead) as well.

Reaction 1

----- 2-phenylpyridine -----

Number of imaginary frequencies : 0

Electronic energy : -478.986785
 Zero-point correction= 0.169248
 Thermal correction to Energy= 0.178078
 Thermal correction to Enthalpy= 0.179023
 Thermal correction to Gibbs Free Energy= 0.134536
 Sum of electronic and zero-point Energies= -478.817537
 Sum of electronic and thermal Energies= -478.808707
 Sum of electronic and thermal Enthalpies= -478.807762
 Sum of electronic and thermal Free Energies= -478.852249

----- Cartesian Coordinates -----

6	-0.721152	0.020439	-0.004413
6	0.759962	0.022351	-0.002495
6	-1.415538	-1.173105	0.225291
6	-2.804102	-1.194967	0.236249
6	-3.525325	-0.025164	0.009332
6	-2.845798	1.165418	-0.231736
6	-1.455835	1.188697	-0.238498
1	-0.845950	-2.082842	0.399314
1	-3.327515	-2.130116	0.424174
1	-4.613059	-0.042329	0.015851
1	-3.400399	2.081538	-0.423402
1	-0.941044	2.123106	-0.453622
6	1.492457	1.186776	0.257328
6	2.878751	1.131448	0.241915
6	3.503925	-0.081333	-0.022468
6	2.696756	-1.190353	-0.251360
7	1.365487	-1.151673	-0.244933
1	0.984861	2.118971	0.490807
1	3.463974	2.025769	0.444141
1	4.586396	-0.171334	-0.043942
1	3.149719	-2.162299	-0.453664

----- Aceticacid -----

Number of imaginary frequencies : 0

Electronic energy : -228.9715094
 Zero-point correction= 0.061960
 Thermal correction to Energy= 0.066504
 Thermal correction to Enthalpy= 0.067448
 Thermal correction to Gibbs Free Energy= 0.034745
 Sum of electronic and zero-point Energies= -228.909549
 Sum of electronic and thermal Energies= -228.905005
 Sum of electronic and thermal Enthalpies= -228.904061
 Sum of electronic and thermal Free Energies= -228.936764

----- Cartesian Coordinates -----

6	-0.090929	0.121158	-0.000009
8	-0.650807	1.193064	0.000001

6	1.385466	-0.100928	-0.000003
8	-0.764133	-1.042871	-0.000002
1	-1.709095	-0.816163	0.000023
1	1.677338	-0.681661	0.881179
1	1.677296	-0.682268	-0.880794
1	1.906763	0.857176	-0.000327

AgOAc-dimer-sol

Number of imaginary frequencies : 0

Electronic energy : -1294.058173
 Zero-point correction= 0.433258
 Thermal correction to Energy= 0.465645
 Thermal correction to Enthalpy= 0.466589
 Thermal correction to Gibbs Free Energy= 0.364081
 Sum of electronic and zero-point Energies= -1293.624915
 Sum of electronic and thermal Energies= -1293.592528
 Sum of electronic and thermal Enthalpies= -1293.591584
 Sum of electronic and thermal Free Energies= -1293.694092

 Cartesian Coordinates

6	-2.042535	3.837674	-0.580020
6	-1.225556	2.573048	-0.471383
8	-1.570348	1.624985	-1.235724
47	-0.907967	-0.541933	-1.096476
8	0.268532	-2.380211	-0.818258
6	1.047542	-2.452402	0.168811
6	1.793921	-3.749126	0.370459
8	-0.284327	2.557859	0.363836
47	0.860086	0.711807	0.744189
8	1.260889	-1.544045	1.022676
8	3.259602	0.279487	1.277817
6	4.169090	0.433465	0.171366
6	3.534677	-0.120139	-1.096545
6	4.400640	1.926757	0.051049
6	5.450058	-0.322576	0.534251
6	6.552946	-0.293820	-0.510514
8	-3.436617	-0.370534	-1.042033
6	-4.039379	-0.628063	0.239028
6	-4.163533	-2.136622	0.322953
6	-3.139933	-0.100426	1.348022
6	-5.403627	0.067203	0.243914
6	-6.231044	-0.102796	1.506712
1	-1.671933	4.620116	0.084925
1	-2.033736	4.195743	-1.614499
1	-3.085763	3.610606	-0.329774
1	2.859038	-3.545741	0.528075
1	1.425048	-4.236986	1.279559
1	1.666126	-4.426997	-0.475753
1	2.962248	-0.649423	1.307926
1	-3.231961	0.580454	-1.103291
1	4.167720	0.062949	-1.972607
1	3.371669	-1.204598	-1.019798
1	2.562557	0.359544	-1.287492
1	5.059661	2.161581	-0.791997
1	3.446696	2.445998	-0.111525
1	4.854197	2.322867	0.967818
1	5.818117	0.092667	1.483471
1	5.170276	-1.368367	0.741577
1	7.441113	-0.823438	-0.148498
1	6.245639	-0.777987	-1.445365
1	6.862213	0.730907	-0.750559
1	-3.549421	-0.329658	2.338838
1	-2.142411	-0.562658	1.290853
1	-3.019742	0.990369	1.277125
1	-4.569356	-2.450489	1.291002
1	-4.819783	-2.516769	-0.469524

1	-3.176037	-2.602113	0.204272
1	-5.229256	1.140674	0.062371
1	-5.963024	-0.306460	-0.625753
1	-7.198134	0.401991	1.404658
1	-6.438553	-1.158450	1.720959
1	-5.734284	0.326207	2.385386

[Pd(OAc)₂]₃

Number of imaginary frequencies : 0

Electronic energy : -1750.6013377
 Zero-point correction= 0.313837
 Thermal correction to Energy= 0.348156
 Thermal correction to Enthalpy= 0.349101
 Thermal correction to Gibbs Free Energy= 0.244827
 Sum of electronic and zero-point Energies= -1750.287501
 Sum of electronic and thermal Energies= -1750.253181
 Sum of electronic and thermal Enthalpies= -1750.252237
 Sum of electronic and thermal Free Energies= -1750.356511

 Cartesian Coordinates

46	-0.010490	-1.799629	0.001857
8	1.114207	-1.975397	1.697655
8	1.621816	-2.125974	-1.208417
6	2.288056	-1.270619	-1.853217
8	2.284275	-0.017073	-1.684234
46	1.565339	0.890861	-0.000949
6	2.204626	-1.360575	1.877974
8	2.634055	-0.367817	1.228190
8	-1.136349	-1.961826	-1.694704
8	-1.646249	-2.106660	1.213143
6	-2.303661	-1.241656	1.853838
8	-2.285231	0.011349	1.680912
46	-1.556588	0.911100	-0.002436
6	-2.220017	-1.335577	-1.878213
8	-2.637951	-0.334431	-1.234462
8	-1.129889	1.985976	-1.685788
8	-1.007137	2.466643	1.228269
6	-0.041829	2.603432	-1.869879
6	0.070878	2.598021	1.870253
8	1.035004	2.455088	-1.229169
8	1.150275	1.965147	1.685887
6	3.100471	-1.886191	2.960294
1	3.878079	-2.502249	2.494322
1	3.591373	-1.061328	3.482201
1	2.540385	-2.506852	3.662454
6	-3.235436	-1.749991	2.913689
1	-4.226006	-1.885297	2.464308
1	-2.895377	-2.711417	3.303528
1	-3.329872	-1.019024	3.720125
6	-3.117409	-1.866469	-2.956565
1	-3.744893	-1.072325	-3.366212
1	-2.528322	-2.337921	-3.746469
1	-3.767423	-2.631584	-2.516641
6	-0.040680	3.648970	-2.945547
1	0.923936	3.669766	-3.457933
1	-0.850495	3.474483	-3.656826
1	-0.196649	4.626711	-2.475394
6	0.087891	3.640106	2.949121
1	0.376857	4.596919	2.499212
1	-0.903804	3.753721	3.392055
1	0.824781	3.388028	3.714894
6	3.212942	-1.794020	-2.911825
1	2.857918	-2.750660	-3.300051
1	3.319147	-1.066550	-3.719973
1	4.200719	-1.944486	-2.461088

phosphonate-methyl

Number of imaginary frequencies : 0

Electronic energy : -647.307926
Zero-point correction= 0.100276
Thermal correction to Energy= 0.108369
Thermal correction to Enthalpy= 0.109313
Thermal correction to Gibbs Free Energy= 0.066401
Sum of electronic and zero-point Energies= -647.207649
Sum of electronic and thermal Energies= -647.199557
Sum of electronic and thermal Enthalpies= -647.198613
Sum of electronic and thermal Free Energies= -647.241525

Cartesian Coordinates

1	-2.227078	-0.227232	1.271575
1	-2.853920	-0.002931	-0.387266
1	-2.692811	-1.642604	0.288041
6	-2.245637	-0.646729	0.260720
8	-0.921532	-0.798423	-0.255944
15	-0.005776	0.516799	-0.381789
8	-0.183174	1.499748	0.708975
1	-0.216337	0.998872	-1.676074
8	1.441807	-0.128010	-0.582072
6	2.039490	-0.786004	0.540389
1	3.056096	-1.056529	0.249004
1	2.078855	-0.118533	1.408601
1	1.481907	-1.693143	0.798630

t-amylalcohol

Number of imaginary frequencies : 0

Electronic energy : -272.8048692
Zero-point correction= 0.163522
Thermal correction to Energy= 0.171434
Thermal correction to Enthalpy= 0.172379
Thermal correction to Gibbs Free Energy= 0.132752
Sum of electronic and zero-point Energies= -272.641348
Sum of electronic and thermal Energies= -272.633435
Sum of electronic and thermal Enthalpies= -272.632491
Sum of electronic and thermal Free Energies= -272.672117

Cartesian Coordinates

6	-0.840426	-0.668282	-0.511356
6	0.430513	0.006308	0.016662
6	-2.137133	-0.035173	-0.039716
1	-3.001452	-0.652958	-0.308296
1	-2.133041	0.084710	1.050113
1	-2.295034	0.954925	-0.484213
1	-0.807219	-1.724044	-0.194804
1	-0.799752	-0.682450	-1.611098
8	0.450785	-0.038599	1.444104
6	1.656041	-0.712594	-0.529504
6	0.483190	1.480730	-0.339616
1	1.429805	1.917677	0.000176
1	0.406338	1.622595	-1.424649
1	-0.331880	2.031690	0.142583
1	2.571398	-0.276725	-0.111619
1	1.632901	-1.779230	-0.264620
1	1.707837	-0.643159	-1.623411
1	0.460710	-0.970175	1.698187

Conformational and Configurational Study of C-H activation

Bimetallic C-H activation (Pd-Ag)

ICH1_Pd-Ag

Number of imaginary frequencies : 1
The smallest frequency is : -1527.0759 cm(-1)

Electronic energy : -2920.7851846
Zero-point correction= 0.502991
Thermal correction to Energy= 0.547576
Thermal correction to Enthalpy= 0.548520
Thermal correction to Gibbs Free Energy= 0.423178
Sum of electronic and zero-point Energies= -2920.282194
Sum of electronic and thermal Energies= -2920.237609
Sum of electronic and thermal Enthalpies= -2920.236665
Sum of electronic and thermal Free Energies= -2920.362007

Cartesian Coordinates

6	2.025940	-0.227583	-1.645933
6	3.357753	-0.462770	-1.223868
6	4.258743	-1.142854	-2.047554
6	3.854267	-1.569847	-3.308107
6	2.559293	-1.318904	-3.760375
6	1.658891	-0.665158	-2.927635
6	3.756922	0.048352	0.099744
6	5.077163	0.366117	0.421160
6	5.373927	0.869124	1.678993
6	4.344558	1.047536	2.594196
6	3.053458	0.712401	2.212247
7	2.760928	0.228565	0.999097
46	0.833514	-0.575126	0.219684
15	-0.794655	-1.812442	-0.830107
8	-0.095021	-2.817697	-1.908688
6	0.945896	-3.672684	-1.460458
15	-0.558656	-0.590181	2.077083
8	-0.617430	-1.943499	2.982252
6	0.557267	-2.740491	3.012280
47	-1.857633	1.146069	-0.469074
8	-1.897344	-1.082363	-1.553143
8	0.155875	0.475966	3.094566
6	-0.587132	0.944387	4.219266
8	-1.991168	-0.127798	1.859867
15	-0.095242	2.756669	-0.955820
8	1.335153	2.246200	-1.241502
8	-1.377610	-2.867195	0.268039
6	-2.425267	-3.739036	-0.159049
8	-0.405084	3.780287	-2.186648
6	-1.690156	4.379550	-2.211214
8	0.017132	3.869084	0.251834
6	0.105255	3.329891	1.559653
1	1.524772	0.985428	-1.334013
1	0.646656	-0.466036	-3.280457
1	2.258185	-1.639322	-4.755512
1	4.559299	-2.098566	-3.946279
1	5.270911	-1.357903	-1.708868
1	5.859533	0.241184	-0.321945
1	6.397914	1.127081	1.937448
1	4.528003	1.443578	3.588409
1	2.210278	0.826059	2.888855
1	0.041063	4.159259	2.270031
1	-0.720636	2.627604	1.760776
1	1.056256	2.799906	1.714804
1	-1.839360	4.803195	-3.208059
1	-2.485562	3.639455	-2.023161
1	-1.771343	5.180698	-1.465852
1	1.375351	-4.155524	-2.342342

1	1.740410	-3.109308	-0.947198
1	0.564626	-4.445429	-0.779576
1	-2.690992	-4.362143	0.698336
1	-3.306161	-3.168251	-0.473334
1	-2.093879	-4.382924	-0.983843
1	0.375764	-3.563739	3.708013
1	0.776569	-3.157392	2.019166
1	1.428421	-2.168501	3.363879
1	0.037774	1.681921	4.731137
1	-1.523958	1.417253	3.904339
1	-0.813727	0.122781	4.910213
8	-4.169226	0.705971	-0.387780
6	-4.624433	-0.401352	-0.112653
8	-4.161460	-1.176466	0.840688
1	-3.327615	-0.791818	1.247439
6	-5.763925	-1.007241	-0.863391
1	-6.362131	-1.664271	-0.227339
1	-6.385828	-0.228103	-1.308526
1	-5.342708	-1.612837	-1.676211

1CH2_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -1501.3717 cm(-1)

Electronic energy : -3339.1217946
 Zero-point correction= 0.542634
 Thermal correction to Energy= 0.590923
 Thermal correction to Enthalpy= 0.591867
 Thermal correction to Gibbs Free Energy= 0.458333
 Sum of electronic and zero-point Energies= -3338.579161
 Sum of electronic and thermal Energies= -3338.530872
 Sum of electronic and thermal Enthalpies= -3338.529927
 Sum of electronic and thermal Free Energies= -3338.663462

 Cartesian Coordinates

6	2.396610	-0.239757	-1.609380
6	3.739921	-0.281400	-1.163250
6	4.715337	-0.963933	-1.894770
6	4.371268	-1.588556	-3.089179
6	3.062100	-1.533154	-3.565632
6	2.090040	-0.873572	-2.822437
6	4.071500	0.438169	0.079215
6	5.351670	0.925414	0.346220
6	5.586088	1.629546	1.517526
6	4.534299	1.836729	2.400659
6	3.286531	1.323253	2.077069
7	3.053878	0.641275	0.949032
46	1.218009	-0.459230	0.282159
15	-0.210237	-2.003919	-0.622121
8	0.648115	-3.100101	-1.474051
6	1.736122	-3.757550	-0.844959
15	-0.112251	-0.501052	2.189106
8	0.179628	-1.733675	3.218848
6	1.520563	-2.181441	3.323028
47	-1.696917	0.828581	-0.704857
8	-1.301515	-1.511421	-1.539490
8	0.456405	0.790449	3.025377
6	-0.326355	1.301110	4.101314
8	-1.611928	-0.354190	2.073426
15	-0.029104	2.542240	-1.293332
8	1.463207	2.183523	-1.476702
8	-0.790532	-2.916405	0.595716
6	-1.772873	-3.901363	0.274220
8	-0.393692	3.411591	-2.623480
6	-1.718160	3.911246	-2.721265
8	-0.110932	3.757874	-0.187216
6	-0.006321	3.350016	1.166432

1	1.776600	0.949085	-1.438089
1	1.065429	-0.831106	-3.192698
1	2.805697	-2.010021	-4.509269
1	5.133759	-2.119091	-3.655754
1	5.739770	-1.025306	-1.531209
1	6.148696	0.772085	-0.375783
1	6.577572	2.020345	1.732488
1	4.667848	2.388812	3.326054
1	2.430862	1.446949	2.735922
1	-0.283136	4.200148	1.797097
1	-0.687419	2.511738	1.389555
1	1.018863	3.040061	1.413664
1	-1.904481	4.160277	-3.769434
1	-2.459699	3.159067	-2.404257
1	-1.847059	4.811530	-2.108044
1	2.243377	-4.352757	-1.609263
1	2.457235	-3.037756	-0.427665
1	1.392080	-4.424429	-0.042719
1	-1.926325	-4.503320	1.173287
1	-2.720422	-3.427339	-0.008638
1	-1.431866	-4.554657	-0.539568
1	1.531554	-3.025455	4.017811
1	1.906434	-2.519925	2.349079
1	2.182679	-1.395515	3.714113
1	0.227762	2.141669	4.529989
1	-1.303589	1.651351	3.750255
1	-0.478468	0.539644	4.877206
15	-3.968611	-0.025503	-0.027276
8	-3.816487	-1.255747	1.000539
8	-4.944182	1.050650	0.682235
8	-5.016364	-0.653021	-1.101451
6	-4.603300	-1.809619	-1.828276
6	-6.216482	0.646248	1.195350
1	-5.168667	-1.828493	-2.763943
1	-3.528421	-1.785887	-2.055453
1	-4.831616	-2.717884	-1.257289
1	-6.530575	1.408024	1.912949
1	-6.953801	0.582919	0.388414
1	-6.150305	-0.320238	1.707488
1	-2.952899	-1.133185	1.482450

1CH3_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -1452.8697 cm(-1)

Electronic energy : -3074.2679481
 Zero-point correction= 0.550609
 Thermal correction to Energy= 0.597489
 Thermal correction to Enthalpy= 0.598433
 Thermal correction to Gibbs Free Energy= 0.468964
 Sum of electronic and zero-point Energies= -3073.717339
 Sum of electronic and thermal Energies= -3073.670459
 Sum of electronic and thermal Enthalpies= -3073.669515
 Sum of electronic and thermal Free Energies= -3073.798984

 Cartesian Coordinates

6	5.595867	-0.487911	-1.007092
6	5.194753	-0.861336	0.275632
6	4.311513	-0.044663	0.981726
6	3.815233	1.124687	0.392749
6	4.167640	1.465861	-0.924182
6	5.078998	0.657119	-1.605422
47	1.721356	-0.142275	-0.151330
15	0.781299	-2.137929	-1.219423
8	1.027859	-3.446051	-0.249876
6	0.964170	-3.206089	1.146438

8	5.623560	-1.999970	0.880064
8	3.667139	2.563154	-1.532853
46	-1.430306	0.354526	0.256295
15	-0.315962	0.502841	2.280235
8	1.183687	0.670829	2.172452
6	-2.219546	-0.043937	-1.809774
6	-3.573113	-0.387843	-1.572950
6	-4.586678	0.062763	-2.422926
6	-4.262478	0.838503	-3.531141
6	-2.934471	1.165960	-3.802966
6	-1.932846	0.735565	-2.940514
6	-3.863805	-1.250188	-0.413856
6	-4.979836	-2.084961	-0.350178
6	-5.163616	-2.898965	0.757496
6	-4.227616	-2.864940	1.783183
6	-3.141738	-2.010133	1.660559
7	-2.958824	-1.224293	0.593191
15	-0.313699	2.303876	-0.295216
8	-0.269601	3.350262	0.949012
6	0.965510	3.801355	1.500838
8	-1.261871	3.130859	-1.323150
6	-2.586872	3.455598	-0.925022
8	1.048483	2.162279	-0.939550
8	-0.854859	1.612410	3.349381
6	-2.250509	1.873678	3.353188
8	-0.655986	-0.908319	3.047587
6	0.204717	-1.314201	4.110026
8	-0.708298	-2.153181	-1.634578
8	1.559502	-2.681356	-2.549094
6	2.976243	-2.613787	-2.511128
1	-1.333486	-1.046053	-1.592969
1	-0.894372	0.990805	-3.153718
1	-2.689179	1.759250	-4.681338
1	-5.053806	1.187309	-4.191458
1	-5.629870	-0.173174	-2.219303
1	-5.683346	-2.110362	-1.177533
1	-6.024683	-3.560342	0.813313
1	-4.326673	-3.489286	2.665944
1	-2.382775	-1.936512	2.435080
1	1.074805	-4.169727	1.652333
1	1.783766	-2.544041	1.474580
1	0.006207	-2.757062	1.449090
1	3.389324	-3.199693	-1.677180
1	3.349571	-3.030970	-3.450351
1	3.325617	-1.572414	-2.425646
1	-3.106531	3.842649	-1.805407
1	-3.126958	2.568202	-0.559977
1	-2.584138	4.223450	-0.141546
1	0.721930	4.620752	2.182442
1	1.452579	2.995916	2.063320
1	1.640390	4.175854	0.721777
1	-2.454183	2.551741	4.186079
1	-2.563464	2.357955	2.416838
1	-2.837266	0.954595	3.496407
1	-0.157312	-2.282913	4.466209
1	1.239817	-1.417020	3.763996
1	0.175481	-0.593207	4.936872
1	3.184168	1.795954	0.974166
1	4.020981	-0.313503	1.995973
1	6.299293	-1.114401	-1.556208
1	5.370452	0.932337	-2.616592
1	6.229018	-2.465211	0.288331
1	2.726131	2.655928	-1.270131

1CH4_Pd-Ag

Number of imaginary frequencies : 1
The smallest frequency is : -1484.7336 cm(-1)

Electronic energy : -3339.1144439
 Zero-point correction= 0.541256
 Thermal correction to Energy= 0.589875
 Thermal correction to Enthalpy= 0.590819
 Thermal correction to Gibbs Free Energy= 0.455977
 Sum of electronic and zero-point Energies= -3338.573188
 Sum of electronic and thermal Energies= -3338.524569
 Sum of electronic and thermal Enthalpies= -3338.523625
 Sum of electronic and thermal Free Energies= -3338.658467

.....
 Cartesian Coordinates

6	2.566324	-0.418806	-1.450211
6	3.850523	-0.554945	-0.869442
6	4.841203	-1.320505	-1.490271
6	4.574768	-1.935371	-2.708945
6	3.328991	-1.788367	-3.318432
6	2.338635	-1.047646	-2.683523
6	4.107807	0.155734	0.395285
6	5.385913	0.557647	0.785244
6	5.552253	1.255795	1.971543
6	4.435679	1.542742	2.746304
6	3.193179	1.112346	2.303117
7	3.026089	0.437933	1.159227
46	1.194898	-0.537570	0.328551
15	-0.283787	-1.974407	-0.686234
8	0.556105	-3.110275	-1.506196
6	1.563168	-3.831996	-0.813867
15	-0.394025	-0.307232	2.003722
8	-0.539923	-1.526739	3.078691
6	0.641190	-2.244319	3.394932
47	-1.454433	0.965488	-0.909169
8	-1.299424	-1.398775	-1.640413
8	0.241012	0.884021	2.942805
6	-0.617886	1.536042	3.872184
8	-1.781930	0.097749	1.567135
15	0.327064	2.553913	-1.398883
8	1.794008	2.064156	-1.417996
8	-0.995946	-2.880487	0.472556
6	-1.893952	-3.902159	0.040850
8	0.182182	3.395798	-2.789287
6	-1.073596	4.004018	-3.040773
8	0.253490	3.822392	-0.351411
6	0.069875	3.480679	1.011675
1	2.012306	0.815173	-1.347731
1	1.364336	-0.933968	-3.159748
1	3.134912	-2.258896	-4.280095
1	5.348113	-2.530885	-3.189803
1	5.814765	-1.454063	-1.021316
1	6.237422	0.342066	0.146038
1	6.542416	1.580421	2.281747
1	4.515510	2.092931	3.678998
1	2.287008	1.301295	2.872770
1	-0.043912	4.411176	1.575812
1	-0.837438	2.868815	1.153319
1	0.928981	2.923724	1.412681
1	-1.112485	4.258723	-4.103386
1	-1.908071	3.319251	-2.815719
1	-1.197757	4.918328	-2.447170
1	2.094430	-4.441080	-1.550247
1	2.285782	-3.155512	-0.331851
1	1.132092	-4.491962	-0.048829
1	-2.441677	-4.243839	0.923018
1	-2.608255	-3.522953	-0.700677
1	-1.349308	-4.749286	-0.395249
1	0.375881	-2.999993	4.139238
1	1.048924	-2.749559	2.507287
1	1.414618	-1.588248	3.820741
1	-0.008366	2.259725	4.421814

1	-1.430805	2.066417	3.361058
1	-1.050891	0.820648	4.583296
8	-3.765097	0.587900	-0.845542
15	-4.214715	-0.537842	0.031453
1	-3.257903	-1.465852	0.419221
8	-4.971356	-0.037181	1.349735
8	-5.285221	-1.521045	-0.634133
6	-4.686703	1.263879	1.881161
6	-6.441574	-0.943416	-1.247845
1	-5.210985	1.327117	2.837373
1	-3.610070	1.391240	2.039745
1	-5.064046	2.043305	1.211263
1	-7.006864	-0.341274	-0.526955
1	-6.157428	-0.323261	-2.104614
1	-7.066877	-1.769659	-1.591376

ICH5_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -1416.5493 cm(-1)

Electronic energy : -3074.2640866
 Zero-point correction= 0.551538
 Thermal correction to Energy= 0.597791
 Thermal correction to Enthalpy= 0.598736
 Thermal correction to Gibbs Free Energy= 0.471487
 Sum of electronic and zero-point Energies= -3073.712548
 Sum of electronic and thermal Energies= -3073.666295
 Sum of electronic and thermal Enthalpies= -3073.665351
 Sum of electronic and thermal Free Energies= -3073.792600

 Cartesian Coordinates

6	-4.562579	-0.585223	1.181683
6	-4.060845	0.556105	0.561074
6	-4.746454	1.112651	-0.517617
6	-5.926646	0.538539	-0.968971
6	-6.437100	-0.600079	-0.343087
6	-5.749215	-1.159245	0.731294
8	-2.923268	1.166178	1.003207
47	-1.067224	1.720401	-0.449110
15	0.975588	2.998202	-0.243038
8	1.189757	3.559502	1.284045
6	1.014483	2.610819	2.323641
8	-7.600524	-1.116727	-0.823586
46	1.058145	-0.679528	0.081372
15	-0.102747	-1.096154	2.062377
8	-1.475740	-0.534836	2.333828
6	2.179315	-0.113275	-1.778760
6	3.433304	-0.749909	-1.603743
6	4.075316	-1.377008	-2.674501
6	3.489965	-1.358841	-3.936352
6	2.270842	-0.714686	-4.141465
6	1.624566	-0.112933	-3.067867
6	4.042432	-0.693362	-0.263500
6	5.421522	-0.765463	-0.062030
6	5.933997	-0.647941	1.220862
6	5.056349	-0.456486	2.279915
6	3.695930	-0.402409	2.012342
7	3.193277	-0.519671	0.777423
15	-0.823744	-1.284611	-1.079676
8	-1.682365	-2.339768	-0.192387
6	-2.886619	-2.845621	-0.773176
8	-0.380485	-2.203352	-2.352774
6	0.463397	-3.321106	-2.125732
8	-1.695685	-0.184767	-1.647157
8	-0.144184	-2.670283	2.493060
6	0.998743	-3.453607	2.195198

8	0.932993	-0.461866	3.167160
6	0.443888	-0.172185	4.472978
8	2.254101	2.235195	-0.657720
8	1.071909	4.416160	-1.033541
6	0.013370	5.338876	-0.822303
1	2.069602	1.066511	-1.108565
1	0.666514	0.381744	-3.230699
1	1.826274	-0.693722	-5.134172
1	3.992210	-1.849100	-4.767756
1	5.022269	-1.894460	-2.530137
1	6.085440	-0.885140	-0.913401
1	7.007072	-0.692994	1.389119
1	5.409781	-0.347509	3.300826
1	2.965979	-0.270028	2.806223
1	0.989639	3.156315	3.271533
1	0.064327	2.059224	2.215274
1	1.837257	1.883916	2.348595
1	0.065950	6.091176	-1.613492
1	-0.969623	4.843597	-0.877033
1	0.106463	5.833698	0.151867
1	0.709853	-3.746637	-3.102239
1	1.399157	-3.023106	-1.628315
1	-0.036575	-4.087299	-1.517726
1	-2.664771	-3.495016	-1.630047
1	-3.393224	-3.429644	-0.000869
1	-3.540207	-2.027078	-1.097432
1	0.770857	-4.485884	2.473966
1	1.237093	-3.424331	1.120215
1	1.879315	-3.119063	2.761981
1	1.284113	0.229597	5.047757
1	-0.361644	0.570116	4.441014
1	0.072961	-1.078688	4.968516
1	-4.339400	1.998806	-1.003162
1	-6.468135	0.963821	-1.810959
1	-6.138362	-2.053161	1.219710
1	-4.008885	-1.031469	2.005949
1	-7.837454	-1.894713	-0.303185
1	-2.408213	0.536947	1.582410

1CH6_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -1506.0234 cm(-1)

Electronic energy : -2691.7798327
 Zero-point correction= 0.440366
 Thermal correction to Energy= 0.478897
 Thermal correction to Enthalpy= 0.479841
 Thermal correction to Gibbs Free Energy= 0.368105
 Sum of electronic and zero-point Energies= -2691.339467
 Sum of electronic and thermal Energies= -2691.300936
 Sum of electronic and thermal Enthalpies= -2691.299991
 Sum of electronic and thermal Free Energies= -2691.411728

 Cartesian Coordinates

6	-3.151741	2.232314	2.044037
6	-2.055493	1.896815	1.247535
7	-1.222627	0.893574	1.602100
6	-1.459762	0.202503	2.723153
6	-2.540377	0.470908	3.549954
6	-3.395493	1.512247	3.203578
6	-1.756253	2.561768	-0.031275
6	-2.119789	3.890190	-0.260177
6	-1.852879	4.477029	-1.493093
6	-1.244225	3.739599	-2.506588
6	-0.876164	2.418714	-2.272575
6	-1.103594	1.800064	-1.034161

46	0.423336	0.663362	0.124335
15	1.893095	-0.442913	1.543983
8	1.614838	0.209160	3.017140
6	2.133905	-0.481541	4.153668
47	-0.044970	-2.283813	0.132091
8	1.637099	-1.955150	1.574383
15	1.776238	0.478509	-1.727999
8	3.309725	-0.002075	-1.446886
6	3.583689	-1.396022	-1.428553
15	-2.017965	-1.919422	-1.207969
8	-2.119344	-2.763737	-2.590683
6	-0.950760	-2.741973	-3.408368
8	1.124783	-0.329888	-2.802050
8	-3.367559	-2.553664	-0.543206
6	-3.681505	-2.082060	0.755923
8	-2.308053	-0.431631	-1.505443
8	2.098848	1.978097	-2.266785
6	2.502125	2.998479	-1.371165
8	3.507675	-0.304969	1.414871
6	4.073005	0.995786	1.491053
1	-1.522324	0.518448	-1.181651
1	-0.414738	1.836270	-3.067942
1	-1.060622	4.197318	-3.476462
1	-2.129370	5.515041	-1.665450
1	-2.592474	4.476382	0.526358
1	-3.818035	3.033319	1.736067
1	-4.252453	1.754311	3.827219
1	-2.699930	-0.122581	4.445037
1	-0.747711	-0.584411	2.966496
1	-4.549235	-2.644959	1.109224
1	-2.848377	-2.251060	1.459364
1	-3.932808	-1.012654	0.748793
1	-1.213165	-3.220625	-4.355098
1	-0.595885	-1.720619	-3.593057
1	-0.134258	-3.312048	-2.939067
1	2.407265	3.951970	-1.899166
1	1.858451	3.032354	-0.477165
1	3.547288	2.865705	-1.061174
1	4.637847	-1.515308	-1.164290
1	2.983558	-1.925266	-0.674325
1	3.402325	-1.842539	-2.413262
1	4.971138	1.010610	0.867025
1	3.380182	1.768380	1.127905
1	4.345101	1.234483	2.527259
1	1.982957	0.164989	5.021550
1	1.605124	-1.429476	4.311324
1	3.205936	-0.689161	4.043455

1CH7_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -1455.1838 cm(-1)

Electronic energy : -2964.6104253
 Zero-point correction= 0.606098
 Thermal correction to Energy= 0.653779
 Thermal correction to Enthalpy= 0.654724
 Thermal correction to Gibbs Free Energy= 0.523814
 Sum of electronic and zero-point Energies= -2964.004327
 Sum of electronic and thermal Energies= -2963.956646
 Sum of electronic and thermal Enthalpies= -2963.955702
 Sum of electronic and thermal Free Energies= -2964.086611

 Cartesian Coordinates

6	2.836459	0.401140	-0.753095
6	3.668503	0.381280	0.397704
6	5.035508	0.116943	0.301528
6	5.606366	-0.127303	-0.943692

6	4.819288	-0.088963	-2.092257
6	3.456252	0.175528	-1.989393
6	3.031884	0.671740	1.690087
6	3.675432	1.314765	2.748656
6	2.958879	1.607002	3.899654
6	1.613997	1.255846	3.974440
6	1.042626	0.601601	2.894105
7	1.733751	0.314769	1.785345
46	0.982608	-0.686636	-0.012959
15	-0.020643	-1.336860	-1.996206
8	1.047401	-1.291611	-3.222684
6	2.023010	-2.319549	-3.336365
15	-0.348935	-2.221405	1.131263
8	-0.176114	-3.746595	0.576858
6	1.132528	-4.216806	0.304952
47	-1.386931	1.149796	-0.389591
8	-1.172145	-0.411561	-2.310291
8	0.437570	-2.309300	2.565106
6	-0.103542	-3.184427	3.553129
8	-1.832648	-2.027473	1.335089
15	0.148743	2.998854	-0.722357
8	1.656124	2.674792	-0.792175
8	-0.462687	-2.896003	-2.129441
6	-1.816246	-3.275526	-1.902801
8	-0.153963	3.884924	-2.056878
6	-1.518948	4.043611	-2.414583
8	-0.033420	4.197234	0.390673
6	0.083142	3.790558	1.741573
1	1.981798	1.445699	-0.766954
1	2.850629	0.228481	-2.892410
1	5.271564	-0.259690	-3.067736
1	6.670309	-0.342317	-1.016732
1	5.653591	0.080319	1.197499
1	4.717438	1.606769	2.650231
1	3.441979	2.118440	4.728477
1	1.015041	1.480521	4.851714
1	0.000505	0.288003	2.910034
1	-0.137966	4.656384	2.371843
1	-0.636965	2.990845	1.985734
1	1.099162	3.437038	1.970944
1	-1.557385	4.737510	-3.258338
1	-1.962942	3.086774	-2.728770
1	-2.113432	4.463650	-1.590979
1	2.737513	-2.008583	-4.104176
1	2.570445	-2.469152	-2.394397
1	1.558861	-3.265501	-3.635973
1	-1.841376	-4.368762	-1.906492
1	-2.182006	-2.924330	-0.930587
1	-2.464544	-2.894722	-2.700626
1	1.051247	-5.035787	-0.415775
1	1.765568	-3.429440	-0.134102
1	1.616947	-4.584152	1.219565
1	0.603836	-3.207106	4.386063
1	-1.074036	-2.822265	3.912503
1	-0.228256	-4.202197	3.161517
8	-3.055519	0.292162	0.923395
6	-4.371054	0.182191	0.343895
6	-5.314192	-0.220263	1.480351
6	-4.694738	1.559228	-0.203942
6	-4.342079	-0.855729	-0.765833
1	-5.693786	1.586529	-0.653364
1	-4.649918	2.312902	0.592712
1	-3.973435	1.840536	-0.986745
1	-5.291100	-0.882247	-1.314487
1	-3.538024	-0.626332	-1.478721
1	-4.157415	-1.856729	-0.352598
6	-6.766182	-0.431234	1.086125
1	-4.916144	-1.146910	1.923303
1	-5.242784	0.552958	2.259310
1	-7.371355	-0.684461	1.963842

1	-7.205869	0.469091	0.639135
1	-6.879874	-1.251625	0.367246
1	-2.703921	-0.609836	1.134604

1CH8_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -1464.4573 cm(-1)

Electronic energy : -3073.0187773
 Zero-point correction= 0.526118
 Thermal correction to Energy= 0.573163
 Thermal correction to Enthalpy= 0.574107
 Thermal correction to Gibbs Free Energy= 0.442444
 Sum of electronic and zero-point Energies= -3072.492659
 Sum of electronic and thermal Energies= -3072.445615
 Sum of electronic and thermal Enthalpies= -3072.444670
 Sum of electronic and thermal Free Energies= -3072.576333

 Cartesian Coordinates

6	2.742596	-0.138653	-1.438908
6	3.991821	-0.436069	-0.842041
6	5.007418	-1.056377	-1.575541
6	4.802516	-1.357537	-2.917760
6	3.594472	-1.040251	-3.538664
6	2.578066	-0.449600	-2.797037
6	4.184969	-0.044445	0.565789
6	5.441761	0.221481	1.110926
6	5.542622	0.625055	2.433836
6	4.384392	0.757374	3.189385
6	3.166161	0.473303	2.588842
7	3.063219	0.084759	1.312317
46	1.275415	-0.637862	0.193810
15	-0.214288	-1.791986	-1.140941
8	0.632206	-2.591534	-2.277851
6	1.617574	-3.526007	-1.860050
15	-0.392759	-0.796480	1.805333
8	-0.612446	-2.250105	2.517464
6	0.535246	-3.066204	2.692616
47	-1.235807	1.132328	-0.590196
8	-1.303542	-1.004558	-1.830602
8	0.157606	0.118469	3.052146
6	-0.770294	0.501883	4.064637
8	-1.759970	-0.304913	1.374682
15	0.561241	2.788093	-0.787532
8	2.022990	2.304138	-0.931635
8	-0.808416	-3.055731	-0.301231
6	-2.210924	-3.233125	-0.137112
8	0.393978	3.903661	-1.967374
6	-0.892265	4.482509	-2.114732
8	0.518165	3.811805	0.502605
6	0.456396	3.188323	1.772840
1	2.208959	1.057858	-1.097486
1	1.633673	-0.201183	-3.282200
1	3.450889	-1.261270	-4.594357
1	5.595421	-1.839028	-3.486402
1	5.953059	-1.320036	-1.104509
1	6.328783	0.134832	0.489776
1	6.515793	0.843043	2.866813
1	4.414250	1.076990	4.226611
1	2.228793	0.548387	3.134996
1	0.268247	3.965893	2.519036
1	-0.359934	2.448714	1.822154
1	1.400055	2.679542	2.019107
1	-0.911880	5.010430	-3.071862
1	-1.682397	3.713478	-2.123043
1	-1.105230	5.196328	-1.308726

1	2.185569	-3.820100	-2.746802
1	2.311575	-3.084457	-1.128295
1	1.151684	-4.415054	-1.417988
1	-2.342446	-4.106814	0.507348
1	-2.661214	-2.361064	0.350051
1	-2.699776	-3.423404	-1.100720
1	0.219366	-3.959632	3.238094
1	0.953244	-3.371957	1.722691
1	1.313996	-2.555261	3.277661
1	-0.234933	1.149676	4.764696
1	-1.617609	1.050616	3.637790
1	-1.148072	-0.375679	4.604599
8	-3.629791	1.691962	-0.511075
6	-4.535598	0.874240	-0.352860
6	-5.789965	1.278601	0.308218
6	-6.787878	0.403855	0.481806
6	-6.670659	-0.996431	0.014208
6	-5.408825	-1.388869	-0.650252
6	-4.406477	-0.516931	-0.822754
1	-5.849675	2.312510	0.640985
1	-7.722897	0.671872	0.968825
8	-7.582023	-1.793684	0.171847
1	-5.346633	-2.422420	-0.985494
1	-3.461065	-0.781160	-1.302685

1CH9_Pd-Ag

Number of imaginary frequencies : 1
The smallest frequency is : -1432.0081 cm(-1)

Electronic energy :	-3073.0195184
Zero-point correction=	0.526043
Thermal correction to Energy=	0.572848
Thermal correction to Enthalpy=	0.573792
Thermal correction to Gibbs Free Energy=	0.443740
Sum of electronic and zero-point Energies=	-3072.493476
Sum of electronic and thermal Energies=	-3072.446670
Sum of electronic and thermal Enthalpies=	-3072.445726
Sum of electronic and thermal Free Energies=	-3072.575778

Cartesian Coordinates

6	-2.076743	0.044808	-1.866102
6	-3.477192	-0.075943	-1.694853
6	-4.362965	0.476115	-2.624513
6	-3.865700	1.130357	-3.746667
6	-2.490726	1.234769	-3.954293
6	-1.614371	0.706145	-3.013792
6	-3.960100	-0.820225	-0.517959
6	-5.198617	-1.461984	-0.490653
6	-5.573292	-2.179731	0.634962
6	-4.700651	-2.244977	1.713589
6	-3.485713	-1.580232	1.625035
7	-3.119345	-0.884934	0.541664
46	-1.349482	0.435275	0.219948
15	0.076285	2.123384	-0.408276
8	-0.659309	3.083638	-1.501861
6	-1.918170	3.646591	-1.165013
15	-0.297117	0.509203	2.291149
8	-0.684794	1.725727	3.306483
6	-2.006056	2.234804	3.226566
47	1.756712	-0.446733	-0.059139
8	1.407944	1.733111	-1.011342
8	-0.939509	-0.789027	3.070416
6	-0.266113	-1.269732	4.230594
8	1.208674	0.378386	2.269014
15	0.603394	-2.400865	-1.009885
8	-0.867988	-2.224583	-1.452449

8	0.253820	3.130941	0.854804
6	1.208152	4.186826	0.719665
8	1.300755	-3.151694	-2.277949
6	2.705296	-3.340508	-2.211400
8	0.639633	-3.650196	0.056764
6	0.404324	-3.310966	1.414015
1	-1.345538	-1.058063	-1.532755
1	-0.539198	0.791080	-3.174662
1	-2.110579	1.733723	-4.843265
1	-4.558219	1.559272	-4.467984
1	-5.439255	0.414765	-2.471587
1	-5.848530	-1.415283	-1.359897
1	-6.532280	-2.690924	0.664311
1	-4.946550	-2.802385	2.612392
1	-2.768446	-1.590765	2.441936
1	0.495077	-4.227783	2.003483
1	1.146945	-2.582024	1.780129
1	-0.600100	-2.888463	1.563592
1	3.009866	-3.859740	-3.123914
1	3.234089	-2.375704	-2.167097
1	2.993349	-3.948805	-1.344310
1	-2.310373	4.130685	-2.063355
1	-2.633244	2.873855	-0.842424
1	-1.821422	4.395541	-0.367447
1	0.957979	4.841046	-0.126122
1	1.170046	4.767690	1.644460
1	2.219426	3.785374	0.577674
1	-2.104194	3.009774	3.991545
1	-2.199802	2.683518	2.241470
1	-2.756562	1.454033	3.419566
1	-0.806471	-2.156702	4.574658
1	0.771250	-1.541488	4.002980
1	-0.269282	-0.515929	5.028376
6	3.888651	0.865813	0.835543
6	4.140249	-0.461195	0.901807
6	4.891862	-1.155265	-0.174163
6	4.389062	1.682706	-0.297878
8	5.205947	-2.331430	-0.077090
8	4.347551	2.901680	-0.268088
6	5.001077	0.958613	-1.433797
6	5.244482	-0.357477	-1.371272
1	3.358912	1.390945	1.628768
1	3.862060	-1.057236	1.771188
1	5.735106	-0.898470	-2.178317
1	5.281354	1.562667	-2.294048

1CH10_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -1495.1691 cm(-1)

Electronic energy : -3073.0195952
 Zero-point correction= 0.526489
 Thermal correction to Energy= 0.573163
 Thermal correction to Enthalpy= 0.574107
 Thermal correction to Gibbs Free Energy= 0.444205
 Sum of electronic and zero-point Energies= -3072.493106
 Sum of electronic and thermal Energies= -3072.446432
 Sum of electronic and thermal Enthalpies= -3072.445488
 Sum of electronic and thermal Free Energies= -3072.575391

 Cartesian Coordinates

6	2.350428	-0.430042	-1.733266
6	3.655305	-0.850111	-1.379212
6	4.417828	-1.631576	-2.251902
6	3.903171	-1.976616	-3.497073
6	2.634297	-1.545233	-3.883267
6	1.869085	-0.792691	-3.000210

6	4.184267	-0.415458	-0.074099
6	5.550571	-0.287465	0.179421
6	5.977758	0.161524	1.419785
6	5.030269	0.477090	2.385463
6	3.687403	0.325287	2.070803
7	3.269365	-0.106974	0.874955
46	1.215528	-0.649383	0.194561
15	-0.613367	-1.665662	-0.758240
8	-0.115425	-2.701358	-1.918604
6	0.842245	-3.688497	-1.564874
15	-0.088040	-0.484435	2.108618
8	-0.255488	-1.819555	3.031018
6	0.848771	-2.710319	3.064314
47	-1.227069	1.367136	-0.244195
8	-1.679034	-0.790433	-1.370477
8	0.820474	0.482072	3.076994
6	0.209379	1.033508	4.240315
8	-1.458425	0.135682	1.933539
15	0.661825	2.780350	-0.901193
8	1.998738	2.105052	-1.286834
8	-1.226704	-2.698882	0.345868
6	-2.353758	-3.481747	-0.043709
8	0.382744	3.826039	-2.122985
6	-0.815413	4.581075	-2.056177
8	0.999237	3.885513	0.271918
6	1.100480	3.366915	1.586358
1	2.023920	0.835940	-1.386212
1	0.877020	-0.454463	-3.301110
1	2.247844	-1.804301	-4.866831
1	4.500310	-2.583385	-4.174714
1	5.405622	-1.985275	-1.960633
1	6.267097	-0.516582	-0.604369
1	7.039375	0.272403	1.626445
1	5.317432	0.838507	3.368272
1	2.902828	0.550118	2.788975
1	1.214587	4.212644	2.270793
1	0.195242	2.804526	1.868636
1	1.969342	2.701439	1.695751
1	-0.982525	5.025931	-3.040909
1	-1.681505	3.944492	-1.808973
1	-0.742587	5.381650	-1.309054
1	1.161576	-4.181931	-2.486756
1	1.724251	-3.241782	-1.080458
1	0.413733	-4.438762	-0.886947
1	-2.772361	-3.919711	0.866362
1	-3.116223	-2.865392	-0.534990
1	-2.057976	-4.290146	-0.724890
1	0.597998	-3.516073	3.759225
1	1.036963	-3.144095	2.071049
1	1.763501	-2.212047	3.417606
1	0.937247	1.709959	4.698355
1	-0.695459	1.596444	3.983839
1	-0.050896	0.245973	4.959046
8	-3.633846	1.713725	-0.440952
6	-4.503531	0.853530	-0.304543
6	-5.808599	1.019658	-0.971752
6	-6.778947	0.110425	-0.822327
6	-6.579690	-1.091081	0.020269
6	-5.268419	-1.244620	0.685358
6	-4.288072	-0.344246	0.529381
1	-5.928966	1.912718	-1.581214
1	-7.749778	0.205616	-1.303677
8	-7.467180	-1.918689	0.158905
1	-5.148098	-2.129983	1.306850
1	-3.313066	-0.432363	1.013952

ICH11_Pd-Ag

Number of imaginary frequencies : 1
The smallest frequency is : -1432.8783 cm(-1)

Electronic energy : -2273.429101
Zero-point correction= 0.400381
Thermal correction to Energy= 0.435736
Thermal correction to Enthalpy= 0.436680
Thermal correction to Gibbs Free Energy= 0.331660
Sum of electronic and zero-point Energies= -2273.028720
Sum of electronic and thermal Energies= -2272.993365
Sum of electronic and thermal Enthalpies= -2272.992421
Sum of electronic and thermal Free Energies= -2273.097441

.....
Cartesian Coordinates
.....

6	-1.925402	-0.850050	-0.537758
6	-2.891262	0.102266	-0.949234
6	-3.876214	-0.235451	-1.880743
6	-3.932659	-1.530568	-2.385499
6	-3.019617	-2.496479	-1.963715
6	-2.022446	-2.148556	-1.059781
6	-2.829821	1.440778	-0.334709
6	-3.937503	2.282306	-0.229181
6	-3.809615	3.501771	0.419124
6	-2.578461	3.857558	0.955503
6	-1.513513	2.980306	0.807841
7	-1.630933	1.807194	0.177276
46	-0.055543	0.354351	-0.394969
15	1.224806	-1.292750	-1.408219
8	0.378327	-1.805705	-2.696642
6	-0.093647	-0.857185	-3.641732
15	1.932598	1.376018	0.211039
8	3.010566	1.800633	-0.934924
6	2.514989	2.466784	-2.084057
47	1.348997	-1.318010	1.695461
8	1.563029	-2.466011	-0.527030
8	1.566331	2.829186	0.869591
6	2.620957	3.558932	1.499013
8	2.703195	0.515000	1.205328
8	-0.371837	-2.307562	2.734115
8	2.538257	-0.714687	-2.174062
6	3.841235	-1.008225	-1.676403
1	-1.304182	-2.900550	-0.732338
1	-3.084680	-3.511960	-2.348715
1	-4.701490	-1.790261	-3.110313
1	-4.592754	0.507297	-2.227409
1	-4.896765	1.967025	-0.629791
1	-4.667719	4.162443	0.514774
1	-2.436496	4.796199	1.482482
1	-0.524270	3.212919	1.192675
1	-0.778966	-1.380167	-4.314209
1	-0.641604	-0.036538	-3.152326
1	0.733451	-0.436568	-4.227603
1	4.543346	-0.405082	-2.258523
1	3.943385	-0.739672	-0.618215
1	4.076697	-2.069983	-1.810008
1	3.296822	2.433566	-2.848132
1	1.617598	1.969110	-2.481468
1	2.272379	3.515300	-1.862419
1	2.201881	4.512609	1.829576
1	3.010181	3.014789	2.366782
1	3.440857	3.751709	0.796102
6	-1.489056	-1.752857	2.821283
8	-1.945461	-0.846947	2.042705
6	-2.420531	-2.176442	3.926013
1	-3.239108	-2.763841	3.494152
1	-1.902571	-2.781031	4.673454
1	-2.870696	-1.297883	4.398302
1	-1.651569	-0.823084	0.803382

1CH12_Pd-Ag

Number of imaginary frequencies : 1
The smallest frequency is : -1681.2372 cm(-1)

Electronic energy : -1855.0759553
Zero-point correction= 0.360372
Thermal correction to Energy= 0.391993
Thermal correction to Enthalpy= 0.392937
Thermal correction to Gibbs Free Energy= 0.296462
Sum of electronic and zero-point Energies= -1854.715583
Sum of electronic and thermal Energies= -1854.683962
Sum of electronic and thermal Enthalpies= -1854.683018
Sum of electronic and thermal Free Energies= -1854.779493

Cartesian Coordinates

6	4.109688	-1.376053	0.688409
6	2.978834	-0.661519	0.300400
6	1.698711	-1.287346	0.280539
6	1.617977	-2.622603	0.709485
6	2.750965	-3.326314	1.108227
6	3.994903	-2.704401	1.089359
6	3.062624	0.762756	-0.054390
7	1.922055	1.460435	0.125271
6	1.874165	2.761248	-0.168845
6	2.977945	3.446592	-0.656176
6	4.163223	2.743247	-0.841683
6	4.209302	1.388927	-0.540812
46	0.227047	0.228528	0.732847
15	-1.622775	-1.073424	0.982222
8	-1.721279	-1.691146	2.488349
6	-1.961048	-0.763876	3.544065
8	-0.871852	1.811028	1.611889
6	-1.590511	2.642295	0.969156
8	-1.793236	2.673582	-0.265990
47	-1.634401	0.825101	-1.520680
8	-1.537006	-1.100882	-2.797318
6	-0.392337	-1.518476	-2.525421
8	0.512593	-0.751230	-2.025147
6	-2.255653	3.688449	1.829844
6	-0.012739	-2.943308	-2.803781
8	-2.891331	-0.385886	0.563353
8	-1.388404	-2.455419	0.158098
6	-2.547954	-3.163881	-0.285839
1	0.789617	-2.966674	-3.549459
1	0.386284	-3.396198	-1.887775
1	-0.863178	-3.525059	-3.165475
1	-3.075328	3.212817	2.381070
1	-1.553716	4.085373	2.568972
1	-2.664056	4.498488	1.221717
1	1.007377	-1.028530	-0.825253
1	0.650724	-3.119307	0.699673
1	2.663358	-4.361115	1.431397
1	4.883036	-3.250765	1.398766
1	5.082821	-0.889116	0.712473
1	5.118905	0.816049	-0.698162
1	5.046143	3.245288	-1.229150
1	2.902028	4.503816	-0.890741
1	0.915956	3.254730	-0.016890
1	-2.209948	-4.151238	-0.612380
1	-3.275162	-3.291371	0.524825
1	-3.020607	-2.642065	-1.125209
1	-1.103417	-0.092428	3.680259
1	-2.860252	-0.165056	3.353440
1	-2.105177	-1.346139	4.457577

1CH13_Pd-Ag

Number of imaginary frequencies : 1
The smallest frequency is : -1503.6365 cm(-1)

Electronic energy : -2273.4170275
Zero-point correction= 0.400594
Thermal correction to Energy= 0.435610
Thermal correction to Enthalpy= 0.436554
Thermal correction to Gibbs Free Energy= 0.332888
Sum of electronic and zero-point Energies= -2273.016434
Sum of electronic and thermal Energies= -2272.981418
Sum of electronic and thermal Enthalpies= -2272.980474
Sum of electronic and thermal Free Energies= -2273.084140

Cartesian Coordinates

6	-4.102398	-1.182551	1.561852
6	-2.984507	-0.656206	0.912999
6	-1.863550	-0.189571	1.642486
6	-1.901648	-0.301673	3.036773
6	-3.014137	-0.825016	3.689719
6	-4.112904	-1.261554	2.950652
6	-2.894927	-0.589555	-0.550450
7	-1.638562	-0.646319	-1.062253
6	-1.449100	-0.547095	-2.386653
6	-2.503847	-0.402030	-3.272729
6	-3.799121	-0.365072	-2.766704
6	-3.994833	-0.456200	-1.396990
46	-0.151340	-0.887861	0.393793
47	1.676957	1.257835	-0.436508
15	-0.109278	2.824178	0.104453
8	-0.691591	3.672811	-1.177438
6	-1.093483	2.895611	-2.290071
8	1.140400	-1.174687	1.980926
6	2.352672	-0.761449	1.993399
8	2.890954	0.006827	1.173639
6	3.189148	-1.329402	3.111769
8	-1.323533	2.202823	0.828479
8	0.317569	4.085547	1.041802
6	1.461852	4.822749	0.643430
1	3.997287	-0.643720	3.377620
1	3.638226	-2.264345	2.752448
1	2.582861	-1.565033	3.989783
1	-1.347528	0.972939	1.161182
1	-1.050407	0.046262	3.620933
1	-3.030693	-0.893667	4.775573
1	-4.980046	-1.676777	3.459487
1	-4.949035	-1.558146	0.988845
1	-4.992110	-0.401975	-0.969239
1	-4.649578	-0.252475	-3.434070
1	-2.303043	-0.318670	-4.336217
1	-0.419772	-0.582450	-2.734370
1	-1.372600	3.582083	-3.094144
1	-0.271859	2.254440	-2.652255
1	-1.960831	2.264061	-2.047506
1	1.761609	5.450835	1.486362
1	2.302831	4.156933	0.389010
1	1.242982	5.463598	-0.219989
15	1.420175	-1.730384	-1.073246
8	2.090752	-0.656548	-1.904074
8	2.477546	-2.688963	-0.300196
8	0.710841	-2.760021	-2.123028
6	-0.021595	-3.858170	-1.592177
6	3.869159	-2.582481	-0.604168
1	4.372645	-3.375848	-0.045361
1	4.061501	-2.724877	-1.674018
1	4.258131	-1.608814	-0.286769
1	-0.580501	-4.307085	-2.417267

1	0.650516	-4.610031	-1.161055
1	-0.733647	-3.530859	-0.819584

ICH14_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -1752.4978 cm(-1)

Electronic energy : -1855.0714946
 Zero-point correction= 0.360192
 Thermal correction to Energy= 0.392004
 Thermal correction to Enthalpy= 0.392948
 Thermal correction to Gibbs Free Energy= 0.294499
 Sum of electronic and zero-point Energies= -1854.711303
 Sum of electronic and thermal Energies= -1854.679491
 Sum of electronic and thermal Enthalpies= -1854.678547
 Sum of electronic and thermal Free Energies= -1854.776996

 Cartesian Coordinates

6	3.611738	1.842095	-1.174517
6	2.714453	0.858571	-0.768348
6	1.470931	1.221868	-0.173545
6	1.188620	2.586801	0.002980
6	2.094537	3.563599	-0.390741
6	3.296204	3.186316	-0.986602
6	2.996334	-0.578955	-0.917328
7	1.910257	-1.381127	-0.867912
6	2.036368	-2.702457	-0.988872
6	3.273799	-3.309271	-1.155437
6	4.403893	-2.500811	-1.201343
6	4.268274	-1.123738	-1.082623
46	0.059790	-0.256160	-0.777674
15	-1.714634	1.184049	-0.757861
8	-3.012132	0.526091	-1.499361
6	-4.240380	0.403519	-0.789134
8	-1.133143	-1.856281	-1.461522
6	-2.099935	-2.296189	-0.762596
8	-2.386213	-1.984719	0.418516
47	-1.348763	-0.498818	1.755520
8	-0.112055	0.304821	3.407622
6	1.130685	0.281774	3.234331
8	1.729046	0.056979	2.133566
6	-3.009139	-3.272158	-1.464659
6	2.019405	0.546279	4.421798
8	-2.105449	1.748551	0.586136
8	-1.320699	2.338699	-1.835989
6	-2.305775	3.341407	-2.087371
1	1.451809	0.549835	5.354763
1	2.813989	-0.204907	4.468933
1	2.506045	1.519810	4.292095
1	-3.807523	-2.697181	-1.950819
1	-2.477193	-3.825810	-2.242109
1	-3.471601	-3.959853	-0.752627
1	1.293952	0.543148	0.933989
1	0.253861	2.866904	0.488055
1	1.869003	4.616460	-0.238899
1	4.002093	3.948658	-1.308867
1	4.550980	1.574086	-1.654607
1	5.141628	-0.477871	-1.102912
1	5.390138	-2.941008	-1.324543
1	3.343548	-4.389132	-1.241955
1	1.112209	-3.275832	-0.952562
1	-1.839549	4.099724	-2.721259
1	-3.172250	2.919791	-2.611405
1	-2.638790	3.811551	-1.153448
1	-4.164008	-0.345852	0.009897
1	-4.553428	1.361594	-0.357953

1 -4.990609 0.075835 -1.514619

ICH15_Pd-Ag

Number of imaginary frequencies : 1
The smallest frequency is : -1709.5344 cm(-1)

Electronic energy : -2273.4112228
Zero-point correction= 0.399479
Thermal correction to Energy= 0.434935
Thermal correction to Enthalpy= 0.435879
Thermal correction to Gibbs Free Energy= 0.330246
Sum of electronic and zero-point Energies= -2273.011744
Sum of electronic and thermal Energies= -2272.976288
Sum of electronic and thermal Enthalpies= -2272.975344
Sum of electronic and thermal Free Energies= -2273.080977

Cartesian Coordinates

6	-3.485097	3.113043	-0.331785
6	-2.721733	1.948855	-0.406059
7	-1.400210	2.012033	-0.674323
6	-0.810802	3.188343	-0.897291
6	-1.514368	4.384287	-0.841566
6	-2.872482	4.339817	-0.550006
6	-3.258067	0.592328	-0.208999
6	-4.620120	0.323032	-0.327885
6	-5.096713	-0.970444	-0.132783
6	-4.224721	-2.007643	0.187762
6	-2.863675	-1.748043	0.292000
6	-2.343141	-0.455818	0.100022
46	-0.468568	0.047633	-0.842640
47	1.818831	-0.374323	1.440757
8	1.086835	-2.538214	0.249281
15	0.363029	-2.066077	-0.987299
8	-0.845712	-3.050791	-1.437798
6	-0.523059	-4.404611	-1.759622
8	1.285883	-2.222854	-2.316887
6	2.686614	-1.975176	-2.277936
8	0.683641	-1.173339	3.299156
6	-0.483125	-0.834737	3.015145
6	-1.646822	-1.449639	3.739675
8	-0.739840	0.072617	2.138350
1	-1.356153	-2.362797	4.263179
1	-2.028755	-0.727964	4.471346
1	-2.467023	-1.658877	3.042933
1	-1.500698	-0.193863	1.067957
1	-2.182346	-2.551765	0.563358
1	-4.606631	-3.012265	0.352761
1	-6.161966	-1.167713	-0.229884
1	-5.318482	1.113753	-0.594084
1	-4.543883	3.059921	-0.094930
1	-3.454030	5.256355	-0.490660
1	-1.001016	5.324296	-1.019834
1	0.255618	3.152481	-1.116817
1	-1.454691	-4.975017	-1.715702
1	-0.102825	-4.474006	-2.768735
1	0.187032	-4.829764	-1.039914
1	2.899338	-0.953096	-2.604005
1	3.092416	-2.130652	-1.270314
1	3.163482	-2.686638	-2.960012
8	1.393462	0.826867	-1.626550
15	2.369273	1.078080	-0.451835
8	2.279739	2.686901	-0.080996
8	3.831090	1.056696	-1.187160
6	4.941025	1.378352	-0.363579
6	1.915176	3.049447	1.242032
1	5.847992	1.079258	-0.895503

1	4.984781	2.455254	-0.156487
1	4.906119	0.835378	0.595227
1	1.721666	4.126774	1.244963
1	1.005941	2.529972	1.580137
1	2.726006	2.837341	1.954199

1CH16_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -1510.7628 cm(-1)

Electronic energy : -1855.0585186
 Zero-point correction= 0.359578
 Thermal correction to Energy= 0.391511
 Thermal correction to Enthalpy= 0.392455
 Thermal correction to Gibbs Free Energy= 0.294176
 Sum of electronic and zero-point Energies= -1854.698940
 Sum of electronic and thermal Energies= -1854.667007
 Sum of electronic and thermal Enthalpies= -1854.666063
 Sum of electronic and thermal Free Energies= -1854.764342

 Cartesian Coordinates

7	1.523438	-0.051510	1.364488
46	0.359953	-1.206324	0.115362
8	-0.616515	-2.364916	-1.260679
6	-1.890668	-2.276950	-1.421422
6	-2.446919	-3.349474	-2.327729
6	2.763618	0.218672	0.887048
6	3.673126	0.938291	1.656194
6	3.291251	1.390079	2.911713
6	2.009150	1.116112	3.377277
6	1.149593	0.381451	2.573797
6	3.015547	-0.302116	-0.457181
6	1.861194	-0.577407	-1.244062
6	2.033015	-1.173427	-2.502541
6	3.306204	-1.431847	-2.994215
6	4.425218	-1.117038	-2.222997
6	4.288302	-0.558463	-0.953844
8	-0.735805	-2.160875	1.650216
6	-1.713737	-1.651736	2.289797
8	-2.189237	-0.503658	2.145809
47	-1.905282	0.598475	0.144756
8	-2.647943	-1.422593	-0.938599
6	-2.347204	-2.566541	3.309934
1	-2.045375	-3.217507	-3.338489
1	-3.537210	-3.298175	-2.363963
1	-2.131927	-4.339062	-1.982280
1	-1.626518	-3.286486	3.705658
1	-2.794427	-1.987711	4.121961
1	-3.148456	-3.128553	2.815475
1	1.095820	0.434018	-1.272364
1	1.154213	-1.405283	-3.100336
1	3.434001	-1.876230	-3.978224
1	5.420715	-1.321647	-2.610240
1	5.171489	-0.355446	-0.350998
1	4.662884	1.147659	1.260136
1	3.987257	1.960771	3.520695
1	1.669454	1.466357	4.346863
1	0.131451	0.147500	2.877033
15	-0.613033	2.282950	-1.024402
8	0.766452	1.790273	-1.487227
8	-1.290804	2.962031	-2.344688
8	-0.389152	3.664258	-0.151110
6	0.071965	3.479915	1.172406
6	-2.616339	3.443264	-2.205778
1	0.140275	4.464519	1.643925
1	-0.624599	2.860383	1.762674

1	1.068082	3.012165	1.195731
1	-3.016579	3.613340	-3.209066
1	-3.261035	2.709115	-1.694887
1	-2.643553	4.386314	-1.645027

1CH17_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -1693.0333 cm(-1)

Electronic energy : -1436.7081461
 Zero-point correction= 0.320013
 Thermal correction to Energy= 0.348399
 Thermal correction to Enthalpy= 0.349343
 Thermal correction to Gibbs Free Energy= 0.258297
 Sum of electronic and zero-point Energies= -1436.388133
 Sum of electronic and thermal Energies= -1436.359747
 Sum of electronic and thermal Enthalpies= -1436.358803
 Sum of electronic and thermal Free Energies= -1436.449849

 Cartesian Coordinates

8	-1.487362	-0.926615	1.948088
6	-0.754172	-1.170283	2.955219
6	-1.478405	-1.700430	4.169087
1	-0.869265	-1.602628	5.070559
1	-2.434520	-1.185447	4.299644
1	-1.700332	-2.762147	4.008836
8	0.490204	-1.032013	3.036825
47	1.634859	-0.049964	1.421699
46	0.079255	0.029711	-0.978426
8	1.064091	-1.608404	-1.709342
6	2.189159	-1.974489	-1.201470
8	2.707565	-1.551059	-0.159751
6	2.888658	-3.035215	-2.018316
1	2.208029	-3.868083	-2.221615
1	3.776984	-3.400158	-1.498332
1	3.182049	-2.614526	-2.986319
8	2.509075	1.754160	0.331815
6	2.498003	1.798126	-0.919936
8	1.661909	1.228750	-1.692812
6	3.579341	2.586659	-1.616657
1	3.231551	2.985236	-2.572882
1	3.943235	3.393430	-0.975648
1	4.419175	1.911247	-1.818799
1	-1.224550	-0.930382	0.573670
6	-1.705791	-1.020777	-0.626090
6	-1.911485	-2.343239	-1.044486
1	-1.096966	-3.058907	-0.956270
6	-3.146906	-2.742336	-1.538415
1	-3.308066	-3.773697	-1.842701
6	-4.183503	-1.815088	-1.647548
1	-5.147363	-2.129503	-2.041128
6	-4.000595	-0.486429	-1.271359
1	-4.811540	0.228220	-1.397867
6	-2.767388	-0.083611	-0.769854
6	-2.458257	1.291702	-0.373238
6	-3.393592	2.264503	-0.034422
6	-2.953678	3.519869	0.361709
6	-1.589219	3.781145	0.418294
6	-0.701946	2.777786	0.058561
7	-1.131445	1.572703	-0.331250
1	-4.453449	2.028620	-0.065079
1	-3.672175	4.286961	0.637806
1	-1.207871	4.743623	0.743974
1	0.375894	2.914928	0.103638

1CH18_Pd-Ag

Number of imaginary frequencies : 1
The smallest frequency is : -1675.7421 cm(-1)

Electronic energy : -1436.7022936
Zero-point correction= 0.320578
Thermal correction to Energy= 0.348796
Thermal correction to Enthalpy= 0.349741
Thermal correction to Gibbs Free Energy= 0.258733
Sum of electronic and zero-point Energies= -1436.381716
Sum of electronic and thermal Energies= -1436.353497
Sum of electronic and thermal Enthalpies= -1436.352553
Sum of electronic and thermal Free Energies= -1436.443560

Cartesian Coordinates

7	-0.186444	-0.494075	1.641559
6	-1.167375	0.404848	1.887177
6	-2.138904	0.130945	2.845402
6	-2.112641	-1.083454	3.512250
6	-1.116378	-2.008871	3.215406
6	-0.158167	-1.673580	2.273765
6	-1.142417	1.583510	1.021368
6	0.057216	1.886775	0.323514
6	0.005108	2.821267	-0.721908
6	-1.168471	3.505038	-1.015236
6	-2.321339	3.240295	-0.281804
6	-2.314228	2.272807	0.718049
46	1.278410	0.147878	0.356477
8	2.330610	-1.660045	0.379923
6	2.048705	-2.573099	-0.466080
8	1.083036	-2.584016	-1.259338
47	-0.663380	-1.215096	-1.394499
8	-2.426159	-0.105785	-2.197444
6	-3.220143	-0.256822	-1.212245
8	-2.943343	-0.886872	-0.169551
8	2.863357	1.036880	-0.640051
6	3.215008	2.112202	-0.054188
6	4.495589	2.748922	-0.501581
6	-4.598605	0.349782	-1.374366
8	2.555750	2.668067	0.866950
6	3.014653	-3.728305	-0.505445
1	1.250095	2.097112	0.831486
1	0.910256	3.052024	-1.279599
1	-1.183808	4.242033	-1.814107
1	-3.244123	3.769263	-0.508692
1	-3.243131	2.014693	1.222373
1	-2.910908	0.865307	3.055627
1	-2.868360	-1.310996	4.259179
1	-1.066839	-2.971798	3.713439
1	0.663142	-2.336824	2.014694
1	2.519433	-4.631978	-0.868075
1	3.823611	-3.478744	-1.201863
1	3.462586	-3.903978	0.475658
1	4.316271	3.803736	-0.730574
1	5.215768	2.712917	0.322855
1	4.914424	2.239227	-1.370566
1	-5.102896	0.458474	-0.409966
1	-4.543750	1.317201	-1.883527
1	-5.206336	-0.311423	-2.004096

1CH19_Pd-Ag

Number of imaginary frequencies : 1
The smallest frequency is : -1609.0364 cm(-1)

Electronic energy : -1436.7028757
 Zero-point correction= 0.320704
 Thermal correction to Energy= 0.348597
 Thermal correction to Enthalpy= 0.349541
 Thermal correction to Gibbs Free Energy= 0.260599
 Sum of electronic and zero-point Energies= -1436.382171
 Sum of electronic and thermal Energies= -1436.354279
 Sum of electronic and thermal Enthalpies= -1436.353335
 Sum of electronic and thermal Free Energies= -1436.442277

 Cartesian Coordinates

7	-1.610906	-0.133512	-1.683958
6	-2.143815	0.727478	-0.799417
6	-3.488766	0.663505	-0.438598
6	-4.289801	-0.331934	-0.983743
6	-3.730595	-1.229055	-1.886172
6	-2.389456	-1.088773	-2.210169
6	-1.265427	1.774279	-0.203750
6	-1.227550	3.027060	-0.813445
6	-0.475590	4.056711	-0.252992
6	0.216512	3.854792	0.938967
6	0.178249	2.608881	1.550239
6	-0.544562	1.538394	0.993177
46	0.514636	-0.350729	1.114665
8	1.650845	-2.098470	1.124819
6	2.129459	-2.566796	0.037819
6	2.965029	-3.814947	0.207802
47	0.673141	-0.276787	-1.730169
8	2.281025	1.298329	-1.144922
6	2.735725	1.310698	0.011290
8	2.277883	0.695399	1.039333
8	1.955448	-2.132328	-1.118280
8	-1.173074	-1.532617	1.356580
6	-2.130078	-1.061546	2.041371
6	-3.270933	-1.986920	2.342034
6	3.944523	2.163743	0.313349
8	-2.173452	0.117579	2.491826
1	-1.790368	3.197288	-1.730191
1	-0.444229	5.027153	-0.743500
1	0.782956	4.668362	1.386660
1	0.724522	2.448129	2.478018
1	-3.884871	1.381396	0.275116
1	-5.338399	-0.405977	-0.705615
1	-4.317691	-2.024476	-2.335161
1	-1.909467	-1.765854	-2.914263
1	-1.215453	0.793688	1.836084
1	3.596802	3.130247	0.699119
1	4.572743	1.705868	1.081589
1	4.525223	2.343086	-0.594496
1	2.328217	-4.689063	0.027894
1	3.769418	-3.831851	-0.532481
1	3.377425	-3.893616	1.216334
1	-4.202749	-1.424146	2.439003
1	-3.361430	-2.752767	1.568129
1	-3.074105	-2.486910	3.297399

1CH20_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -925.2300 cm(-1)

Electronic energy : -1436.6848689
 Zero-point correction= 0.321331
 Thermal correction to Energy= 0.349118
 Thermal correction to Enthalpy= 0.350062
 Thermal correction to Gibbs Free Energy= 0.260865
 Sum of electronic and zero-point Energies= -1436.363538

Sum of electronic and thermal Energies= -1436.335751
 Sum of electronic and thermal Enthalpies= -1436.334807
 Sum of electronic and thermal Free Energies= -1436.424004

 Cartesian Coordinates

7	1.028761	1.259558	1.124970
6	2.181093	0.949156	0.481579
6	3.165004	1.948131	0.375301
6	3.013480	3.181088	0.981894
6	1.859186	3.434395	1.711342
6	0.889848	2.452161	1.736081
6	2.479980	-0.384802	-0.122945
6	3.840290	-0.744454	-0.129018
6	4.296133	-1.874345	-0.795336
6	3.395794	-2.685507	-1.474706
6	2.040960	-2.382839	-1.401280
6	1.533846	-1.259663	-0.719653
47	-0.256270	-0.315129	-1.724743
8	-2.582111	-0.802387	-1.344306
6	-3.145846	-0.878415	-0.243279
8	-2.665149	-0.543274	0.904155
46	-0.814315	0.300511	1.010194
8	-1.571185	2.020063	0.185511
6	-1.309371	2.508192	-0.973760
6	-1.808864	3.922905	-1.141415
8	-0.278152	-1.273853	2.257752
6	-0.284496	-2.440438	1.780627
8	-0.187819	-2.706916	0.540380
6	-0.405688	-3.595463	2.721745
8	-0.694587	1.962631	-1.903168
6	-4.556444	-1.410757	-0.154618
1	4.566310	-0.142843	0.413059
1	5.356022	-2.118327	-0.774734
1	3.740580	-3.562588	-2.018721
1	1.326423	-3.074666	-1.850374
1	4.051223	1.752076	-0.218044
1	3.788494	3.936567	0.880969
1	1.690859	4.374841	2.226136
1	-0.053624	2.618424	2.248385
1	-4.596734	-2.252394	0.544380
1	-5.221498	-0.634124	0.237653
1	-4.909747	-1.731608	-1.136957
1	-2.818200	4.029618	-0.734253
1	-1.153633	4.593760	-0.572596
1	-1.792921	4.217412	-2.192941
1	0.383962	-1.831226	-0.070093
1	-0.429852	-3.262132	3.760549
1	-1.329185	-4.139199	2.493465
1	0.425991	-4.289137	2.565348

Monometallic C-H activation (Pd)

1CH1_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -1559.4937 cm(-1)

Electronic energy : -1899.1965442
 Zero-point correction= 0.349017
 Thermal correction to Energy= 0.376803
 Thermal correction to Enthalpy= 0.377747
 Thermal correction to Gibbs Free Energy= 0.290451
 Sum of electronic and zero-point Energies= -1898.847527
 Sum of electronic and thermal Energies= -1898.819742
 Sum of electronic and thermal Enthalpies= -1898.818797
 Sum of electronic and thermal Free Energies= -1898.906093

Cartesian Coordinates

```

-----
 7  -1.613471  1.379403 -0.279092
 6  -2.806491  0.750780 -0.378668
 6  -3.931568  1.441166 -0.831667
 6  -3.821242  2.781174 -1.172195
 6  -2.588563  3.413668 -1.056180
 6  -1.503867  2.672805 -0.612781
 6  -2.851598 -0.658883  0.057779
 6  -1.724106 -1.508959 -0.087884
 6  -1.802707 -2.766996  0.533596
 6  -2.936730 -3.200986  1.214957
 6  -4.042311 -2.364407  1.306096
 6  -3.992360 -1.095823  0.739262
46  0.041015 -0.013906 -0.067314
15  1.344542 -1.730289 -0.735109
 8  1.885912 -2.815361  0.320491
 6  2.777835 -2.367459  1.344304
 8  2.669986 -1.500619 -1.618208
 6  2.597842 -0.555829 -2.683270
 8  0.247172 -2.404500 -1.601481
 1 -0.956533 -3.447246  0.439552
 1 -2.956951 -4.189287  1.669649
 1 -4.936204 -2.685727  1.836075
 1 -4.836733 -0.420322  0.867600
 1 -4.878373  0.917932 -0.932875
 1 -4.690451  3.325547 -1.533234
 1 -2.459680  4.460262 -1.314799
 1 -0.504300  3.100555 -0.518350
 1 -0.766799 -1.833246 -1.068981
 1  2.085880  0.365506 -2.371143
 1  3.623229 -0.307823 -2.966190
 1  2.071707 -0.984805 -3.543613
 1  3.752053 -2.096640  0.923105
 1  2.360720 -1.503102  1.877853
 1  2.899619 -3.197365  2.043619
15  1.698358  1.476289  0.445845
 8  1.602722  2.832837 -0.185537
 8  1.665175  1.574054  2.084867
 8  3.163039  0.800278  0.282266
 6  4.299521  1.626694  0.536465
 6  0.565083  2.264180  2.662015
 1  5.185574  1.004297  0.388803
 1  4.333847  2.473907 -0.157708
 1  4.292370  2.002042  1.566765
 1  0.755547  2.343829  3.735563
 1  0.459978  3.272892  2.242493
 1 -0.374872  1.712374  2.514728

```

1CH2_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -1272.9880 cm(-1)

Electronic energy : -1480.8464852
 Zero-point correction= 0.309666
 Thermal correction to Energy= 0.333551
 Thermal correction to Enthalpy= 0.334495
 Thermal correction to Gibbs Free Energy= 0.255347
 Sum of electronic and zero-point Energies= -1480.536819
 Sum of electronic and thermal Energies= -1480.512934
 Sum of electronic and thermal Enthalpies= -1480.511990
 Sum of electronic and thermal Free Energies= -1480.591138

 Cartesian Coordinates

```

 6  1.844145  1.121973  0.079941
 6  2.724872  0.018256  0.167583

```

6	3.961738	0.144624	0.808369
6	4.340219	1.353757	1.379001
6	3.473868	2.441038	1.334881
6	2.242469	2.313595	0.698682
6	2.282867	-1.298085	-0.313895
6	3.160965	-2.294975	-0.736354
6	2.665143	-3.523024	-1.146700
6	1.293386	-3.739394	-1.126903
6	0.461332	-2.713641	-0.706508
7	0.943858	-1.526546	-0.310836
46	-0.201149	0.171778	0.070200
15	-2.247667	-0.852763	0.359216
8	-2.499548	-0.739135	1.958528
6	-3.682531	-1.346064	2.480979
8	-1.185710	2.026723	0.041302
6	-0.744590	2.734857	-0.908743
8	0.304710	2.460748	-1.575787
6	-1.515814	3.956416	-1.295299
8	-2.475132	-2.234141	-0.180647
8	-3.407432	0.177989	-0.152836
6	-3.495990	0.394230	-1.549696
1	0.980495	1.609791	-0.916190
1	1.584938	3.182122	0.653502
1	3.756937	3.385692	1.794419
1	5.303063	1.438105	1.877627
1	4.618684	-0.718182	0.902938
1	4.227713	-2.091992	-0.760371
1	3.344959	-4.300968	-1.484818
1	0.860824	-4.684867	-1.438939
1	-0.623748	-2.822636	-0.667170
1	-2.244262	4.222400	-0.527408
1	-0.835281	4.790234	-1.487480
1	-2.049068	3.746375	-2.230127
1	-4.075884	1.308337	-1.708149
1	-2.503840	0.527646	-2.009265
1	-3.998924	-0.442618	-2.051118
1	-3.662419	-1.209079	3.564966
1	-4.582134	-0.866037	2.077065
1	-3.708789	-2.417716	2.252401

1CH3_Pd

Number of imaginary frequencies : 1
The smallest frequency is : -1262.1989 cm(-1)

Electronic energy : -1480.8462661
Zero-point correction= 0.310021
Thermal correction to Energy= 0.333701
Thermal correction to Enthalpy= 0.334645
Thermal correction to Gibbs Free Energy= 0.256630
Sum of electronic and zero-point Energies= -1480.536245
Sum of electronic and thermal Energies= -1480.512565
Sum of electronic and thermal Enthalpies= -1480.511621
Sum of electronic and thermal Free Energies= -1480.589637

Cartesian Coordinates

6	-3.315646	2.196815	-0.537023
6	-2.365705	1.229341	-0.214439
7	-1.044152	1.543335	-0.215461
6	-0.649172	2.789353	-0.515307
6	-1.554748	3.788191	-0.837305
6	-2.909550	3.484239	-0.853617
6	-2.712452	-0.147489	0.163130
6	-3.915737	-0.401053	0.829765
6	-4.203109	-1.674438	1.305424
6	-3.279104	-2.700304	1.136582
6	-2.082068	-2.446398	0.472752

6	-1.773686	-1.183232	-0.048755
46	0.216711	-0.108658	-0.030140
8	1.296636	-1.897682	-0.250791
6	0.847873	-2.564256	-1.226552
6	1.598756	-3.782196	-1.661457
8	-0.223543	-2.280145	-1.852145
1	-0.919151	-1.523389	-1.108511
1	-1.381795	-3.269725	0.326322
1	-3.491318	-3.696660	1.518746
1	-5.139606	-1.858474	1.826940
1	-4.616629	0.410115	1.018721
1	-4.367302	1.925784	-0.557458
1	-3.645213	4.240551	-1.115167
1	-1.190967	4.782998	-1.074863
1	0.425359	2.971650	-0.471282
1	1.775936	-3.738335	-2.740327
1	2.547094	-3.875347	-1.130080
1	0.980927	-4.666678	-1.470782
15	2.177557	1.040062	0.377271
8	2.244460	2.525281	0.206090
8	2.606028	0.714914	1.922188
8	3.318720	0.270082	-0.497087
6	2.741594	-0.635465	2.341924
6	4.644586	0.789471	-0.400437
1	3.127052	-0.617029	3.365069
1	1.774811	-1.156249	2.341186
1	3.441271	-1.189368	1.703692
1	5.288307	0.146355	-1.006128
1	4.696490	1.815522	-0.782363
1	5.002322	0.777187	0.637746

1CH4_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -1916.5669 cm(-1)

Electronic energy : -1480.828839
 Zero-point correction= 0.308484
 Thermal correction to Energy= 0.332823
 Thermal correction to Enthalpy= 0.333768
 Thermal correction to Gibbs Free Energy= 0.253269
 Sum of electronic and zero-point Energies= -1480.520355
 Sum of electronic and thermal Energies= -1480.496016
 Sum of electronic and thermal Enthalpies= -1480.495071
 Sum of electronic and thermal Free Energies= -1480.575570

 Cartesian Coordinates

6	1.243644	-1.424386	0.074680
6	2.553569	-0.869089	-0.019290
6	3.618496	-1.657383	-0.452244
6	3.417275	-2.983717	-0.825506
6	2.140042	-3.528429	-0.798933
6	1.073137	-2.750570	-0.360166
6	2.758384	0.578554	0.167147
6	3.969672	1.164362	0.533147
6	4.059585	2.548182	0.601028
6	2.944953	3.325396	0.304119
6	1.764670	2.680255	-0.035039
7	1.683439	1.349643	-0.101018
46	-0.156176	0.228005	-0.126434
15	-1.732451	-1.131644	0.723773
8	-3.031112	-0.448973	1.390940
6	-2.820731	0.645269	2.288298
8	-1.289466	1.955687	-0.325846
6	-2.294156	1.928819	-1.144368
6	-3.090821	3.215785	-1.134563
8	-2.617031	0.982895	-1.859133

8	-0.811129	-1.794683	1.769741
8	-2.422585	-2.304632	-0.124414
6	-3.465178	-2.008973	-1.063797
1	0.084617	-3.200909	-0.292366
1	1.973573	-4.556479	-1.111415
1	4.261507	-3.581274	-1.161479
1	4.611222	-1.222884	-0.552712
1	4.825503	0.541520	0.778071
1	4.996413	3.018012	0.889843
1	2.980608	4.409566	0.347478
1	0.843362	3.218211	-0.252352
1	-3.832322	3.218111	-1.936791
1	-3.607276	3.312699	-0.171713
1	-2.431252	4.083459	-1.234278
1	0.354095	-1.433009	1.094028
1	-2.312611	1.473549	1.779274
1	-3.806781	0.973759	2.624276
1	-2.233031	0.326683	3.157410
1	-4.421361	-1.907885	-0.539322
1	-3.246590	-1.086852	-1.614695
1	-3.517549	-2.854142	-1.754152

1CH5_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -1668.5492 cm(-1)

Electronic energy : -1062.4850607
 Zero-point correction= 0.268778
 Thermal correction to Energy= 0.289212
 Thermal correction to Enthalpy= 0.290156
 Thermal correction to Gibbs Free Energy= 0.218621
 Sum of electronic and zero-point Energies= -1062.216282
 Sum of electronic and thermal Energies= -1062.195849
 Sum of electronic and thermal Enthalpies= -1062.194905
 Sum of electronic and thermal Free Energies= -1062.266440

 Cartesian Coordinates

6	3.679118	-0.533889	-0.092255
6	2.347258	-0.177386	0.115903
6	1.323831	-1.152342	-0.013518
6	1.683499	-2.440783	-0.426766
6	3.013665	-2.786556	-0.642403
6	4.010964	-1.835415	-0.455167
6	1.961082	1.225489	0.297936
7	0.688122	1.516778	-0.062102
6	0.230922	2.772867	-0.020005
6	1.032236	3.820895	0.404122
6	2.337266	3.543792	0.796659
6	2.807544	2.239731	0.738667
46	-0.506576	-0.105344	-0.434616
8	-2.093682	1.051323	-1.051865
6	-2.975914	1.206190	-0.108305
8	-2.860507	0.811972	1.048630
8	-1.711755	-1.790944	-0.442151
6	-1.573354	-2.415443	0.658428
8	-0.638713	-2.211146	1.480299
6	-2.616407	-3.440302	0.987325
6	-4.193807	1.977046	-0.569595
1	0.316525	-1.394805	0.805913
1	0.909688	-3.198952	-0.532710
1	3.271207	-3.797546	-0.948616
1	5.053674	-2.098870	-0.615528
1	4.464263	0.215651	-0.016762
1	3.823902	2.002470	1.038738
1	2.987653	4.341169	1.146491
1	0.631303	4.828970	0.431981

1	-0.797910	2.911867	-0.343407
1	-3.909430	3.007171	-0.814385
1	-4.607107	1.534076	-1.481276
1	-4.955801	1.992540	0.213459
1	-3.019037	-3.895051	0.079390
1	-2.214089	-4.203358	1.656938
1	-3.439340	-2.929925	1.501375

1CH6_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -1679.1479 cm(-1)

Electronic energy : -1062.4849887
 Zero-point correction= 0.269118
 Thermal correction to Energy= 0.289500
 Thermal correction to Enthalpy= 0.290445
 Thermal correction to Gibbs Free Energy= 0.218865
 Sum of electronic and zero-point Energies= -1062.215871
 Sum of electronic and thermal Energies= -1062.195488
 Sum of electronic and thermal Enthalpies= -1062.194544
 Sum of electronic and thermal Free Energies= -1062.266124

 Cartesian Coordinates

6	3.447934	0.612798	0.713118
6	2.229106	0.283696	0.120510
6	1.158367	1.216125	0.134585
6	1.341195	2.424119	0.818896
6	2.558047	2.741569	1.413479
6	3.616050	1.841503	1.342704
6	1.967983	-1.075117	-0.362087
7	0.660536	-1.427477	-0.382700
6	0.283615	-2.660398	-0.739563
6	1.211285	-3.622235	-1.105280
6	2.559285	-3.279480	-1.107756
6	2.941798	-1.999621	-0.733382
46	-0.663934	0.098372	-0.043371
8	-2.283596	-1.181385	-0.091801
6	-2.538505	-1.639943	1.097031
6	-3.686352	-2.624282	1.117757
8	-1.916196	-1.348880	2.115739
1	0.356386	1.578309	-0.861864
1	0.529366	3.148561	0.847831
1	2.680706	3.691762	1.927590
1	4.570716	2.083485	1.803510
1	4.259727	-0.111509	0.731569
1	3.988720	-1.710464	-0.738061
1	3.310942	-4.006109	-1.404669
1	0.875522	-4.613192	-1.393796
1	-0.788468	-2.845450	-0.735496
1	-3.948387	-2.885902	2.145717
1	-4.560456	-2.210719	0.605033
1	-3.398819	-3.534938	0.578714
8	-0.434550	2.507442	-1.584948
6	-1.536333	2.581057	-0.972072
8	-1.922597	1.750685	-0.089808
6	-2.461267	3.713353	-1.304194
1	-2.872503	3.547895	-2.306185
1	-3.282623	3.781337	-0.588952
1	-1.901345	4.652410	-1.332907

1CH7_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -1499.0091 cm(-1)

Electronic energy : -1335.3097379
 Zero-point correction= 0.434020
 Thermal correction to Energy= 0.463643
 Thermal correction to Enthalpy= 0.464587
 Thermal correction to Gibbs Free Energy= 0.372227
 Sum of electronic and zero-point Energies= -1334.875718
 Sum of electronic and thermal Energies= -1334.846095
 Sum of electronic and thermal Enthalpies= -1334.845151
 Sum of electronic and thermal Free Energies= -1334.937511

 Cartesian Coordinates

6	1.523439	3.530816	-0.572736
6	1.081980	2.300771	-0.091816
7	1.654214	1.154471	-0.535912
6	2.643763	1.184520	-1.433859
6	3.121480	2.380689	-1.946552
6	2.549279	3.569300	-1.506482
6	0.039069	2.105478	0.919170
6	-0.372723	3.110216	1.792709
6	-1.280386	2.814854	2.806575
6	-1.761616	1.517423	2.976044
6	-1.360121	0.513778	2.100476
6	-0.492937	0.794675	1.037802
46	0.876783	-0.589282	0.221426
8	-0.072738	-2.254582	0.974304
8	2.416232	-1.759193	-0.542288
6	3.452169	-1.745778	0.236694
8	3.534885	-1.141114	1.304575
6	4.619198	-2.538871	-0.312974
1	-1.732898	-0.503127	2.221274
1	-2.444514	1.292617	3.791891
1	-1.595550	3.601984	3.487555
1	0.037582	4.115461	1.715983
1	1.060035	4.447026	-0.218465
1	2.898454	4.523674	-1.891666
1	3.921558	2.371829	-2.680069
1	3.036743	0.215054	-1.733568
1	5.413344	-2.624554	0.432861
1	4.296663	-3.535926	-0.629329
1	5.017697	-2.034220	-1.201514
1	-0.972692	0.307606	-0.110411
8	-1.631034	0.006324	-1.253376
1	-1.445943	-0.980509	-1.293706
6	-0.862168	-2.887317	0.188235
8	-1.165466	-2.557576	-0.975435
6	-1.501349	-4.111287	0.792790
1	-2.446700	-3.808180	1.261546
1	-1.733547	-4.842117	0.014033
1	-0.871170	-4.561584	1.563377
6	-3.060900	0.264923	-1.364970
6	-3.422677	0.028891	-2.820170
6	-3.795851	-0.692981	-0.425698
6	-3.245419	1.720575	-0.981127
1	-4.479536	0.251270	-3.006950
1	-2.818958	0.673053	-3.469708
1	-3.237502	-1.016262	-3.100480
1	-4.263307	2.054544	-1.209222
1	-3.064240	1.880515	0.089938
1	-2.549050	2.348583	-1.550729
6	-5.301736	-0.500518	-0.361553
1	-3.560911	-1.720668	-0.739885
1	-3.366541	-0.570665	0.580735
1	-5.751802	-1.230422	0.320123
1	-5.572829	0.496746	0.005533
1	-5.775905	-0.637875	-1.340944

1CH8_Pd

Number of imaginary frequencies : 1
The smallest frequency is : -1706.1042 cm(-1)

Electronic energy : -1215.9669491
Zero-point correction= 0.315533
Thermal correction to Energy= 0.338319
Thermal correction to Enthalpy= 0.339263
Thermal correction to Gibbs Free Energy= 0.261895
Sum of electronic and zero-point Energies= -1215.651416
Sum of electronic and thermal Energies= -1215.628631
Sum of electronic and thermal Enthalpies= -1215.627686
Sum of electronic and thermal Free Energies= -1215.705055

Cartesian Coordinates

6	3.594637	2.205979	0.798548
6	2.741588	1.205662	0.336118
7	1.498985	1.528839	-0.091815
6	1.069812	2.794610	-0.089029
6	1.880548	3.829410	0.350401
6	3.158876	3.523602	0.806321
6	3.090375	-0.215195	0.213620
6	4.422012	-0.613369	0.090233
6	4.739856	-1.936421	-0.198166
6	3.728083	-2.870337	-0.394483
6	2.398181	-2.481798	-0.266496
6	2.047197	-1.167993	0.067698
46	0.272745	-0.069469	-0.509630
8	-0.994191	-1.737665	-0.541150
6	-0.950897	-2.306797	0.593308
6	-2.061752	-3.261106	0.909391
8	-1.202766	1.178330	-1.166415
8	-0.053249	-2.095250	1.459946
1	0.956862	-1.364243	0.823969
1	1.611927	-3.226048	-0.382801
1	3.973792	-3.900740	-0.640596
1	5.782399	-2.231007	-0.292015
1	5.220863	0.120606	0.176152
1	4.586866	1.948281	1.157412
1	3.815139	4.309842	1.170615
1	1.508728	4.849104	0.342148
1	0.052162	2.935837	-0.451038
1	-1.843909	-3.845262	1.805195
1	-2.973994	-2.674563	1.072198
1	-2.249241	-3.921655	0.058373
6	-2.403362	0.913830	-0.662793
6	-2.668190	0.999289	0.720043
6	-3.934756	0.759214	1.230802
6	-4.986020	0.433954	0.370180
6	-4.748244	0.345138	-1.001382
6	-3.473141	0.569447	-1.506645
1	-1.844454	1.253701	1.388971
1	-4.132609	0.823323	2.299095
8	-6.210915	0.214490	0.920763
1	-5.566727	0.089085	-1.675421
1	-3.281455	0.489329	-2.575102
1	-6.835380	-0.003841	0.217350

1CH9_Pd

Number of imaginary frequencies : 1
The smallest frequency is : -1668.7758 cm(-1)

Electronic energy : -1480.8128825
Zero-point correction= 0.307959
Thermal correction to Energy= 0.331991

Thermal correction to Enthalpy= 0.332935
 Thermal correction to Gibbs Free Energy= 0.252928
 Sum of electronic and zero-point Energies= -1480.504923
 Sum of electronic and thermal Energies= -1480.480892
 Sum of electronic and thermal Enthalpies= -1480.479947
 Sum of electronic and thermal Free Energies= -1480.559955

 Cartesian Coordinates

6	-1.591279	3.374098	-0.861292
6	-1.398068	2.056737	-0.454502
7	-0.178625	1.483900	-0.588062
6	0.861772	2.164931	-1.077722
6	0.726735	3.483348	-1.484614
6	-0.521463	4.088319	-1.383393
6	-2.401601	1.209587	0.196644
6	-3.468533	1.769355	0.898152
6	-4.293144	0.968721	1.682357
6	-4.040433	-0.393693	1.800234
6	-2.982896	-0.961810	1.097347
6	-2.169301	-0.190219	0.258369
46	-0.102803	-0.524917	-0.208336
8	-0.202578	-2.594183	-0.139726
6	-1.143879	-3.021083	-0.882298
6	-1.197659	-4.495936	-1.143525
8	1.918989	-0.550594	-0.560722
8	-2.020234	-2.282726	-1.411886
1	-1.934452	-1.027095	-0.740331
1	-2.814388	-2.034961	1.162952
1	-4.668779	-1.015158	2.433500
1	-5.120770	1.419575	2.224571
1	-3.632385	2.844949	0.877028
1	-2.574724	3.827074	-0.774626
1	-0.662344	5.115707	-1.709009
1	1.584923	4.014986	-1.883316
1	1.795107	1.605426	-1.124992
1	-0.912581	-4.676241	-2.185918
1	-0.516989	-5.043085	-0.489184
1	-2.221985	-4.857952	-1.018238
15	2.746911	-0.846331	0.760385
8	4.307784	-0.841304	0.194780
8	2.685134	0.700265	1.431129
6	3.458170	0.866840	2.597402
6	4.725191	0.191716	-0.680341
1	3.100276	1.753899	3.131189
1	3.376345	0.004190	3.279589
1	4.525257	1.008982	2.365747
1	5.819097	0.167545	-0.730102
1	4.325655	0.047693	-1.692698
1	4.413945	1.181169	-0.317538

1CH10_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -1636.3152 cm(-1)

Electronic energy : -1106.3029855
 Zero-point correction= 0.370753
 Thermal correction to Energy= 0.394447
 Thermal correction to Enthalpy= 0.395391
 Thermal correction to Gibbs Free Energy= 0.317662
 Sum of electronic and zero-point Energies= -1105.932233
 Sum of electronic and thermal Energies= -1105.908539
 Sum of electronic and thermal Enthalpies= -1105.907595
 Sum of electronic and thermal Free Energies= -1105.985323

 Cartesian Coordinates

6	-2.611213	2.886689	-0.576060
6	-1.981894	1.683946	-0.259712

7	-0.630341	1.623330	-0.229239
6	0.120137	2.699913	-0.476141
6	-0.454141	3.922464	-0.787203
6	-1.841402	4.009203	-0.845510
6	-2.669190	0.444151	0.117669
6	-3.963808	0.480546	0.638873
6	-4.544221	-0.665431	1.170533
6	-3.824135	-1.854734	1.209784
6	-2.538249	-1.899826	0.680359
6	-1.941394	-0.773890	0.099878
46	0.172174	-0.257840	0.010379
8	0.825969	-2.251239	-0.092539
6	0.230788	-2.862185	-1.034285
6	0.773613	-4.205087	-1.417726
8	1.978516	0.621699	0.057831
6	3.087141	0.070792	0.708545
8	-0.764850	-2.396742	-1.658548
1	-1.221525	-1.336412	-0.896958
1	-1.999707	-2.846187	0.679209
1	-4.265457	-2.748284	1.645364
1	-5.552495	-0.621258	1.575314
1	-4.511504	1.420196	0.672942
1	-3.695646	2.934360	-0.617608
1	-2.324121	4.949523	-1.099588
1	0.177615	4.782306	-0.987032
1	1.195034	2.525528	-0.404814
1	0.069586	-4.750350	-2.048919
1	1.708409	-4.058093	-1.971238
1	1.013188	-4.785464	-0.522473
6	4.039193	1.252716	0.988593
6	2.698393	-0.548317	2.050914
6	3.778210	-0.978903	-0.163930
1	3.580752	-0.907748	2.598579
1	2.185851	0.196252	2.675022
1	2.024033	-1.400474	1.902002
1	4.728680	-1.311996	0.277423
1	3.127328	-1.851938	-0.286732
1	3.986640	-0.571085	-1.160532
1	4.885109	0.885637	1.591116
6	4.558091	1.966715	-0.246960
1	3.485578	1.963271	1.621301
1	5.113759	2.873065	0.021905
1	5.237299	1.333828	-0.831700
1	3.731412	2.260341	-0.905024

1CH11_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -1561.2436 cm(-1)

Electronic energy : -1480.8054462
 Zero-point correction= 0.307482
 Thermal correction to Energy= 0.331703
 Thermal correction to Enthalpy= 0.332647
 Thermal correction to Gibbs Free Energy= 0.253112
 Sum of electronic and zero-point Energies= -1480.497965
 Sum of electronic and thermal Energies= -1480.473744
 Sum of electronic and thermal Enthalpies= -1480.472799
 Sum of electronic and thermal Free Energies= -1480.552334

 Cartesian Coordinates

7	-2.082054	0.010907	-0.374093
6	-2.347453	-1.311168	-0.254682

6	-3.613648	-1.797085	-0.570821
6	-4.594541	-0.912923	-0.996296
6	-4.301121	0.443123	-1.096747
6	-3.022190	0.871929	-0.779156
6	-1.235437	-2.108096	0.265804
6	0.079834	-1.579835	0.163687
6	1.108152	-2.220207	0.868671
6	0.865396	-3.379024	1.599380
6	-0.417301	-3.915290	1.643394
6	-1.466706	-3.275915	0.990463
46	-0.131981	0.550633	-0.082706
8	-0.621010	2.563588	-0.166888
6	-0.619371	3.092788	1.017719
8	-0.296077	2.505460	2.050484
6	-1.083701	4.530628	1.031132
1	2.122531	-1.833835	0.782640
1	1.680769	-3.869554	2.125690
1	-0.610616	-4.823906	2.208723
1	-2.477962	-3.664570	1.093097
1	-3.816213	-2.861753	-0.494775
1	-5.584455	-1.281096	-1.252704
1	-5.043109	1.162406	-1.428359
1	-2.710949	1.912587	-0.842217
1	-0.915259	4.979458	2.012903
1	-0.569129	5.113183	0.260568
1	-2.155039	4.568001	0.801397
8	1.926692	1.011035	-0.247523
15	2.802805	0.069464	-1.470448
8	3.696152	-0.866939	-0.417201
8	1.630563	-0.839436	-1.897438
6	5.068894	-0.553107	-0.263209
1	5.265166	-0.177552	0.749215
1	5.666900	-1.457617	-0.421747
1	5.402818	0.208491	-0.983854
1	0.646726	-1.132189	-0.907552
6	2.659819	1.551087	0.848900
1	3.570533	2.043847	0.481565
1	2.026137	2.289050	1.347116
1	2.930252	0.766507	1.567238

1CH12_Pd

Number of imaginary frequencies : 1
The smallest frequency is : -124.6489 cm(-1)

Electronic energy : -1062.457204
Zero-point correction= 0.267686
Thermal correction to Energy= 0.288164
Thermal correction to Enthalpy= 0.289108
Thermal correction to Gibbs Free Energy= 0.217466
Sum of electronic and zero-point Energies= -1062.189518
Sum of electronic and thermal Energies= -1062.169040
Sum of electronic and thermal Enthalpies= -1062.168096
Sum of electronic and thermal Free Energies= -1062.239738

Cartesian Coordinates

6	3.357987	1.613513	0.662958
6	2.310814	0.820623	0.186161
6	1.046612	1.412265	0.062272
6	0.792731	2.731759	0.368903
6	1.857203	3.498953	0.848462
6	3.127184	2.944087	0.989802
6	2.401121	-0.590854	-0.158589
7	1.213698	-1.139569	-0.506635
6	1.099764	-2.430015	-0.827010
6	2.207503	-3.261978	-0.832048
6	3.443861	-2.723926	-0.486200

6	3.545244	-1.382795	-0.144516
46	-0.405664	0.123696	-0.446742
8	-1.098227	-1.232170	1.095574
6	-2.255231	-1.202020	1.668188
6	-2.493666	-2.384124	2.588407
8	-3.127131	-0.343345	1.520585
1	0.183365	0.925608	-1.623931
1	-0.203295	3.156344	0.244310
1	1.685689	4.544077	1.106505
1	3.947712	3.557012	1.360772
1	4.352817	1.183499	0.788960
1	4.503795	-0.947586	0.135803
1	4.333206	-3.353976	-0.479852
1	2.095119	-4.310231	-1.101313
1	0.096328	-2.780447	-1.075364
1	-2.544790	-3.305028	1.993334
1	-1.659450	-2.501541	3.289822
1	-3.429414	-2.264912	3.142657
8	-2.571421	-0.333172	-1.602178
6	-2.843260	0.777983	-1.116385
8	-1.938027	1.481865	-0.513338
6	-4.208864	1.379919	-1.174858
1	-4.153885	2.458958	-1.354706
1	-4.810205	0.894953	-1.949289
1	-4.687900	1.224496	-0.199561

1CH13_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -115.8878 cm(-1)

Electronic energy : -1062.4538518
 Zero-point correction= 0.269370
 Thermal correction to Energy= 0.289784
 Thermal correction to Enthalpy= 0.290728
 Thermal correction to Gibbs Free Energy= 0.219255
 Sum of electronic and zero-point Energies= -1062.184482
 Sum of electronic and thermal Energies= -1062.164068
 Sum of electronic and thermal Enthalpies= -1062.163123
 Sum of electronic and thermal Free Energies= -1062.234597

 Cartesian Coordinates

6	3.264374	1.805652	0.378600
6	2.208251	0.937174	0.089571
6	0.899706	1.446657	0.112757
6	0.628169	2.772389	0.391704
6	1.699311	3.621304	0.675969
6	3.006561	3.140258	0.667087
6	2.357552	-0.484842	-0.203864
7	1.184893	-1.142833	-0.369924
6	1.144515	-2.451864	-0.637015
6	2.309346	-3.191382	-0.758012
6	3.529004	-2.541952	-0.591579
6	3.557014	-1.183352	-0.312270
46	-0.499288	0.021401	-0.129044
8	-1.898247	-1.732375	-0.205204
6	-1.844066	-1.890200	1.059462
6	-2.711805	-2.942570	1.684104
8	-1.094528	-1.173709	1.770618
1	-0.138501	0.762974	-1.417644
1	-0.397218	3.132630	0.400892
1	1.505783	4.666882	0.904679
1	3.832715	3.810775	0.889383
1	4.288211	1.437175	0.387154
1	4.501310	-0.663463	-0.177945
1	4.460298	-3.095064	-0.680354
1	2.254134	-4.252326	-0.978975

1	0.152847	-2.884860	-0.749533
1	-2.417650	-3.133873	2.718407
1	-3.751802	-2.597119	1.671235
1	-2.669753	-3.868139	1.102103
8	-3.974543	2.175343	-0.306270
6	-3.041687	1.458128	-0.632091
8	-2.016622	1.308022	0.180343
6	-3.016380	0.738526	-1.956818
1	-2.905350	-0.340090	-1.801883
1	-3.942415	0.939338	-2.500823
1	-2.167289	1.078748	-2.562754

1CH14_Pd

Number of imaginary frequencies : 1
The smallest frequency is : -172.5265 cm(-1)

Electronic energy : -1062.4354291
Zero-point correction= 0.270042
Thermal correction to Energy= 0.290689
Thermal correction to Enthalpy= 0.291633
Thermal correction to Gibbs Free Energy= 0.218478
Sum of electronic and zero-point Energies= -1062.165387
Sum of electronic and thermal Energies= -1062.144740
Sum of electronic and thermal Enthalpies= -1062.143796
Sum of electronic and thermal Free Energies= -1062.216951

Cartesian Coordinates

6	-0.873292	1.236389	0.740535
6	-2.033560	0.903360	-0.007362
6	-3.029166	1.847544	-0.229395
6	-2.866476	3.139204	0.265457
6	-1.712561	3.497890	0.961750
6	-0.719323	2.553416	1.191375
6	-2.056293	-0.445929	-0.576329
6	-3.185652	-1.203549	-0.869534
6	-3.022065	-2.482253	-1.385351
6	-1.741507	-2.984942	-1.594729
6	-0.652266	-2.180341	-1.293249
7	-0.825587	-0.947387	-0.816077
46	0.744364	0.273712	-0.378862
8	2.482218	-0.158555	-1.638587
6	3.096546	0.712169	-0.961521
6	4.558289	0.941897	-1.125941
8	2.441392	1.390911	-0.093876
8	1.363973	-1.653261	1.136268
6	0.662081	-1.648610	2.175383
6	0.947870	-2.694548	3.239413
8	-0.272642	-0.834401	2.445756
1	-0.421003	0.356144	1.407402
1	0.180465	2.816721	1.743953
1	-1.594807	4.515959	1.324507
1	-3.640854	3.881975	0.088154
1	-3.908685	1.595059	-0.819414
1	-4.173002	-0.795067	-0.672158
1	-3.892551	-3.092173	-1.612759
1	-1.582370	-3.987883	-1.977294
1	0.380283	-2.501542	-1.412352
1	4.863619	0.703392	-2.147439
1	4.811820	1.974851	-0.875402
1	5.097622	0.279464	-0.440605
1	0.012353	-3.088171	3.648837
1	1.487642	-2.221027	4.067346
1	1.562552	-3.504489	2.837892

Conformational and Configurational Study of Reductive Elimination (RE)

Bimetallic Reductive Elimination (Pd-Ag)

IRE1_Pd-Ag

Number of imaginary frequencies : 1

The smallest frequency is : -88.9079 cm(-1)

Electronic energy : -2691.7729306
Zero-point correction= 0.442930
Thermal correction to Energy= 0.482256
Thermal correction to Enthalpy= 0.483200
Thermal correction to Gibbs Free Energy= 0.367175
Sum of electronic and zero-point Energies= -2691.330000
Sum of electronic and thermal Energies= -2691.290675
Sum of electronic and thermal Enthalpies= -2691.289731
Sum of electronic and thermal Free Energies= -2691.405755

Cartesian Coordinates

6	4.155117	-1.685450	-1.975598
6	3.384891	-0.882675	-1.132524
6	2.047492	-1.252089	-0.863968
6	1.519347	-2.405594	-1.445488
6	2.295548	-3.186220	-2.303292
6	3.613936	-2.828994	-2.559442
6	3.927881	0.363975	-0.561665
7	3.045195	1.369603	-0.414944
6	3.449796	2.518728	0.128178
6	4.761247	2.737459	0.532840
6	5.680174	1.705475	0.374603
6	5.261805	0.500031	-0.173477
46	0.785304	0.400005	-0.506224
47	-1.606989	-0.914475	0.168655
15	-4.014034	-0.585697	-0.083796
8	-4.602811	-0.797524	-1.567305
6	-5.923190	-0.342008	-1.882921
15	-0.830178	2.112860	-0.141808
8	0.031453	3.422871	0.337623
6	-0.678120	4.620846	0.630390
15	1.194587	-1.093928	1.218006
8	0.105506	-2.146963	1.314009
8	-1.293709	2.700055	-1.630821
6	-2.211455	1.898302	-2.339966
8	-2.090518	2.021576	0.722050
8	2.597463	-1.678427	1.803292
6	3.045785	-2.987649	1.479919
8	1.042336	0.086581	2.329847
6	1.161802	-0.255065	3.714015
8	-4.368145	0.912247	0.332566
8	-5.089819	-1.463522	0.765017
6	-4.884083	-1.500968	2.173357
1	0.506129	-2.717587	-1.196804
1	1.870280	-4.078462	-2.757546
1	4.226029	-3.436305	-3.222228
1	5.177221	-1.390611	-2.209553
1	5.950458	-0.335042	-0.277797
1	6.713716	1.833504	0.687605
1	5.050475	3.692211	0.962540
1	2.682909	3.286288	0.235177
1	2.213057	-0.342470	4.006434
1	0.640362	-1.192279	3.943169
1	0.693110	0.556265	4.276716
1	3.586507	-3.367442	2.351905
1	3.731531	-2.962062	0.623356
1	2.209902	-3.662536	1.264043
1	0.058869	5.370975	0.931186
1	-1.220119	4.988299	-0.250124
1	-1.391161	4.470164	1.449446

1	-2.260441	2.263481	-3.370557
1	-1.894336	0.839631	-2.369454
1	-3.220006	1.944928	-1.902361
1	-3.508775	1.432477	0.488978
1	-5.516303	-2.294978	2.577102
1	-3.834806	-1.729794	2.417801
1	-5.159706	-0.547228	2.638804
1	-6.085397	-0.549913	-2.942638
1	-6.673590	-0.876310	-1.290464
1	-6.015297	0.735408	-1.706634

IRE2_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -101.1168 cm(-1)

Electronic energy : -2654.680998
 Zero-point correction= 0.491519
 Thermal correction to Energy= 0.533882
 Thermal correction to Enthalpy= 0.534826
 Thermal correction to Gibbs Free Energy= 0.414979
 Sum of electronic and zero-point Energies= -2654.189479
 Sum of electronic and thermal Energies= -2654.147116
 Sum of electronic and thermal Enthalpies= -2654.146172
 Sum of electronic and thermal Free Energies= -2654.266019

 Cartesian Coordinates

6	2.015617	-0.975571	0.553190
6	3.276609	-0.518246	0.094618
6	4.344956	-1.413616	0.031683
6	4.189825	-2.739700	0.432514
6	2.961911	-3.183779	0.906906
6	1.880992	-2.305230	0.963263
6	3.425984	0.883349	-0.332294
6	4.640796	1.572727	-0.291498
6	4.676559	2.897636	-0.700448
6	3.503500	3.515645	-1.123510
6	2.330883	2.772927	-1.118675
7	2.298973	1.491853	-0.746204
46	0.421190	0.103131	-0.539754
15	0.841598	0.225553	1.838727
8	2.123119	0.497518	2.818909
6	2.768341	-0.564332	3.504616
15	-1.448872	1.621537	-0.722955
8	-2.125614	1.396767	-2.207826
6	-3.168350	2.266203	-2.634381
47	-2.012366	-0.807030	1.145983
8	-4.271222	-1.274772	0.823338
6	-5.095489	-0.627355	0.178124
6	-6.454249	-1.161673	-0.137421
8	-2.583836	1.569164	0.326085
8	-1.054249	3.217396	-0.931645
6	-0.903909	4.064576	0.193523
8	-0.147713	-0.698489	2.530028
8	0.347468	1.788626	1.880319
6	-0.173934	2.266578	3.122259
8	-4.892151	0.577142	-0.291519
1	0.925071	-2.645397	1.359471
1	2.835903	-4.216580	1.225809
1	5.033650	-3.422813	0.370548
1	5.302395	-1.081644	-0.366256
1	5.537595	1.082318	0.077627
1	5.613077	3.449493	-0.677442
1	3.493420	4.552240	-1.447115
1	1.375280	3.201886	-1.424226
1	0.502417	2.048004	3.956146
1	-1.158542	1.826489	3.322915

1	-0.278598	3.351202	3.027764
1	3.203040	-0.140720	4.415257
1	3.575880	-0.993073	2.897978
1	2.062560	-1.353236	3.789775
1	0.051525	3.886347	0.705992
1	-0.925700	5.097728	-0.168905
1	-1.724521	3.924334	0.908396
1	-3.832121	1.698170	-3.293699
1	-3.757925	2.646608	-1.791376
1	-2.755492	3.118365	-3.186703
1	-3.979218	0.944710	-0.037966
1	-7.214847	-0.513889	0.311214
1	-6.616438	-1.146123	-1.220089
1	-6.565387	-2.178779	0.240711
6	-0.750718	-1.408427	-1.837382
6	0.236608	-0.952048	-2.689445
6	1.445203	-1.739186	-2.942451
8	2.362259	-1.339395	-3.654497
6	1.498173	-3.090726	-2.334114
6	0.543977	-3.543836	-1.508863
6	-0.612350	-2.704347	-1.138124
8	-1.416880	-3.072224	-0.282507
1	0.597847	-4.523569	-1.037147
1	2.379823	-3.683337	-2.573253
1	0.078526	-0.076552	-3.316388
1	-1.751517	-0.978390	-1.852709

IRE3_Pd-Ag

Number of imaginary frequencies : 1
The smallest frequency is : -140.9178 cm(-1)

Electronic energy : -2313.0795875
Zero-point correction= 0.492275
Thermal correction to Energy= 0.535409
Thermal correction to Enthalpy= 0.536353
Thermal correction to Gibbs Free Energy= 0.411922
Sum of electronic and zero-point Energies= -2312.587313
Sum of electronic and thermal Energies= -2312.544179
Sum of electronic and thermal Enthalpies= -2312.543234
Sum of electronic and thermal Free Energies= -2312.667665

Cartesian Coordinates

6	2.345772	-0.281211	1.049479
6	2.232540	-1.686093	0.893364
6	2.698609	-2.518915	1.911561
6	3.254317	-1.997112	3.077558
6	3.412523	-0.624643	3.214945
6	2.988695	0.221950	2.192788
6	1.792277	-2.330625	-0.369426
6	2.652974	-3.244841	-0.988370
6	2.283328	-3.834201	-2.186722
6	1.059821	-3.497042	-2.756496
6	0.258006	-2.587874	-2.087652
7	0.607445	-2.023766	-0.920619
47	-1.104544	-0.933446	0.091327
8	-2.515279	-0.159410	-1.876498
6	-2.999518	0.960980	-1.937650
6	-3.381339	1.626554	-3.218526
46	0.754752	1.073228	0.818619
8	-0.798578	0.988417	2.645839
6	-2.011150	0.864062	2.445917
6	-3.009005	1.270486	3.498279
15	2.511871	0.887865	-0.684834
8	3.610425	-0.202650	-1.191062
6	3.978476	-0.197081	-2.565671
8	-0.532862	2.902301	0.271011

6	-0.838938	3.317171	-0.845086
8	-0.382765	2.827031	-1.973905
6	-1.747896	4.488352	-1.031898
8	1.680478	1.250167	-1.909691
8	3.545472	2.084108	-0.279131
6	2.999124	3.381518	-0.069249
8	-2.526413	0.383231	1.357548
8	-3.213743	1.727783	-0.878809
1	3.173928	1.291616	2.273289
1	3.877569	-0.209179	4.106094
1	3.587648	-2.670357	3.863846
1	2.615526	-3.597973	1.788498
1	3.617664	-3.457181	-0.535115
1	2.948240	-4.541001	-2.677231
1	0.729040	-3.926782	-3.697146
1	-0.712140	-2.294996	-2.486920
1	-3.642308	2.076015	3.109816
1	-3.670553	0.427658	3.729005
1	-2.512165	1.608237	4.409966
1	0.353763	2.144844	-1.842785
1	3.838460	4.056014	0.118136
1	2.450660	3.728897	-0.954337
1	2.325098	3.399398	0.799867
1	3.119436	-0.419005	-3.208887
1	4.406669	0.767924	-2.865820
1	4.738444	-0.974153	-2.689324
1	-2.393079	4.349404	-1.903472
1	-1.135581	5.380432	-1.210408
1	-2.350574	4.647631	-0.136330
1	-2.903031	1.273928	-0.050436
1	-4.264198	2.258487	-3.091919
1	-2.545117	2.267140	-3.525834
1	-3.549696	0.881558	-3.998216
8	-2.903041	-2.671023	0.366026
6	-4.093822	-2.408537	0.463529
8	-4.563271	-1.258052	0.911740
6	-5.181021	-3.366024	0.095661
1	-3.812925	-0.647072	1.157007
1	-5.804396	-3.574691	0.971452
1	-5.830814	-2.915493	-0.661843
1	-4.756804	-4.295929	-0.285535

IRE4_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -87.6190 cm(-1)

Electronic energy : -2273.4289189
 Zero-point correction= 0.403880
 Thermal correction to Energy= 0.439510
 Thermal correction to Enthalpy= 0.440454
 Thermal correction to Gibbs Free Energy= 0.332543
 Sum of electronic and zero-point Energies= -2273.025038
 Sum of electronic and thermal Energies= -2272.989409
 Sum of electronic and thermal Enthalpies= -2272.988465
 Sum of electronic and thermal Free Energies= -2273.096376

 Cartesian Coordinates

6	4.827451	1.054846	-0.392772
6	3.519800	0.718150	-0.748503
7	2.519159	1.615436	-0.697528
6	2.782927	2.854249	-0.279498
6	4.056132	3.273545	0.087052
6	5.095579	2.351482	0.024549
6	3.141986	-0.644309	-1.166199
6	4.001871	-1.425140	-1.940780
6	3.619817	-2.695598	-2.365597

6	2.375248	-3.204988	-2.013230
6	1.514696	-2.446249	-1.219467
6	1.880760	-1.165543	-0.800465
46	0.366040	0.287964	-0.618965
15	-1.585064	1.600412	-0.275377
8	-2.705377	1.133985	0.688741
47	-1.799896	-1.265169	0.539355
8	0.197607	-2.048298	1.569199
15	1.089058	-0.856376	1.266778
8	0.767137	0.426330	2.221250
6	0.907633	0.263928	3.635419
8	-3.931070	-1.903436	-0.094742
6	-4.876259	-1.167188	-0.386073
8	-4.885408	0.130049	-0.236690
8	2.584800	-1.115030	1.861553
6	3.236176	-2.366218	1.691424
8	-1.180921	3.131445	0.181434
6	-2.016405	3.919717	1.015695
8	-2.296586	1.842291	-1.746973
6	-3.355234	2.783746	-1.844215
6	-6.149350	-1.705639	-0.952496
1	0.564694	-2.866034	-0.893128
1	2.075313	-4.197556	-2.342067
1	4.297707	-3.285117	-2.978588
1	4.965876	-1.019320	-2.245292
1	5.611293	0.301545	-0.417753
1	6.105058	2.636221	0.311692
1	4.224229	4.295904	0.413371
1	1.933661	3.536640	-0.244399
1	1.959998	0.306925	3.934129
1	0.472260	-0.685105	3.971278
1	0.362027	1.088302	4.101635
1	3.858212	-2.529968	2.576435
1	3.882046	-2.349986	0.803600
1	2.518106	-3.190137	1.609845
1	-1.372858	4.537312	1.651255
1	-2.654533	4.583890	0.416731
1	-2.654395	3.295460	1.651256
1	-3.944990	2.541236	-2.733737
1	-4.022116	2.746258	-0.972010
1	-2.961998	3.803401	-1.952945
1	-4.010636	0.497753	0.137970
1	-6.091163	-2.788082	-1.073378
1	-6.983644	-1.449879	-0.291011
1	-6.349327	-1.233087	-1.919747

IRE5_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -95.0032 cm(-1)

Electronic energy : -2654.6763543
 Zero-point correction= 0.491692
 Thermal correction to Energy= 0.534079
 Thermal correction to Enthalpy= 0.535023
 Thermal correction to Gibbs Free Energy= 0.414956
 Sum of electronic and zero-point Energies= -2654.184663
 Sum of electronic and thermal Energies= -2654.142275
 Sum of electronic and thermal Enthalpies= -2654.141331
 Sum of electronic and thermal Free Energies= -2654.261398

 Cartesian Coordinates

6	1.988535	-0.572356	-1.238670
6	3.206046	0.113705	-1.048144
6	4.126121	0.170635	-2.098703
6	3.851399	-0.440053	-3.319167
6	2.656945	-1.131371	-3.499491

6	1.733317	-1.202268	-2.457660
6	3.475261	0.786254	0.235607
6	4.765883	0.937653	0.749330
6	4.931790	1.571750	1.972165
6	3.812210	2.025234	2.662639
6	2.562351	1.818413	2.092852
7	2.398289	1.228823	0.908337
46	0.353378	0.324655	-0.134168
15	1.168164	-1.830474	0.411641
8	2.672116	-2.413458	0.679159
6	3.374787	-3.144417	-0.314728
15	-1.372141	0.434014	1.532647
8	-2.205271	1.849074	1.424449
6	-3.256594	2.111141	2.340208
47	-1.701179	-1.850101	-0.555064
8	-3.660439	-1.222505	-1.550642
6	-4.535665	-0.512252	-1.048196
6	-5.696284	-0.013263	-1.842087
8	-2.414414	-0.711704	1.560275
8	-0.782033	0.594287	3.058470
6	-1.147653	-0.294703	4.096184
8	0.332343	-2.885557	-0.308461
8	0.775822	-1.766345	2.000850
6	0.634127	-3.011454	2.683365
8	-4.583876	-0.170576	0.212089
1	0.810534	-1.767096	-2.586696
1	2.443036	-1.618099	-4.448846
1	4.572462	-0.371868	-4.130473
1	5.051105	0.731472	-1.972657
1	5.621198	0.540096	0.208747
1	5.927449	1.698745	2.390641
1	3.901641	2.522384	3.624243
1	1.649588	2.134680	2.598279
1	1.470291	-3.688141	2.472435
1	-0.307503	-3.500621	2.401636
1	0.620522	-2.792850	3.754929
1	4.017664	-3.860402	0.206697
1	4.006589	-2.480624	-0.918974
1	2.692585	-3.699748	-0.968706
1	-0.293364	-0.392104	4.775158
1	-2.001081	0.101470	4.665896
1	-1.422128	-1.283087	3.711808
1	-3.985534	2.756272	1.836972
1	-3.770042	1.191966	2.650744
1	-2.875697	2.625146	3.232186
1	-3.751792	-0.435180	0.722834
1	-6.605347	-0.531462	-1.516227
1	-5.837720	1.054492	-1.654820
1	-5.538053	-0.194778	-2.906083
6	-0.927783	1.424427	-1.897199
6	0.351219	1.907383	-1.975904
6	0.718989	3.221018	-1.400465
8	1.854218	3.665438	-1.504091
6	-0.354055	3.988094	-0.736000
6	-1.618689	3.548675	-0.713489
6	-2.015287	2.265784	-1.341784
8	-3.190531	1.958298	-1.472261
1	-2.425539	4.114109	-0.252346
1	-0.060846	4.937767	-0.292788
1	1.104018	1.439974	-2.606551
1	-1.247645	0.549519	-2.463619

IRE6_Pd-Ag

Number of imaginary frequencies : 1
The smallest frequency is : -152.4598 cm(-1)

Electronic energy : -2084.083448

Zero-point correction= 0.429324
 Thermal correction to Energy= 0.466418
 Thermal correction to Enthalpy= 0.467363
 Thermal correction to Gibbs Free Energy= 0.357401
 Sum of electronic and zero-point Energies= -2083.654124
 Sum of electronic and thermal Energies= -2083.617030
 Sum of electronic and thermal Enthalpies= -2083.616085
 Sum of electronic and thermal Free Energies= -2083.726047

.....
 Cartesian Coordinates

6	-2.484199	3.033392	0.337816
6	-1.585853	2.030868	0.712953
7	-0.283421	2.119342	0.390443
6	0.149327	3.169225	-0.326015
6	-0.690070	4.187089	-0.747119
6	-2.034496	4.118027	-0.400200
6	-2.109094	0.855747	1.459242
6	-2.690053	1.079031	2.707303
6	-3.310630	0.045329	3.406080
6	-3.409646	-1.218133	2.835800
6	-2.876512	-1.447142	1.570231
6	-2.182284	-0.437478	0.885255
46	-0.522631	-1.345690	-0.007155
8	1.131052	-1.940587	-1.566142
6	1.712886	-1.015028	-2.130257
6	3.189535	-1.051849	-2.357672
15	-2.317614	-0.472759	-1.205923
8	-1.492415	0.165239	-2.311428
47	1.292758	0.633711	0.915004
8	2.779579	-0.983755	1.206271
6	2.282874	-2.160999	1.344544
6	3.279503	-3.290908	1.388053
8	1.068122	-2.407689	1.415618
8	-3.092960	-1.828755	-1.676067
6	-2.312546	-2.928441	-2.135938
8	-3.650444	0.449857	-1.022401
6	-4.183084	1.067419	-2.189291
8	1.124770	0.073328	-2.568501
1	-3.009684	-2.417986	1.095316
1	-3.916186	-2.022103	3.364930
1	-3.738831	0.238998	4.386801
1	-2.651523	2.079407	3.136910
1	-3.532558	2.930232	0.605277
1	-2.727618	4.896913	-0.708302
1	-0.292741	5.012585	-1.329771
1	1.213467	3.180859	-0.558534
1	3.539771	-3.554680	0.354744
1	4.201053	-2.995614	1.897811
1	2.850566	-4.175436	1.864701
1	0.127612	0.051043	-2.409656
1	-3.008983	-3.655455	-2.561926
1	-1.597698	-2.618919	-2.908101
1	-1.763345	-3.401204	-1.308549
1	-3.467493	1.772509	-2.627694
1	-4.462196	0.323098	-2.946085
1	-5.081454	1.607315	-1.876371
1	3.445186	-1.940425	-2.943756
1	3.680969	-1.156032	-1.382886
1	3.554473	-0.157164	-2.866506
8	3.381906	1.868028	0.035991
6	4.525223	1.445620	-0.074079
8	4.924496	0.265494	0.363884
1	4.154471	-0.249701	0.746414
6	5.626680	2.212735	-0.731366
1	6.481585	2.299688	-0.053161
1	5.971872	1.664789	-1.615411
1	5.280600	3.204313	-1.026333

IRE7_Pd-Ag

Number of imaginary frequencies : 1
The smallest frequency is : -98.5100 cm(-1)

Electronic energy : -2084.0805832
Zero-point correction= 0.428713
Thermal correction to Energy= 0.466411
Thermal correction to Enthalpy= 0.467355
Thermal correction to Gibbs Free Energy= 0.354728
Sum of electronic and zero-point Energies= -2083.651870
Sum of electronic and thermal Energies= -2083.614172
Sum of electronic and thermal Enthalpies= -2083.613228
Sum of electronic and thermal Free Energies= -2083.725855

Cartesian Coordinates

6	-3.874793	2.193153	-0.385958
6	-3.149880	1.004897	-0.288182
6	-1.803138	1.050984	0.153770
6	-1.235935	2.292164	0.488631
6	-1.967811	3.469746	0.355636
6	-3.288559	3.418323	-0.076248
6	-3.786155	-0.281548	-0.633479
7	-3.046946	-1.159805	-1.331467
6	-3.581403	-2.346879	-1.624438
6	-4.869527	-2.717015	-1.256916
6	-5.636069	-1.805812	-0.538477
6	-5.089159	-0.571640	-0.217784
46	-0.524610	-0.220507	-0.881596
8	0.854432	-1.482162	-2.078381
6	2.093383	-1.357769	-2.089913
6	2.924826	-2.336374	-2.873089
15	-1.085311	-0.438789	1.403531
8	-1.003991	-2.054003	1.211928
6	-1.018013	-2.875394	2.384223
47	1.905039	0.096449	0.776300
8	2.209555	2.501534	0.130647
6	1.896144	2.868459	-0.994635
8	1.941330	2.086380	-2.058699
8	0.064896	0.122185	2.219696
8	2.740612	-0.441180	-1.461178
8	4.099884	-0.591610	1.483848
6	5.102850	-0.867353	0.833585
6	6.420314	-1.176326	1.464799
8	-2.436150	-0.470247	2.322355
6	-2.847863	0.687512	3.032644
8	5.142395	-0.920873	-0.480696
6	1.410621	4.243752	-1.312409
1	-0.222434	2.325418	0.884772
1	-1.506999	4.423387	0.605105
1	-3.868422	4.333158	-0.174271
1	-4.903069	2.160499	-0.743283
1	-5.647415	0.152369	0.371646
1	-6.645256	-2.058451	-0.221735
1	-5.257899	-3.694468	-1.529148
1	-2.947995	-3.031520	-2.188071
1	-2.036935	-2.990691	2.767548
1	-0.376552	-2.458847	3.170145
1	-0.627304	-3.852106	2.087487
1	3.607967	-1.800156	-3.539959
1	2.301066	-3.022037	-3.449561
1	3.544650	-2.914410	-2.176876
1	-3.436513	0.348825	3.890208
1	-3.479638	1.330651	2.404366
1	-1.991397	1.264203	3.401652
1	4.243035	-0.719507	-0.876625
1	6.769899	-2.159196	1.132653
1	6.339424	-1.156917	2.552325

1	7.163295	-0.442124	1.135562
1	2.232632	1.171766	-1.797988
1	2.033490	4.693601	-2.092397
1	0.390205	4.181978	-1.708380
1	1.422990	4.867809	-0.417251

IRE8_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -94.9068 cm(-1)

Electronic energy : -1855.0827291
 Zero-point correction= 0.364790
 Thermal correction to Energy= 0.396901
 Thermal correction to Enthalpy= 0.397845
 Thermal correction to Gibbs Free Energy= 0.297027
 Sum of electronic and zero-point Energies= -1854.717939
 Sum of electronic and thermal Energies= -1854.685829
 Sum of electronic and thermal Enthalpies= -1854.684884
 Sum of electronic and thermal Free Energies= -1854.785702

 Cartesian Coordinates

6	4.927480	0.413284	0.166484
6	3.630315	0.556175	-0.335530
7	2.895477	1.657904	-0.109777
6	3.428751	2.637149	0.623105
6	4.712223	2.583218	1.153861
6	5.473923	1.444170	0.917233
6	2.996341	-0.528711	-1.110797
6	3.738976	-1.246701	-2.049822
6	3.158503	-2.273600	-2.790331
6	1.824771	-2.611112	-2.589238
6	1.073117	-1.921839	-1.640884
6	1.636282	-0.866310	-0.907693
46	0.370647	0.746564	-0.610584
47	-2.075629	-0.628097	0.171707
8	-2.941162	1.266802	-0.809225
6	-2.273910	2.349037	-0.855765
6	-3.062805	3.606372	-1.117551
15	0.837946	-0.838920	1.046755
8	-0.325303	-1.819418	1.096406
8	-1.032764	2.440383	-0.718343
8	2.161563	-1.542760	1.691302
6	2.573863	-2.836240	1.275840
8	0.729673	0.329112	2.176852
6	0.653467	-0.063359	3.551273
8	-4.411464	-1.209224	0.451565
6	-5.424045	-0.557831	0.211413
8	-5.426618	0.633833	-0.342239
6	-6.796624	-1.050594	0.535963
1	0.047416	-2.222546	-1.437512
1	1.368821	-3.416729	-3.160148
1	3.753468	-2.809868	-3.525941
1	4.778326	-0.973859	-2.226833
1	5.481992	-0.506112	-0.007801
1	6.478736	1.354500	1.323383
1	5.100232	3.413453	1.737324
1	2.798910	3.511446	0.786044
1	-3.477323	3.564973	-2.131227
1	-3.910165	3.667752	-0.426138
1	-2.442314	4.499536	-1.021741
1	-4.490244	0.939089	-0.545766
1	-7.424398	-1.027630	-0.360448
1	-6.755671	-2.063894	0.937710
1	-7.259134	-0.381580	1.269687
1	0.277529	0.801431	4.103736
1	-0.039059	-0.902813	3.687339

1	1.640976	-0.340785	3.933922
1	3.103422	-3.292648	2.117254
1	1.719666	-3.471782	1.014068
1	3.260925	-2.773351	0.420909

IRE9_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -85.6847 cm(-1)

Electronic energy : -2273.4247924
 Zero-point correction= 0.406003
 Thermal correction to Energy= 0.441003
 Thermal correction to Enthalpy= 0.441947
 Thermal correction to Gibbs Free Energy= 0.336551
 Sum of electronic and zero-point Energies= -2273.018789
 Sum of electronic and thermal Energies= -2272.983789
 Sum of electronic and thermal Enthalpies= -2272.982845
 Sum of electronic and thermal Free Energies= -2273.088242

 Cartesian Coordinates

6	1.783202	0.069691	1.197057
6	3.167146	-0.176645	1.008434
6	4.008097	-0.198274	2.121038
6	3.502716	-0.003134	3.404491
6	2.144804	0.231217	3.595584
6	1.291943	0.283825	2.497025
6	3.711391	-0.397387	-0.344870
6	4.920655	0.183309	-0.737320
6	5.380477	-0.034412	-2.028202
6	4.620255	-0.815298	-2.892204
6	3.424462	-1.344019	-2.421264
7	2.976631	-1.151961	-1.179051
46	0.562379	-1.208812	0.092833
15	0.744332	1.126929	-0.171876
8	0.450043	0.920204	-1.761126
6	0.078667	2.059371	-2.542161
47	-2.374668	0.311859	-0.000177
8	-3.478533	2.363265	-0.253752
6	-3.118727	3.535503	-0.172765
6	-4.043984	4.680707	-0.411159
8	-0.451635	1.767963	0.535302
8	1.894676	2.268713	-0.389755
6	2.354733	3.042003	0.708809
8	-1.899319	3.911205	0.139756
1	0.240754	0.533803	2.625837
1	1.749164	0.384703	4.596898
1	4.175655	-0.037604	4.258029
1	5.068131	-0.405967	1.982260
1	5.472588	0.814826	-0.044691
1	6.316728	0.408130	-2.360107
1	4.943477	-1.013429	-3.910315
1	2.797771	-1.959795	-3.065753
1	-1.314415	3.111209	0.298498
1	-5.013480	4.324826	-0.761767
1	-4.173669	5.238430	0.522769
1	-3.608286	5.370859	-1.140235
1	-0.373018	1.676057	-3.460461
1	-0.658680	2.682712	-2.019146
1	0.954804	2.667320	-2.789497
1	2.755389	3.974626	0.301538
1	1.542530	3.285082	1.404886
1	3.156186	2.523406	1.252865
15	-2.336094	-2.102982	-0.172453
8	-0.971864	-2.649337	-0.614320
8	-3.507911	-2.774716	-1.087377
8	-2.746424	-2.821501	1.259090

6	-3.505505	-4.189236	-1.260602
6	-1.990632	-2.444890	2.389595
1	-4.252304	-4.424779	-2.023762
1	-2.526245	-4.547977	-1.599095
1	-3.773899	-4.700689	-0.328376
1	-2.484907	-2.850922	3.277670
1	-0.963322	-2.835863	2.349864
1	-1.941455	-1.346823	2.496943

IRE10_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -94.1850 cm(-1)

Electronic energy : -2008.5457912
 Zero-point correction= 0.410713
 Thermal correction to Energy= 0.445417
 Thermal correction to Enthalpy= 0.446361
 Thermal correction to Gibbs Free Energy= 0.338916
 Sum of electronic and zero-point Energies= -2008.135078
 Sum of electronic and thermal Energies= -2008.100374
 Sum of electronic and thermal Enthalpies= -2008.099430
 Sum of electronic and thermal Free Energies= -2008.206876

 Cartesian Coordinates

6	1.628268	0.094333	1.153241
1	0.500477	1.767192	1.912000
6	1.218356	0.986788	2.157595
6	1.757110	0.912860	3.439087
1	1.420575	1.603043	4.209196
6	2.735144	-0.034510	3.723846
1	3.164948	-0.092459	4.721069
6	3.163637	-0.918667	2.736014
1	3.906353	-1.678770	2.974057
6	2.615995	-0.877211	1.454251
6	3.039930	-1.841309	0.422782
6	4.382475	-2.193107	0.261540
1	5.142114	-1.752075	0.903152
6	4.725213	-3.079488	-0.749698
1	5.763618	-3.365086	-0.900477
6	3.724890	-3.582709	-1.574780
1	3.950284	-4.277956	-2.378484
6	2.416017	-3.174914	-1.347338
1	1.601682	-3.544470	-1.969641
7	2.071826	-2.333274	-0.370291
46	0.066142	-0.685987	-0.000937
15	1.567577	0.996569	-0.686245
8	3.186866	1.213910	-0.762082
6	3.856063	1.984537	0.223140
1	4.787259	2.342908	-0.224977
1	4.102438	1.375028	1.103674
1	3.261206	2.852202	0.534499
8	1.435628	0.395572	-2.193004
6	2.013781	1.120890	-3.283141
1	3.091635	0.940504	-3.343502
1	1.827383	2.197584	-3.191563
1	1.530835	0.753892	-4.192426
8	0.884947	2.345115	-0.560512
47	-1.741825	1.310164	-0.713892
8	-2.339126	3.445757	-0.285485
6	-1.717638	4.315825	0.327261
6	-2.375900	5.558816	0.820874
1	-1.953511	6.423100	0.297080
1	-3.452415	5.517213	0.651541
1	-2.165480	5.694097	1.886453
8	-0.439040	4.259805	0.600918
1	0.016474	3.474570	0.172183

8	-1.851174	-0.900294	-1.171293
6	-2.774375	-1.601324	-0.514829
6	-3.799057	-2.261526	-1.217097
6	-4.756890	-3.024075	-0.555277
6	-4.727795	-3.151231	0.832707
6	-3.725019	-2.503604	1.551541
6	-2.770907	-1.741279	0.887187
8	-5.645147	-3.885681	1.528788
1	-1.989190	-1.224048	1.454795
1	-3.705881	-2.602082	2.635454
1	-5.538049	-3.528641	-1.126073
1	-3.824163	-2.170973	-2.301874
1	-6.271222	-4.270726	0.903524

IRE11_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -99.0183 cm(-1)

Electronic energy : -1898.8881472
 Zero-point correction= 0.465265
 Thermal correction to Energy= 0.500796
 Thermal correction to Enthalpy= 0.501740
 Thermal correction to Gibbs Free Energy= 0.393723
 Sum of electronic and zero-point Energies= -1898.422882
 Sum of electronic and thermal Energies= -1898.387352
 Sum of electronic and thermal Enthalpies= -1898.386407
 Sum of electronic and thermal Free Energies= -1898.494424

 Cartesian Coordinates

6	-1.220460	-1.041882	0.956239
6	-0.421475	-1.818333	1.813960
1	0.602970	-2.044050	1.523414
6	-0.938207	-2.336791	2.997904
1	-0.301143	-2.922376	3.656838
6	-2.272859	-2.118204	3.323851
1	-2.685139	-2.528668	4.242716
6	-3.085580	-1.364971	2.478700
1	-4.120780	-1.168484	2.754809
6	-2.576343	-0.810645	1.305004
6	-3.422648	0.035422	0.443591
6	-4.738049	-0.320626	0.134968
1	-5.159886	-1.241975	0.530146
6	-5.473594	0.500740	-0.707908
1	-6.497536	0.243298	-0.968575
6	-4.877330	1.646168	-1.225261
1	-5.417650	2.315237	-1.889131
6	-3.562544	1.921565	-0.869062
1	-3.055606	2.807987	-1.251102
7	-2.849599	1.148214	-0.048118
46	-0.261066	0.684726	0.254808
15	-0.663439	-1.282243	-0.977771
8	-1.875969	-2.336035	-1.315074
6	-1.964842	-3.564305	-0.614815
1	-2.565660	-4.243479	-1.226971
1	-2.464542	-3.435251	0.355498
1	-0.977062	-4.016613	-0.458686
8	-0.945466	-0.340245	-2.272893
6	-1.053077	-0.945492	-3.564616
1	-2.050594	-1.370809	-3.714607
1	-0.298607	-1.728364	-3.706761
1	-0.880962	-0.151297	-4.295786
8	0.659539	-2.018816	-1.076566
47	2.447993	0.221186	-0.467264
8	3.946935	-1.427620	-0.259444
6	3.781573	-2.599932	0.085905
6	4.909033	-3.444251	0.574718

1	5.062627	-4.279562	-0.116868
1	5.824564	-2.856857	0.652629
1	4.653516	-3.874362	1.548326
8	2.635727	-3.228026	0.058167
1	1.893535	-2.686767	-0.358931
8	1.295732	2.059881	-0.538925
6	1.620698	3.121224	0.319613
6	2.924858	3.752762	-0.162070
6	0.457824	4.125092	0.225290
6	1.793947	2.637175	1.758404
1	2.083127	3.439805	2.450514
1	0.856916	2.187686	2.127682
1	2.577536	1.864965	1.796659
1	3.249848	4.593700	0.464806
1	3.724540	2.997576	-0.149888
1	2.815452	4.111454	-1.193712
6	0.556238	5.376477	1.082444
1	0.362100	4.403351	-0.835070
1	-0.461972	3.570355	0.479493
1	-0.303851	6.035129	0.911928
1	0.573573	5.140541	2.154086
1	1.457870	5.960576	0.856900

Monometallic Reductive Elimination (Pd)

IRE1_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -81.1109 cm(-1)

Electronic energy : -1633.1243536
 Zero-point correction= 0.337300
 Thermal correction to Energy= 0.362971
 Thermal correction to Enthalpy= 0.363915
 Thermal correction to Gibbs Free Energy= 0.281319
 Sum of electronic and zero-point Energies= -1632.787054
 Sum of electronic and thermal Energies= -1632.761383
 Sum of electronic and thermal Enthalpies= -1632.760439
 Sum of electronic and thermal Free Energies= -1632.843034

 Cartesian Coordinates

6	-2.286206	-0.313985	2.713790
6	-1.725059	-0.041332	1.463680
6	-0.553665	-0.726306	1.080369
6	0.039819	-1.638381	1.944749
6	-0.526465	-1.887098	3.195581
6	-1.694773	-1.234524	3.572197
6	-2.273275	0.997381	0.578964
6	-3.590502	1.454548	0.628840
6	-3.990861	2.457894	-0.242108
6	-3.077696	2.983691	-1.150506
6	-1.787623	2.473149	-1.152183
7	-1.399319	1.513212	-0.309538
46	0.539972	0.349239	-0.332101
15	-0.342476	-1.626405	-1.174883
8	-0.016092	-1.353683	-2.609868
8	-1.915598	-1.894446	-0.942243
6	-2.594068	-2.627255	-1.969342
8	0.283237	-3.024860	-0.658304
6	1.639081	-3.325256	-0.997207
1	-2.124238	-3.604412	-2.133680
1	-3.617112	-2.777958	-1.617666
1	-2.607472	-2.065771	-2.908758
1	1.804241	-3.229446	-2.076206
1	2.339955	-2.674423	-0.456354
1	1.814035	-4.361224	-0.696609
1	0.937795	-2.173217	1.642580
1	-0.053628	-2.598396	3.869213

1	-2.141282	-1.428769	4.544445
1	-3.174086	0.227456	3.035926
1	-4.296271	1.016286	1.329115
1	-5.014354	2.823600	-0.216527
1	-3.354581	3.770798	-1.845087
1	-1.030554	2.843759	-1.842073
6	2.678446	0.218139	-0.819720
6	2.240286	1.516077	-1.122329
6	2.361397	2.609580	-0.143490
6	3.277172	-0.091127	0.493167
8	3.747887	-1.191810	0.763948
8	2.063459	3.769276	-0.405969
6	3.295916	1.004516	1.492786
6	2.874188	2.243942	1.201576
1	2.912828	3.051818	1.930411
1	3.696719	0.744774	2.471018
1	2.834092	-0.517557	-1.607839
1	2.027732	1.813564	-2.148661

IRE2_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -121.5073 cm(-1)

Electronic energy : -1899.2105614
 Zero-point correction= 0.352537
 Thermal correction to Energy= 0.380262
 Thermal correction to Enthalpy= 0.381206
 Thermal correction to Gibbs Free Energy= 0.293166
 Sum of electronic and zero-point Energies= -1898.858025
 Sum of electronic and thermal Energies= -1898.830300
 Sum of electronic and thermal Enthalpies= -1898.829356
 Sum of electronic and thermal Free Energies= -1898.917395

 Cartesian Coordinates

6	1.588012	-0.876104	-0.691037
6	2.577415	0.124829	-0.826763
6	3.757866	-0.172043	-1.507703
6	3.955192	-1.428458	-2.075032
6	2.973631	-2.405873	-1.963264
6	1.801465	-2.134969	-1.258176
6	2.333452	1.480385	-0.300743
7	1.073649	1.937933	-0.418314
6	0.780900	3.148996	0.059053
6	1.722600	3.976348	0.657876
6	3.027700	3.509127	0.773792
6	3.340048	2.244409	0.294399
46	-0.383382	-0.128826	-0.791664
15	0.447569	-1.058632	1.186764
8	1.920603	-1.028083	1.867581
6	1.978981	-1.153556	3.289085
15	-2.642577	0.237406	-0.365204
8	-3.331869	1.635250	-0.854751
6	-4.152133	2.441294	-0.016121
8	-3.691018	-0.889362	-0.901165
6	-5.080952	-0.777143	-0.611589
8	-2.900939	0.278214	1.225610
8	0.170168	-2.663499	1.207046
6	-1.153367	-3.107323	0.932613
8	-0.493741	-0.341652	2.139975
1	1.486737	-2.073361	3.627794
1	3.038242	-1.199068	3.554562
1	1.514706	-0.294041	3.782793
1	-1.874203	-2.672299	1.636488
1	-1.455118	-2.848610	-0.093044
1	-1.154889	-4.194700	1.042854
1	1.062585	-2.921229	-1.118435
1	3.122475	-3.386655	-2.409653

1	4.876022	-1.637726	-2.614709
1	4.512831	0.603452	-1.631085
1	4.343118	1.838237	0.398980
1	3.793830	4.120331	1.245024
1	1.437411	4.958992	1.022595
1	-0.255748	3.468416	-0.053425
1	-2.037677	0.059134	1.678881
1	-4.435308	3.320071	-0.602191
1	-5.064563	1.920284	0.299042
1	-3.610056	2.767529	0.878229
1	-5.559006	-1.703440	-0.941054
1	-5.257581	-0.654225	0.464249
1	-5.529138	0.061274	-1.159269

IRE3_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -63.9633 cm(-1)

Electronic energy : -1633.1208044
 Zero-point correction= 0.336994
 Thermal correction to Energy= 0.362746
 Thermal correction to Enthalpy= 0.363690
 Thermal correction to Gibbs Free Energy= 0.281191
 Sum of electronic and zero-point Energies= -1632.783811
 Sum of electronic and thermal Energies= -1632.758059
 Sum of electronic and thermal Enthalpies= -1632.757115
 Sum of electronic and thermal Free Energies= -1632.839614

 Cartesian Coordinates

6	3.675130	-0.675302	-1.178782
6	2.479230	-0.187212	-0.644980
6	1.312839	-0.971904	-0.753642
6	1.357723	-2.200050	-1.404069
6	2.555998	-2.662862	-1.947768
6	3.715925	-1.906879	-1.822415
6	2.392552	1.155245	-0.054582
6	3.471901	1.829642	0.516393
6	3.274967	3.103654	1.030169
6	2.010046	3.679536	0.969831
6	0.979892	2.945330	0.398185
7	1.170366	1.722627	-0.101199
46	-0.416507	0.178588	-0.665912
15	-0.176552	-1.243668	1.171751
8	-1.342263	-0.749000	1.970109
8	1.219898	-1.105874	1.969617
6	1.180328	-1.385304	3.372996
8	-0.234488	-2.846679	0.947421
6	-1.470737	-3.405209	0.504745
1	0.816334	-2.402439	3.561907
1	2.206720	-1.300368	3.736914
1	0.543595	-0.667448	3.899725
1	-2.242335	-3.310896	1.276257
1	-1.831060	-2.916488	-0.410246
1	-1.282751	-4.461864	0.297201
1	0.464057	-2.815268	-1.473757
1	2.578969	-3.622243	-2.460037
1	4.652892	-2.267818	-2.239675
1	4.575371	-0.065070	-1.125702
1	4.445764	1.351196	0.575268
1	4.103925	3.641721	1.483445
1	1.819588	4.675256	1.358771
1	-0.031940	3.346487	0.320675
6	-2.083573	1.229743	-1.601853
6	-2.497027	-0.098563	-1.449183
6	-3.418027	-0.467635	-0.352968
6	-2.482642	2.273825	-0.640871

8	-2.121056	3.441498	-0.761383
8	-3.934137	-1.575320	-0.283226
6	-3.337578	1.853775	0.490371
6	-3.753104	0.588777	0.631516
1	-4.379585	0.273316	1.462990
1	-3.604046	2.633612	1.201299
1	-1.662686	1.586257	-2.543262
1	-2.444465	-0.804993	-2.276570

IRE4_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -49.9671 cm(-1)

Electronic energy : -1709.8545766
 Zero-point correction= 0.376077
 Thermal correction to Energy= 0.405852
 Thermal correction to Enthalpy= 0.406796
 Thermal correction to Gibbs Free Energy= 0.312085
 Sum of electronic and zero-point Energies= -1709.478500
 Sum of electronic and thermal Energies= -1709.448725
 Sum of electronic and thermal Enthalpies= -1709.447781
 Sum of electronic and thermal Free Energies= -1709.542491

 Cartesian Coordinates

6	1.042072	0.673892	-1.145685
6	1.791673	1.503534	-0.271242
6	2.059808	2.813796	-0.664577
6	1.603430	3.307186	-1.884833
6	0.879678	2.495628	-2.748388
6	0.604298	1.180865	-2.380128
6	2.286278	0.986383	1.024723
7	1.647742	-0.083506	1.517479
6	2.059115	-0.624046	2.660380
6	3.122846	-0.114185	3.398223
6	3.793847	0.991840	2.891096
6	3.382572	1.546865	1.685998
46	-0.785694	0.073620	-0.231861
8	-2.639631	-0.925625	0.399190
6	-2.690942	-2.072360	0.965267
6	-4.031725	-2.444034	1.546911
15	0.917249	-1.289490	-0.918957
8	2.526993	-1.413239	-0.985358
6	3.177409	-2.653377	-0.732335
8	-1.976896	2.116775	0.308711
6	-3.158199	2.263187	0.599586
8	-4.009564	1.271124	0.758587
6	-3.785412	3.603757	0.807138
8	0.529985	-1.816955	-2.408981
6	-0.797007	-2.287697	-2.629214
8	0.617750	-2.531982	0.047456
8	-1.737972	-2.866206	1.055430
1	-4.340964	-1.686254	2.276162
1	-3.997752	-3.422577	2.030266
1	-4.789167	-2.452884	0.755261
1	-0.314901	-2.565847	0.441008
1	2.732046	-3.473784	-1.309291
1	4.218487	-2.527603	-1.040202
1	3.141484	-2.905326	0.333663
1	-1.052801	-3.096359	-1.933243
1	-1.533135	-1.478372	-2.521531
1	-0.832384	-2.671436	-3.651715
1	0.069930	0.526904	-3.065393
1	0.528919	2.879140	-3.703398
1	1.815071	4.339071	-2.155736
1	2.603750	3.477373	0.003799
1	3.924045	2.386363	1.258566

1	4.642221	1.415908	3.423106
1	3.416636	-0.576733	4.336116
1	1.509029	-1.501848	3.001532
1	-3.544122	0.390844	0.625272
1	-4.204833	3.664570	1.816834
1	-3.050409	4.396965	0.663129
1	-4.615900	3.735720	0.105597

IRE5_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -134.8069 cm(-1)

Electronic energy : -1480.8606674
 Zero-point correction= 0.312870
 Thermal correction to Energy= 0.337089
 Thermal correction to Enthalpy= 0.338033
 Thermal correction to Gibbs Free Energy= 0.256945
 Sum of electronic and zero-point Energies= -1480.547798
 Sum of electronic and thermal Energies= -1480.523579
 Sum of electronic and thermal Enthalpies= -1480.522634
 Sum of electronic and thermal Free Energies= -1480.603723

 Cartesian Coordinates

6	3.221381	1.832227	0.288143
6	2.130464	1.202745	-0.319385
7	0.981116	1.856666	-0.565338
6	0.887334	3.138253	-0.205121
6	1.923436	3.841559	0.396679
6	3.114950	3.168684	0.644878
6	2.181478	-0.223937	-0.694335
6	1.047360	-1.055584	-0.519151
6	1.125145	-2.405016	-0.892486
6	2.287179	-2.922952	-1.459004
6	3.399439	-2.104899	-1.621510
6	3.346637	-0.768328	-1.234365
46	-0.749750	-0.140298	-0.994175
8	-2.852564	0.511411	-1.355699
6	-3.653259	0.903673	-0.505648
8	-3.405909	0.996393	0.774727
15	-0.206983	-0.769139	1.173668
8	1.144819	-0.820683	2.068906
6	0.998243	-0.663026	3.480630
8	-0.773214	-2.274668	1.440025
6	-2.127861	-2.523318	1.084033
8	-1.128281	0.261764	1.812510
6	-5.038806	1.326843	-0.867989
1	-5.215240	2.351063	-0.523792
1	-5.764981	0.686689	-0.355962
1	-5.189943	1.266472	-1.946455
1	-2.476023	0.705764	1.050471
1	0.322816	-1.419655	3.898483
1	1.992163	-0.796865	3.915074
1	0.620857	0.333639	3.730712
1	-2.813545	-1.914290	1.686204
1	-2.305773	-2.313669	0.016967
1	-2.322033	-3.581714	1.275267
1	0.277705	-3.060218	-0.703208
1	2.325890	-3.968109	-1.757936
1	4.313557	-2.504597	-2.054605
1	4.212859	-0.126649	-1.389645
1	4.126731	1.268961	0.500409
1	3.949181	3.676388	1.123349
1	1.796250	4.887444	0.661536
1	-0.062582	3.628174	-0.418450

IRE6_Pd

Number of imaginary frequencies : 1
The smallest frequency is : -87.9333 cm(-1)

Electronic energy : -1633.1090467
Zero-point correction= 0.336594
Thermal correction to Energy= 0.362522
Thermal correction to Enthalpy= 0.363467
Thermal correction to Gibbs Free Energy= 0.279842
Sum of electronic and zero-point Energies= -1632.772453
Sum of electronic and thermal Energies= -1632.746524
Sum of electronic and thermal Enthalpies= -1632.745580
Sum of electronic and thermal Free Energies= -1632.829205

Cartesian Coordinates

6	-2.364690	2.683652	-0.923533
6	-1.893045	1.410587	-0.596342
6	-0.513935	1.234502	-0.358176
6	0.355718	2.315974	-0.448193
6	-0.133024	3.579469	-0.780782
6	-1.491159	3.762211	-1.014329
6	-2.791642	0.247797	-0.526315
6	-4.155423	0.344445	-0.241204
6	-4.914703	-0.815058	-0.173663
6	-4.302245	-2.047695	-0.377572
6	-2.940531	-2.067000	-0.646238
7	-2.209958	-0.951983	-0.727681
46	0.102350	-0.706670	-0.776554
15	0.055379	-0.157611	1.476705
8	0.167702	-1.563755	1.976608
8	1.293274	-2.053883	-1.940832
8	-1.163934	0.601386	2.227496
6	-2.171724	-0.179335	2.870851
8	1.323411	0.774445	1.811104
6	1.987735	0.546656	3.058233
1	-1.784237	-0.649369	3.780940
1	-2.979059	0.510572	3.130204
1	-2.567014	-0.961147	2.210642
1	2.322354	-0.492668	3.141572
1	2.853604	1.212407	3.077923
1	1.326882	0.786038	3.900984
1	1.414128	2.179308	-0.239189
1	0.554180	4.419603	-0.852665
1	-1.873410	4.745444	-1.277910
1	-3.421268	2.826199	-1.143570
1	-4.607693	1.314258	-0.051371
1	-5.977258	-0.758136	0.049663
1	-4.862641	-2.976381	-0.328050
1	-2.408253	-3.002464	-0.810662
6	2.156117	-1.310638	-1.350124
6	2.687264	-0.104050	-1.992386
6	3.680059	0.609284	-1.425408
6	4.290194	0.205685	-0.150509
6	3.814080	-1.055413	0.437621
6	2.812436	-1.761425	-0.117273
1	2.233608	0.182878	-2.940827
1	4.068095	1.517381	-1.882199
8	5.158084	0.884848	0.395042
1	4.302368	-1.375177	1.356328
1	2.439342	-2.686080	0.319549

IRE7_Pd

Number of imaginary frequencies : 1
The smallest frequency is : -78.3227 cm(-1)

Electronic energy : -1633.1040227
 Zero-point correction= 0.335864
 Thermal correction to Energy= 0.362212
 Thermal correction to Enthalpy= 0.363156
 Thermal correction to Gibbs Free Energy= 0.277401
 Sum of electronic and zero-point Energies= -1632.768159
 Sum of electronic and thermal Energies= -1632.741811
 Sum of electronic and thermal Enthalpies= -1632.740867
 Sum of electronic and thermal Free Energies= -1632.826622

 Cartesian Coordinates

7	-0.501788	1.559288	0.276425
6	0.584481	2.305537	-0.010860
6	-1.489767	2.058574	1.018340
6	-1.460712	3.354226	1.513496
6	-0.345989	4.137486	1.231261
6	0.686840	3.612533	0.467272
6	1.601639	1.643303	-0.841072
6	1.601364	0.237328	-0.940785
6	2.504772	-0.409853	-1.774344
6	3.418003	0.333496	-2.522940
6	3.436555	1.720222	-2.421717
6	2.531734	2.370140	-1.589985
46	-0.218757	-0.576504	-0.359650
15	1.436360	-1.164160	1.130259
8	2.436985	-0.022800	1.666121
6	2.970195	-0.206280	2.984023
8	-1.175219	-2.440614	-1.033588
6	-2.133716	-1.638103	-0.767935
8	2.486469	-2.271186	0.594015
6	1.941478	-3.535163	0.208369
8	0.528398	-1.695551	2.194779
1	3.531881	-1.145491	3.053390
1	3.648767	0.630184	3.164056
1	2.173734	-0.200775	3.734737
1	1.096701	-3.411604	-0.483027
1	2.740736	-4.085491	-0.293769
1	1.603491	-4.095804	1.086499
1	2.514846	-1.496263	-1.832484
1	4.120087	-0.177675	-3.178189
1	4.149207	2.301455	-3.001900
1	2.527344	3.458086	-1.551628
1	1.574238	4.203654	0.258818
1	-0.277300	5.153389	1.612305
1	-2.287447	3.731872	2.107225
1	-2.331249	1.390392	1.213078
6	-2.753538	-0.817339	-1.812254
6	-3.830487	-0.050079	-1.549812
6	-4.443512	-0.004364	-0.213853
6	-3.813532	-0.832181	0.825404
6	-2.737023	-1.603767	0.564998
1	-2.305836	-0.869301	-2.804178
1	-4.298434	0.562416	-2.317793
8	-5.429806	0.691838	0.021853
1	-4.269069	-0.800561	1.813170
1	-2.269060	-2.229706	1.323653

IRE8_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -141.0057 cm(-1)

Electronic energy : -1524.6838145
 Zero-point correction= 0.414817
 Thermal correction to Energy= 0.442750
 Thermal correction to Enthalpy= 0.443694

Thermal correction to Gibbs Free Energy= 0.354167
 Sum of electronic and zero-point Energies= -1524.268998
 Sum of electronic and thermal Energies= -1524.241064
 Sum of electronic and thermal Enthalpies= -1524.240120
 Sum of electronic and thermal Free Energies= -1524.329647

 Cartesian Coordinates

6	-1.163411	1.238235	-0.388251
6	-2.404504	0.676497	-0.781186
6	-3.347280	1.479011	-1.425321
6	-3.068673	2.810289	-1.721898
6	-1.839693	3.359322	-1.371686
6	-0.901740	2.582810	-0.696956
6	-2.691045	-0.754482	-0.557308
7	-1.679836	-1.617251	-0.764775
6	-1.896964	-2.919227	-0.556930
6	-3.122468	-3.434257	-0.153475
6	-4.170499	-2.543382	0.056909
6	-3.954380	-1.187691	-0.142311
46	0.423935	-0.028421	-0.877925
15	-0.167777	0.486289	1.307777
8	-1.591861	0.122977	2.021924
6	-1.703701	-1.059443	2.803629
8	2.409675	-1.162721	-0.348909
6	3.645380	-0.444887	-0.534467
6	3.769097	-0.234720	-2.030745
6	3.576290	0.886153	0.196720
6	4.760313	-1.338453	0.015617
6	6.168844	-0.777430	-0.086742
8	0.156433	1.985014	1.853478
6	0.651913	2.085713	3.184375
8	0.866025	-0.476146	1.871147
1	-1.032236	-1.042596	3.669559
1	-2.739718	-1.107755	3.152148
1	-1.483427	-1.956161	2.210487
1	-0.038490	1.621165	3.901483
1	1.636551	1.615667	3.282701
1	0.731245	3.151244	3.415450
1	0.031121	3.030603	-0.363413
1	-1.614968	4.397163	-1.608297
1	-3.810795	3.414372	-2.239062
1	-4.293878	1.041362	-1.739973
1	-4.743058	-0.462927	0.044116
1	-5.144583	-2.900987	0.382682
1	-3.248768	-4.503854	-0.011428
1	-1.048473	-3.579583	-0.734167
1	4.524970	-1.549560	1.070557
1	4.699727	-2.300259	-0.514034
1	4.670082	0.335322	-2.283761
1	3.808071	-1.197369	-2.555631
1	2.898957	0.326023	-2.401358
1	4.469342	1.493077	0.007154
1	2.697603	1.455733	-0.139887
1	3.486859	0.732951	1.280763
1	6.899424	-1.494497	0.304414
1	6.450325	-0.562538	-1.125145
1	6.284463	0.148504	0.489832
1	2.117119	-1.068645	0.585174

IRE9_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -149.5259 cm(-1)

Electronic energy : -1634.3350366
 Zero-point correction= 0.359328
 Thermal correction to Energy= 0.386352

Thermal correction to Enthalpy= 0.387296
 Thermal correction to Gibbs Free Energy= 0.300716
 Sum of electronic and zero-point Energies= -1633.975709
 Sum of electronic and thermal Energies= -1633.948684
 Sum of electronic and thermal Enthalpies= -1633.947740
 Sum of electronic and thermal Free Energies= -1634.034321

 Cartesian Coordinates

7	-0.446602	1.896161	0.461518
6	-0.176922	3.106871	-0.036657
1	0.862779	3.281401	-0.319364
6	-1.140744	4.094556	-0.190642
1	-0.869896	5.069200	-0.586745
6	-2.450147	3.797373	0.177547
1	-3.238107	4.538391	0.063986
6	-2.743557	2.537917	0.679957
1	-3.761813	2.266235	0.947341
6	-1.712768	1.603557	0.813619
6	-1.934798	0.252111	1.360023
6	-2.784086	0.076823	2.456646
1	-3.327721	0.934101	2.851845
6	-2.887560	-1.156697	3.089008
1	-3.540852	-1.269180	3.951231
6	-2.136975	-2.236565	2.632164
1	-2.202738	-3.200650	3.132068
6	-1.321527	-2.089167	1.515190
1	-0.793349	-2.953106	1.117053
6	-1.211466	-0.855842	0.859347
46	0.664155	-0.300493	0.128789
15	-0.982659	-1.123471	-1.323904
8	-1.927723	0.131214	-1.775285
6	-1.381077	1.080303	-2.679714
1	-2.086865	1.914525	-2.735631
1	-0.409988	1.463077	-2.335178
1	-1.253380	0.647163	-3.678722
8	-2.121432	-2.280667	-1.155336
6	-2.597624	-2.857494	-2.368864
1	-3.410371	-3.537099	-2.098599
1	-1.808269	-3.417173	-2.881851
1	-2.990467	-2.089700	-3.048394
8	-0.045987	-1.515747	-2.433645
6	2.695112	0.368735	-0.999320
6	2.758850	-0.992723	-0.643098
6	3.326252	1.336711	-0.196526
8	3.263641	2.627618	-0.621748
6	3.977781	0.949976	0.964233
6	4.013033	-0.398058	1.339547
6	3.421884	-1.368670	0.544487
8	3.510684	-2.665991	0.932715
1	2.281485	0.664837	-1.962007
1	2.412630	-1.749466	-1.346642
1	4.521897	-0.703481	2.250809
1	4.464337	1.697608	1.590044
1	3.724138	3.191600	0.013789
1	3.026075	-3.216374	0.303323

IRE10_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -146.7751 cm(-1)

Electronic energy : -1899.1867833
 Zero-point correction= 0.351035
 Thermal correction to Energy= 0.379224
 Thermal correction to Enthalpy= 0.380169
 Thermal correction to Gibbs Free Energy= 0.289813
 Sum of electronic and zero-point Energies= -1898.835748

Sum of electronic and thermal Energies= -1898.807559
 Sum of electronic and thermal Enthalpies= -1898.806615
 Sum of electronic and thermal Free Energies= -1898.896970

 Cartesian Coordinates

7	0.543559	2.036785	-0.226784
6	1.863471	1.851862	-0.048091
6	2.634068	2.739854	0.710480
6	2.022179	3.842522	1.288414
6	0.656579	4.030810	1.104935
6	-0.034054	3.096069	0.344110
6	2.477105	0.659215	-0.669579
6	3.731809	0.764725	-1.271006
6	4.329293	-0.333551	-1.883858
6	3.683667	-1.564583	-1.887750
6	2.445584	-1.697628	-1.264094
6	1.815558	-0.595693	-0.665829
46	-0.202451	-0.456158	-1.052293
8	-2.461847	-0.247317	-1.290423
15	-3.030292	0.437072	-0.083411
8	-3.952278	-0.511877	0.808934
6	-3.554995	-1.876178	1.024043
15	0.643235	-1.138828	1.028068
8	0.837620	-2.761591	1.014367
6	-0.239877	-3.544247	0.524494
8	-0.606852	-0.739647	1.775042
8	1.939681	-0.736738	1.929579
6	1.800426	-0.869155	3.342360
8	-4.003326	1.659763	-0.397951
6	-5.101255	1.448481	-1.295719
1	1.559661	-1.901995	3.624731
1	2.764906	-0.599050	3.780583
1	1.024120	-0.201568	3.730949
1	-1.057664	-3.595608	1.254860
1	-0.633401	-3.139131	-0.423137
1	0.143803	-4.552663	0.344617
1	1.972922	-2.675834	-1.209725
1	4.147814	-2.426696	-2.362012
1	5.300576	-0.222819	-2.360759
1	4.232567	1.731858	-1.291151
1	3.692974	2.546959	0.863778
1	2.603165	4.541670	1.885408
1	0.136438	4.880022	1.539012
1	-1.106359	3.207822	0.173108
1	-2.103831	1.056162	0.749212
1	-5.606840	2.408949	-1.408747
1	-4.743171	1.109439	-2.273547
1	-5.803029	0.715940	-0.882096
1	-3.476614	-2.406605	0.068795
1	-2.596748	-1.906489	1.554520
1	-4.338937	-2.334016	1.630838

IRE11_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -113.8951 cm(-1)

Electronic energy : -1634.3358043
 Zero-point correction= 0.359692
 Thermal correction to Energy= 0.386600
 Thermal correction to Enthalpy= 0.387545
 Thermal correction to Gibbs Free Energy= 0.301940
 Sum of electronic and zero-point Energies= -1633.976112
 Sum of electronic and thermal Energies= -1633.949204
 Sum of electronic and thermal Enthalpies= -1633.948260
 Sum of electronic and thermal Free Energies= -1634.033865

Cartesian Coordinates

```

-----
1 -2.875176 -0.827207 -2.151970
6 -2.971557 -0.084060 -1.361019
6 -2.303262 1.153019 -1.479737
46 -0.522675 0.026633 -0.606769
15 0.211987 -1.065947 1.303472
8 -0.498666 -0.198129 2.298664
7 1.321869 1.802792 -0.230597
6 1.347406 2.977377 0.403621
6 2.502338 3.529069 0.942653
6 3.687088 2.810734 0.824465
6 3.668232 1.576569 0.191104
6 2.462279 1.094096 -0.327186
6 2.375637 -0.239558 -0.954812
6 3.440987 -0.739517 -1.708957
6 3.379330 -2.002547 -2.288221
6 2.249667 -2.793453 -2.108371
6 1.182327 -2.317395 -1.349251
6 1.222262 -1.038606 -0.789681
8 1.742481 -1.332181 1.777508
6 1.951132 -1.458391 3.184561
8 -0.331667 -2.605939 1.323909
6 -1.730195 -2.790681 1.147924
1 0.393087 3.498613 0.479232
1 2.468835 4.492625 1.442939
1 4.614427 3.199149 1.238995
1 4.569780 0.972649 0.125932
1 4.321931 -0.118262 -1.865660
1 4.216082 -2.367807 -2.879267
1 2.199302 -3.786935 -2.549257
1 0.319917 -2.955919 -1.170099
1 3.012225 -1.678991 3.325789
1 1.698498 -0.531039 3.709122
1 1.358216 -2.281214 3.603216
1 -1.941954 -3.847865 1.328715
1 -2.034713 -2.532163 0.122713
1 -2.307909 -2.178237 1.851127
6 -2.525358 2.160483 -0.518251
6 -3.412203 1.930708 0.525560
8 -1.920464 3.373643 -0.605347
1 -3.581415 2.718603 1.255194
6 -4.079580 0.710797 0.629122
6 -3.857985 -0.300012 -0.298214
1 -4.777743 0.531479 1.443151
8 -4.521462 -1.475980 -0.137415
1 -1.762082 1.391487 -2.400738
1 -1.252657 3.341113 -1.304531
1 -4.321536 -2.058657 -0.881517

```

IRE12_Pd

Number of imaginary frequencies : 1
The smallest frequency is : -146.8368 cm(-1)

Electronic energy : -1634.3325495
Zero-point correction= 0.359725
Thermal correction to Energy= 0.386597
Thermal correction to Enthalpy= 0.387542
Thermal correction to Gibbs Free Energy= 0.299511
Sum of electronic and zero-point Energies= -1633.972824
Sum of electronic and thermal Energies= -1633.945952
Sum of electronic and thermal Enthalpies= -1633.945008
Sum of electronic and thermal Free Energies= -1634.033038

Cartesian Coordinates

```

-----
7 -2.057414 -1.621967 -0.755278

```

6	-3.042156	-0.744569	-0.485476
6	-2.264439	-2.916226	-0.501040
6	-3.458955	-3.411704	0.005733
6	-4.483990	-2.509245	0.269898
6	-4.274519	-1.159307	0.027910
6	-2.751708	0.681159	-0.735224
6	-1.472422	1.219975	-0.440619
6	-1.218189	2.567826	-0.733486
6	-2.195605	3.368527	-1.318592
6	-3.454695	2.841545	-1.583166
6	-3.729439	1.508904	-1.287064
46	0.037452	-0.126562	-0.926641
15	-0.417210	0.537491	1.266817
8	-1.785079	0.741721	2.114102
6	-1.745544	0.408464	3.502106
8	1.729453	-1.737319	-0.193777
6	2.987493	-1.201380	-0.204609
6	3.572540	-0.903407	-1.432023
6	4.849433	-0.354439	-1.483174
6	5.548992	-0.094575	-0.304700
6	4.962233	-0.396017	0.923738
6	3.690842	-0.955287	0.974158
8	6.795439	0.447323	-0.294221
8	0.374037	1.903647	1.667157
6	1.757297	1.976601	1.345405
8	0.308503	-0.673925	1.835140
1	-0.959842	0.968590	4.024000
1	-2.716542	0.688164	3.918359
1	-1.579048	-0.663681	3.647774
1	2.349460	1.318873	1.992597
1	1.943729	1.699862	0.293977
1	2.070604	3.013206	1.496489
1	-0.257542	3.001341	-0.465421
1	-1.975950	4.408251	-1.551188
1	-4.226223	3.464941	-2.029269
1	-4.706623	1.092150	-1.527400
1	-5.042155	-0.425129	0.259360
1	-5.433387	-2.852564	0.674074
1	-3.579518	-4.476235	0.185496
1	-1.434761	-3.586299	-0.726057
1	3.229464	-1.188088	1.932819
1	5.517349	-0.191648	1.836518
1	5.303052	-0.122457	-2.446642
1	3.015077	-1.101031	-2.346537
1	7.081315	0.600886	-1.203726
1	1.296942	-1.548523	0.679107

Reaction 2

----- Palladium Acetate -----

Electronic energy =	-1750.5747527
Zero-point correction=	0.315721
Thermal correction to Energy=	0.349705
Thermal correction to Enthalpy=	0.350649
Thermal correction to Gibbs Free Energy=	0.246602
Sum of electronic and zero-point Energies=	-1750.259032
Sum of electronic and thermal Energies=	-1750.225048
Sum of electronic and thermal Enthalpies=	-1750.224104
Sum of electronic and thermal Free Energies=	-1750.328150

----- Cartesian Coordinates -----

46	1.559035	0.928517	-0.001488
----	----------	----------	-----------

8	2.288923	0.035252	-1.687034
8	2.647810	-0.307196	1.230488
6	2.237852	-1.316717	1.863936
8	1.167666	-1.961743	1.678836
46	0.023737	-1.809013	-0.005073
6	2.293813	-1.213951	-1.872974
8	1.643995	-2.088608	-1.240602
8	1.120996	1.989960	1.685653
8	0.987207	2.468096	-1.238768
6	-0.097361	2.595324	-1.866543
8	-1.177729	1.970201	-1.674795
46	-1.584820	0.884526	0.004864
6	0.023807	2.584005	1.881424
8	-1.056839	2.431772	1.252415
8	-2.292781	-0.036957	1.684456
8	-2.637837	-0.371235	-1.237573
6	-2.258254	-1.285451	1.868666
6	-2.201317	-1.367915	-1.873886
8	-1.586267	-2.139524	1.230445
8	-1.115962	-1.986975	-1.689102
6	3.211151	-1.714134	-2.954887
1	4.199556	-1.887528	-2.516001
1	2.841569	-2.655559	-3.365126
1	3.317398	-0.959696	-3.737086
6	-0.122294	3.635851	-2.952546
1	-0.414397	4.592791	-2.507050
1	0.869100	3.748847	-3.395060
1	-0.863054	3.373592	-3.710443
6	0.023199	3.615209	2.976519
1	-0.981084	3.739540	3.385116
1	0.731771	3.332599	3.757816
1	0.350759	4.570526	2.552863
6	-3.146914	-1.821616	2.957425
1	-2.653964	-2.649816	3.470838
1	-3.413996	-1.029053	3.658558
1	-4.064058	-2.205113	2.497903
6	-3.091996	-1.901625	-2.962005
1	-3.830490	-2.570382	-2.507229
1	-3.626653	-1.083020	-3.447853
1	-2.508398	-2.473340	-3.685744
6	3.144000	-1.833096	2.947659
1	3.668482	-1.005114	3.428560
1	2.574304	-2.412780	3.676207
1	3.889797	-2.491563	2.489745

Substrate (PhCONHOMe)

Electronic energy : -515.0817023
 Zero-point correction= 0.159293
 Thermal correction to Energy= 0.169439
 Thermal correction to Enthalpy= 0.170384
 Thermal correction to Gibbs Free Energy= 0.122620
 Sum of electronic and zero-point Energies= -514.922410
 Sum of electronic and thermal Energies= -514.912263
 Sum of electronic and thermal Enthalpies= -514.911319
 Sum of electronic and thermal Free Energies= -514.959083

 Cartesian Coordinates

6	-3.387049	-0.361599	0.061904
6	-2.484408	-1.418704	0.138155

6	-1.117329	-1.171796	0.102251
6	-0.646390	0.139694	-0.013224
6	-1.556715	1.197433	-0.073693
6	-2.921660	0.946905	-0.041727
1	-4.456622	-0.557989	0.090619
1	-2.846449	-2.439528	0.235949
1	-0.421520	-2.003290	0.197288
1	-1.174651	2.213100	-0.147486
1	-3.626241	1.773692	-0.094669
6	0.800380	0.485104	-0.054167
8	1.228142	1.598331	0.223516
7	1.635106	-0.554081	-0.380992
1	1.316335	-1.301251	-0.989247
8	2.954214	-0.228668	-0.626646
6	3.726211	-0.395761	0.557164
1	3.687600	-1.433130	0.913249
1	4.752181	-0.141118	0.277529
1	3.386541	0.283108	1.348768

AgOAc.2AcOH

Solvent SP on SMD(AcOH)/M06/6-31G**(LANL2DZ) with ultrafine grid optimized job

Electronic energy : -832.1608226

Cartesian Coordinates

47	-0.091540	-0.930489	-0.031313
8	-2.405716	0.110800	-0.795095
8	-2.186734	-1.580697	0.637871
6	-2.889152	-0.744852	0.005979
6	-4.381118	-0.758223	0.202400
1	-4.875598	-0.884926	-0.766649
1	-4.695972	-1.551779	0.883546
1	-4.702723	0.211726	0.597982
8	2.198991	-1.304681	-0.125773
8	0.517127	1.469311	-0.117257
6	3.170392	-0.563086	-0.002357
6	-0.177421	2.482174	-0.001072
8	3.089725	0.746701	0.112615
8	-1.478384	2.469630	-0.131196
6	0.382982	3.826310	0.306514
1	0.003095	4.162500	1.277575
1	1.473481	3.795684	0.328159
1	0.039927	4.548992	-0.440324
6	4.572615	-1.064151	0.019933
1	5.091661	-0.679745	0.903528
1	4.588482	-2.154673	0.015704
1	5.103842	-0.682864	-0.858951
1	-1.822591	1.549779	-0.358709
1	2.148909	1.060761	0.052134

Phenyl Iodide

Electronic energy : -242.8150829

Zero-point correction= 0.089671

Thermal correction to Energy= 0.095589

Thermal correction to Enthalpy= 0.096533

Thermal correction to Gibbs Free Energy= 0.057914

Sum of electronic and zero-point Energies= -242.725412

Sum of electronic and thermal Energies= -242.719494

Sum of electronic and thermal Enthalpies= -242.718550

Sum of electronic and thermal Free Energies= -242.757169

Cartesian Coordinates

6 0.000000 -2.648097 1.204085
6 0.000000 -1.255538 1.212547
6 0.000000 -0.575425 0.000000
6 0.000000 -1.255538 -1.212547
6 0.000000 -2.648097 -1.204085
6 0.000000 -3.345256 0.000000
1 0.000000 -3.187157 2.149107
1 0.000000 -0.711318 2.153613
1 0.000000 -0.711318 -2.153613
1 0.000000 -3.187157 -2.149107
1 0.000000 -4.432778 0.000000
53 0.000000 1.558442 0.000000

Acetic Acid

Electronic energy : -228.967229
Zero-point correction= 0.061735
Thermal correction to Energy= 0.066385
Thermal correction to Enthalpy= 0.067329
Thermal correction to Gibbs Free Energy= 0.033140
Sum of electronic and zero-point Energies= -228.905494
Sum of electronic and thermal Energies= -228.900844
Sum of electronic and thermal Enthalpies= -228.899900
Sum of electronic and thermal Free Energies= -228.934089

Cartesian Coordinates

6 0.089606 0.119473 -0.000575
8 0.643350 1.199011 0.000103
8 0.768287 -1.038735 -0.000111
1 1.717156 -0.827410 0.001390
6 -1.383198 -0.106674 -0.000213
1 -1.668110 -0.709713 -0.868616
1 -1.671563 -0.670788 0.893088
1 -1.909024 0.848908 -0.021066

Conformational and Configurational Study of C-H activation

Monometallic C-H activation (Pd)

2CH1_Pd

Number of imaginary frequencies : 1
Imaginary frequency : -1587.3969 cm(-1)

Electronic energy : -1098.5705762
Zero-point correction= 0.258874 (hartree/particle)
Thermal correction to Energy= 0.280040
Thermal correction to Enthalpy= 0.280984
Thermal correction to Gibbs Free Energy= 0.208549
Sum of electronic and zero-point Energies= -1098.311702

Sum of electronic and thermal Energies= -1098.290536
 Sum of electronic and thermal Enthalpies= -1098.289592
 Sum of electronic and thermal Free Energies= -1098.362027

 Cartesian Coordinates

6	-1.782957	0.057837	-0.125744
6	-2.060310	-1.317918	0.026194
6	-3.285940	-1.842052	-0.350562
6	-4.238503	-1.012095	-0.939454
6	-3.956152	0.331403	-1.170676
6	-2.733500	0.863629	-0.774984
6	-0.961021	-2.246498	0.418657
7	0.223983	-1.633349	0.191789
46	0.312056	0.341333	-0.161619
8	2.443628	0.680116	-0.320857
6	3.413330	0.017087	-0.700602
6	4.727131	0.651285	-0.982592
8	-1.125229	-3.400431	0.813839
8	1.355445	-2.405703	0.411225
6	1.815758	-2.275342	1.759432
8	0.199436	2.439513	-0.202222
6	-0.522593	2.877054	0.750069
8	-1.245728	2.145211	1.483028
6	-0.544524	4.358915	0.970079
8	3.404145	-1.279814	-0.879986
1	2.015982	-1.222132	1.999545
1	1.072086	-2.684171	2.452011
1	2.740762	-2.855630	1.819545
1	-3.467398	-2.906936	-0.218015
1	-5.198344	-1.423005	-1.244171
1	-4.694336	0.970058	-1.649657
1	-2.537404	1.926101	-0.908521
1	-1.363650	0.854481	0.810089
1	-0.736206	4.586938	2.021079
1	0.389650	4.817787	0.639022
1	-1.364338	4.781808	0.377327
1	4.649789	1.736689	-0.912607
1	5.464962	0.281755	-0.262053
1	5.071894	0.356674	-1.978877
1	2.556201	-1.699264	-0.571891

2CH2_Pd

Number of imaginary frequencies : 1
 Imaginary frequency : -1513.9825 cm(-1)

Electronic energy : -1327.5605064
 Zero-point correction= 0.322051 (hartree/particle)
 Thermal correction to Energy= 0.348398
 Thermal correction to Enthalpy= 0.349342
 Thermal correction to Gibbs Free Energy= 0.264746
 Sum of electronic and zero-point Energies= -1327.238455
 Sum of electronic and thermal Energies= -1327.212109
 Sum of electronic and thermal Enthalpies= -1327.211165
 Sum of electronic and thermal Free Energies= -1327.295760

 Cartesian Coordinates

6	-1.092215	-2.269270	-0.532098
8	-1.295772	-3.470788	-0.701922
7	0.055751	-1.693337	-0.078581
8	1.136899	-2.564350	-0.015155
6	1.682365	-2.578611	1.302839

1	1.999037	-1.571988	1.612799
1	0.945202	-2.976631	2.010261
1	2.551042	-3.241960	1.260165
6	-2.093638	-1.197330	-0.793508
6	-3.302893	-1.487459	-1.405943
6	-4.177405	-0.445110	-1.702124
6	-3.846639	0.876341	-1.395179
6	-2.631162	1.169430	-0.790413
6	-1.748134	0.130865	-0.448729
1	-3.536275	-2.518513	-1.664875
1	-5.127192	-0.660503	-2.187012
1	-4.544158	1.676993	-1.629882
1	-2.385790	2.198083	-0.532307
1	-1.462255	0.213504	0.853351
46	0.321984	0.276424	-0.432309
8	0.386472	2.322636	-0.832375
6	0.170516	3.129000	0.131361
6	0.158668	4.590328	-0.217841
1	-0.882025	4.935650	-0.240028
1	0.676381	5.163653	0.556571
1	0.610222	4.775828	-1.194915
8	-0.063998	2.798807	1.316898
8	2.503073	0.437747	-0.574687
6	3.371112	-0.274923	-1.083485
8	3.215526	-1.547771	-1.361217
6	4.715914	0.249120	-1.439619
1	4.789616	1.310869	-1.202653
1	5.484792	-0.313713	-0.900170
1	4.890973	0.091024	-2.509165
1	2.350704	-1.900549	-1.021164
8	-1.575356	-0.061864	2.149134
1	0.250060	1.489578	2.008523
6	-0.550072	-0.065917	2.863023
8	0.453366	0.731528	2.680392
6	-0.432065	-1.001393	4.010237
1	-1.014832	-1.905636	3.822809
1	0.615835	-1.237613	4.213594
1	-0.840669	-0.508231	4.900686

2CH3_Pd

Number of imaginary frequencies : 1
 Imaginary frequency : -1721.8556 cm(-1)

Electronic energy : -1327.5549137
 Zero-point correction= 0.322210 (hartree/particle)
 Thermal correction to Energy= 0.348523
 Thermal correction to Enthalpy= 0.349467
 Thermal correction to Gibbs Free Energy= 0.265665
 Sum of electronic and zero-point Energies= -1327.232704
 Sum of electronic and thermal Energies= -1327.206391
 Sum of electronic and thermal Enthalpies= -1327.205446
 Sum of electronic and thermal Free Energies= -1327.289249

 Cartesian Coordinates

6	-1.800506	0.398175	-0.319186
6	-2.405796	-0.853718	-0.573310
6	-3.669213	-0.934070	-1.139481
6	-4.331206	0.239780	-1.488525
6	-3.732598	1.486234	-1.291417
6	-2.465782	1.567240	-0.730115
6	-1.602852	-2.083384	-0.339957
7	-0.342843	-1.728594	0.060057

46	0.279840	0.123155	-0.399816
8	2.449950	-0.111638	-0.504101
6	3.177515	-0.958478	-1.026816
6	4.617015	-0.708150	-1.295408
8	-2.019107	-3.228429	-0.489464
8	0.567899	-2.768911	0.019155
6	1.172936	-2.955626	1.301884
8	0.810008	2.119589	-0.931587
6	0.948417	3.083010	-0.160547
8	0.538633	3.120250	1.070260
6	1.635097	4.322614	-0.614991
8	2.773223	-2.153478	-1.389723
8	-0.928608	1.208778	2.059733
6	-0.202244	0.370626	2.767288
6	-0.980316	-0.709714	3.459805
8	1.022320	0.452501	2.839608
1	1.544636	-2.002872	1.702729
1	0.448836	-3.397927	1.995171
1	2.004407	-3.647647	1.141355
1	-4.107302	-1.911482	-1.331094
1	-5.321166	0.185029	-1.935847
1	-4.263993	2.392407	-1.572214
1	-2.012636	2.539737	-0.541170
1	-1.337003	0.650266	0.863230
1	2.592293	4.403706	-0.087459
1	1.815398	4.292245	-1.690243
1	1.041487	5.201774	-0.347946
1	4.875036	0.326128	-1.065943
1	5.220904	-1.387098	-0.683405
1	4.838031	-0.932965	-2.343753
1	1.852051	-2.331823	-1.068994
1	0.034678	2.295867	1.397160
1	-1.783037	-0.269786	4.060773
1	-1.459611	-1.343444	2.701388
1	-0.333123	-1.323642	4.091008

Bimetallic C-H Activation (Pd-Ag)

2CH1_Pd-Ag

Number of imaginary frequencies : 1
Imaginary frequency : -1695.7368 cm(-1)

Electronic energy : -1701.7959398
Zero-point correction= 0.377398 (hartree/particle)
Thermal correction to Energy= 0.410381
Thermal correction to Enthalpy= 0.411325
Thermal correction to Gibbs Free Energy= 0.313746
Sum of electronic and zero-point Energies= -1701.418542
Sum of electronic and thermal Energies= -1701.385559
Sum of electronic and thermal Enthalpies= -1701.384615
Sum of electronic and thermal Free Energies= -1701.482194

Cartesian Coordinates

6	1.860173	3.752368	-0.072449
6	2.257188	2.419615	-0.132701
6	1.599912	1.437686	0.623858
6	0.452122	1.818997	1.354907
6	0.071280	3.151732	1.430675
6	0.789239	4.122373	0.735274

46	1.438516	-0.638273	0.158963
8	3.310508	-0.794021	-0.807740
6	4.223772	-0.348456	-0.043630
8	3.997254	0.292309	1.024556
6	-0.492693	0.781596	1.861084
7	-0.133947	-0.438356	1.387933
8	-1.046566	-1.444206	1.586288
6	-0.658631	-2.297981	2.652825
8	1.039399	-2.664687	-0.259805
6	-0.008694	-3.067828	-0.844334
8	-0.819256	-2.351851	-1.497279
47	-0.823892	-0.037941	-1.475672
8	-3.094869	-0.364644	-0.368550
6	-3.401658	-1.332768	0.330237
8	-3.117993	-2.568223	-0.029070
6	-0.327949	-4.529742	-0.702764
8	-1.486154	1.022309	2.552203
6	-4.132251	-1.202336	1.617623
6	5.649507	-0.582542	-0.434404
1	-5.076691	-0.674714	1.450232
1	-4.322555	-2.172784	2.080333
1	-3.517541	-0.581941	2.282039
1	-1.044516	-4.636896	0.123063
1	-0.804144	-4.912966	-1.609219
1	0.562003	-5.114547	-0.460050
1	3.131818	2.147614	-0.721162
1	2.401384	4.504698	-0.641396
1	0.491344	5.166859	0.798733
1	-0.819405	3.406199	2.003271
1	6.148593	0.384017	-0.561127
1	6.162055	-1.107763	0.378086
1	5.723144	-1.162670	-1.355928
1	-2.489405	-2.547160	-0.794589
1	2.616689	0.690975	1.009338
1	-1.435147	-3.068542	2.708932
1	0.313136	-2.768205	2.447862
1	-0.616865	-1.741663	3.598796
8	-1.348395	2.206645	-1.593564
6	-2.153787	2.848530	-0.919734
8	-3.000488	2.316367	-0.065805
6	-2.289125	4.328038	-1.031260
1	-2.419824	4.783128	-0.044975
1	-1.425976	4.752438	-1.546945
1	-3.193720	4.547781	-1.611048
1	-2.993507	1.322732	-0.086599

2CHI_Pd-Ag-PRC

Number of imaginary frequencies : 0

Electronic energy : HF=-1701.8174316
Zero-point correction= 0.381856
Thermal correction to Energy= 0.415851
Thermal correction to Enthalpy= 0.416795
Thermal correction to Gibbs Free Energy= 0.316040
Sum of electronic and zero-point Energies= -1701.435576
Sum of electronic and thermal Energies= -1701.401580
Sum of electronic and thermal Enthalpies= -1701.400636
Sum of electronic and thermal Free Energies= -1701.501392

.....
Cartesian Coordinates
.....

6	2.524631	3.047987	0.901549
6	2.917468	1.929101	1.603660
6	1.957919	0.996089	2.049814
6	0.580141	1.243245	1.793740
6	0.198515	2.431539	1.131719
6	1.158570	3.305253	0.674255
46	1.329174	-0.534895	0.445877
8	2.534639	0.194348	-1.089720
6	3.790420	-0.042253	-0.889596
8	4.240777	-0.665196	0.078181
6	-0.495601	0.258921	2.130946
7	0.041716	-1.001485	1.993721
8	-0.956889	-1.923605	1.778339
6	-0.507878	-3.229953	2.108029
8	1.197126	-2.380369	-0.568625
6	0.235705	-2.695015	-1.326442
8	-0.641588	-1.905184	-1.776278
47	-0.749897	0.357101	-1.341913
8	-3.015957	-0.316569	-0.416972
6	-3.281346	-1.394262	0.119989
8	-2.858252	-2.537780	-0.377027
6	0.104833	-4.149623	-1.679028
8	-1.666698	0.563024	2.335158
6	-4.091525	-1.503416	1.359511
6	4.703202	0.561606	-1.925519
1	-5.055837	-1.007525	1.210384
1	-4.244804	-2.542437	1.657605
1	-3.554983	-0.959591	2.147521
1	-0.761470	-4.548336	-1.134668
1	-0.097674	-4.264790	-2.747697
1	0.992746	-4.718441	-1.396068
1	3.967369	1.745033	1.816074
1	3.269434	3.753509	0.541282
1	0.859243	4.203201	0.137300
1	-0.864009	2.629251	1.012197
1	4.793944	1.636702	-1.725578
1	5.697010	0.110059	-1.871864
1	4.289213	0.449706	-2.931961
1	-2.219929	-2.353529	-1.114705
1	2.260386	0.200437	2.729134
1	-1.334198	-3.897569	1.844902
1	0.386502	-3.497977	1.530583
1	-0.293179	-3.309961	3.181066
8	-1.759258	2.438172	-1.604403
6	-2.550610	2.975136	-0.830324
8	-3.254309	2.325885	0.073897
6	-2.774341	4.446332	-0.795208
1	-2.411674	4.835953	0.163994
1	-2.243437	4.935085	-1.613182
1	-3.844842	4.667272	-0.845755
1	-3.156048	1.339831	-0.010053

2CH2_Pd-Ag

Number of imaginary frequencies : 1

Imaginary frequency : -1809.8073 cm(-1)

Electronic energy : -1701.7872361
Zero-point correction= 0.374794 (hartree/particle)
Thermal correction to Energy= 0.408617
Thermal correction to Enthalpy= 0.409561
Thermal correction to Gibbs Free Energy= 0.308278
Sum of electronic and zero-point Energies= -1701.412442
Sum of electronic and thermal Energies= -1701.378619
Sum of electronic and thermal Enthalpies= -1701.377675
Sum of electronic and thermal Free Energies= -1701.478958

Cartesian Coordinates


```

-----
1 -0.676617 5.289504 -0.226629
1 -1.302775 4.486992 -1.702402
1 0.433345 4.714281 -1.497906
6 -0.498291 4.501041 -0.960435
6 -0.373966 3.159991 -0.298188
8 -0.234635 3.092893 0.940565
8 -2.289679 1.271778 -2.715683
6 -2.428258 0.008980 -2.393247
8 -1.737161 -0.568379 -1.547916
8 -0.385673 2.152321 -1.091780
6 -3.491415 -0.695119 -3.157754
1 -3.554393 -1.740560 -2.850899
1 -3.258147 -0.635756 -4.226641
1 -4.454351 -0.195150 -3.011143
46 0.202008 0.118920 -0.723762
47 -0.706621 1.075646 1.867415
8 -0.221912 -1.051555 2.568533
6 0.981798 -1.421075 2.463180
6 1.304648 -2.868090 2.676885
1 0.605990 -3.327408 3.380810
1 2.335277 -2.995098 3.017279
1 1.201653 -3.380894 1.710256
8 1.934523 -0.632259 2.169299
1 1.806996 0.062558 1.006919
6 2.185961 0.454077 -0.173155
8 2.787158 -3.010707 -1.061329
1 2.229862 2.565453 0.304508
6 2.777311 1.732982 -0.137322
6 4.076697 1.907088 -0.588912
1 4.549540 2.884604 -0.530068
6 4.790087 0.822652 -1.110825
1 5.805704 0.975752 -1.469634
6 4.221953 -0.446550 -1.183256
1 4.767703 -1.290649 -1.599882
6 2.921865 -0.620315 -0.735464
6 2.232569 -1.937148 -0.824670
7 0.904750 -1.750712 -0.578759
8 0.067293 -2.823581 -0.711785
6 -0.089846 -3.232967 -2.071788
1 -0.874013 -3.994511 -2.060606
1 -0.409069 -2.385640 -2.691423
1 0.840423 -3.660136 -2.463270
1 -1.580447 1.704982 -2.163563
8 -2.901732 0.090188 1.236953
6 -3.116030 -1.084913 0.955758
8 -2.331671 -2.085499 1.304760
6 -4.321526 -1.540247 0.205225
1 -4.864062 -0.684053 -0.200666
1 -4.023128 -2.227559 -0.593154
1 -4.978373 -2.095999 0.884009
1 -1.548976 -1.765352 1.830823

```

2CH3_Pd-Ag

Number of imaginary frequencies : 1
Imaginary frequency : -1518.5210 cm(-1)

Electronic energy : -1701.7825852
Zero-point correction= 0.373792 (hartree/particle)
Thermal correction to Energy= 0.407725
Thermal correction to Enthalpy= 0.408669
Thermal correction to Gibbs Free Energy= 0.306383
Sum of electronic and zero-point Energies= -1701.408793

Sum of electronic and thermal Energies= -1701.374861
Sum of electronic and thermal Enthalpies= -1701.373916
Sum of electronic and thermal Free Energies= -1701.476203

Cartesian Coordinates

6	-0.507954	-2.834451	-1.107263
6	-0.371168	-1.828337	-0.136834
6	0.799978	-1.809201	0.659177
6	1.771317	-2.795639	0.531706
6	1.588801	-3.805253	-0.407212
6	0.457217	-3.826123	-1.225758
46	-1.001780	0.158699	-0.298383
47	1.749631	1.286340	-0.607014
8	3.580700	0.009690	-0.807403
6	4.499523	-0.440877	-0.121135
6	5.836224	-0.758935	-0.694723
6	0.996680	-0.653775	1.569794
8	2.024179	-0.477711	2.255088
7	-0.065624	0.187911	1.523493
8	0.168310	1.379966	2.177408
6	-1.013735	1.807619	2.837897
8	-1.559708	2.211653	-0.368144
6	-0.743250	3.177988	-0.449019
8	0.501311	3.100067	-0.606927
8	-1.855053	-0.032758	-2.192952
6	-2.957381	-0.665470	-2.279957
6	-3.538123	-0.804363	-3.658148
6	-1.348998	4.549915	-0.312463
8	-3.583055	-1.164221	-1.314191
8	4.411462	-0.706461	1.158326
8	-3.734358	-0.439691	1.106838
6	-3.142353	-1.220105	1.950533
8	-2.282053	-2.067337	1.622939
6	-3.559160	-1.079357	3.367135
1	-1.829259	1.973485	2.120929
1	-1.321811	1.078312	3.599668
1	-0.755812	2.754977	3.319419
1	2.664229	-2.764041	1.152634
1	2.340313	-4.585059	-0.510107
1	0.331520	-4.625054	-1.952937
1	-1.404108	-2.868909	-1.725912
1	-1.485719	-1.796244	0.616791
1	-2.793985	-0.608876	-4.433502
1	-3.965067	-1.803886	-3.784024
1	-4.356302	-0.082958	-3.767063
1	-2.310932	4.598827	-0.830384
1	-1.535962	4.741340	0.751635
1	-0.673110	5.319483	-0.692341
1	-3.546787	-0.692826	0.123550
1	-2.725850	-1.319504	4.031101
1	-3.945678	-0.075451	3.559099
1	-4.366876	-1.795679	3.561061
1	5.899557	-0.422470	-1.730170
1	6.619238	-0.287114	-0.092836
1	5.999966	-1.841123	-0.646734
1	3.491413	-0.558165	1.530709

2CH4_Pd-Ag

Number of imaginary frequencies : 1
Imaginary frequency : -1657.5400 cm(-1)

Electronic energy : -1472.790192

Zero-point correction= 0.310312 (hartree/particle)
 Thermal correction to Energy= 0.339176
 Thermal correction to Enthalpy= 0.340120
 Thermal correction to Gibbs Free Energy= 0.248186
 Sum of electronic and zero-point Energies= -1472.479880
 Sum of electronic and thermal Energies= -1472.451016
 Sum of electronic and thermal Enthalpies= -1472.450072
 Sum of electronic and thermal Free Energies= -1472.542006

 Cartesian Coordinates

6	2.682798	1.282493	-1.718815
6	2.147257	1.000471	-0.454760
6	1.718707	2.080192	0.342913
6	1.892635	3.393303	-0.069299
6	2.456447	3.652088	-1.317457
6	2.832234	2.599515	-2.146600
46	1.042315	-0.740621	0.125141
8	-0.228888	-2.321511	0.704608
6	-1.384563	-2.365854	0.186343
6	-2.254624	-3.531347	0.558183
6	0.953180	1.794077	1.589458
8	0.917913	2.519922	2.573418
7	0.240631	0.617992	1.433523
47	-1.527443	0.855662	-0.069089
8	-1.826715	-1.512219	-0.630914
8	-0.417311	0.171252	2.572891
8	-3.673472	1.166556	-0.847049
6	-4.549007	0.319032	-1.038064
6	-5.966204	0.684659	-1.315614
8	-4.341902	-0.975014	-1.023302
8	2.105409	-2.111635	-1.060460
6	3.356877	-1.991149	-0.868603
6	4.260575	-3.021458	-1.470294
8	3.881468	-1.038914	-0.222153
1	-6.263207	0.280341	-2.289144
1	-6.615175	0.222437	-0.564224
1	-6.095209	1.767654	-1.306060
1	-2.243915	-4.252832	-0.267003
1	-1.895035	-4.027269	1.462126
1	-3.289269	-3.198602	0.692825
1	3.033441	0.468178	-2.350960
1	3.257300	2.802880	-3.126764
1	2.588809	4.679176	-1.649424
1	1.561542	4.202055	0.579709
1	3.695121	-3.865390	-1.869199
1	4.835606	-2.553208	-2.276817
1	4.975336	-3.366733	-0.717484
1	-3.371039	-1.211425	-0.875409
1	2.869993	-0.030122	-0.065618
6	0.475620	-0.491984	3.462459
1	-0.145709	-0.870226	4.278651
1	0.972109	-1.333261	2.960138
1	1.224639	0.201141	3.865276

2CH5_Pd-Ag

Number of imaginary frequencies : 1
 Imaginary frequency : -1784.7088 cm(-1)

Electronic energy : -1472.788921
 Zero-point correction= 0.310664 (hartree/particle)
 Thermal correction to Energy= 0.339526
 Thermal correction to Enthalpy= 0.340470

Thermal correction to Gibbs Free Energy= 0.247649
 Sum of electronic and zero-point Energies= -1472.478257
 Sum of electronic and thermal Energies= -1472.449395
 Sum of electronic and thermal Enthalpies= -1472.448451
 Sum of electronic and thermal Free Energies= -1472.541272

 Cartesian Coordinates

1	4.334273	-2.685570	-1.457751
1	4.484311	-0.948458	-1.835839
1	3.461314	-1.966755	-2.849963
6	3.799966	-1.806135	-1.821949
6	2.632943	-1.474308	-0.938343
8	2.487290	-2.097701	0.136296
8	3.028924	1.858123	-1.525483
6	2.483372	2.500994	-0.518736
8	1.516464	2.080674	0.124197
8	1.870414	-0.539759	-1.367538
6	3.116802	3.812007	-0.225684
1	2.732321	4.221259	0.709550
1	2.886884	4.501145	-1.046610
1	4.204604	3.706653	-0.183574
46	0.176642	0.420086	-0.453316
47	1.062473	-1.363622	1.646205
8	-0.526918	-0.437676	2.861220
6	-1.669116	-0.703234	2.404318
6	-2.856009	-0.027930	3.024688
1	-2.676243	0.189711	4.080530
1	-3.759693	-0.630438	2.903119
1	-3.013606	0.928157	2.505808
8	-1.883685	-1.501325	1.428500
1	-1.318794	-1.194822	0.222859
6	-1.301379	-0.921635	-1.045679
8	-3.702048	1.713032	-0.409618
1	-0.143266	-2.645507	-1.657096
6	-1.032413	-2.045613	-1.849693
6	-1.932886	-2.419017	-2.836549
1	-1.745191	-3.302312	-3.442377
6	-3.090636	-1.663376	-3.051410
1	-3.784208	-1.963057	-3.834142
6	-3.366697	-0.532050	-2.287610
1	-4.258411	0.066820	-2.460914
6	-2.461433	-0.153371	-1.309454
6	-2.652925	1.073019	-0.488857
7	-1.489273	1.342343	0.165954
8	-1.419322	2.475996	0.924939
6	-1.406348	3.661862	0.127966
1	-1.220167	4.484070	0.823466
1	-0.598755	3.616272	-0.614102
1	-2.370407	3.806218	-0.373166
1	2.599793	0.968247	-1.648716

2CH6_Pd-Ag

Number of imaginary frequencies : 1
 Imaginary frequency : -1452.2815 cm(-1)

Electronic energy : -1701.7814949
 Zero-point correction= 0.374037 (hartree/particle)
 Thermal correction to Energy= 0.408108
 Thermal correction to Enthalpy= 0.409052
 Thermal correction to Gibbs Free Energy= 0.306514
 Sum of electronic and zero-point Energies= -1701.407458
 Sum of electronic and thermal Energies= -1701.373387

Sum of electronic and thermal Enthalpies= -1701.372443
Sum of electronic and thermal Free Energies= -1701.474981

Cartesian Coordinates

1 0.090783 -4.460507 -2.711623
1 -0.787739 -3.325935 -3.792153
1 -1.634287 -4.115550 -2.456435
6 -0.674663 -3.683001 -2.765163
6 -0.345825 -2.549061 -1.832465
8 0.402033 -2.758858 -0.855382
8 1.786188 1.291933 -0.545427
6 1.393213 1.602706 -1.703110
8 0.300745 1.205953 -2.215445
8 -0.918859 -1.441676 -2.118787
6 2.250106 2.514654 -2.530455
1 1.850906 2.645667 -3.538180
1 3.270409 2.117781 -2.578546
1 2.306430 3.488460 -2.030388
46 -0.978467 0.198769 -0.864822
47 1.569024 -1.035552 0.148076
1 -1.189697 -0.679436 1.137747
6 -2.323423 -0.639835 0.569368
8 -3.422591 2.805770 0.860056
1 -2.148226 -2.773170 0.317546
6 -2.829483 -1.949658 0.530359
6 -4.160203 -2.199310 0.838148
1 -4.537964 -3.218800 0.833751
6 -5.017582 -1.143972 1.158398
1 -6.060252 -1.349054 1.388854
6 -4.556760 0.168103 1.168270
1 -5.226581 0.999338 1.376022
6 -3.221233 0.414916 0.870594
6 -2.756474 1.807233 0.742431
7 -1.344558 1.861140 0.359063
8 -0.912256 3.121835 -0.013403
6 -1.501886 3.572695 -1.235981
1 -0.819343 4.336428 -1.617796
1 -1.565238 2.752306 -1.960669
1 -2.489711 4.012193 -1.064482
1 3.354436 1.287155 -0.153476
8 3.795594 -0.775324 0.937410
6 4.620429 0.102305 0.685969
8 4.335146 1.223301 0.061894
6 6.053917 -0.000052 1.080082
1 6.694616 0.235848 0.224797
1 6.264142 0.742936 1.857501
1 6.277574 -0.998125 1.459585
8 -0.099347 -0.993555 2.002309
6 0.305759 -0.016971 2.738668
8 -0.083090 1.162109 2.619679
6 1.343261 -0.363639 3.768234
1 1.112265 -1.319983 4.246335
1 2.312015 -0.473968 3.262683
1 1.428677 0.428117 4.516307
1 -0.769359 1.613298 1.228119

2CH7_Pd-Ag

Number of imaginary frequencies : 1
Imaginary frequency : -1729.8795 cm(-1)

Electronic energy : -1701.7766241
Zero-point correction= 0.374569 (hartree/particle)

Thermal correction to Energy= 0.408257
 Thermal correction to Enthalpy= 0.409201
 Thermal correction to Gibbs Free Energy= 0.307248
 Sum of electronic and zero-point Energies= -1701.402055
 Sum of electronic and thermal Energies= -1701.368367
 Sum of electronic and thermal Enthalpies= -1701.367423
 Sum of electronic and thermal Free Energies= -1701.469376

 Cartesian Coordinates

6	0.841413	1.826375	-0.886241
6	-0.415315	2.428187	-0.650690
6	-0.945806	3.346775	-1.545693
6	-0.232298	3.660750	-2.699954
6	0.995514	3.053404	-2.969429
6	1.521106	2.126649	-2.077818
6	-1.215678	1.959462	0.506143
7	-0.649877	0.861727	1.054590
46	0.778803	-0.092343	0.010690
8	0.723724	-1.980766	0.996713
6	0.425841	-3.024757	0.335340
6	1.078078	-4.297649	0.797367
8	-2.267437	2.509943	0.879387
8	-1.415275	0.202743	1.983720
6	-0.729144	0.145830	3.234015
8	2.246409	-1.056407	-1.206307
6	3.443726	-1.191500	-0.901579
8	4.090245	-0.427347	-0.075419
6	4.259709	-2.287158	-1.490394
8	-0.330471	-3.067068	-0.669678
8	2.886728	1.721391	0.805700
6	2.620606	1.580568	2.089098
6	1.921853	2.749424	2.720026
8	2.907026	0.563377	2.712817
1	0.263765	-0.309568	3.121604
1	-0.633064	1.150965	3.664789
1	-1.350118	-0.477297	3.882727
1	-1.922644	3.783686	-1.349132
1	-0.644298	4.376433	-3.407945
1	1.540372	3.309705	-3.875051
1	2.494442	1.672399	-2.265251
1	1.750431	1.782315	0.047737
1	3.648121	-2.925549	-2.129407
1	5.088202	-1.860564	-2.065220
1	4.701203	-2.876004	-0.679316
1	0.582528	-5.176374	0.378947
1	2.122734	-4.283083	0.461452
1	1.090195	-4.348860	1.889657
1	3.559255	0.365072	0.282429
1	2.511723	3.661116	2.576335
1	0.958670	2.910368	2.217468
1	1.754502	2.578299	3.786178
47	-1.632214	-1.293609	-1.009674
8	-3.365965	0.121118	-0.702864
6	-4.122756	-0.076993	0.256284
8	-4.242486	0.776724	1.239460
6	-4.945505	-1.307275	0.412533
1	-5.911028	-1.077740	0.871064
1	-5.081502	-1.802295	-0.551566
1	-4.414745	-1.988825	1.089436
1	-3.538529	1.488910	1.151579

2CH8_Pd-Ag

Number of imaginary frequencies : 1
Imaginary frequency : -1612.5787 cm(-1)

Electronic energy : -1472.7807873
Zero-point correction= 0.311396 (hartree/particle)
Thermal correction to Energy= 0.339910
Thermal correction to Enthalpy= 0.340854
Thermal correction to Gibbs Free Energy= 0.251633
Sum of electronic and zero-point Energies= -1472.469391
Sum of electronic and thermal Energies= -1472.440878
Sum of electronic and thermal Enthalpies= -1472.439933
Sum of electronic and thermal Free Energies= -1472.529154

Cartesian Coordinates

1	2.020798	3.855705	2.551327
1	1.294304	2.815370	3.818391
1	0.254984	3.793684	2.778933
6	1.179675	3.205437	2.802614
6	1.068812	2.079224	1.807619
8	1.690528	2.116603	0.738264
8	2.963615	-0.769128	-0.510213
6	2.877011	-1.257129	0.637404
8	1.871920	-1.198954	1.422941
8	0.267672	1.137375	2.186742
6	4.050775	-2.040626	1.164739
1	4.987734	-1.606929	0.805636
1	3.983880	-3.064206	0.775195
1	4.045613	-2.086916	2.256098
46	-0.010478	-0.428226	0.895180
47	1.441108	0.640799	-1.350420
8	-0.084369	1.844709	-2.423435
6	-0.846518	2.537622	-1.698200
6	-1.333210	3.859787	-2.227957
1	-2.401327	3.782502	-2.460941
1	-0.788622	4.154296	-3.127828
1	-1.227165	4.629666	-1.457123
8	-1.269069	2.212284	-0.545854
1	-1.363450	0.866327	-0.074434
6	-2.077199	-0.009787	0.545185
1	-2.468425	1.578131	1.934777
6	-2.893482	0.722611	1.413496
6	-4.242296	0.407857	1.556639
1	-4.871543	0.999651	2.216886
6	-4.787583	-0.660219	0.851476
1	-5.840144	-0.906721	0.966050
6	-3.988520	-1.438926	0.015766
1	-4.416919	-2.312370	-0.472710
6	-2.644919	-1.118305	-0.132394
6	-1.712278	-1.994206	-0.842437
7	-0.473249	-1.886723	-0.461701
8	-2.055387	-2.880657	-1.752659
1	-2.959188	-2.740685	-2.075825
8	0.442787	-2.670217	-1.119097
6	0.777980	-3.800910	-0.312151
1	-0.085510	-4.471991	-0.212423
1	1.586071	-4.310545	-0.841978
1	1.120499	-3.477773	0.678991

2CH9_Pd-Ag

Number of imaginary frequencies : 1
Imaginary frequency : -1655.5627 cm(-1)

Electronic energy : -1472.7756447
 Zero-point correction= 0.310750 (hartree/particle)
 Thermal correction to Energy= 0.339850
 Thermal correction to Enthalpy= 0.340794
 Thermal correction to Gibbs Free Energy= 0.248659
 Sum of electronic and zero-point Energies= -1472.464895
 Sum of electronic and thermal Energies= -1472.435795
 Sum of electronic and thermal Enthalpies= -1472.434851
 Sum of electronic and thermal Free Energies= -1472.526986

.....
 Cartesian Coordinates

1	3.978733	-2.944367	-1.248000
1	3.816595	-1.997852	-2.744193
1	2.671210	-3.305141	-2.422791
6	3.262285	-2.514640	-1.952273
6	2.376294	-1.519770	-1.249778
8	2.723436	-0.994427	-0.187578
8	1.985900	2.392660	0.212299
6	1.911440	2.418828	-1.036768
8	1.275877	1.600216	-1.780473
8	1.272652	-1.284662	-1.889754
6	2.660614	3.502232	-1.764924
1	2.529541	4.457399	-1.248319
1	2.340231	3.588060	-2.805422
1	3.729205	3.259509	-1.742627
46	0.044128	0.086298	-1.045555
47	1.441608	0.597047	1.426309
8	0.656850	-0.982487	2.778695
6	0.459182	-2.125016	2.287987
6	0.627901	-3.324535	3.183075
1	1.105979	-4.141814	2.635137
1	-0.363020	-3.675860	3.494248
1	1.208982	-3.076212	4.074280
8	0.097498	-2.371180	1.095704
1	-0.569623	-1.456059	0.237264
6	-1.519091	-1.281180	-0.626999
8	-1.283362	1.393769	-0.064164
1	-0.821329	-3.107810	-1.511951
6	-1.697805	-2.507448	-1.274347
6	-2.975382	-2.970861	-1.574156
1	-3.104039	-3.930867	-2.068377
6	-4.090559	-2.204385	-1.248199
1	-5.086927	-2.564297	-1.492232
6	-3.941916	-0.963199	-0.632631
1	-4.819621	-0.350142	-0.436950
6	-2.666293	-0.505422	-0.322622
6	-2.388560	0.846574	0.184827
1	-4.151672	1.040083	1.255577
7	-3.332754	1.500059	0.867175
8	-3.026842	2.706737	1.432728
6	-3.378998	3.781523	0.555070
1	-3.108632	4.690152	1.097700
1	-2.807481	3.725132	-0.378676
1	-4.455092	3.777579	0.344904

.....
2CH10_Pd-Ag

Number of imaginary frequencies : 1
 Imaginary frequency : -1704.6012 cm(-1)

Electronic energy : -1701.7602424
 Zero-point correction= 0.373936 (hartree/particle)
 Thermal correction to Energy= 0.408352

Thermal correction to Enthalpy= 0.409297
 Thermal correction to Gibbs Free Energy= 0.304595
 Sum of electronic and zero-point Energies= -1701.386306
 Sum of electronic and thermal Energies= -1701.351890
 Sum of electronic and thermal Enthalpies= -1701.350946
 Sum of electronic and thermal Free Energies= -1701.455647

 Cartesian Coordinates

6	-2.075937	-1.654074	-0.332702
6	-0.874696	-2.396552	-0.455928
6	-0.868614	-3.658651	-1.029926
6	-2.062912	-4.189041	-1.511480
6	-3.251397	-3.460852	-1.438512
6	-3.256663	-2.192074	-0.874337
6	0.388462	-1.732905	-0.066723
7	0.149894	-0.449334	0.286527
46	-1.544904	0.383587	-0.400217
8	-1.005454	2.498926	-0.487137
6	-0.006327	3.151501	-0.802005
6	-0.061780	4.620374	-1.017960
8	1.494588	-2.305674	-0.082603
8	1.282639	0.326220	0.412474
6	1.384546	0.887988	1.730830
8	-3.374357	1.125672	-1.175241
6	-4.409373	1.364185	-0.528027
8	-4.632778	0.986678	0.691431
6	-5.518017	2.142333	-1.142363
8	1.190295	2.642304	-0.970548
8	-3.041122	-0.651948	1.930253
6	-2.222615	-0.018002	2.741076
6	-1.381251	-0.907567	3.609833
8	-2.145132	1.208281	2.782217
1	0.455865	1.408966	1.993493
1	1.601045	0.094315	2.455131
1	2.221665	1.589650	1.677326
1	0.068542	-4.202362	-1.124148
1	-2.066085	-5.177912	-1.963739
1	-4.174397	-3.890551	-1.819806
1	-4.192687	-1.642260	-0.783386
1	-2.402339	-1.151204	0.806084
1	-5.609083	3.098289	-0.614657
1	-5.322841	2.325683	-2.199764
1	-6.463970	1.608078	-1.011698
1	-1.090447	4.977842	-0.964221
1	0.545932	5.116471	-0.253516
1	0.378662	4.864667	-1.989842
1	1.220209	1.692163	-0.701386
1	-3.910773	0.411089	1.127653
1	-2.028868	-1.522719	4.244699
1	-0.805085	-1.601247	2.983687
1	-0.702675	-0.322590	4.235428
47	3.422996	-1.115584	-0.047045
8	5.484285	-0.308693	-0.025652
6	5.286152	0.948278	-0.162796
8	4.158709	1.476398	-0.257114
6	6.527276	1.803273	-0.247097
1	6.296456	2.857143	-0.071790
1	7.284254	1.460687	0.464770
1	6.957662	1.703980	-1.250837

2CH11_Pd-Ag

Number of imaginary frequencies : 1

Imaginary frequency : -562.7437 cm(-1)

Electronic energy : -1472.7620895
Zero-point correction= 0.312083 (hartree/particle)
Thermal correction to Energy= 0.340329
Thermal correction to Enthalpy= 0.341273
Thermal correction to Gibbs Free Energy= 0.251223
Sum of electronic and zero-point Energies= -1472.450007
Sum of electronic and thermal Energies= -1472.421760
Sum of electronic and thermal Enthalpies= -1472.420816
Sum of electronic and thermal Free Energies= -1472.510866

Cartesian Coordinates

1 -4.730723 -1.376669 -1.127434
6 -4.109744 -2.221722 -0.806413
1 -4.151719 -3.010382 -1.559895
1 -4.521869 -2.583727 0.140780
6 -2.702582 -1.742355 -0.599155
8 -2.561335 -0.868784 0.333346
8 -1.790477 -2.192813 -1.324509
47 0.315269 -1.541438 -1.081515
46 -0.793222 0.284572 0.693178
8 -0.424538 -0.710561 2.487083
6 0.633491 -1.319007 2.772941
6 0.770279 -1.906599 4.137224
1 1.602597 -1.412917 4.650597
1 1.020389 -2.969077 4.056119
1 -0.147004 -1.775966 4.713321
8 1.640608 -1.498895 1.997439
1 1.631491 -1.081960 0.978550
6 2.182585 -0.555080 -0.444601
6 3.123781 -1.394991 -1.078157
1 3.006143 -2.477605 -0.997667
6 4.221650 -0.907963 -1.787026
1 4.918612 -1.595754 -2.262983
6 4.421533 0.463834 -1.867123
1 5.272822 0.866927 -2.412036
6 3.546851 1.325111 -1.215315
1 3.728939 2.396979 -1.222131
6 2.437328 0.839465 -0.514665
1 -3.230213 0.652287 -0.216523
8 -3.411836 1.417344 -0.824100
6 -2.304040 1.878579 -1.346791
6 -2.485763 2.976122 -2.326024
1 -2.566179 3.914546 -1.762271
1 -1.617765 3.043059 -2.983798
1 -3.407478 2.843987 -2.897034
8 -1.171737 1.478428 -1.036262
8 2.115286 3.069282 0.258585
6 1.711449 1.903826 0.267486
7 0.718093 1.502825 1.135488
8 0.269112 2.506408 1.974468
6 -0.609672 3.446135 1.356925
1 -0.698796 4.273975 2.065492
1 -0.204522 3.813293 0.407904
1 -1.604335 3.001106 1.201384

2CH12_Pd-Ag

Number of imaginary frequencies : 1
Imaginary frequency : -69.2070 cm(-1)

Electronic energy : -1701.7509779
 Zero-point correction= 0.379696 (hartree/particle)
 Thermal correction to Energy= 0.412966
 Thermal correction to Enthalpy= 0.413911
 Thermal correction to Gibbs Free Energy= 0.314275
 Sum of electronic and zero-point Energies= -1701.371281
 Sum of electronic and thermal Energies= -1701.338012
 Sum of electronic and thermal Enthalpies= -1701.337067
 Sum of electronic and thermal Free Energies= -1701.436703

.....
 Cartesian Coordinates

6	-0.034372	3.944526	-1.716596
6	0.127951	4.258643	-0.370352
6	-0.260332	3.340282	0.598917
6	-0.806373	2.120572	0.196107
6	-0.974206	1.734297	-1.158792
6	-0.561331	2.707966	-2.092974
6	-1.232411	1.174928	1.256385
8	-0.472165	0.658900	2.122763
46	1.076987	-0.485728	1.261588
8	-0.543980	-1.767665	0.752971
6	-0.596855	-2.862897	0.182453
6	0.276240	-4.026206	0.464318
47	0.434482	0.073128	-1.509584
8	2.630787	1.293036	-0.627263
6	2.924000	1.537022	0.545417
6	3.880889	2.646815	0.888465
7	-2.537423	0.920459	1.253647
8	-3.034297	-0.153146	1.944265
6	-3.669938	0.277844	3.149467
8	1.823558	-1.722837	-1.573653
6	2.612003	-2.053155	-0.666657
8	2.556871	-1.693490	0.565883
6	3.761285	-2.969518	-0.980967
8	2.442785	0.937321	1.594850
8	-1.502930	-3.065956	-0.746127
8	-2.661937	-0.574240	-1.445583
6	-3.942564	-0.387465	-1.147917
6	-4.736474	-1.650789	-1.162995
8	-4.400573	0.705193	-0.846945
1	-0.640574	2.489796	-3.159544
1	0.270162	4.661062	-2.478046
1	0.553472	5.215620	-0.075308
1	-0.143258	3.564996	1.659123
1	-3.166213	1.284105	0.528650
1	-0.347359	-4.881611	0.745934
1	0.810924	-4.309561	-0.450009
1	0.981522	-3.794812	1.264126
1	4.654466	2.715015	0.119028
1	3.318016	3.587680	0.885566
1	4.332975	2.515624	1.874206
1	3.538204	-3.565141	-1.869721
1	4.646958	-2.357707	-1.188092
1	3.991991	-3.618022	-0.131502
1	-4.047622	-0.633203	3.619453
1	-2.946806	0.766508	3.813188
1	-4.503843	0.956552	2.931909
1	-2.082107	0.297533	-1.401232
1	-1.955500	-2.207749	-0.945099
1	-4.506494	-2.208122	-0.245285
1	-5.804721	-1.427507	-1.176358
1	-4.464302	-2.281943	-2.014064

Conformational and Configurational Study of Reductive Elimination (RE)

Monometallic Reductive Elimination (Pd)

2RE1_Pd

Number of imaginary frequencies : 1
Imaginary frequency : -285.9995 cm(-1)

Electronic energy : -1341.420413
Zero-point correction= 0.355293 (hartree/particle)
Thermal correction to Energy= 0.384431
Thermal correction to Enthalpy= 0.385375
Thermal correction to Gibbs Free Energy= 0.293475
Sum of electronic and zero-point Energies= -1341.065120
Sum of electronic and thermal Energies= -1341.035982
Sum of electronic and thermal Enthalpies= -1341.035038
Sum of electronic and thermal Free Energies= -1341.126938

Cartesian Coordinates

6	0.404339	2.570369	1.099810
8	0.042881	3.669126	1.504751
7	-0.060029	1.359064	1.573911
8	-1.238232	1.471976	2.266156
6	-1.206925	0.659035	3.437706
1	-0.906020	-0.367380	3.194651
1	-0.511373	1.085046	4.169905
1	-2.223996	0.664769	3.837503
6	1.432759	2.344348	0.058792
6	2.141454	3.427296	-0.460101
6	2.989663	3.243931	-1.541098
6	3.103824	1.981907	-2.125983
6	2.398878	0.894304	-1.623447
6	1.582994	1.065460	-0.506452
1	1.985024	4.409284	-0.017424
1	3.548746	4.083742	-1.946044
1	3.755940	1.837629	-2.984498
1	2.512154	-0.081973	-2.085871
46	-0.092336	-0.009349	0.026394
53	-0.449243	-1.593615	-2.228323
6	1.831873	-0.636837	0.682212
6	2.399147	-1.721380	0.006599
6	2.239687	-0.341780	1.983915
6	3.341698	-2.519643	0.648026
1	2.116440	-1.957134	-1.014864
6	3.194167	-1.143216	2.607095
1	1.824530	0.508317	2.515168
6	3.743441	-2.237140	1.949403
1	3.765153	-3.366854	0.112560
1	3.502543	-0.899745	3.621873
1	4.483944	-2.861645	2.443627
6	-2.978297	1.756798	-0.652791
8	-1.845685	1.397047	-0.947387
8	-3.404208	1.882628	0.593944
1	-2.666508	1.686802	1.218766
6	-4.023091	2.096185	-1.658049
8	-1.962764	-1.004835	0.941267
6	-1.959914	-2.136178	1.419089
8	-1.002089	-3.019426	1.195504
1	-0.369401	-2.666981	0.536437
6	-3.023328	-2.643683	2.323082
1	-3.733933	-1.849070	2.554748

1	-2.569915	-3.030477	3.241851
1	-3.542729	-3.478404	1.840187
1	-4.863666	1.401773	-1.550523
1	-3.614709	2.025840	-2.666916
1	-4.408118	3.103902	-1.472252

2RE2_Pd

Number of imaginary frequencies : 1
Imaginary frequency : -263.8446 cm(-1)

Electronic energy : -883.4321368
Zero-point correction= 0.226614 (hartree/particle)
Thermal correction to Energy= 0.244604
Thermal correction to Enthalpy= 0.245548
Thermal correction to Gibbs Free Energy= 0.178332
Sum of electronic and zero-point Energies= -883.205523
Sum of electronic and thermal Energies= -883.187533
Sum of electronic and thermal Enthalpies= -883.186589
Sum of electronic and thermal Free Energies= -883.253805

Cartesian Coordinates

6	2.418475	-1.409896	-0.137300
8	3.290283	-2.258079	-0.241030
7	1.583427	-1.012908	-1.184833
8	1.373461	-1.998922	-2.092767
6	1.265181	-1.442725	-3.408557
1	0.472170	-0.685727	-3.443128
1	2.221479	-0.998052	-3.704896
1	1.013649	-2.278890	-4.063643
6	2.100305	-0.643969	1.082104
6	2.880234	-0.777325	2.231063
6	2.456538	-0.203319	3.419225
6	1.235693	0.472395	3.471353
6	0.439214	0.606328	2.338026
6	0.895286	0.071360	1.138301
1	3.793184	-1.366781	2.176481
1	3.061835	-0.297424	4.316981
1	0.896441	0.908981	4.407959
1	-0.501376	1.146904	2.392557
46	-0.257316	-0.488095	-0.468238
53	-2.864017	-0.589675	0.310665
6	0.403358	1.502339	-0.388138
6	-0.582239	2.408696	-0.001142
6	1.521281	1.905517	-1.109828
6	-0.445836	3.743776	-0.371372
1	-1.447527	2.092226	0.573829
6	1.643955	3.249577	-1.457290
1	2.285697	1.194237	-1.405861
6	0.664542	4.167344	-1.095352
1	-1.218757	4.452259	-0.082106
1	2.517125	3.569933	-2.021628
1	0.765623	5.213264	-1.375205

Bimetallic Reductive Elimination (Pd-Ag)

2RE1_Pd-Ag

Number of imaginary frequencies : 1
Imaginary frequency : -220.9112 cm(-1)

Electronic energy : -1944.6542771
 Zero-point correction= 0.473242 (hartree/particle)
 Thermal correction to Energy= 0.513966
 Thermal correction to Enthalpy= 0.514910
 Thermal correction to Gibbs Free Energy= 0.398673
 Sum of electronic and zero-point Energies= -1944.181035
 Sum of electronic and thermal Energies= -1944.140311
 Sum of electronic and thermal Enthalpies= -1944.139367
 Sum of electronic and thermal Free Energies= -1944.255604

.....
 Cartesian Coordinates

6	-6.197803	-0.496914	-0.027560
6	-5.459155	-1.038342	1.019070
6	-4.084162	-0.828710	1.100093
6	-3.467185	-0.081691	0.105053
6	-4.180561	0.477415	-0.948859
6	-5.556507	0.255421	-1.004559
46	-1.402388	-0.420622	-0.125666
53	-0.074270	-2.512916	-1.507533
47	1.576500	-0.606996	-0.235898
8	3.449621	0.045753	1.599504
6	3.889401	-1.039380	1.995306
6	5.312787	-1.429124	1.824940
6	-1.917337	1.253660	0.961924
6	-1.668509	2.411149	0.228007
6	-1.619278	3.640663	0.880335
6	-1.790460	3.697194	2.259094
6	-1.998542	2.525911	2.984614
6	-2.068578	1.290523	2.340372
6	-1.368730	2.298952	-1.221387
7	-1.314950	0.994203	-1.593901
8	-1.073475	0.731406	-2.912795
6	0.300844	0.904646	-3.262668
8	-1.182423	3.263980	-1.965880
8	-1.368473	-1.719901	1.557095
6	-0.313383	-1.752076	2.264176
6	-0.276624	-2.767225	3.369874
8	0.691609	-1.012811	2.087292
8	3.115016	-1.933442	2.560142
1	-1.424255	4.536494	0.292209
1	-2.261189	0.387229	2.914234
1	-2.122316	2.568921	4.064536
1	-1.750658	4.654379	2.773537
1	0.933110	0.168400	-2.745492
1	0.350291	0.723079	-4.339868
1	0.629543	1.925097	-3.037930
1	-3.515685	-1.266508	1.913922
1	-3.696846	1.055140	-1.728823
1	-5.947199	-1.631207	1.789920
1	-6.120467	0.679779	-1.832483
1	-7.271116	-0.662773	-0.081958
1	0.104805	-2.309242	4.287824
1	-1.258391	-3.210945	3.547271
1	0.422392	-3.562948	3.083112
1	5.481720	-1.611444	0.755523
1	5.959017	-0.597624	2.120412
1	5.565574	-2.329633	2.387082
1	2.168068	-1.592607	2.533631
8	3.647117	-0.075166	-1.500790
8	1.544706	1.821623	-0.286467
6	1.606436	2.589511	0.665069
6	4.057604	1.079164	-1.436528

8	1.613403	2.182468	1.926623
8	4.496391	1.625045	-0.311648
6	4.097729	2.020080	-2.589443
1	3.413291	2.851650	-2.380293
1	5.100055	2.446069	-2.701023
1	3.796418	1.514280	-3.508443
6	1.732540	4.063481	0.502158
1	1.418069	4.605792	1.396817
1	2.791865	4.286744	0.318572
1	1.163573	4.382944	-0.375685
1	1.674159	1.204925	1.957127
1	4.300370	1.009048	0.441582

2RE2_Pd-Ag

Number of imaginary frequencies : 1
 Imaginary frequency : -165.0513 cm(-1)

Electronic energy : -1715.6529075
 Zero-point correction= 0.407476 (hartree/particle)
 Thermal correction to Energy= 0.443696
 Thermal correction to Enthalpy= 0.444640
 Thermal correction to Gibbs Free Energy= 0.337076
 Sum of electronic and zero-point Energies= -1715.245432
 Sum of electronic and thermal Energies= -1715.209212
 Sum of electronic and thermal Enthalpies= -1715.208268
 Sum of electronic and thermal Free Energies= -1715.315831

 Cartesian Coordinates

6	5.703405	-1.385816	0.348051
6	5.240005	-0.685071	-0.760987
6	3.904865	-0.297358	-0.845477
6	3.045250	-0.640780	0.189605
6	3.484071	-1.328102	1.317074
6	4.826888	-1.702919	1.378208
46	0.996464	-0.623897	-0.242902
53	-1.039329	-2.331670	-1.206552
47	-1.756818	0.383220	-0.470408
8	-1.731839	2.647812	0.352643
6	-1.271248	3.684779	-0.112883
6	-1.366133	4.995518	0.592067
6	1.662242	1.132821	0.601946
6	1.285936	1.210709	1.938910
6	1.282363	2.444373	2.582287
6	1.637229	3.586277	1.872202
6	2.010719	3.488738	0.532684
6	2.047056	2.252200	-0.116081
6	0.889768	-0.042842	2.621528
7	0.527966	-0.982090	1.698647
8	0.461219	-2.275838	2.157724
6	-0.833457	-2.580250	2.669269
8	0.871457	-0.207496	3.839262
8	1.385226	-0.073278	-2.247349
6	0.635112	0.789816	-2.810727
6	1.055151	1.228504	-4.184587
8	-0.390821	1.299469	-2.299535
8	-0.695093	3.768826	-1.297626
1	0.988086	2.488472	3.629399
1	2.366167	2.189886	-1.154135
1	2.283420	4.383527	-0.023954
1	1.627316	4.557045	2.362349
1	-1.617714	-2.245832	1.978378

1	-0.871692	-3.668210	2.770368
1	-0.979663	-2.108037	3.648624
1	3.547025	0.242520	-1.716509
1	2.828729	-1.599025	2.138040
1	5.916305	-0.429460	-1.574051
1	5.175973	-2.252072	2.250088
1	6.748049	-1.681683	0.408989
1	1.930059	0.679179	-4.537785
1	0.221878	1.090978	-4.881052
1	1.281737	2.300897	-4.158180
1	-1.409798	4.837042	1.671761
1	-0.535897	5.655133	0.326601
1	-2.296467	5.484852	0.278957
1	-0.652553	2.877779	-1.736168
8	-4.012738	0.393577	0.382530
6	-4.570457	-0.538591	0.945808
8	-4.131937	-1.791592	0.894714
6	-5.804209	-0.403400	1.765145
1	-6.177914	0.620053	1.722098
1	-6.565504	-1.103425	1.406992
1	-5.577942	-0.670997	2.803156
1	-3.338958	-1.851043	0.322277

2RE3_Pd-Ag

Number of imaginary frequencies : 1
 Imaginary frequency : -222.0651 cm(-1)

Electronic energy : -1486.6586579
 Zero-point correction= 0.343486 (hartree/particle)
 Thermal correction to Energy= 0.373966
 Thermal correction to Enthalpy= 0.374910
 Thermal correction to Gibbs Free Energy= 0.279616
 Sum of electronic and zero-point Energies= -1486.315172
 Sum of electronic and thermal Energies= -1486.284692
 Sum of electronic and thermal Enthalpies= -1486.283748
 Sum of electronic and thermal Free Energies= -1486.379042

 Cartesian Coordinates

6	0.444676	-2.724428	-2.756477
6	0.661386	-3.024046	-1.416077
6	0.039521	-2.284459	-0.413407
6	-0.797598	-1.235659	-0.778403
6	-1.042077	-0.921530	-2.115758
6	-0.400219	-1.676157	-3.098995
46	-1.119433	0.335309	0.578253
7	-2.619447	1.077208	-0.529573
8	-2.280384	1.977148	-1.498768
6	-2.776458	3.279147	-1.183669
8	0.292103	-0.563466	1.976707
6	1.115589	-0.015498	2.724554
8	1.218962	1.277091	2.874727
6	-2.446760	-1.241724	0.667184
6	-3.650784	-0.940886	0.040280
6	-4.782112	-1.703655	0.305034
6	-4.699238	-2.740854	1.227846
6	-3.496369	-3.001289	1.881776
6	-2.347474	-2.258799	1.602764
6	-3.659890	0.230443	-0.858593
8	-4.485196	0.466530	-1.729028
8	-0.462459	2.359404	1.136968
6	0.105532	3.145650	0.289220

8	0.700564	2.768664	-0.739415
47	1.660648	0.726461	-0.735750
53	3.818666	-0.864699	-0.257569
6	2.069833	-0.807965	3.538211
6	0.060315	4.612947	0.604729
1	-5.712405	-1.460020	-0.205236
1	-1.413202	-2.480508	2.112188
1	-3.441753	-3.799133	2.619225
1	-5.576382	-3.343343	1.449604
1	-2.514139	3.560201	-0.156260
1	-2.307142	3.960543	-1.898202
1	-3.866730	3.302842	-1.302779
1	0.561036	1.761756	2.302558
1	2.034002	-1.860064	3.252381
1	3.080174	-0.410454	3.396055
1	1.817249	-0.697875	4.598807
1	-0.718639	4.847313	1.333793
1	1.030112	4.905794	1.024377
1	-0.084835	5.190761	-0.312494
1	0.241487	-2.518604	0.626464
1	-1.683655	-0.102897	-2.425845
1	1.329588	-3.833483	-1.131073
1	-0.576253	-1.426670	-4.142941
1	0.935824	-3.305811	-3.532689

2RE4_Pd-Ag

Number of imaginary frequencies : 1
Imaginary frequency : -166.4579 cm(-1)

Electronic energy : -1715.6493543
Zero-point correction= 0.408686 (hartree/particle)
Thermal correction to Energy= 0.444431
Thermal correction to Enthalpy= 0.445375
Thermal correction to Gibbs Free Energy= 0.338831
Sum of electronic and zero-point Energies= -1715.240668
Sum of electronic and thermal Energies= -1715.204923
Sum of electronic and thermal Enthalpies= -1715.203979
Sum of electronic and thermal Free Energies= -1715.310523

Cartesian Coordinates

46	1.388062	0.156786	0.340291
8	1.946627	1.878699	-0.925198
6	2.513566	2.921867	-0.565828
6	3.023166	3.906290	-1.555992
6	2.772709	-1.158354	-0.441015
6	2.854986	-2.322475	0.310287
6	3.940948	-3.176000	0.143193
6	4.941669	-2.832220	-0.758198
6	4.852214	-1.645316	-1.483280
6	3.754158	-0.792724	-1.345110
6	1.758882	-2.588741	1.262388
8	1.480955	-3.668772	1.762439
47	-1.764247	0.233103	0.800116
8	1.343641	1.538510	2.032770
6	0.293904	2.024230	2.608724
6	0.566869	3.167670	3.545551
7	1.106535	-1.409605	1.559966
8	-0.155078	-1.552478	2.073632
6	-0.166743	-1.363508	3.493131
8	2.731496	3.250242	0.676322
8	-0.862090	1.606411	2.452315

1	3.982412	-4.091659	0.730755
1	3.688611	0.116805	-1.936375
1	5.642152	-1.375273	-2.180732
1	5.796913	-3.487985	-0.898688
1	0.352857	-0.440263	3.770485
1	-1.221532	-1.302652	3.774471
1	0.307421	-2.223738	3.980346
1	2.307189	2.589166	1.306995
1	2.580193	4.888156	-1.359591
1	4.106122	4.011513	-1.428329
1	2.799496	3.587023	-2.575190
1	-0.355369	3.526405	4.006485
1	1.270185	2.848161	4.321875
1	1.043939	3.987254	2.995098
6	0.718420	-0.883854	-1.331362
6	0.867118	-0.261828	-2.567693
6	-0.177828	-1.932831	-1.144400
6	0.067911	-0.677366	-3.628813
1	1.576117	0.547582	-2.709098
6	-0.967619	-2.331776	-2.225384
1	-0.307487	-2.445470	-0.196240
6	-0.850790	-1.709994	-3.460815
1	0.170105	-0.182303	-4.592569
1	-1.686272	-3.134451	-2.076411
1	-1.471209	-2.030148	-4.294169
53	-4.085858	-0.824287	-0.237084
8	-0.980188	2.261330	-0.599441
6	-1.220492	2.322084	-1.796863
8	-2.072145	1.515411	-2.416415
6	-0.596438	3.304816	-2.727334
1	0.080838	3.963631	-2.181359
1	-0.055982	2.775553	-3.520823
1	-1.378410	3.896396	-3.214894
1	-2.500267	0.908106	-1.773664

2RE5_Pd-Ag

Number of imaginary frequencies : 1
 Imaginary frequency : -174.1632 cm(-1)

Electronic energy : -1944.634891
 Zero-point correction= 0.473698 (hartree/particle)
 Thermal correction to Energy= 0.514460
 Thermal correction to Enthalpy= 0.515405
 Thermal correction to Gibbs Free Energy= 0.399419
 Sum of electronic and zero-point Energies= -1944.161192
 Sum of electronic and thermal Energies= -1944.120431
 Sum of electronic and thermal Enthalpies= -1944.119486
 Sum of electronic and thermal Free Energies= -1944.235472

 Cartesian Coordinates

46	1.653321	-0.171995	0.534125
8	2.231045	1.940482	0.893778
6	2.446753	2.497676	1.982048
6	3.220859	3.764938	2.053585
6	3.246125	-0.439828	-0.739333
6	3.506766	-1.791576	-0.932980
6	4.728893	-2.191546	-1.463126
6	5.681675	-1.227661	-1.773199
6	5.409423	0.121820	-1.555263

6	4.177921	0.537924	-1.044462
6	2.438411	-2.744239	-0.575812
8	2.347658	-3.899929	-0.963618
47	-1.441974	-0.335694	-0.151680
8	0.875776	-0.197592	2.580878
6	-0.372600	-0.277571	2.921814
6	-0.678856	0.260944	4.291514
7	1.545268	-2.163300	0.305086
8	0.308532	-2.735229	0.317366
6	0.098208	-3.498813	1.508283
8	2.055623	2.028523	3.131329
8	-1.274835	-0.729061	2.207021
1	4.912846	-3.253321	-1.618622
1	3.968352	1.593769	-0.893740
1	6.160787	0.871349	-1.794015
1	6.641926	-1.526249	-2.185825
1	0.339146	-2.908407	2.399119
1	-0.963155	-3.760998	1.502280
1	0.718898	-4.403047	1.475368
1	1.587810	1.137207	3.012746
1	2.823232	4.423173	2.830646
1	4.252409	3.513887	2.330010
1	3.234746	4.266300	1.084183
1	-1.669404	-0.056149	4.625646
1	0.083580	-0.037729	5.017113
1	-0.665626	1.357801	4.226897
6	1.225167	0.172896	-1.475848
6	1.222404	1.513602	-1.851195
6	0.601903	-0.807162	-2.250560
6	0.553737	1.880414	-3.016717
1	1.713692	2.272145	-1.249443
6	-0.051928	-0.411244	-3.419486
1	0.596110	-1.859946	-1.987387
6	-0.078230	0.922556	-3.804093
1	0.532002	2.930467	-3.300510
1	-0.553829	-1.169270	-4.016212
1	-0.597294	1.217592	-4.712689
53	-3.494702	0.787102	-1.736935
8	-0.929610	1.988301	1.158230
6	-0.814938	3.103654	0.676312
8	-1.211859	3.411611	-0.554184
6	-0.223357	4.270458	1.390976
1	0.148616	3.960494	2.370905
1	0.581037	4.709387	0.789776
1	-0.986377	5.045767	1.519852
1	-1.666996	2.636128	-0.951852
8	-2.865625	-2.542928	0.415412
6	-3.632421	-2.263766	1.322962
8	-4.373690	-1.157114	1.331435
6	-3.817111	-3.092508	2.547919
1	-3.107632	-2.734713	3.304635
1	-4.826027	-2.993242	2.955532
1	-3.590859	-4.138159	2.327669
1	-4.182604	-0.640419	0.517878

Reaction 3

Silyl-Alkyne

Number of imaginary frequencies : 0

Electronic energy : -734.0450444
Zero-point correction= 0.292018
Thermal correction to Energy= 0.310689
Thermal correction to Enthalpy= 0.311633
Thermal correction to Gibbs Free Energy= 0.245335
Sum of electronic and zero-point Energies= -733.753027
Sum of electronic and thermal Energies= -733.734355
Sum of electronic and thermal Enthalpies= -733.733411
Sum of electronic and thermal Free Energies= -733.799709

Cartesian Coordinates

6	1.920894	0.002001	-0.141712
6	0.701557	-0.003383	-0.148286
14	-1.154124	0.013264	-0.132705
6	-1.665042	1.551771	-1.122098
6	-1.779516	-1.530901	-1.057121
6	-1.672535	0.006106	1.692660
1	-2.772917	-0.069899	1.703448
1	-1.320325	1.306715	-2.142465
1	-1.880996	-1.198727	-2.104886
6	-0.800498	-2.703171	-1.031705
1	0.170714	-2.443755	-1.468405
1	-0.611194	-3.050672	-0.006454
1	-1.200871	-3.559489	-1.593057
6	-3.159342	-1.980345	-0.573429
1	-3.553212	-2.784531	-1.210470
1	-3.114859	-2.378818	0.449361
1	-3.903294	-1.172896	-0.574513
6	-3.181771	1.726142	-1.169811
1	-3.461635	2.600414	-1.774625
1	-3.687383	0.856029	-1.608073
1	-3.604674	1.884517	-0.167036
6	-0.973356	2.846132	-0.704243
1	0.113666	2.726949	-0.613014
1	-1.158996	3.642232	-1.439139
1	-1.346144	3.212762	0.261009
6	-1.268680	1.283642	2.425596
1	-1.496036	1.205342	3.498494
1	-0.189142	1.474316	2.338769
1	-1.791674	2.170370	2.048279
6	-1.097699	-1.213714	2.413502
1	-1.403586	-1.223654	3.469240
1	-1.422479	-2.163722	1.970627
1	0.001315	-1.202135	2.395791
35	3.761354	0.002208	-0.145004

Silver Triflate

Electronic energy : -2214.0676636
Zero-point correction= 0.060004
Thermal correction to Energy= 0.079931
Thermal correction to Enthalpy= 0.080875
Thermal correction to Gibbs Free Energy= 0.003389
Sum of electronic and zero-point Energies= -2214.007659
Sum of electronic and thermal Energies= -2213.987733
Sum of electronic and thermal Enthalpies= -2213.986789
Sum of electronic and thermal Free Energies= -2214.064274

Cartesian Coordinates

47	0.000136	1.454842	-0.000872
----	----------	----------	-----------

8	2.184585	1.243047	-0.025828
16	2.814444	0.000023	0.521835
8	2.184645	-1.243231	-0.025396
8	3.065319	0.000266	1.950535
6	4.437749	0.000039	-0.334728
9	4.248009	0.000202	-1.641031
9	5.110798	1.079384	0.017272
9	5.110793	-1.079379	0.017078
47	0.000128	-1.454975	-0.000866
8	-3.071230	0.000254	-1.950799
16	-2.815824	0.000014	-0.522911
8	-2.184203	1.243044	0.022704
8	-2.184282	-1.243249	0.022285
6	-4.436645	0.000049	0.338389
9	-5.110744	1.079375	-0.011664
9	-5.110753	-1.079340	-0.011471
9	-4.243171	0.000210	1.644143

Silver_Acetate

Electronic energy : -748.4010127
 Zero-point correction= 0.103564
 Thermal correction to Energy= 0.116829
 Thermal correction to Enthalpy= 0.117773
 Thermal correction to Gibbs Free Energy= 0.059878
 Sum of electronic and zero-point Energies= -748.297449
 Sum of electronic and thermal Energies= -748.284184
 Sum of electronic and thermal Enthalpies= -748.283240
 Sum of electronic and thermal Free Energies= -748.341135

 Cartesian Coordinates

1	-4.571548	-0.562933	0.880646
6	-4.217632	-0.017185	0.000048
6	-2.709705	0.004223	-0.000053
1	-4.571777	-0.565516	-0.878836
1	-4.634962	0.991099	-0.001295
8	-2.148670	-1.128268	0.000033
8	-2.152351	1.136666	-0.000082
47	0.000002	1.392480	0.000012
47	-0.000002	-1.386182	-0.000019
1	4.571738	-0.565060	-0.879145
6	4.217631	-0.017192	0.000040
6	2.709705	0.004220	-0.000029
1	4.571585	-0.563399	0.880329
1	4.634966	0.991086	-0.000821
8	2.148667	-1.128268	0.000040
8	2.152355	1.136665	-0.000065

Phenyl-amide

Electronic energy : -479.2382814
 Zero-point correction= 0.182872
 Thermal correction to Energy= 0.193194
 Thermal correction to Enthalpy= 0.194138
 Thermal correction to Gibbs Free Energy= 0.147043
 Sum of electronic and zero-point Energies= -479.055409
 Sum of electronic and thermal Energies= -479.045087
 Sum of electronic and thermal Enthalpies= -479.044143
 Sum of electronic and thermal Free Energies= -479.091238

 Cartesian Coordinates

6	1.226334	1.156876	-0.435260
6	2.600702	0.960390	-0.518516
6	0.401148	0.163157	0.096180

6	0.971275	-1.031865	0.542522
6	2.343612	-1.223103	0.447137
8	-1.575628	-1.666397	-0.580676
1	2.774445	-2.157657	0.800066
1	0.791377	2.085958	-0.798029
1	3.228824	1.744643	-0.935431
6	3.166268	-0.231389	-0.080275
1	4.240379	-0.387255	-0.147231
7	-0.998789	0.400701	0.210799
6	-1.425570	1.744505	0.575866
1	-0.639438	2.220643	1.166832
1	-1.635477	2.379441	-0.296506
1	-2.322927	1.710616	1.199235
6	-1.911761	-0.557802	-0.199823
6	-3.365473	-0.156825	-0.153193
1	-3.564263	0.766901	-0.707845
1	-3.944119	-0.970274	-0.594013
1	-3.707832	-0.003724	0.877065
1	0.336370	-1.806695	0.957847

Conformational and Configurational Study of C-H activation

Bimetallic C-H activation (Pd-Ag)

3CH1_Pd-Ag

Number of imaginary frequencies : 1
The smallest frequency is : -1495.8715 cm(-1)

Electronic energy : -2902.6340408
Zero-point correction= 0.292545
Thermal correction to Energy= 0.327416
Thermal correction to Enthalpy= 0.328360
Thermal correction to Gibbs Free Energy= 0.224194
Sum of electronic and zero-point Energies= -2902.341496
Sum of electronic and thermal Energies= -2902.306625
Sum of electronic and thermal Enthalpies= -2902.305681
Sum of electronic and thermal Free Energies= -2902.409847

Cartesian Coordinates

6	3.431230	-3.081566	-0.149886
6	3.845492	-3.476594	1.116985
6	2.331685	-2.239680	-0.290833
6	1.670428	-1.735631	0.865286
1	1.765291	-0.413825	0.806079
6	2.106336	-2.181014	2.132713
8	-0.281371	-2.115894	-1.187250
1	-2.048608	0.666866	4.560043
6	-1.000994	0.880399	4.318402
6	-0.785846	0.591152	2.856317
1	-0.811497	1.936421	4.524063
1	-0.373273	0.247399	4.949636
8	-0.999154	1.492327	2.029295
8	-0.412957	-0.615599	2.614580
46	-0.341013	-1.347166	0.713298
1	1.579306	-1.809033	3.008989
1	3.947522	-3.460616	-1.027989
1	4.689191	-4.156857	1.205006
6	3.190226	-3.030282	2.263834
1	3.526145	-3.348848	3.246701
7	1.950787	-1.833262	-1.595322
6	3.007032	-1.603350	-2.589753
1	3.915282	-1.296697	-2.070586
1	3.194344	-2.501218	-3.189527
1	2.720397	-0.777223	-3.242268
6	0.648336	-1.830973	-1.975851

6	0.296680	-1.501256	-3.384955
1	0.871354	-2.082579	-4.112118
1	-0.770914	-1.681182	-3.519982
1	0.495506	-0.435582	-3.559101
47	-0.721142	1.421413	-0.216254
8	-3.684951	-1.785515	-1.634938
16	-3.062050	-0.723651	-0.864691
8	-2.173566	0.195337	-1.618693
8	-2.497206	-1.130891	0.467006
6	-4.426908	0.376948	-0.320065
9	-5.067727	0.846113	-1.380198
9	-5.275523	-0.288429	0.444667
9	-3.930709	1.400428	0.369148
8	1.330097	1.365801	-1.547474
16	2.463644	1.420188	-0.599519
8	3.754409	0.974474	-1.096438
8	2.085226	0.866133	0.760244
6	2.645530	3.205541	-0.191032
9	2.994932	3.853754	-1.288353
9	1.492205	3.688513	0.252730
9	3.573446	3.361055	0.732035

3CH2_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -1214.7637 cm(-1)

Electronic energy : -2169.7921256
 Zero-point correction= 0.314154
 Thermal correction to Energy= 0.346028
 Thermal correction to Enthalpy= 0.346972
 Thermal correction to Gibbs Free Energy= 0.249367
 Sum of electronic and zero-point Energies= -2169.477971
 Sum of electronic and thermal Energies= -2169.446098
 Sum of electronic and thermal Enthalpies= -2169.445153
 Sum of electronic and thermal Free Energies= -2169.542758

 Cartesian Coordinates

6	-1.942341	3.796623	0.139390
6	-2.010213	4.284841	1.439131
6	-1.202707	2.647498	-0.130952
6	-0.547413	1.954062	0.913107
1	-0.974997	0.659144	0.872369
6	-0.630334	2.483577	2.214756
8	1.065490	1.726166	-1.461827
1	2.562871	-1.543668	4.133293
6	1.485923	-1.504292	3.934146
6	1.278714	-1.070169	2.504777
1	1.065921	-2.500073	4.091938
1	1.046219	-0.789038	4.633957
8	1.090183	-1.926839	1.629617
8	1.349604	0.205870	2.343985
46	1.237492	0.991576	0.466880
8	3.230827	0.450822	0.051237
6	3.606007	-0.275599	-0.923056
8	2.896401	-1.046207	-1.609513
6	5.069462	-0.179709	-1.281709
1	5.162544	0.349669	-2.236661
1	5.639000	0.358556	-0.521618
1	5.482373	-1.182820	-1.423694
1	-0.119527	1.950743	3.014587
1	-2.447112	4.325783	-0.665495
1	-2.575907	5.192888	1.634527
6	-1.359741	3.631115	2.483212
1	-1.423184	4.018577	3.496687
7	-1.188277	2.146653	-1.464125
6	-2.428977	2.224034	-2.243133
1	-3.272101	2.250099	-1.552962

1	-2.449601	3.113523	-2.883857
1	-2.540065	1.326698	-2.854996
6	-0.033922	1.759143	-2.058830
6	-0.058904	1.365405	-3.498328
1	-0.543666	2.113565	-4.133111
1	0.969957	1.210218	-3.826868
1	-0.606226	0.420289	-3.606270
47	0.920366	-1.617231	-0.684386
8	-1.323178	-1.087406	-1.423461
16	-2.310971	-0.929850	-0.335383
8	-3.575283	-0.311674	-0.694436
8	-1.683442	-0.396968	0.937346
6	-2.698963	-2.650070	0.180186
9	-3.293106	-3.259300	-0.832274
9	-1.583832	-3.294726	0.486525
9	-3.504086	-2.638708	1.224976

3CH3_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -1593.9595 cm(-1)

Electronic energy : -3635.4650459
 Zero-point correction= 0.271041
 Thermal correction to Energy= 0.309023
 Thermal correction to Enthalpy= 0.309967
 Thermal correction to Gibbs Free Energy= 0.199456
 Sum of electronic and zero-point Energies= -3635.194005
 Sum of electronic and thermal Energies= -3635.156023
 Sum of electronic and thermal Enthalpies= -3635.155079
 Sum of electronic and thermal Free Energies= -3635.265590

 Cartesian Coordinates

6	-3.951279	-0.629542	-2.849388
6	-3.964244	0.430485	-3.748592
6	-2.895007	-0.770920	-1.954465
6	-1.858877	0.211534	-1.920167
1	-1.959429	0.718870	-0.718177
6	-1.901052	1.264423	-2.868104
8	-0.701275	-2.267742	-1.165363
46	0.024513	-0.389495	-1.391390
1	-1.103376	2.003431	-2.847745
1	-4.752363	-1.363180	-2.873268
1	-4.782963	0.503870	-4.460409
6	-2.948261	1.386069	-3.760290
1	-2.978965	2.214200	-4.462296
7	-2.941274	-1.829763	-1.017486
6	-4.254991	-2.239968	-0.499693
1	-4.910619	-1.368511	-0.477637
1	-4.696645	-3.029484	-1.117665
1	-4.153269	-2.592992	0.527142
6	-1.832630	-2.540673	-0.699095
6	-1.934922	-3.719521	0.203197
1	-2.751138	-4.393991	-0.069610
1	-0.984728	-4.255293	0.173852
1	-2.100824	-3.364792	1.228544
47	0.527671	-0.293502	1.566381
8	1.249171	1.797204	0.820914
16	1.108972	2.472024	-0.483182
8	0.311429	3.682966	-0.525733
8	0.811088	1.525939	-1.630818
6	2.830201	2.955357	-0.899700
9	3.269485	3.809290	0.010508
9	3.604697	1.886784	-0.911063
9	2.850764	3.531565	-2.090082
8	1.550618	-2.343081	1.105199
16	2.398410	-2.267921	-0.112271

8	2.041890	-1.105056	-0.994073
8	2.653865	-3.523054	-0.793730
6	4.009333	-1.680851	0.545399
9	3.819290	-0.554441	1.225116
9	4.514562	-2.593913	1.359380
9	4.857340	-1.455256	-0.441584
8	-2.303576	1.264452	0.450797
16	-2.725297	0.370367	1.592553
8	-1.829573	-0.799987	1.742619
8	-4.149870	0.096252	1.657017
6	-2.321042	1.435286	3.036995
9	-1.017814	1.699366	3.042173
9	-2.999049	2.561214	2.973014
9	-2.633916	0.784594	4.143523

3CH4_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -1269.9971 cm(-1)

Electronic energy : -2902.6270766
 Zero-point correction= 0.293357
 Thermal correction to Energy= 0.327973
 Thermal correction to Enthalpy= 0.328917
 Thermal correction to Gibbs Free Energy= 0.225951
 Sum of electronic and zero-point Energies= -2902.333719
 Sum of electronic and thermal Energies= -2902.299104
 Sum of electronic and thermal Enthalpies= -2902.298160
 Sum of electronic and thermal Free Energies= -2902.401125

 Cartesian Coordinates

6	3.403455	-2.618286	1.656931
6	3.033102	-2.938480	2.958117
6	2.515489	-1.932168	0.832077
6	1.250522	-1.528231	1.325096
1	1.132570	-0.204748	1.160546
6	0.905513	-1.881334	2.646548
8	0.938397	-2.092693	-1.478890
46	-0.346935	-1.482459	-0.003557
8	-2.000505	-1.890229	-1.220009
6	-2.390135	-1.296356	-2.274976
8	-1.876520	-0.291759	-2.817479
6	-3.632293	-1.884569	-2.895693
1	-3.577202	-2.976449	-2.905073
1	-4.492930	-1.605664	-2.276168
1	-3.783531	-1.500249	-3.906551
1	-0.066854	-1.568236	3.021717
1	4.375417	-2.930336	1.283790
1	3.729649	-3.492318	3.582973
6	1.788893	-2.566985	3.462927
1	1.514867	-2.813132	4.485106
7	2.943336	-1.581841	-0.479682
6	4.354147	-1.214480	-0.662628
1	4.729944	-0.794905	0.270791
1	4.959604	-2.081781	-0.950237
1	4.446712	-0.437276	-1.422370
6	2.139071	-1.735694	-1.556223
6	2.690460	-1.486288	-2.919900
1	3.650170	-1.983828	-3.087413
1	1.960844	-1.833744	-3.653067
1	2.836881	-0.406939	-3.057015
47	-0.367862	0.909660	-1.730533
8	1.847470	1.390542	-1.216203
16	2.163537	1.724406	0.194573
8	3.562831	1.614503	0.564939
8	1.192390	1.085479	1.162752
6	1.664657	3.486824	0.348577

9	2.424208	4.207377	-0.459278
9	0.397997	3.607907	-0.012362
9	1.821455	3.895992	1.590126
8	-1.882058	1.359469	0.164087
16	-2.161428	0.666888	1.428103
8	-1.945736	1.388249	2.668902
8	-1.611484	-0.750135	1.481804
6	-3.964477	0.322805	1.355481
9	-4.624639	1.471108	1.351231
9	-4.259934	-0.349557	0.254135
9	-4.331692	-0.386945	2.410524

3CH5_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -1329.3402 cm(-1)

Electronic energy : -2169.7879165
 Zero-point correction= 0.314998
 Thermal correction to Energy= 0.346435
 Thermal correction to Enthalpy= 0.347379
 Thermal correction to Gibbs Free Energy= 0.250655
 Sum of electronic and zero-point Energies= -2169.472918
 Sum of electronic and thermal Energies= -2169.441482
 Sum of electronic and thermal Enthalpies= -2169.440537
 Sum of electronic and thermal Free Energies= -2169.537261

 Cartesian Coordinates

6	-4.288050	0.276872	-1.677296
6	-4.717218	1.599931	-1.729383
6	-3.049534	-0.020824	-1.123578
6	-2.244244	1.007636	-0.553562
1	-2.030254	0.615013	0.626275
6	-2.710506	2.339194	-0.645567
8	-0.558396	-0.956105	-1.811809
46	-0.201426	0.816991	-0.823732
1	-2.082354	3.125994	-0.233721
1	-4.905709	-0.515997	-2.093062
1	-5.676016	1.824307	-2.191037
6	-3.935146	2.635140	-1.216927
1	-4.286144	3.662036	-1.267659
7	-2.652320	-1.376594	-1.013827
6	-3.632277	-2.355811	-0.533922
1	-4.456660	-1.819902	-0.060110
1	-4.023835	-2.973106	-1.349759
1	-3.171105	-2.996949	0.223299
6	-1.403386	-1.766546	-1.365917
6	-1.021282	-3.200137	-1.249266
1	-1.738282	-3.870843	-1.733130
1	-0.028939	-3.323880	-1.686796
1	-0.967199	-3.462231	-0.184111
1	-3.044080	-1.497687	4.175753
6	-3.310230	-1.721260	3.135757
6	-2.264199	-1.109167	2.235607
1	-3.332905	-2.809190	3.027441
1	-4.297189	-1.289641	2.948739
8	-1.279918	-1.825988	1.912429
8	-2.450267	0.099994	1.899984
47	0.584881	-0.574979	1.583864
8	2.006607	-1.610677	-0.062212
16	2.586847	-0.749141	-1.115748
8	1.908722	0.588642	-1.240218
8	2.902847	-1.399572	-2.376842
6	4.190839	-0.227674	-0.392601
9	3.986412	0.366468	0.775244
9	4.958709	-1.292153	-0.203579
9	4.809710	0.613675	-1.206448

1	2.228491	4.221130	1.034460
6	1.345040	3.948098	1.622853
6	0.897431	2.574631	1.199285
1	1.617037	3.948378	2.680544
1	0.571742	4.695015	1.425940
8	1.249077	1.588395	1.864024
8	0.176253	2.572813	0.131636

3CH6_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -1459.8720 cm(-1)

Electronic energy : -2169.7846479
 Zero-point correction= 0.313999
 Thermal correction to Energy= 0.345807
 Thermal correction to Enthalpy= 0.346751
 Thermal correction to Gibbs Free Energy= 0.250020
 Sum of electronic and zero-point Energies= -2169.470649
 Sum of electronic and thermal Energies= -2169.438841
 Sum of electronic and thermal Enthalpies= -2169.437897
 Sum of electronic and thermal Free Energies= -2169.534628

 Cartesian Coordinates

6	-3.883529	2.064677	-1.128743
6	-3.556520	3.413292	-1.236207
6	-2.906033	1.157155	-0.740581
6	-1.598941	1.588822	-0.415482
1	-1.289190	1.042979	0.687394
6	-1.303317	2.961279	-0.537650
8	-1.462973	-0.971766	-1.770499
46	-0.037167	0.335721	-1.041032
8	1.462892	-0.734635	-2.006973
6	1.836662	-1.918551	-1.721424
8	1.404165	-2.654491	-0.807797
6	2.952725	-2.442875	-2.589052
1	2.864009	-2.069269	-3.612079
1	3.903353	-2.078133	-2.182041
1	2.968386	-3.534999	-2.578349
1	-0.298252	3.294966	-0.288281
1	-4.887244	1.720473	-1.368639
1	-4.316829	4.117606	-1.565366
6	-2.271940	3.867078	-0.939191
1	-2.034150	4.924343	-1.019552
7	-3.261413	-0.210273	-0.576646
6	-4.463139	-0.521230	0.203567
1	-4.726836	0.356958	0.796278
1	-5.310302	-0.789405	-0.437432
1	-4.249798	-1.340018	0.896600
6	-2.522064	-1.192918	-1.129427
6	-2.970872	-2.606922	-0.980065
1	-4.027747	-2.747481	-1.225963
1	-2.350526	-3.235815	-1.621156
1	-2.816671	-2.913560	0.064707
1	-1.889132	-0.716314	4.627618
6	-2.553262	-0.299854	3.862031
6	-1.844811	-0.344990	2.531791
1	-3.445522	-0.934178	3.833835
1	-2.819886	0.721232	4.142083
8	-1.697004	-1.486175	2.008222
8	-1.457806	0.759002	2.053137
47	0.104622	-1.892157	0.807350
8	1.964878	-0.241357	1.375387
16	2.188835	1.160743	1.011247
8	2.202612	2.158901	2.065563
8	1.375046	1.612975	-0.194334
6	3.885644	1.170401	0.309708

9	4.746465	0.845043	1.263090
9	3.985406	0.294456	-0.677976
9	4.178046	2.377947	-0.148264

3CH7_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -1021.3132 cm(-1)

Electronic energy : -2902.620477
 Zero-point correction= 0.293058
 Thermal correction to Energy= 0.328029
 Thermal correction to Enthalpy= 0.328974
 Thermal correction to Gibbs Free Energy= 0.224682
 Sum of electronic and zero-point Energies= -2902.327419
 Sum of electronic and thermal Energies= -2902.292448
 Sum of electronic and thermal Enthalpies= -2902.291503
 Sum of electronic and thermal Free Energies= -2902.395795

 Cartesian Coordinates

6	-4.397824	0.415705	-2.032370
6	-4.440356	1.694798	-2.581062
6	-3.297690	0.030931	-1.278837
6	-2.241370	0.952425	-1.013557
1	-2.131456	0.979625	0.228006
6	-2.322946	2.240405	-1.598542
8	-1.141593	-1.685032	-1.264064
46	-0.327633	0.167962	-1.025912
1	-1.514255	2.941948	-1.406287
1	-5.207393	-0.285992	-2.217750
1	-5.292514	1.973890	-3.196275
6	-3.413165	2.612929	-2.362305
1	-3.470324	3.609713	-2.789897
7	-3.301767	-1.248030	-0.670718
6	-4.542646	-1.710141	-0.039076
1	-5.133395	-0.836696	0.243914
1	-5.128562	-2.346433	-0.711517
1	-4.305742	-2.264668	0.872136
6	-2.211012	-2.043465	-0.711787
6	-2.268101	-3.409522	-0.122842
1	-3.127030	-3.983868	-0.483989
1	-1.341784	-3.930892	-0.373346
1	-2.343765	-3.328571	0.969399
1	-3.566046	0.670662	4.237244
6	-3.952661	0.215498	3.317769
6	-2.816474	0.099010	2.332315
1	-4.348180	-0.770092	3.577846
1	-4.743515	0.865840	2.935310
8	-2.154506	-0.976917	2.339262
8	-2.601612	1.101645	1.592244
47	-0.016850	-0.812780	1.735920
8	1.300768	1.214168	1.508219
16	1.115978	2.385987	0.639054
8	0.528507	3.582267	1.213971
8	0.513545	2.037557	-0.716862
6	2.822042	2.844041	0.138544
9	3.496348	3.219871	1.213840
9	3.423710	1.813618	-0.422126
9	2.774959	3.850053	-0.720942
8	1.637440	-2.140639	0.776455
16	2.033224	-1.988951	-0.644541
8	1.659585	-0.649589	-1.219003
8	1.779603	-3.133178	-1.504166
6	3.858796	-1.811406	-0.566369
9	4.191854	-0.799563	0.215346
9	4.377869	-2.929552	-0.081149
9	4.336231	-1.601754	-1.782525

3CH8_Pd-Ag

Number of imaginary frequencies : 1
The smallest frequency is : -1656.7714 cm(-1)

Electronic energy : -1436.9468554
Zero-point correction= 0.335369
Thermal correction to Energy= 0.364169
Thermal correction to Enthalpy= 0.365113
Thermal correction to Gibbs Free Energy= 0.274663
Sum of electronic and zero-point Energies= -1436.611487
Sum of electronic and thermal Energies= -1436.582686
Sum of electronic and thermal Enthalpies= -1436.581742
Sum of electronic and thermal Free Energies= -1436.672192

Cartesian Coordinates

6	-3.851850	0.989356	-1.104916
6	-4.153628	2.292559	-0.720538
6	-2.617127	0.447000	-0.768831
6	-1.677076	1.184113	-0.014277
1	-1.234185	0.411806	0.915408
6	-2.015129	2.499843	0.352955
8	-0.295355	-0.425585	-2.014152
1	3.078071	3.324261	2.233951
6	2.258406	2.788203	2.725384
6	1.720924	1.745864	1.775695
1	2.639730	2.313718	3.632040
1	1.489599	3.523964	2.976694
8	2.029408	0.558153	1.921796
8	0.971263	2.246617	0.849797
46	0.329804	0.978686	-0.604627
8	2.216333	1.028302	-1.492303
6	2.989034	0.017686	-1.577149
8	2.847890	-1.097177	-1.033249
6	4.186918	0.224993	-2.474088
1	3.901912	-0.024245	-3.502836
1	4.512213	1.268060	-2.461978
1	5.005979	-0.434208	-2.176918
1	-1.289294	3.073404	0.925819
1	-4.566240	0.405468	-1.681549
1	-5.112765	2.720462	-1.002938
6	-3.240270	3.051206	0.009040
1	-3.488398	4.067458	0.304400
7	-2.342687	-0.907771	-1.111574
6	-3.359494	-1.913946	-0.798043
1	-4.054463	-1.489515	-0.070617
1	-3.919499	-2.223475	-1.688024
1	-2.889441	-2.788403	-0.338816
6	-1.188618	-1.255282	-1.725257
6	-0.968289	-2.688238	-2.075593
1	-1.814645	-3.135060	-2.606135
1	-0.065121	-2.759746	-2.684022
1	-0.810239	-3.247645	-1.143023
1	-1.551278	-2.603829	3.905501
6	-2.166325	-2.410723	3.018704
6	-1.332534	-1.654946	2.012891
1	-2.468584	-3.381687	2.615293
1	-3.039637	-1.832459	3.330086
8	-0.592688	-2.335124	1.252446
8	-1.432531	-0.391891	2.033803
47	1.349785	-1.370765	0.641501

Monometallic C-H activation (Pd)

3CH1_Pd

Number of imaginary frequencies : 1
The smallest frequency is : -1394.7439 cm(-1)

Electronic energy : -1795.5641717
Zero-point correction= 0.261435
Thermal correction to Energy= 0.286375
Thermal correction to Enthalpy= 0.287320
Thermal correction to Gibbs Free Energy= 0.204719
Sum of electronic and zero-point Energies= -1795.302736
Sum of electronic and thermal Energies= -1795.277796
Sum of electronic and thermal Enthalpies= -1795.276852
Sum of electronic and thermal Free Energies= -1795.359453

Cartesian Coordinates

6 3.960078 -0.062592 1.475976
6 3.868372 0.936967 2.437581
6 2.983796 -0.171985 0.488392
6 1.934708 0.771252 0.420949
1 1.698620 1.332405 -0.695691
6 1.855979 1.753586 1.430147
8 0.884617 -1.856048 -0.197103
46 0.097540 0.059979 -0.283317
8 1.373660 2.370675 -1.640825
6 0.172046 2.648268 -1.405682
8 -0.613556 1.936161 -0.693076
6 -0.432255 3.887585 -1.995812
1 0.345646 4.599760 -2.276438
1 -0.992267 3.602713 -2.893328
1 -1.140087 4.338509 -1.296588
1 1.041442 2.474171 1.388839
1 4.772216 -0.783662 1.525931
1 4.626636 0.995163 3.214800
6 2.809355 1.842271 2.429252
1 2.737056 2.612580 3.191924
7 3.082623 -1.252392 -0.433546
6 4.409434 -1.588716 -0.953528
1 5.009161 -0.677615 -0.992492
1 4.920382 -2.332906 -0.330971
1 4.324801 -1.975838 -1.971121
6 2.032468 -2.090120 -0.630218
6 2.260134 -3.368098 -1.368148
1 3.119261 -3.923487 -0.979335
1 1.357603 -3.974510 -1.282340
1 2.439876 -3.166671 -2.430945
8 -3.570937 -2.299008 -0.336410
16 -2.638913 -1.316036 0.194534
8 -1.753745 -0.740737 -0.896311
8 -1.917371 -1.609616 1.428177
6 -3.678938 0.135384 0.619232
9 -4.268776 0.623012 -0.463320
9 -4.614515 -0.226090 1.490075
9 -2.936190 1.088572 1.170815

3CH2_Pd

Electronic energy : -1062.7167959
Zero-point correction= 0.282599
Thermal correction to Energy= 0.304473
Thermal correction to Enthalpy= 0.305417
Thermal correction to Gibbs Free Energy= 0.230659
Sum of electronic and zero-point Energies= -1062.434197
Sum of electronic and thermal Energies= -1062.412323
Sum of electronic and thermal Enthalpies= -1062.411379
Sum of electronic and thermal Free Energies= -1062.486137

Cartesian Coordinates

6 3.374424 0.171152 1.080862

6	3.367068	1.194922	2.020222
6	2.280166	-0.007410	0.236132
6	1.172192	0.854967	0.303417
1	0.617503	1.343749	-0.775203
6	1.187805	1.866131	1.281110
8	0.270508	-1.916993	-0.046327
1	-2.181151	3.453603	-2.738383
6	-1.883011	3.651546	-1.702949
6	-1.109380	2.469230	-1.200146
1	-1.246712	4.540610	-1.709108
1	-2.778549	3.823467	-1.103799
8	0.065719	2.293847	-1.623240
8	-1.701024	1.705402	-0.374861
46	-0.711303	-0.073677	-0.048919
8	-2.485734	-1.076902	-0.239692
6	-2.991814	-1.297302	0.935429
8	-2.486392	-0.953328	2.000212
6	-4.303678	-2.049274	0.878835
1	-5.021017	-1.512610	0.249321
1	-4.151239	-3.034367	0.424701
1	-4.714733	-2.170798	1.883995
1	0.330146	2.533718	1.348612
1	4.220374	-0.510567	1.029591
1	4.220472	1.316709	2.682951
6	2.268361	2.043114	2.130942
1	2.258596	2.835333	2.875054
7	2.322406	-1.110346	-0.674613
6	3.561412	-1.327049	-1.421233
1	4.062886	-0.365729	-1.547868
1	4.241300	-2.018752	-0.908509
1	3.339077	-1.721250	-2.415507
6	1.346285	-2.050170	-0.666570
6	1.578523	-3.324929	-1.413256
1	2.544071	-3.779117	-1.169736
1	0.772388	-4.016421	-1.164986
1	1.554961	-3.141807	-2.494082

3CH3_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -1505.6817 cm(-1)

Electronic energy : -2528.3849438
 Zero-point correction= 0.239509
 Thermal correction to Energy= 0.267490
 Thermal correction to Enthalpy= 0.268434
 Thermal correction to Gibbs Free Energy= 0.178444
 Sum of electronic and zero-point Energies= -2528.145435
 Sum of electronic and thermal Energies= -2528.117454
 Sum of electronic and thermal Enthalpies= -2528.116510
 Sum of electronic and thermal Free Energies= -2528.206499

 Cartesian Coordinates

6	3.557877	-1.927333	1.521182
6	3.651538	-1.142547	2.664069
6	2.584521	-1.649281	0.563394
6	1.749856	-0.513520	0.715506
1	1.924887	0.371052	-0.241729
6	1.841188	0.230494	1.915750
8	0.177025	-2.538890	-0.505208
46	-0.114433	-0.539614	-0.156308
1	1.172200	1.078154	2.049596
1	4.212422	-2.787458	1.407783
1	4.398360	-1.392392	3.413602
6	2.788724	-0.067495	2.876477
1	2.861653	0.527069	3.782405
7	2.470717	-2.514005	-0.553654
6	3.699747	-3.071311	-1.126752
1	4.513282	-2.361479	-0.968813

1	3.962266	-4.034389	-0.674469
1	3.578029	-3.201666	-2.203309
6	1.258556	-2.970683	-0.961067
6	1.201070	-4.073099	-1.965067
1	1.843026	-4.915986	-1.691095
1	0.165830	-4.407310	-2.044639
1	1.522954	-3.707828	-2.947852
8	-0.205294	1.599058	-0.122343
16	0.780758	2.220786	-1.070655
8	0.317048	2.582608	-2.389721
8	2.077722	1.445839	-1.027749
6	1.192832	3.781288	-0.190893
9	0.104203	4.515986	-0.092873
9	1.652939	3.498671	1.016408
9	2.115706	4.429011	-0.875538
8	-4.192470	-1.898906	-0.699656
16	-3.092689	-1.254490	-0.000640
8	-2.063528	-0.683299	-0.960312
8	-2.483467	-1.926279	1.144714
6	-3.803369	0.282869	0.707132
9	-4.284702	1.063205	-0.248209
9	-4.784343	-0.023890	1.546803
9	-2.864539	0.947507	1.374389

3CH4_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -1190.8161 cm(-1)

Electronic energy : -1795.5399744
 Zero-point correction= 0.260916
 Thermal correction to Energy= 0.285978
 Thermal correction to Enthalpy= 0.286922
 Thermal correction to Gibbs Free Energy= 0.203951
 Sum of electronic and zero-point Energies= -1795.279059
 Sum of electronic and thermal Energies= -1795.253996
 Sum of electronic and thermal Enthalpies= -1795.253052
 Sum of electronic and thermal Free Energies= -1795.336024

 Cartesian Coordinates

6	-2.734581	-2.539902	1.091749
6	-2.064599	-3.033088	2.204560
6	-2.146006	-1.544228	0.313332
6	-0.858858	-1.060469	0.619606
1	0.034835	-1.125152	-0.415510
6	-0.221168	-1.562625	1.771111
8	-2.445512	1.160888	-0.321706
46	-0.434548	0.937048	0.144132
8	-0.160277	2.932155	-0.186786
6	0.256484	3.459936	0.925304
8	0.367717	2.837128	1.980129
6	0.615022	4.919221	0.804226
1	-0.168685	5.467530	0.272339
1	0.771887	5.354594	1.794062
1	1.535862	5.018145	0.218682
1	0.765520	-1.182344	2.031701
1	-3.730375	-2.905693	0.852256
1	-2.540814	-3.797050	2.814401
6	-0.807758	-2.543725	2.554324
1	-0.294369	-2.927114	3.432022
7	-2.883286	-1.041390	-0.799273
6	-3.613388	-2.006719	-1.623664
1	-3.112139	-2.973047	-1.549465
1	-4.656350	-2.118001	-1.304023
1	-3.591551	-1.701177	-2.671927
6	-3.049152	0.289196	-0.986411
6	-4.029141	0.750588	-2.015870

1	-4.993394	0.239748	-1.933186
1	-4.168756	1.825756	-1.897051
1	-3.632531	0.565843	-3.021583
8	1.724856	0.558723	0.148955
16	2.102682	-0.332190	-0.987124
8	2.659272	0.264947	-2.179832
8	0.989387	-1.335982	-1.237445
6	3.417441	-1.381600	-0.247765
9	4.412747	-0.613597	0.149045
9	2.922439	-2.041205	0.786590
9	3.847128	-2.241185	-1.152680

Conformational and Configurational Study of Reductive Elimination (RE)

Bimetallic Reductive Elimination (Pd-Ag)

3RE1_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -317.7310 cm(-1)

Electronic energy : -2903.8931055
 Zero-point correction= 0.613372
 Thermal correction to Energy= 0.665192
 Thermal correction to Enthalpy= 0.666136
 Thermal correction to Gibbs Free Energy= 0.526605
 Sum of electronic and zero-point Energies= -2903.279734
 Sum of electronic and thermal Energies= -2903.227914
 Sum of electronic and thermal Enthalpies= -2903.226969
 Sum of electronic and thermal Free Energies= -2903.366501

 Cartesian Coordinates

8	-5.122680	-2.055873	-0.667601
6	-5.223154	-1.324167	0.407630
6	-6.607605	-1.238132	0.955464
8	-4.274117	-0.742766	0.941818
1	-7.009912	-2.243827	1.111464
1	-7.252252	-0.743365	0.221036
1	-6.618823	-0.677398	1.890630
6	-2.490626	2.406893	1.385412
6	-2.552637	3.309089	2.440517
6	-1.875328	3.035845	3.622405
6	-1.131978	1.870928	3.744861
6	-1.040472	0.953691	2.692978
6	-1.747179	1.238059	1.515615
7	-0.196974	-0.178480	2.878262
6	1.017601	-0.009021	3.687661
46	-2.157274	-0.275774	0.184490
35	-3.039062	1.038468	-1.762772
6	-0.492568	0.740802	-0.081137
6	0.543502	1.319945	-0.434914
14	2.006058	2.445673	-0.749501
6	2.892312	2.478534	0.932722
6	-0.523664	-1.398967	2.421495
8	-1.474355	-1.598246	1.622645
6	0.239848	-2.596568	2.870680
6	3.132768	1.685904	-2.077542
6	1.213360	4.092575	-1.289880
1	-3.008986	2.619334	0.455511
1	-0.610227	1.661444	4.674697
1	-1.923252	3.728315	4.458442
1	1.345105	1.028837	3.605697
1	0.837301	-0.250340	4.741666
1	1.813120	-0.634969	3.280660
1	0.460390	-2.576423	3.941481
1	-0.341869	-3.486461	2.624801
1	1.187263	-2.630322	2.315969

1	2.015358	4.850493	-1.232044
1	2.940606	1.410943	1.209599
1	3.701173	0.917855	-1.525451
1	-3.129227	4.223339	2.327903
47	0.720146	-1.070682	-1.114740
1	-4.152157	-2.098498	-0.946443
8	-2.583303	-2.067715	-1.080894
6	-1.924949	-2.528996	-2.082861
6	-2.753662	-3.276573	-3.093887
8	-0.703289	-2.405188	-2.264290
1	-3.341547	-4.058754	-2.601695
1	-2.126784	-3.718063	-3.870494
1	-3.461408	-2.573988	-3.551263
8	3.010193	-1.723915	-1.148198
16	3.531393	-1.438807	0.215218
6	4.181080	-3.065215	0.759123
8	2.442199	-1.170630	1.182476
8	4.678121	-0.537679	0.280208
9	4.618747	-2.976939	2.010497
9	3.216851	-3.981144	0.713471
9	5.178364	-3.453723	-0.018991
6	2.432954	0.990490	-3.243583
1	1.668527	0.264425	-2.927691
1	1.931860	1.704664	-3.909240
1	3.161330	0.433243	-3.848336
6	4.130937	2.714382	-2.616703
1	4.862860	2.230340	-3.277784
1	3.630607	3.491435	-3.211263
1	4.697467	3.221293	-1.826139
6	4.321569	3.009707	0.865042
1	4.778315	3.014795	1.865219
1	4.963428	2.393234	0.225355
1	4.355846	4.045782	0.494990
6	2.102363	3.220757	2.006672
1	1.053450	2.892641	2.071898
1	2.561667	3.080094	2.997063
1	2.098306	4.303702	1.817999
6	0.050422	4.537859	-0.402799
1	-0.367949	5.486295	-0.769178
1	-0.760803	3.795748	-0.431315
1	0.326337	4.685561	0.646683
6	0.713697	4.007352	-2.733318
1	0.206202	4.938622	-3.022755
1	1.516732	3.838085	-3.459549
1	-0.020777	3.195332	-2.847257

3RE2_Pd-Ag

Number of imaginary frequencies : 1

The smallest frequency is : -198.4147 cm(-1)

Electronic energy : -2903.8912166
 Zero-point correction= 0.613102
 Thermal correction to Energy= 0.665185
 Thermal correction to Enthalpy= 0.666129
 Thermal correction to Gibbs Free Energy= 0.525163
 Sum of electronic and zero-point Energies= -2903.278115
 Sum of electronic and thermal Energies= -2903.226032
 Sum of electronic and thermal Enthalpies= -2903.225087
 Sum of electronic and thermal Free Energies= -2903.366054

 Cartesian Coordinates

8	-4.089555	1.741283	1.944622
6	-3.165964	2.107515	2.799398
6	-3.729477	2.651372	4.070134
8	-1.957098	2.027374	2.598290
1	-4.394559	1.910877	4.525581

1	-4.334770	3.537438	3.851891
1	-2.928446	2.912046	4.762418
6	-0.431744	-3.834609	-0.767750
6	0.208273	-4.917877	-1.361145
6	0.943628	-4.731852	-2.524413
6	1.056000	-3.468372	-3.085920
6	0.442744	-2.354390	-2.499787
6	-0.327144	-2.581934	-1.355238
7	0.653180	-1.079520	-3.097177
6	1.942238	-0.812120	-3.749290
46	-1.676419	-1.153671	-0.743579
35	-2.272629	-1.980887	1.558439
6	0.136140	-0.920714	-0.020015
6	1.182890	-0.690745	0.591764
14	2.798936	-0.692207	1.528537
6	4.061104	0.108871	0.372935
6	-0.334735	-0.168933	-3.204328
8	-1.429642	-0.277320	-2.601405
6	-0.163593	0.989568	-4.125339
8	-3.770755	-1.287498	-1.342295
6	-4.125086	-0.174991	-0.860458
6	-5.561711	0.237935	-0.922426
8	-3.277815	0.579872	-0.291509
6	2.569253	0.296889	3.133986
6	3.075720	-2.566848	1.729709
1	-6.015026	0.058060	0.060131
1	-6.109792	-0.339721	-1.669187
1	-5.640378	1.307842	-1.134018
1	-0.999156	-3.965753	0.148153
1	1.622718	-3.336815	-4.004034
1	1.436650	-5.572867	-3.004577
1	2.685192	-1.504816	-3.353413
1	1.879206	-0.937468	-4.836395
1	2.266913	0.200601	-3.495113
1	0.110653	0.655515	-5.131914
1	-1.098438	1.549795	-4.155492
1	0.628381	1.648278	-3.749766
1	2.943511	-2.947353	0.699987
1	3.548771	1.027542	0.050839
1	2.685151	1.347885	2.817004
1	0.124571	-5.900595	-0.904686
47	-0.610270	1.213475	0.921588
1	-3.702782	1.359941	1.105240
9	0.604438	5.108864	-0.849653
6	1.392296	4.339097	-1.588023
16	1.262421	2.590307	-1.051685
9	1.020955	4.441781	-2.860680
9	2.641790	4.768058	-1.470880
8	1.656626	2.607530	0.369153
8	-0.181421	2.300580	-1.243037
8	2.159584	1.871875	-1.966811
6	2.009855	-3.226589	2.601074
1	2.123565	-2.945471	3.657488
1	0.991906	-2.953476	2.290788
1	2.085982	-4.322710	2.554706
6	4.481368	-2.945405	2.191496
1	4.597486	-4.037794	2.240926
1	5.257906	-2.567054	1.514552
1	4.700176	-2.555321	3.194646
6	1.195439	0.150640	3.785352
1	0.975257	-0.891182	4.055618
1	1.139520	0.745120	4.708273
1	0.374188	0.494028	3.139440
6	3.662586	-0.022000	4.156627
1	3.609998	0.669825	5.008904
1	3.543619	-1.035769	4.564477
1	4.676988	0.050296	3.744303
6	5.387246	0.503954	1.015692
1	6.048429	0.977474	0.275888
1	5.251457	1.225110	1.831078

1	5.931406	-0.361061	1.421241
6	4.274523	-0.760244	-0.862554
1	3.317364	-1.091571	-1.289723
1	4.811474	-0.209744	-1.648254
1	4.863665	-1.659100	-0.628675

3RE3_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -153.2775 cm(-1)

Electronic energy : -3636.718743
 Zero-point correction= 0.591956
 Thermal correction to Energy= 0.647065
 Thermal correction to Enthalpy= 0.648009
 Thermal correction to Gibbs Free Energy= 0.499134
 Sum of electronic and zero-point Energies= -3636.126787
 Sum of electronic and thermal Energies= -3636.071678
 Sum of electronic and thermal Enthalpies= -3636.070734
 Sum of electronic and thermal Free Energies= -3636.219609

 Cartesian Coordinates

8	-0.012570	4.861269	-1.254743
6	0.973751	4.217227	-1.841496
6	1.765402	5.079418	-2.766304
8	1.241407	3.036626	-1.647208
1	2.390203	5.754654	-2.170741
1	1.103413	5.700032	-3.376424
1	2.407995	4.464969	-3.398066
6	0.173612	-4.013273	-0.474844
6	-0.467824	-5.209912	-0.165635
6	-1.164742	-5.331648	1.028523
6	-1.232836	-4.264438	1.911893
6	-0.609389	-3.041739	1.630726
6	0.109020	-2.972371	0.435979
7	-0.764569	-1.978816	2.562272
6	-2.017719	-1.914692	3.320342
46	1.443432	-1.427353	0.130586
35	1.839700	-1.576326	-2.328718
6	-0.380209	-0.940653	-0.374535
6	-1.492729	-0.606483	-0.793203
14	-3.236925	-0.327679	-1.427407
6	-4.295998	-1.089629	-0.040286
6	0.253473	-1.146882	2.865964
8	1.295633	-1.078747	2.173927
6	0.190576	-0.302755	4.091459
6	-3.466007	1.540081	-1.651819
6	-3.326738	-1.238169	-3.095173
1	0.705609	-3.902491	-1.413260
1	-1.776504	-4.374882	2.846166
1	-1.666360	-6.262070	1.279909
1	-2.837073	-2.222760	2.664230
1	-1.994547	-2.559528	4.206339
1	-2.210066	-0.887335	3.629348
1	-0.135011	-0.879805	4.962536
1	1.181698	0.119455	4.263507
1	-0.498721	0.535063	3.938905
1	-2.901507	-0.523595	-3.820686
1	-3.860976	-0.645631	0.867940
1	-3.422947	1.979401	-0.641534
1	-0.415987	-6.034435	-0.871377
47	0.365307	1.344981	-0.285304
1	-0.494682	4.273174	-0.619665
9	6.338237	-0.633625	-0.174766
6	5.329224	0.167456	-0.479496
16	3.981448	-0.054674	0.751896
9	5.740428	1.425989	-0.437231

9	4.905268	-0.110613	-1.698504
8	3.578522	-1.501459	0.537618
8	4.594476	0.219577	2.038052
8	2.895495	0.835521	0.289119
8	0.075110	2.234457	2.150441
16	-1.114710	3.065640	1.875526
6	-2.491725	1.951385	2.362885
8	-1.295627	4.267548	2.671578
8	-1.368266	3.206897	0.410023
9	-2.312041	0.751689	1.795524
9	-2.499051	1.776965	3.683619
9	-3.669340	2.421015	1.987434
6	-4.808046	1.894822	-2.295597
1	-5.671896	1.471050	-1.770226
1	-4.945758	2.984267	-2.321435
1	-4.849244	1.546747	-3.337381
6	-2.337989	2.151632	-2.481474
1	-2.321726	1.743852	-3.502442
1	-2.470819	3.238795	-2.569138
1	-1.343237	1.983893	-2.046084
6	-2.489793	-2.515047	-3.153288
1	-2.551370	-2.972392	-4.150773
1	-1.430131	-2.327463	-2.939186
1	-2.848693	-3.264758	-2.434231
6	-4.771151	-1.530474	-3.507929
1	-5.407012	-0.636254	-3.523531
1	-4.804702	-1.967628	-4.515624
1	-5.240595	-2.257878	-2.831303
6	-5.776140	-0.716158	-0.060161
1	-6.309566	-1.217680	0.760301
1	-5.927571	0.362273	0.072346
1	-6.272863	-1.016019	-0.992659
6	-4.112124	-2.605413	0.048418
1	-4.583902	-3.005574	0.959221
1	-4.585064	-3.122040	-0.798514
1	-3.054435	-2.908098	0.065218

3RE4_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -205.3933 cm(-1)

Electronic energy : -2903.887945
 Zero-point correction= 0.616997
 Thermal correction to Energy= 0.667689
 Thermal correction to Enthalpy= 0.668633
 Thermal correction to Gibbs Free Energy= 0.533227
 Sum of electronic and zero-point Energies= -2903.270948
 Sum of electronic and thermal Energies= -2903.220256
 Sum of electronic and thermal Enthalpies= -2903.219312
 Sum of electronic and thermal Free Energies= -2903.354718

 Cartesian Coordinates

8	3.554534	-3.499534	-0.331174
6	2.650697	-3.840522	-1.223813
6	3.078411	-4.990731	-2.072523
8	1.567719	-3.281828	-1.360310
1	3.343481	-5.842140	-1.437787
1	3.976751	-4.716353	-2.635696
1	2.281131	-5.270356	-2.761692
6	-3.155925	2.228118	-1.066072
6	-3.679691	3.502125	-0.877442
6	-3.618349	4.092246	0.378199
6	-3.025545	3.419457	1.435784
6	-2.476843	2.140844	1.272670
6	-2.589313	1.553851	0.007564
7	-1.835638	1.547629	2.400551

6	-1.220754	2.443098	3.385516
46	-2.289219	-0.477828	-0.206562
35	-2.302633	-0.730165	-2.705314
6	-0.665691	0.621973	-0.438236
6	0.417779	1.138553	-0.734341
14	1.911751	2.136738	-1.261144
6	1.989986	3.615262	-0.063694
6	-1.941600	0.231318	2.683101
8	-2.368388	-0.611617	1.865217
6	-1.584574	-0.262591	4.044537
8	-3.827552	-1.972536	-0.096145
6	-3.038167	-2.975853	-0.056999
6	-3.639185	-4.344719	0.044451
8	-1.794184	-2.833601	-0.130591
6	3.417470	1.005837	-1.062573
6	1.526446	2.733660	-3.027898
1	-3.659658	-4.786619	-0.958193
1	-4.660564	-4.305641	0.428869
1	-3.015144	-4.980653	0.677637
1	-3.187259	1.760356	-2.044999
1	-2.989038	3.891306	2.413761
1	-4.032045	5.083711	0.542024
1	-0.809986	3.311363	2.865865
1	-1.941436	2.779160	4.140248
1	-0.392074	1.935350	3.879872
1	-2.029425	0.353398	4.831986
1	-1.927539	-1.294156	4.131353
1	-0.496380	-0.267208	4.166299
1	0.955682	3.668751	-2.889144
1	2.482759	3.240040	0.849181
1	3.298671	0.616729	-0.037434
1	-4.131713	4.022568	-1.717590
47	0.523516	-1.468085	-0.336956
1	3.243174	-2.738046	0.222207
8	0.615447	-1.571413	2.288127
16	2.067158	-1.342173	2.429050
6	2.155421	0.437470	2.885430
8	2.752432	-2.031603	3.511432
8	2.764445	-1.354239	1.109300
9	1.402850	1.172290	2.066656
9	1.686888	0.599850	4.125852
9	3.397314	0.890161	2.838096
6	3.408854	-0.195030	-2.005420
1	2.445308	-0.728047	-2.013820
1	3.626613	0.099275	-3.041811
1	4.178029	-0.923195	-1.709985
6	4.760148	1.732629	-1.124314
1	4.843034	2.518542	-0.363209
1	5.584181	1.027655	-0.945361
1	4.939161	2.192388	-2.105813
6	2.806592	4.782752	-0.615329
1	2.888493	5.587048	0.129481
1	3.828021	4.500190	-0.898241
1	2.327658	5.222286	-1.501696
6	0.584273	4.085639	0.306003
1	0.009207	4.388265	-0.583060
1	0.010425	3.290695	0.796191
1	0.615689	4.955617	0.978859
6	0.643809	1.766964	-3.814909
1	-0.339430	1.633185	-3.348741
1	0.483398	2.132945	-4.839207
1	1.094012	0.767106	-3.895376
6	2.793634	3.071023	-3.814719
1	3.389075	2.170378	-4.017413
1	2.539547	3.509016	-4.790290
1	3.443182	3.788043	-3.297317

3RE5_Pd-Ag

Number of imaginary frequencies : 1
The smallest frequency is : -127.8819 cm(-1)

Electronic energy : -2903.8846724
Zero-point correction= 0.615973
Thermal correction to Energy= 0.666966
Thermal correction to Enthalpy= 0.667910
Thermal correction to Gibbs Free Energy= 0.531131
Sum of electronic and zero-point Energies= -2903.268699
Sum of electronic and thermal Energies= -2903.217706
Sum of electronic and thermal Enthalpies= -2903.216762
Sum of electronic and thermal Free Energies= -2903.353541

Cartesian Coordinates

8 3.145198 -3.250870 -1.597493
6 1.993633 -3.756059 -1.198861
6 1.908238 -5.231914 -1.387744
8 1.080795 -3.087601 -0.726996
1 2.732410 -5.723962 -0.861595
1 2.017793 -5.468858 -2.451371
1 0.950332 -5.605608 -1.024674
6 -3.851206 1.453702 0.907598
6 -4.375790 2.335022 1.851924
6 -3.786137 2.437712 3.106274
6 -2.676499 1.668702 3.433556
6 -2.122145 0.780150 2.506169
6 -2.760384 0.692703 1.273852
7 -0.946169 0.057948 2.848339
6 0.065498 0.731715 3.671451
46 -2.306603 -0.822387 -0.008063
35 -3.998426 -2.701645 -0.203595
6 -0.954696 0.646568 -0.100547
6 -0.163017 1.563583 -0.347416
14 0.875860 3.060837 -0.750148
6 1.784948 3.471483 0.865752
6 -0.754128 -1.219078 2.467119
8 -1.474610 -1.799449 1.616760
6 0.355888 -2.010620 3.067544
8 -3.045814 0.009106 -1.709529
6 -2.297897 -0.407061 -2.689828
6 -2.726947 0.080433 -4.043720
8 -1.324644 -1.151421 -2.540472
6 2.127682 2.570366 -2.094611
6 -0.422998 4.324523 -1.339443
1 -3.509556 0.839245 -3.983643
1 -3.096414 -0.774660 -4.619233
1 -1.853601 0.480949 -4.567865
1 -4.276011 1.367226 -0.089295
1 -2.227480 1.754306 4.420391
1 -4.191523 3.124868 3.843955
1 -0.018775 1.807871 3.507765
1 -0.066683 0.514510 4.737467
1 1.063447 0.431359 3.342533
1 0.445193 -1.854116 4.146172
1 0.177712 -3.065107 2.850129
1 1.302073 -1.714510 2.592247
1 0.098153 5.291871 -1.448479
1 2.133914 2.480970 1.205686
1 2.923101 2.060571 -1.524263
1 -5.240344 2.940232 1.592609
47 0.731799 -0.777248 -0.846162
1 3.181167 -2.286288 -1.389372
8 3.181098 -0.629268 -0.815626
16 3.513650 -0.116209 0.554710
8 2.320275 -0.018592 1.416687
8 4.426712 1.017597 0.566554
6 4.441383 -1.520431 1.291422
9 5.474800 -1.849451 0.533871

9	4.870642	-1.189594	2.499462
9	3.634009	-2.576271	1.400358
6	1.633220	1.595294	-3.162329
1	2.478028	1.201193	-3.743489
1	1.090788	0.727686	-2.754904
1	0.951919	2.082098	-3.872259
6	2.745237	3.798564	-2.769405
1	2.008417	4.335570	-3.383062
1	3.163376	4.519260	-2.056169
1	3.561206	3.500580	-3.442128
6	0.873025	4.053124	1.942653
1	-0.070126	3.497292	2.051955
1	1.378241	4.057118	2.919442
1	0.612771	5.097722	1.718996
6	3.013152	4.358615	0.679772
1	3.487163	4.565911	1.649784
1	3.775697	3.886511	0.049388
1	2.750645	5.332028	0.238512
6	-1.584104	4.497277	-0.359660
1	-1.275184	4.895441	0.611731
1	-2.335870	5.185360	-0.772040
1	-2.090698	3.536686	-0.177940
6	-0.981645	3.907085	-2.701327
1	-1.435468	2.904520	-2.648467
1	-1.770882	4.599371	-3.026962
1	-0.221098	3.887920	-3.490378

3RE6_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -272.8297 cm(-1)

Electronic energy : -2903.8832731
 Zero-point correction= 0.614698
 Thermal correction to Energy= 0.665866
 Thermal correction to Enthalpy= 0.666810
 Thermal correction to Gibbs Free Energy= 0.530034
 Sum of electronic and zero-point Energies= -2903.268575
 Sum of electronic and thermal Energies= -2903.217407
 Sum of electronic and thermal Enthalpies= -2903.216463
 Sum of electronic and thermal Free Energies= -2903.353239

 Cartesian Coordinates

8	4.867408	1.115205	0.586064
6	5.008764	-0.185396	0.456482
6	6.367060	-0.665907	0.833185
8	4.126202	-0.942096	0.056682
1	6.643995	-0.273371	1.816369
1	7.096146	-0.278591	0.113273
1	6.398629	-1.755657	0.835966
6	1.608882	-3.402429	0.676894
6	1.525715	-4.451593	1.587720
6	1.127945	-4.200163	2.896343
6	0.819569	-2.908636	3.303991
6	0.904757	-1.836501	2.410866
6	1.304725	-2.120091	1.103470
7	0.541575	-0.538155	2.870711
6	-0.562999	-0.435429	3.829691
46	1.863154	-0.598109	-0.157037
35	2.448741	1.708967	-1.573374
6	-0.067203	-0.950807	-0.060590
6	-1.280663	-1.145175	-0.118072
14	-3.065112	-1.651009	-0.263357
6	-3.735023	-1.755923	1.510429
6	1.202767	0.570034	2.493769
8	2.016615	0.583569	1.532248
6	1.027294	1.838688	3.251424

6	-3.947238	-0.323986	-1.286981
6	-2.949771	-3.384570	-1.046414
1	1.890854	-3.572123	-0.359030
1	0.518494	-2.724700	4.332326
1	1.059173	-5.013364	3.614020
1	-1.286338	-1.224177	3.607053
1	-0.216856	-0.535626	4.864959
1	-1.069050	0.522711	3.701490
1	1.007620	1.674495	4.332430
1	1.844591	2.512495	2.987895
1	0.084207	2.304097	2.937471
1	-3.972633	-3.672166	-1.345497
1	-2.944811	-2.295821	2.065058
1	-3.714085	0.620883	-0.765386
1	1.764103	-5.462271	1.266679
47	-0.337775	1.129142	-1.432247
1	3.997466	1.399090	0.222920
8	1.887061	-1.756810	-1.799448
6	1.188000	-1.491666	-2.873235
6	1.511211	-2.465890	-3.982361
8	0.381319	-0.588481	-3.044706
1	1.824333	-3.438346	-3.596211
1	2.333708	-2.049805	-4.574198
1	0.637128	-2.571294	-4.629413
8	-1.345702	1.834374	1.355240
16	-2.071349	2.856828	0.575234
6	-0.963068	4.310937	0.725169
8	-2.057683	2.592061	-0.893060
8	-3.357827	3.293571	1.102026
9	-0.870082	4.676506	2.003207
9	0.254444	3.999157	0.290587
9	-1.422906	5.335009	0.022980
6	-3.893679	-0.367170	2.126533
1	-4.151614	-0.433515	3.194156
1	-2.987380	0.245741	2.032380
1	-4.705280	0.192601	1.641184
6	-5.031544	-2.556141	1.633598
1	-4.952765	-3.569761	1.220616
1	-5.331810	-2.655010	2.686446
1	-5.861612	-2.059070	1.115082
6	-2.048297	-3.424242	-2.280514
1	-2.345134	-2.711650	-3.058666
1	-1.009864	-3.193599	-1.999851
1	-2.048416	-4.426661	-2.731540
6	-2.434813	-4.394816	-0.018515
1	-3.112818	-4.530007	0.832623
1	-2.291128	-5.382859	-0.479035
1	-1.457101	-4.085286	0.385217
6	-3.422715	-0.199358	-2.715565
1	-3.737079	-1.055510	-3.330012
1	-3.820416	0.706350	-3.193572
1	-2.325470	-0.143452	-2.773781
6	-5.463716	-0.511512	-1.298617
1	-5.907549	-0.409248	-0.300895
1	-5.940432	0.241941	-1.940907
1	-5.752292	-1.496718	-1.695460

3RE7_Pd-Ag

Number of imaginary frequencies : 1
The smallest frequency is : -338.1456 cm(-1)

Electronic energy : -2171.0400416
Zero-point correction= 0.634278
Thermal correction to Energy= 0.683105
Thermal correction to Enthalpy= 0.684049
Thermal correction to Gibbs Free Energy= 0.550493
Sum of electronic and zero-point Energies= -2170.405764

Sum of electronic and thermal Energies= -2170.356937
 Sum of electronic and thermal Enthalpies= -2170.355993
 Sum of electronic and thermal Free Energies= -2170.489549

 Cartesian Coordinates

8	-5.150830	-0.819071	-0.993481
6	-5.119656	0.126172	-0.093545
6	-6.451763	0.737857	0.182816
8	-4.097281	0.509754	0.480813
1	-7.211946	-0.039449	0.299869
1	-6.740190	1.348882	-0.680174
1	-6.408697	1.369813	1.070699
6	-1.366982	2.986021	0.718138
6	-1.207984	4.032195	1.619048
6	-0.764341	3.773361	2.910309
6	-0.461937	2.474576	3.293271
6	-0.591994	1.408717	2.398455
6	-1.067413	1.683253	1.106293
7	-0.171812	0.122640	2.840298
6	1.026017	0.036262	3.688799
46	-1.875949	0.155269	-0.012347
35	-2.095067	1.316760	-2.224936
6	0.045133	0.512658	-0.201280
6	1.238850	0.626383	-0.509101
14	3.025403	1.047701	-0.826344
6	3.816045	1.026137	0.905654
6	-0.856621	-0.992592	2.537968
8	-1.812607	-0.998935	1.719316
6	-0.493319	-2.280176	3.188260
8	2.789111	-3.021093	-0.193847
6	3.055234	-2.721518	1.001787
6	4.395279	-3.143108	1.562006
8	2.291158	-2.050353	1.751859
6	3.821984	-0.297753	-1.905015
6	2.952964	2.753586	-1.671806
1	5.057626	-2.267086	1.585393
1	4.866241	-3.915796	0.949720
1	4.290112	-3.492364	2.593806
1	-1.710784	3.183514	-0.292626
1	-0.121178	2.275034	4.306253
1	-0.653793	4.581292	3.628658
1	1.632207	0.926394	3.513094
1	0.761802	-0.017994	4.751457
1	1.623051	-0.831070	3.390127
1	-0.399044	-2.179464	4.274147
1	-1.255481	-3.020619	2.941128
1	0.476212	-2.609392	2.781997
1	3.979277	3.161391	-1.641589
1	3.431744	0.082540	1.337701
1	4.059946	-1.103218	-1.189390
1	-1.437851	5.046907	1.304565
47	0.785588	-1.808106	-0.331564
1	-4.223169	-1.198203	-1.119917
8	-2.708849	-1.624394	-1.041330
6	-2.245591	-2.820247	-0.939162
6	-3.225546	-3.900971	-1.324582
8	-1.101482	-3.130850	-0.579442
1	-4.144222	-3.802637	-0.735479
1	-2.793650	-4.892265	-1.174345
1	-3.502974	-3.782166	-2.377766
6	5.341356	0.962964	0.879212
1	5.748205	0.923793	1.900262
1	5.720117	0.080509	0.348399
1	5.775810	1.852493	0.398420
6	3.357373	2.181815	1.790482
1	3.706445	2.047120	2.825544
1	3.774595	3.138118	1.442877
1	2.262135	2.290975	1.815615
6	2.512062	2.623273	-3.131144

1	3.205930	2.037798	-3.744577
1	1.522936	2.145399	-3.197913
1	2.419786	3.614042	-3.598736
6	2.005860	3.729826	-0.972313
1	2.024477	4.709110	-1.471508
1	0.971520	3.359906	-1.027384
1	2.236591	3.894301	0.085548
6	5.127080	0.182394	-2.543512
1	5.657571	-0.654286	-3.018989
1	4.942752	0.926598	-3.329404
1	5.819724	0.637616	-1.824437
6	2.907441	-0.912559	-2.962127
1	3.415008	-1.742949	-3.472822
1	1.983332	-1.324402	-2.530982
1	2.612309	-0.186048	-3.730825

3RE8_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -245.7971 cm(-1)

Electronic energy : -3636.7123105
 Zero-point correction= 0.592753
 Thermal correction to Energy= 0.647829
 Thermal correction to Enthalpy= 0.648774
 Thermal correction to Gibbs Free Energy= 0.500021
 Sum of electronic and zero-point Energies= -3636.119557
 Sum of electronic and thermal Energies= -3636.064481
 Sum of electronic and thermal Enthalpies= -3636.063537
 Sum of electronic and thermal Free Energies= -3636.212290

 Cartesian Coordinates

8	-6.550850	-1.401186	0.282493
6	-6.312892	-0.177233	-0.133466
6	-7.545880	0.522339	-0.601323
8	-5.207049	0.348760	-0.141248
1	-8.318971	0.476633	0.171831
1	-7.941033	0.007094	-1.483525
1	-7.321295	1.559554	-0.852321
6	1.365950	0.407904	2.832026
6	1.154526	-0.497256	3.868889
6	0.743678	-1.793653	3.587914
6	0.577729	-2.204355	2.273466
6	0.818776	-1.332069	1.206090
6	1.160101	-0.020096	1.530783
7	0.728233	-1.845517	-0.117047
6	1.133078	-3.236610	-0.323636
46	0.762347	1.463523	0.151385
35	1.950285	3.403795	1.159142
6	2.512377	0.659347	-0.041157
6	3.597070	0.130300	-0.267896
14	5.158639	-0.844422	-0.483562
6	6.461287	0.324833	-1.206035
6	0.064314	-1.192547	-1.081685
8	-0.253042	0.023186	-0.977803
6	-0.323445	-1.893008	-2.337730
6	5.625589	-1.387605	1.275138
6	4.672698	-2.343694	-1.543115
1	1.676227	1.425389	3.042046
1	0.233499	-3.211811	2.055337
1	0.548073	-2.495868	4.393356
1	1.957289	-3.462151	0.357262
1	0.303361	-3.928776	-0.137190
1	1.491416	-3.369618	-1.346764
1	-0.781657	-2.865711	-2.139296
1	-1.033578	-1.261794	-2.876461
1	0.558275	-2.037618	-2.975925

1	3.987374	-2.901687	-0.879727
1	6.403822	1.213499	-0.554818
1	6.600241	-1.899817	1.205366
1	1.302747	-0.168505	4.893969
47	-2.864924	0.234320	-0.200316
1	-5.715351	-1.852828	0.564823
9	-1.040189	5.218704	0.357149
6	-2.022023	4.687377	-0.343838
16	-1.561677	2.987519	-0.866088
9	-3.117211	4.636069	0.394685
9	-2.247194	5.418757	-1.421930
8	-0.304350	3.110681	-1.615795
8	-1.312273	2.273960	0.448494
8	-2.742052	2.455466	-1.554487
8	-2.109504	-1.991330	0.226454
16	-3.310050	-2.834697	-0.042019
6	-2.619047	-4.527451	0.112948
8	-4.319011	-2.763707	1.030515
8	-3.810988	-2.745927	-1.410130
9	-1.790425	-4.768049	-0.905676
9	-1.931597	-4.646968	1.244302
9	-3.584561	-5.426722	0.094018
6	3.893648	-1.991868	-2.807720
1	3.508098	-2.897565	-3.299891
1	3.043431	-1.328251	-2.595179
1	4.523882	-1.476883	-3.544648
6	5.862167	-3.248680	-1.854979
1	5.536927	-4.184471	-2.331193
1	6.560755	-2.765516	-2.551967
1	6.431257	-3.521313	-0.955505
6	4.609453	-2.364996	1.861132
1	3.599047	-1.925622	1.879198
1	4.558846	-3.307258	1.299017
1	4.861596	-2.621426	2.899769
6	5.777164	-0.166896	2.182150
1	4.823884	0.376848	2.268795
1	6.079125	-0.461472	3.196861
1	6.526268	0.544685	1.811773
6	6.131464	0.770729	-2.628287
1	6.805842	1.574874	-2.953553
1	6.252882	-0.052458	-3.345919
1	5.104194	1.147173	-2.722121
6	7.877398	-0.241898	-1.118552
1	7.988086	-1.152386	-1.724356
1	8.612240	0.482803	-1.496145
1	8.168219	-0.493125	-0.090450

3RE9_Pd-Ag

Number of imaginary frequencies : 1

The smallest frequency is : -262.8339 cm(-1)

Electronic energy : -3636.7097612
 Zero-point correction= 0.593002
 Thermal correction to Energy= 0.647725
 Thermal correction to Enthalpy= 0.648669
 Thermal correction to Gibbs Free Energy= 0.501400
 Sum of electronic and zero-point Energies= -3636.116759
 Sum of electronic and thermal Energies= -3636.062037
 Sum of electronic and thermal Enthalpies= -3636.061092
 Sum of electronic and thermal Free Energies= -3636.208361

 Cartesian Coordinates

8	-3.848464	-3.201723	0.889631
6	-4.287585	-2.107728	1.469254
6	-5.545748	-2.313458	2.236098
8	-3.737003	-1.010108	1.388770

1	-5.454972	-3.192897	2.880411
1	-6.360278	-2.511181	1.530743
1	-5.782867	-1.427867	2.826157
6	-1.838890	1.866412	2.549318
6	-1.713137	2.473179	3.794293
6	-0.875475	1.914207	4.753098
6	-0.159417	0.756893	4.479208
6	-0.260903	0.126078	3.234061
6	-1.121000	0.707949	2.300329
7	0.529077	-1.034603	2.993240
6	1.837967	-1.148065	3.652158
46	-1.704752	-0.347996	0.632752
35	-2.032985	-2.018385	-1.598595
6	-0.012993	0.635121	0.442703
6	0.998716	1.285836	0.178951
14	2.567504	2.291022	-0.022270
6	3.677517	1.595716	1.357090
6	0.095494	-2.059193	2.248953
8	-0.933701	-1.998677	1.516707
6	0.780082	-3.378377	2.315344
6	3.276265	1.971208	-1.752794
6	2.027791	4.103811	0.203514
1	-2.467168	2.295127	1.773213
1	0.482446	0.327212	5.243880
1	-0.776161	2.378557	5.730485
1	2.196744	-0.145664	3.885459
1	1.777030	-1.737919	4.573336
1	2.550500	-1.598112	2.956609
1	0.939811	-3.690227	3.352389
1	0.171448	-4.116746	1.791468
1	1.750251	-3.305425	1.812464
1	1.643297	4.406467	-0.785820
1	3.520315	0.506386	1.266890
1	3.734954	0.968755	-1.715458
1	-2.265379	3.385557	4.002780
47	0.415451	-0.726199	-1.610889
1	-3.093149	-2.997109	0.293361
8	2.434909	-1.647319	0.471604
16	3.213712	-1.954550	-0.746727
6	2.883438	-3.743289	-0.984362
8	2.620038	-1.370937	-1.982414
8	4.661359	-1.828829	-0.642856
9	3.372874	-4.440263	0.039916
9	1.567530	-3.946756	-1.037475
9	3.432972	-4.186178	-2.102769
8	-1.232332	1.306330	-2.345450
16	-2.089179	2.052727	-1.432487
6	-3.672231	2.297284	-2.345039
8	-2.668658	1.201577	-0.274051
8	-1.673355	3.368027	-0.976437
9	-3.424584	3.062618	-3.395120
9	-4.149125	1.136134	-2.746446
9	-4.556128	2.895393	-1.564491
6	3.209853	2.035103	2.742851
1	3.766397	1.508150	3.533416
1	3.381888	3.108284	2.905625
1	2.136298	1.850646	2.904883
6	5.169153	1.864246	1.175497
1	5.748137	1.379607	1.974626
1	5.547952	1.469964	0.224677
1	5.405597	2.936940	1.216657
6	3.200332	5.019070	0.561633
1	2.877853	6.069537	0.586990
1	3.597904	4.785464	1.559161
1	4.033657	4.953625	-0.148045
6	0.891547	4.282399	1.210253
1	1.196699	3.978958	2.221828
1	0.593613	5.339081	1.268428
1	0.001323	3.705316	0.933228
6	2.203281	1.962128	-2.838707

1	1.487083	1.137103	-2.727915
1	1.613566	2.890601	-2.849557
1	2.659813	1.852911	-3.832329
6	4.354757	2.993634	-2.119534
1	4.832206	2.720926	-3.070570
1	3.919730	3.993632	-2.258164
1	5.152141	3.077789	-1.370311

3RE10_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -311.7321 cm(-1)

Electronic energy : -3636.7131327
 Zero-point correction= 0.593727
 Thermal correction to Energy= 0.647700
 Thermal correction to Enthalpy= 0.648644
 Thermal correction to Gibbs Free Energy= 0.506488
 Sum of electronic and zero-point Energies= -3636.119406
 Sum of electronic and thermal Energies= -3636.065433
 Sum of electronic and thermal Enthalpies= -3636.064489
 Sum of electronic and thermal Free Energies= -3636.206645

 Cartesian Coordinates

8	0.927045	4.750279	-0.668874
6	-0.330389	4.874597	-0.301845
6	-0.695311	6.282101	0.026370
8	-1.125025	3.941650	-0.233669
1	-0.410094	6.947107	-0.794201
1	-0.131376	6.597815	0.910800
1	-1.764189	6.362278	0.226266
6	-0.157000	-2.608354	-2.340927
6	-0.664862	-3.726016	-2.992927
6	-1.201954	-4.772836	-2.253968
6	-1.259585	-4.693443	-0.870726
6	-0.784846	-3.566752	-0.186757
6	-0.206211	-2.558053	-0.956890
7	-0.965341	-3.507191	1.227735
6	-2.106873	-4.246796	1.781512
46	1.144618	-1.275706	-0.068437
35	3.432286	-2.424981	-0.198020
6	-0.788963	-0.684585	-0.194345
6	-1.924388	-0.184281	-0.266512
14	-3.670892	0.407737	-0.576406
6	-4.736557	-1.148468	-0.360789
6	-0.081027	-2.932540	2.063285
8	0.889789	-2.224787	1.701490
6	-0.201204	-3.137264	3.537684
6	-4.030417	1.805115	0.653952
6	-3.699507	1.094717	-2.350805
1	0.284839	-1.790304	-2.899958
1	-1.682943	-5.519459	-0.307043
1	-1.582076	-5.660743	-2.751409
1	-2.936688	-4.187508	1.073356
1	-1.856903	-5.297547	1.966589
1	-2.435742	-3.789279	2.714493
1	-0.324760	-4.194217	3.791012
1	0.703163	-2.744990	4.003516
1	-1.059607	-2.579794	3.930170
1	-3.517218	2.177361	-2.232531
1	-5.759295	-0.884639	-0.676786
1	-3.438551	2.651168	0.263039
1	-0.623871	-3.771835	-4.077624
47	-0.562863	1.686686	0.113438
1	1.148217	3.815189	-0.874081
8	1.466910	2.087070	-1.277214
16	1.950599	1.092877	-2.251210

6	3.778808	1.096866	-2.043133
8	1.552453	-0.329343	-1.895575
8	1.698854	1.345433	-3.657093
9	4.233589	2.273002	-2.450089
9	4.093688	0.911945	-0.782912
9	4.295975	0.140454	-2.791796
8	2.169159	0.414291	1.351637
16	1.822780	1.465961	2.333037
6	0.801202	0.574369	3.576013
8	2.934868	2.004421	3.098684
8	0.854873	2.472646	1.823998
9	-0.265231	0.008905	2.991502
9	1.501566	-0.383773	4.169699
9	0.362367	1.416229	4.500293
6	-4.220427	-2.274654	-1.256194
1	-3.178919	-2.526856	-1.005743
1	-4.818602	-3.189074	-1.130245
1	-4.239901	-2.016627	-2.322782
6	-2.596533	0.530099	-3.245813
1	-1.592490	0.771672	-2.873496
1	-2.657120	-0.565252	-3.329143
1	-2.674121	0.938510	-4.262905
6	-5.071300	0.913757	-3.003088
1	-5.893761	1.312282	-2.393967
1	-5.111461	1.424552	-3.974651
1	-5.287368	-0.147321	-3.189990
6	-4.778600	-1.604391	1.095795
1	-5.316952	-2.558683	1.194964
1	-3.763599	-1.754631	1.497727
1	-5.281349	-0.880554	1.747815
6	-5.504762	2.206751	0.599633
1	-5.706970	3.052933	1.270506
1	-5.817044	2.513594	-0.407527
1	-6.162469	1.383932	0.914284
6	-3.577063	1.558849	2.091133
1	-4.167909	0.772693	2.579583
1	-2.519934	1.263991	2.160050
1	-3.697349	2.470490	2.692130

3RE11 Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -316.2617 cm(-1)

Electronic energy : -2171.0361234
 Zero-point correction= 0.635037
 Thermal correction to Energy= 0.683399
 Thermal correction to Enthalpy= 0.684343
 Thermal correction to Gibbs Free Energy= 0.552726
 Sum of electronic and zero-point Energies= -2170.401086
 Sum of electronic and thermal Energies= -2170.352724
 Sum of electronic and thermal Enthalpies= -2170.351780
 Sum of electronic and thermal Free Energies= -2170.483397

 Cartesian Coordinates

8	-1.125488	4.817666	-0.982395
6	0.140447	4.583070	-0.722788
6	1.018786	5.763094	-0.979294
8	0.578531	3.509877	-0.318163
1	0.643457	6.638208	-0.439835
1	0.991379	6.006788	-2.046859
1	2.045407	5.544574	-0.683304
6	1.537254	-3.176134	0.952324
6	1.366966	-4.106597	1.970973
6	1.029254	-3.679658	3.249038
6	0.828471	-2.329619	3.497155
6	0.964049	-1.377360	2.481814

6	1.362127	-1.820084	1.212235
7	0.620940	-0.028447	2.792172
6	-0.499973	0.197886	3.714398
46	2.265731	-0.480921	-0.082052
35	2.473562	-1.913414	-2.125313
6	0.315352	-0.746013	-0.210622
6	-0.892975	-0.847587	-0.487684
14	-2.679444	-1.358696	-0.691235
6	-2.542960	-3.167721	-1.255777
6	1.325816	1.023881	2.332191
8	2.230298	0.919663	1.469225
6	1.035114	2.386474	2.868104
8	-2.641114	2.753796	-0.328107
6	-2.894276	2.593051	0.916647
6	-4.279678	2.970096	1.378359
8	-2.068810	2.139214	1.738254
6	-3.371046	-1.185723	1.071106
6	-3.522172	-0.163539	-1.898992
1	-5.028006	2.597097	0.671335
1	-4.374217	4.062246	1.391868
1	-4.482532	2.584388	2.380609
1	1.801509	-3.502873	-0.048761
1	0.557157	-2.001387	4.497554
1	0.914066	-4.396139	4.057880
1	-1.152851	-0.676237	3.687085
1	-0.150829	0.351837	4.742149
1	-1.091233	1.052896	3.377789
1	1.069423	2.406554	3.962581
1	1.765618	3.082639	2.454408
1	0.029873	2.698509	2.551071
1	-3.735922	0.730844	-1.287222
1	-1.856063	-3.616672	-0.516437
1	-2.971796	-0.212320	1.412355
1	1.508807	-5.162799	1.756838
47	-0.597172	1.469574	-0.291391
1	-1.694123	4.021622	-0.762663
8	3.387103	1.108308	-1.285040
6	4.460441	0.702965	-0.766790
6	5.760552	1.358143	-1.128098
8	4.464145	-0.278861	0.037419
1	5.607463	2.419231	-1.339403
1	6.145864	0.883588	-2.037723
1	6.499233	1.228766	-0.333802
6	-4.893731	-1.122973	1.159024
1	-5.218945	-0.956477	2.196197
1	-5.313645	-0.308864	0.554481
1	-5.364521	-2.058633	0.824669
6	-2.810547	-2.274666	1.983644
1	-3.098046	-2.103024	3.031924
1	-3.194259	-3.267448	1.709252
1	-1.711998	-2.330716	1.943526
6	-3.867035	-3.927805	-1.201580
1	-3.719552	-4.988883	-1.448210
1	-4.338326	-3.886433	-0.210703
1	-4.590387	-3.529646	-1.925964
6	-1.890825	-3.298345	-2.630490
1	-2.538739	-2.896690	-3.422055
1	-0.927960	-2.772695	-2.689063
1	-1.703872	-4.353196	-2.876826
6	-2.623730	0.279485	-3.052221
1	-2.348250	-0.562209	-3.702822
1	-3.135980	1.022892	-3.678919
1	-1.686808	0.737385	-2.705859
6	-4.844336	-0.710122	-2.439655
1	-5.373126	0.060102	-3.018308
1	-4.680079	-1.558547	-3.118431
1	-5.528173	-1.048018	-1.650245

3RE12_Pd-Ag

Number of imaginary frequencies : 1
The smallest frequency is : -273.7904 cm(-1)

Electronic energy : -2171.0382824
Zero-point correction= 0.635542
Thermal correction to Energy= 0.683307
Thermal correction to Enthalpy= 0.684252
Thermal correction to Gibbs Free Energy= 0.555722
Sum of electronic and zero-point Energies= -2170.402741
Sum of electronic and thermal Energies= -2170.354975
Sum of electronic and thermal Enthalpies= -2170.354031
Sum of electronic and thermal Free Energies= -2170.482560

Cartesian Coordinates

8	-2.567176	-3.555736	-1.474917
6	-3.234226	-3.337988	-0.368578
6	-4.666009	-3.758233	-0.453420
8	-2.760406	-2.834483	0.647359
1	-4.728883	-4.834792	-0.642601
1	-5.148693	-3.256565	-1.299959
1	-5.188760	-3.513128	0.472547
6	2.214764	2.814349	0.660155
6	2.477870	4.118458	0.250850
6	2.315476	4.476557	-1.082495
6	1.878545	3.539648	-2.009637
6	1.590909	2.227929	-1.621800
6	1.794204	1.892532	-0.283272
7	1.044313	1.336125	-2.589826
6	0.040161	1.880491	-3.506925
46	1.977055	-0.080660	0.244683
35	4.439628	-0.774469	0.463892
6	0.106804	0.653023	0.155641
6	-1.094794	0.945338	0.173090
14	-2.869486	1.475095	0.204460
6	-2.937165	3.216503	-0.569566
6	1.427520	0.045924	-2.668358
8	2.132456	-0.508676	-1.793278
6	1.026752	-0.794090	-3.832282
8	1.321210	-2.577979	0.199933
6	1.006067	-2.970275	-0.956064
6	2.022183	-3.791878	-1.706950
8	-0.099507	-2.699915	-1.517772
6	-3.836952	0.217071	-0.838089
6	-3.411943	1.458744	2.021683
1	1.630814	-4.161143	-2.658895
1	2.344676	-4.635886	-1.088809
1	2.909493	-3.172365	-1.881173
1	2.344381	2.505138	1.693077
1	1.748056	3.823874	-3.051550
1	2.530068	5.490875	-1.407935
1	-0.483973	2.695655	-3.000408
1	0.487996	2.263222	-4.431325
1	-0.696312	1.113483	-3.753451
1	0.744390	-0.231726	-4.723031
1	1.869146	-1.449511	-4.070139
1	0.206624	-1.448635	-3.500933
1	-4.425294	1.895092	2.046491
1	-3.085262	3.048701	-1.651498
1	-3.827367	-0.715260	-0.250504
1	2.818127	4.847260	0.981923
47	-0.806320	-1.527270	0.746401
1	-1.610901	-3.252916	-1.408248
8	1.996492	0.352970	2.230696
6	1.181534	-0.194911	3.084492
6	1.514540	0.228790	4.496962
8	0.260218	-0.972598	2.860677
1	0.676433	-0.006500	5.156543

1	1.750681	1.295165	4.545153
1	2.400569	-0.323006	4.828369
6	-3.165758	-0.066048	-2.180057
1	-3.078664	0.848422	-2.787233
1	-2.158431	-0.491966	-2.056865
1	-3.751262	-0.782552	-2.774563
6	-5.289077	0.650751	-1.025075
1	-5.865234	-0.112076	-1.568269
1	-5.799831	0.820831	-0.067307
1	-5.358762	1.579779	-1.609495
6	-3.484377	0.043304	2.591973
1	-2.487780	-0.425402	2.619062
1	-3.850465	0.059890	3.628209
1	-4.146591	-0.619026	2.019835
6	-4.128273	4.024335	-0.054026
1	-4.208039	4.985691	-0.580901
1	-5.086486	3.503964	-0.180163
1	-4.019448	4.254558	1.014767
6	-1.639171	4.003509	-0.391474
1	-1.395528	4.157200	0.669372
1	-0.776453	3.493177	-0.839286
1	-1.716125	4.999375	-0.851871
6	-2.488878	2.323895	2.879574
1	-2.472401	3.373886	2.558986
1	-2.801703	2.308990	3.933093
1	-1.455209	1.947410	2.843132

3RE13_Pd-Ag

Number of imaginary frequencies : 1

The smallest frequency is : -149.1161 cm(-1)

Electronic energy : -2903.8689525
 Zero-point correction= 0.613951
 Thermal correction to Energy= 0.665555
 Thermal correction to Enthalpy= 0.666500
 Thermal correction to Gibbs Free Energy= 0.527538
 Sum of electronic and zero-point Energies= -2903.255002
 Sum of electronic and thermal Energies= -2903.203397
 Sum of electronic and thermal Enthalpies= -2903.202453
 Sum of electronic and thermal Free Energies= -2903.341415

Cartesian Coordinates

8	-1.430784	4.604981	0.319043
6	-0.212641	4.501650	-0.163057
6	0.233408	5.727348	-0.889881
8	0.505135	3.515908	-0.027880
1	0.350654	6.547732	-0.173477
1	-0.527941	6.037169	-1.612552
1	1.184128	5.546975	-1.392891
6	0.444334	-3.737731	-1.166130
6	-0.120948	-5.007464	-1.072466
6	-0.803383	-5.378987	0.078052
6	-0.912637	-4.498131	1.144591
6	-0.354602	-3.215964	1.087148
6	0.327676	-2.881973	-0.083598
7	-0.504620	-2.365490	2.215545
6	-1.758725	-2.388547	2.976410
46	1.474352	-1.171876	-0.130767
35	1.644975	-0.773371	-2.585406
6	-0.409539	-0.792844	-0.426176
6	-1.559109	-0.433950	-0.683605
14	-3.298685	0.066671	-1.119733
6	-4.288159	-0.250578	0.473713
6	0.519217	-1.611580	2.662210
8	1.519829	-1.353187	1.950420
6	0.502138	-1.082705	4.051293

8	-1.391518	0.839611	2.692597
6	-2.316803	1.696416	2.591441
6	-3.411471	1.643956	3.633480
8	-2.387416	2.564240	1.685518
6	-3.273876	1.918983	-1.535206
6	-3.753266	-1.054576	-2.591064
1	-2.989071	1.889173	4.614527
1	-3.814131	0.625321	3.705674
1	-4.219920	2.343302	3.408535
1	0.955344	-3.427202	-2.071039
1	-1.424412	-4.806901	2.052877
1	-1.249321	-6.366722	0.156544
1	-2.540379	-2.812886	2.345615
1	-1.672193	-2.984739	3.891901
1	-2.035819	-1.354262	3.213888
1	0.210463	-1.850369	4.774397
1	1.497128	-0.701148	4.286127
1	-0.217276	-0.254695	4.091595
1	-4.845822	-0.958546	-2.724735
1	-3.591915	0.100198	1.253589
1	-3.261429	2.395949	-0.540280
1	-0.029310	-5.690934	-1.912128
47	-0.125615	1.394214	0.743178
1	-1.693529	3.792920	0.836599
9	6.156526	0.398219	-0.512995
6	5.020882	1.080176	-0.518868
16	3.855207	0.320137	0.682339
9	5.259251	2.331212	-0.152466
9	4.514897	1.076206	-1.738044
8	3.657080	-1.073843	0.126901
8	4.543986	0.384024	1.959125
8	2.598166	1.088300	0.524061
6	-5.574157	0.562672	0.575530
1	-6.278875	0.306354	-0.229697
1	-6.092850	0.360443	1.524337
1	-5.388540	1.642573	0.532365
6	-4.567359	-1.726160	0.735817
1	-4.952686	-1.875569	1.756212
1	-5.329249	-2.118071	0.047093
1	-3.668818	-2.349301	0.620679
6	-4.541060	2.362076	-2.268782
1	-5.462463	2.078129	-1.744360
1	-4.559984	3.454759	-2.383453
1	-4.595479	1.936398	-3.280306
6	-2.027545	2.387965	-2.284696
1	-2.021331	3.485091	-2.365804
1	-1.092675	2.086909	-1.790641
1	-1.986497	1.992072	-3.307765
6	-3.413008	-2.527553	-2.357269
1	-3.957149	-2.973391	-1.518334
1	-3.648073	-3.121436	-3.252029
1	-2.336862	-2.655186	-2.160761
6	-3.058415	-0.585452	-3.869808
1	-3.345484	0.429666	-4.166422
1	-1.964513	-0.602520	-3.752181
1	-3.301141	-1.251493	-4.709730

3RE14_Pd-Ag

Number of imaginary frequencies : 1
The smallest frequency is : -59.3125 cm(-1)

Electronic energy : -2171.0324987
Zero-point correction= 0.635397
Thermal correction to Energy= 0.683571
Thermal correction to Enthalpy= 0.684515
Thermal correction to Gibbs Free Energy= 0.553683
Sum of electronic and zero-point Energies= -2170.397101

Sum of electronic and thermal Energies= -2170.348928
 Sum of electronic and thermal Enthalpies= -2170.347983
 Sum of electronic and thermal Free Energies= -2170.478816

 Cartesian Coordinates

6	-2.039991	1.307454	-2.551763
6	-2.591200	2.412797	-3.197656
6	-3.099833	3.470385	-2.455808
6	-3.052938	3.422727	-1.071880
6	-2.512696	2.332596	-0.375183
6	-2.058044	1.279864	-1.169589
7	-2.483173	2.406929	1.039230
6	-1.241679	2.757452	1.710304
35	-3.278819	-2.497446	-0.893256
6	-0.017880	0.508680	-0.123471
6	1.092909	1.038153	-0.002494
14	2.756383	1.864882	0.022948
6	3.038874	2.412961	1.819328
6	-3.663861	2.163877	1.717309
8	-4.707483	1.932517	1.134955
6	-3.572612	2.228659	3.219529
8	0.675099	-2.503821	-1.077790
6	0.259920	-2.039805	-2.160911
6	0.839298	-2.516440	-3.462494
8	-0.677009	-1.176207	-2.268005
6	3.959430	0.500205	-0.540587
6	2.575139	3.386194	-1.107267
1	-1.629180	0.483337	-3.124831
1	-3.439141	4.242949	-0.469901
1	-3.526236	4.337717	-2.953003
1	-0.555763	3.190960	0.976382
1	-1.416109	3.512622	2.484449
1	-0.746146	1.885851	2.164347
1	-3.406136	3.257517	3.561646
1	-4.520511	1.877923	3.632263
1	-2.751152	1.616029	3.608755
1	2.211723	4.178641	-0.428175
1	2.120205	2.976907	2.062575
1	3.820779	-0.276350	0.233152
1	-2.609634	2.430893	-4.284455
1	0.744518	-1.759450	-4.243988
1	0.283076	-3.406601	-3.777861
1	1.888308	-2.798989	-3.331701
46	-1.596537	-0.644254	-0.474417
47	0.940848	-1.286931	1.118163
8	3.115450	-3.426549	-0.673252
6	3.572931	-3.094263	0.510462
6	4.989435	-3.510890	0.728243
8	2.928844	-2.483388	1.361284
1	5.275269	-3.362821	1.770270
1	5.638003	-2.904675	0.084240
1	5.131663	-4.555421	0.436727
8	-1.022497	-1.756545	2.316201
6	-2.104306	-1.150051	2.274267
6	-3.099441	-1.323426	3.390909
8	-2.516206	-0.372984	1.332542
1	-3.934660	-0.625051	3.306705
1	-2.601100	-1.223680	4.359700
1	-3.491385	-2.344705	3.320528
1	2.171100	-3.123225	-0.812654
6	3.549352	-0.105415	-1.882543
1	4.146624	-1.000753	-2.112766
1	2.491329	-0.402100	-1.893337
1	3.703488	0.605150	-2.707306
6	5.435475	0.891530	-0.544881
1	6.064650	0.031831	-0.817725
1	5.646781	1.681780	-1.276470
1	5.783006	1.245728	0.433788
6	4.222347	3.362122	1.994892

1	5.178439	2.871175	1.766792
1	4.146427	4.250079	1.354062
1	4.289045	3.717691	3.032642
6	3.133824	1.232710	2.782557
1	4.027591	0.622238	2.592495
1	3.196303	1.574649	3.825163
1	2.260136	0.565108	2.716189
6	3.904712	3.849573	-1.701847
1	4.285496	3.125830	-2.436214
1	3.783454	4.804840	-2.231495
1	4.686447	3.993747	-0.944405
6	1.529075	3.200696	-2.206689
1	1.476810	4.092521	-2.847229
1	1.764033	2.346345	-2.857950
1	0.525763	3.024697	-1.797702

3RE15_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -216.1064 cm(-1)

Electronic energy : -2903.8724991
 Zero-point correction= 0.615740
 Thermal correction to Energy= 0.666594
 Thermal correction to Enthalpy= 0.667538
 Thermal correction to Gibbs Free Energy= 0.532251
 Sum of electronic and zero-point Energies= -2903.256759
 Sum of electronic and thermal Energies= -2903.205905
 Sum of electronic and thermal Enthalpies= -2903.204961
 Sum of electronic and thermal Free Energies= -2903.340248

 Cartesian Coordinates

8	-4.240416	0.027757	-3.166971
6	-3.512355	1.118228	-3.215330
6	-4.238119	2.276731	-3.816300
8	-2.359635	1.208181	-2.806277
1	-4.831955	1.961382	-4.678503
1	-3.534034	3.060902	-4.099414
1	-4.934166	2.675872	-3.068770
6	1.425656	-1.236757	-2.140850
6	0.819508	-2.296677	-2.814948
6	0.395836	-3.412404	-2.105123
6	0.582152	-3.479054	-0.733626
6	1.166334	-2.425411	-0.021853
6	1.586003	-1.323151	-0.762954
7	1.266492	-2.533128	1.390550
6	0.252187	-3.346439	2.072165
46	3.025152	-0.022587	-0.048862
35	5.519885	-0.319273	-0.437630
6	1.168291	0.462995	0.477338
6	0.217630	1.031624	1.019898
14	-1.145925	1.974367	1.887372
6	-0.235897	3.239400	2.984960
6	2.312952	-2.029558	2.071759
8	3.207582	-1.318467	1.556259
6	2.452312	-2.326711	3.528874
6	-2.212234	2.711347	0.499042
6	-2.107721	0.711286	2.931359
1	1.757870	-0.356692	-2.681501
1	0.259397	-4.364645	-0.194265
1	-0.084471	-4.240515	-2.618178
1	-0.704709	-3.202799	1.565268
1	0.524508	-4.408092	2.068832
1	0.133853	-3.012720	3.102891
1	2.364934	-3.395698	3.744433
1	3.424652	-1.962671	3.862797
1	1.670628	-1.796630	4.088041

1	-2.798231	0.215297	2.228921
1	0.048221	2.666710	3.885661
1	-2.422288	1.834716	-0.141282
1	0.688980	-2.232378	-3.891619
47	-0.706666	0.383433	-1.363862
1	-3.779433	-0.696304	-2.664049
8	-3.119283	-1.921607	-1.686602
16	-3.055486	-1.459665	-0.280545
6	-3.597634	-2.913138	0.693481
8	-1.668297	-1.270600	0.203855
8	-3.994156	-0.393940	0.066812
9	-4.839956	-3.247753	0.391216
9	-2.800132	-3.951096	0.444389
9	-3.524936	-2.630072	1.990544
8	1.130376	1.772637	-2.259167
6	2.219450	2.221131	-1.904407
6	2.627600	3.630678	-2.255317
8	3.142352	1.617993	-1.218336
1	2.385687	4.274115	-1.400365
1	2.061585	3.973565	-3.124294
1	3.702007	3.707226	-2.436815
6	-1.474561	3.752951	-0.340658
1	-0.516842	3.383747	-0.735762
1	-2.081076	4.055162	-1.206469
1	-1.268180	4.663700	0.239743
6	-3.570550	3.234982	0.959594
1	-4.168576	3.556237	0.094471
1	-4.153491	2.468331	1.484255
1	-3.474668	4.104869	1.623390
6	1.044121	3.790394	2.357184
1	0.833141	4.343148	1.431034
1	1.541189	4.491649	3.042258
1	1.764985	3.002475	2.108243
6	-1.143451	4.390673	3.420722
1	-0.616480	5.059961	4.115453
1	-1.447184	5.002025	2.559252
1	-2.056587	4.052382	3.926358
6	-1.172863	-0.351206	3.504084
1	-1.733037	-1.093677	4.092008
1	-0.643395	-0.877886	2.701791
1	-0.420631	0.094507	4.174649
6	-2.917490	1.359834	4.052676
1	-3.624928	2.116280	3.690364
1	-3.504093	0.604319	4.594128
1	-2.263435	1.843891	4.792433

3RE16_Pd-Ag

Number of imaginary frequencies : 1

The smallest frequency is : -167.1978 cm(-1)

Electronic energy : -2171.027719
 Zero-point correction= 0.635677
 Thermal correction to Energy= 0.683700
 Thermal correction to Enthalpy= 0.684644
 Thermal correction to Gibbs Free Energy= 0.554690
 Sum of electronic and zero-point Energies= -2170.392042
 Sum of electronic and thermal Energies= -2170.344019
 Sum of electronic and thermal Enthalpies= -2170.343075
 Sum of electronic and thermal Free Energies= -2170.473029

 Cartesian Coordinates

8	-3.732870	-2.710471	0.661261
6	-2.509750	-2.902754	0.205928
6	-1.747230	-3.971393	0.907298
8	-2.040684	-2.236560	-0.712510
1	-2.362986	-4.525220	1.618608

1	-0.901436	-3.490193	1.422394
1	-1.314195	-4.653934	0.168366
6	-1.388629	3.293645	-0.102057
6	-1.309446	4.514886	0.562524
6	-1.029694	4.542272	1.923101
6	-0.824092	3.362106	2.624097
6	-0.885704	2.117630	1.984994
6	-1.200083	2.136174	0.627380
7	-0.629888	0.941499	2.744670
6	0.320290	1.012627	3.858188
46	-1.789779	0.429231	-0.319502
35	-4.372501	0.399674	-0.574230
6	0.191635	0.589896	-0.230848
6	1.419589	0.661605	-0.300541
14	3.277633	0.702954	-0.326658
6	3.759162	0.310618	1.473465
6	-1.305671	-0.208341	2.550173
8	-2.034158	-0.416814	1.551151
6	-1.221975	-1.293534	3.565617
8	1.993403	-3.171940	0.026113
6	1.918113	-2.876254	1.256509
6	2.974519	-3.479477	2.160769
8	1.034781	-2.139793	1.765804
6	3.885201	-0.682100	-1.478375
6	3.723032	2.457847	-0.924480
1	3.076081	-2.909718	3.089586
1	3.938441	-3.538279	1.645836
1	2.684214	-4.504757	2.420555
1	-1.596281	3.237471	-1.166553
1	-0.623580	3.399450	3.691859
1	-0.973218	5.490065	2.451596
1	0.998172	1.849259	3.693377
1	-0.185641	1.145941	4.821323
1	0.921574	0.099209	3.875478
1	-1.255826	-0.918402	4.591843
1	-2.050867	-1.985005	3.397286
1	-0.277086	-1.830655	3.391070
1	4.798321	2.603071	-0.718623
1	3.044092	-0.489415	1.742354
1	3.733951	-1.589426	-0.865546
1	-1.467750	5.435657	0.007483
47	0.378640	-1.804726	-0.856693
1	-4.098487	-1.910442	0.217973
8	-1.625505	1.191200	-2.188542
6	-1.064544	0.415498	-3.073104
6	-1.012813	1.039568	-4.444314
8	-0.598995	-0.703213	-2.874580
1	-1.577228	1.971581	-4.505265
1	-1.398520	0.320403	-5.172457
1	0.037726	1.230692	-4.690274
6	5.372324	-0.549031	-1.811134
1	5.727598	-1.430818	-2.362744
1	5.563070	0.322713	-2.452933
1	6.009346	-0.444309	-0.925011
6	3.082173	-0.874203	-2.764123
1	3.337657	-1.832681	-3.236994
1	1.994797	-0.869239	-2.604956
1	3.297353	-0.086802	-3.498612
6	5.178203	-0.214336	1.666877
1	5.368255	-0.441617	2.726285
1	5.374053	-1.132423	1.100686
1	5.929111	0.531294	1.363913
6	3.515060	1.494289	2.404522
1	2.526462	1.949572	2.249053
1	3.587311	1.191482	3.459815
1	4.268708	2.279945	2.249466
6	3.489921	2.583630	-2.431067
1	3.688951	3.610131	-2.770564
1	4.126309	1.916528	-3.024027
1	2.442777	2.359113	-2.686045

6	2.933132	3.558199	-0.212698
1	1.849301	3.403743	-0.329108
1	3.142434	3.618913	0.859842
1	3.166586	4.540512	-0.647833

3RE17_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -121.9508 cm(-1)

Electronic energy : -2903.8559868
 Zero-point correction= 0.612501
 Thermal correction to Energy= 0.664861
 Thermal correction to Enthalpy= 0.665805
 Thermal correction to Gibbs Free Energy= 0.524638
 Sum of electronic and zero-point Energies= -2903.243486
 Sum of electronic and thermal Energies= -2903.191126
 Sum of electronic and thermal Enthalpies= -2903.190181
 Sum of electronic and thermal Free Energies= -2903.331349

 Cartesian Coordinates

8	2.582354	-3.468290	-1.582288
6	3.717439	-2.838967	-1.358010
6	4.807921	-3.253039	-2.287437
8	3.865743	-1.990136	-0.485002
1	4.528338	-2.979032	-3.310938
1	4.932083	-4.339893	-2.265087
1	5.742261	-2.758739	-2.019350
6	0.157895	1.355233	2.388278
6	-0.383469	1.579972	3.654782
6	-1.465061	2.436831	3.797554
6	-2.022446	3.058942	2.688098
6	-1.522882	2.828597	1.399724
6	-0.396053	2.019524	1.316115
7	-2.184729	3.427165	0.289190
6	-3.628221	3.660197	0.399298
46	0.768569	1.976580	-0.369948
35	1.999928	0.667891	-2.415146
6	-0.693038	0.685561	-0.606803
6	-1.600403	-0.129330	-0.766012
14	-2.985071	-1.339952	-0.987561
6	-3.845350	-0.700539	-2.560982
6	-1.511092	3.898790	-0.777559
8	-0.295458	3.684611	-0.986463
6	-2.224273	4.747389	-1.780761
8	2.382109	3.281540	-0.135178
6	3.317210	2.735588	0.558021
6	4.544495	3.569601	0.771519
8	3.248596	1.581961	1.022695
6	-2.168412	-3.029972	-1.192115
6	-4.051295	-1.299121	0.593123
1	4.305557	4.636094	0.781199
1	5.236944	3.385055	-0.057863
1	5.041305	3.278123	1.700214
1	0.985021	0.659437	2.271570
1	-2.860471	3.738546	2.818492
1	-1.896175	2.617097	4.778680
1	-4.050412	2.917356	1.077298
1	-3.850273	4.664591	0.778021
1	-4.105872	3.525556	-0.573835
1	-2.829584	5.526792	-1.309405
1	-1.481394	5.202342	-2.437431
1	-2.881766	4.119373	-2.395117
1	-3.549735	-2.015248	1.265158
1	-3.012559	-0.598659	-3.277964
1	-1.499830	-3.086530	-0.319965
1	0.043591	1.059781	4.508076

47	2.191043	-0.393833	0.043499
1	1.914435	-3.220200	-0.894679
8	1.714327	-1.405802	2.130574
16	1.069791	-2.706777	1.798014
6	-0.590891	-2.526515	2.563443
8	0.759474	-2.807582	0.348623
8	1.647818	-3.886601	2.421970
9	-0.471969	-2.444825	3.881070
9	-1.189020	-1.422089	2.123507
9	-1.354513	-3.569999	2.262519
6	-1.284367	-3.073347	-2.434515
1	-0.568895	-2.238856	-2.456881
1	-0.700655	-4.004347	-2.469701
1	-1.876325	-3.028438	-3.360664
6	-3.122784	-4.218989	-1.121872
1	-3.847122	-4.225565	-1.948339
1	-2.566210	-5.165088	-1.179109
1	-3.691998	-4.238406	-0.182624
6	-4.442797	0.688672	-2.345872
1	-5.281301	0.660644	-1.634630
1	-3.693729	1.392295	-1.952810
1	-4.832016	1.105539	-3.286108
6	-4.869918	-1.656068	-3.166197
1	-5.302079	-1.236193	-4.086243
1	-4.426328	-2.623827	-3.431623
1	-5.704748	-1.853185	-2.481206
6	-5.481690	-1.785286	0.363571
1	-6.015706	-1.897489	1.317998
1	-6.057391	-1.067991	-0.238613
1	-5.528232	-2.755024	-0.148558
6	-4.055003	0.061492	1.285087
1	-4.641584	0.032648	2.215423
1	-3.041161	0.398553	1.539103
1	-4.512477	0.825079	0.637910

3RE18_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -62.2151 cm(-1)

Electronic energy : -2903.8609558
 Zero-point correction= 0.616129
 Thermal correction to Energy= 0.666965
 Thermal correction to Enthalpy= 0.667910
 Thermal correction to Gibbs Free Energy= 0.530880
 Sum of electronic and zero-point Energies= -2903.244827
 Sum of electronic and thermal Energies= -2903.193990
 Sum of electronic and thermal Enthalpies= -2903.193046
 Sum of electronic and thermal Free Energies= -2903.330076

 Cartesian Coordinates

8	1.890701	0.173330	-1.762231
6	1.270833	-0.517518	-2.580472
6	1.362249	-0.269363	-4.057535
8	0.476556	-1.480282	-2.244369
1	1.051886	-1.141502	-4.634985
1	2.384512	0.017328	-4.315939
1	0.700597	0.568676	-4.302791
6	-1.598820	-3.452103	-1.518400
6	-2.626449	-4.393463	-1.568257
6	-3.453369	-4.577393	-0.466629
6	-3.269058	-3.825622	0.686591
6	-2.253530	-2.867006	0.764901
6	-1.433140	-2.737362	-0.350925
7	-2.131499	-2.081945	1.943124
6	-3.362863	-1.668048	2.619568
46	0.284206	-1.661086	-0.230045

35	2.515154	-3.038849	-0.082761
6	-1.206329	-0.400078	-0.401989
6	-2.098019	0.434383	-0.502090
14	-3.496233	1.643976	-0.546431
6	-4.048305	1.884148	1.260699
6	-0.925157	-1.735306	2.430971
8	0.139559	-1.951922	1.803130
6	-0.812293	-1.087046	3.766888
8	3.633138	2.274467	-1.799573
6	4.704548	1.946340	-1.100257
6	5.581909	3.118821	-0.809241
8	4.941310	0.810667	-0.709483
6	-2.862722	3.244222	-1.346181
6	-4.846207	0.793062	-1.590637
1	5.119250	3.680380	0.010813
1	5.649405	3.785484	-1.672260
1	6.570719	2.783538	-0.494755
1	-0.947295	-3.273430	-2.368789
1	-3.915758	-3.982491	1.546393
1	-4.251384	-5.313569	-0.499558
1	-4.152316	-1.578862	1.869119
1	-3.670438	-2.387092	3.387019
1	-3.221454	-0.685642	3.076447
1	-1.517687	-1.481325	4.501563
1	0.214069	-1.211201	4.114428
1	-0.973749	-0.007693	3.638738
1	-4.532496	0.927843	-2.640351
1	-4.607687	0.964470	1.515258
1	-2.331967	3.789443	-0.548715
1	-2.772279	-4.973398	-2.475333
47	3.163274	-0.412905	0.389769
1	3.033269	1.493218	-1.888116
8	0.763315	0.734039	1.621339
16	1.582948	1.943065	1.822967
6	0.949164	3.122313	0.567081
8	1.403346	2.638509	3.093850
8	2.994828	1.748202	1.389308
9	1.034690	2.604978	-0.650849
9	-0.330406	3.407807	0.808693
9	1.648181	4.249336	0.602861
6	-4.914667	-0.707398	-1.304086
1	-3.964149	-1.215950	-1.505207
1	-5.175716	-0.891880	-0.249328
1	-5.694568	-1.189605	-1.909963
6	-6.233964	1.409948	-1.416310
1	-6.255672	2.487677	-1.616603
1	-6.959750	0.934863	-2.090769
1	-6.602981	1.255390	-0.392521
6	-2.856069	2.012298	2.210789
1	-3.180602	1.966020	3.261245
1	-2.085503	1.247282	2.043080
1	-2.355294	2.979528	2.078354
6	-1.862068	2.939446	-2.460760
1	-1.514799	3.866629	-2.937391
1	-0.984366	2.399910	-2.087606
1	-2.322602	2.324245	-3.248695
6	-3.990238	4.129574	-1.878656
1	-3.589321	5.070387	-2.279878
1	-4.523148	3.633146	-2.702182
1	-4.732001	4.389475	-1.112772
6	-4.980749	3.081212	1.453134
1	-5.292829	3.169267	2.503011
1	-4.465575	4.016894	1.195254
1	-5.889848	3.024114	0.842743

3RE19_Pd-Ag

Number of imaginary frequencies : 1

The smallest frequency is : -291.1971 cm(-1)

Electronic energy : -2171.0223317
Zero-point correction= 0.635531
Thermal correction to Energy= 0.683634
Thermal correction to Enthalpy= 0.684578
Thermal correction to Gibbs Free Energy= 0.555003
Sum of electronic and zero-point Energies= -2170.386801
Sum of electronic and thermal Energies= -2170.338698
Sum of electronic and thermal Enthalpies= -2170.337754
Sum of electronic and thermal Free Energies= -2170.467329

.....
Cartesian Coordinates

.....
8 4.977135 -1.036695 -0.631684
6 5.002355 0.194007 -0.172101
6 6.335909 0.842090 -0.313344
8 4.039606 0.766874 0.333750
1 6.668552 0.782052 -1.354384
1 7.068700 0.298379 0.292057
1 6.289690 1.882420 0.009251
6 1.270528 3.181079 0.482994
6 1.111067 4.468650 -0.018802
6 0.790623 4.653015 -1.359259
6 0.623126 3.559366 -2.199135
6 0.760723 2.254685 -1.715682
6 1.095209 2.099541 -0.366564
7 0.501545 1.172364 -2.602307
6 -0.615549 1.288793 -3.550046
46 1.809691 0.293708 0.316749
35 2.336330 -2.410402 0.787085
6 -0.136122 0.495173 0.297157
6 -1.360030 0.483398 0.414025
14 -3.201056 0.629624 0.575548
6 -3.777984 1.070968 -1.187067
6 1.243256 0.052425 -2.595966
8 2.077636 -0.203413 -1.687297
6 1.102989 -0.935872 -3.696833
8 -2.161028 -3.071509 -0.913026
6 -2.326650 -2.361342 -1.945223
6 -3.559840 -2.628541 -2.783576
8 -1.533628 -1.460387 -2.326477
6 -3.955607 -1.031931 1.104971
6 -3.437048 2.009615 1.872634
1 -4.353743 -3.095328 -2.193330
1 -3.297155 -3.317585 -3.595450
1 -3.923860 -1.704652 -3.246172
1 1.513081 3.005149 1.527685
1 0.384894 3.712042 -3.249426
1 0.675401 5.655500 -1.762794
1 -1.292896 2.064782 -3.190134
1 -0.268058 1.553602 -4.555173
1 -1.168178 0.342386 -3.559187
1 1.062329 -0.465290 -4.683454
1 1.938652 -1.635921 -3.644744
1 0.164664 -1.485369 -3.521129
1 -4.488601 2.339676 1.795760
1 -3.182561 0.377444 -1.810247
1 -3.971702 -1.621538 0.172195
1 1.239416 5.321737 0.642330
47 -0.298754 -2.061740 -0.015583
1 4.109171 -1.460381 -0.435496
8 1.747183 0.847939 2.238652
6 0.972377 0.239220 3.119017
6 1.108286 0.922236 4.464577
8 0.232645 -0.701721 2.927661
1 2.158927 1.028226 4.748603
1 0.570946 0.341852 5.217575
1 0.677002 1.927925 4.402156
6 -3.188180 1.474110 3.283320

1	-3.891577	0.685766	3.574857
1	-2.172815	1.057053	3.369149
1	-3.271204	2.279331	4.027672
6	-2.520093	3.211508	1.643828
1	-1.466714	2.913549	1.755333
1	-2.623992	3.666347	0.652757
1	-2.714411	3.995276	2.390116
6	-3.422389	2.500327	-1.587120
1	-3.623149	2.673595	-2.655442
1	-4.029089	3.230065	-1.031624
1	-2.365400	2.744198	-1.399803
6	-5.258024	0.809933	-1.452270
1	-5.514714	1.048025	-2.495332
1	-5.540167	-0.236804	-1.284402
1	-5.902240	1.437191	-0.817458
6	-5.392823	-0.862399	1.604316
1	-6.029178	-0.291374	0.917005
1	-5.870288	-1.841189	1.752012
1	-5.422225	-0.346613	2.574327
6	-3.141422	-1.836677	2.115128
1	-3.595111	-2.826334	2.266621
1	-2.107104	-2.005965	1.788324
1	-3.091714	-1.344224	3.095318

3RE20_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -144.9152 cm(-1)

Electronic energy : -3636.69393
 Zero-point correction= 0.593022
 Thermal correction to Energy= 0.647750
 Thermal correction to Enthalpy= 0.648694
 Thermal correction to Gibbs Free Energy= 0.503447
 Sum of electronic and zero-point Energies= -3636.100908
 Sum of electronic and thermal Energies= -3636.046180
 Sum of electronic and thermal Enthalpies= -3636.045236
 Sum of electronic and thermal Free Energies= -3636.190483

 Cartesian Coordinates

8	1.571351	4.723373	-0.778341
6	0.312422	4.852992	-1.137762
6	0.061679	6.071510	-1.959728
8	-0.575761	4.065108	-0.827920
1	0.723815	6.072051	-2.831491
1	0.301193	6.963517	-1.371433
1	-0.979980	6.105935	-2.279567
6	-1.021544	-1.060185	2.073225
6	-1.058963	-1.708211	3.309434
6	-0.842344	-3.076601	3.376033
6	-0.575117	-3.806677	2.224546
6	-0.503398	-3.183889	0.972639
6	-0.796627	-1.825574	0.950519
7	-0.148528	-3.964889	-0.163638
6	0.785189	-5.076591	0.041799
46	-1.352694	-0.904104	-0.805244
35	-1.033489	0.923131	-2.802065
6	0.581489	-0.865798	-0.609932
6	1.810837	-0.818983	-0.561853
14	3.668390	-0.847116	-0.563370
6	4.090549	-1.892578	-2.099369
6	-0.757286	-3.807320	-1.355229
8	-1.518418	-2.850330	-1.622758
6	-0.536126	-4.820415	-2.430678
6	4.255474	0.954300	-0.601836
6	4.271151	-1.680705	1.042668
1	-1.150720	0.018604	2.017697

1	-0.418871	-4.880590	2.291164
1	-0.865322	-3.588223	4.334411
1	1.437323	-4.830168	0.881297
1	0.259447	-6.014629	0.254569
1	1.411351	-5.205702	-0.843760
1	-0.655127	-5.843806	-2.063314
1	-1.246861	-4.631266	-3.236035
1	0.478244	-4.712604	-2.836361
1	4.357621	-0.848361	1.761196
1	5.187691	-2.003652	-2.116581
1	3.975338	1.335286	0.395467
1	-1.236030	-1.119009	4.205235
47	-0.643419	1.774402	-0.330590
1	1.681831	3.946234	-0.173897
8	-5.154958	1.029054	-1.005336
16	-4.109823	0.348857	-0.265404
6	-4.964106	-0.513475	1.113698
8	-3.490817	-0.819978	-1.005116
8	-3.077764	1.162238	0.404124
9	-5.538406	0.376065	1.905778
9	-5.884281	-1.331714	0.629908
9	-4.087167	-1.218940	1.819121
8	-0.272101	1.982031	1.924558
16	1.103355	2.519257	2.156830
6	1.925181	1.138598	3.045528
8	1.873318	2.600347	0.891305
8	1.189159	3.659662	3.052854
9	1.325956	0.932104	4.209065
9	1.857060	0.020982	2.328616
9	3.202367	1.429378	3.251823
6	3.300974	-2.705502	1.627590
1	2.289469	-2.301734	1.763297
1	3.227259	-3.588220	0.975946
1	3.652856	-3.062924	2.606042
6	5.654869	-2.309039	0.873834
1	6.397983	-1.613723	0.463777
1	6.042906	-2.666374	1.837985
1	5.620646	-3.178340	0.202754
6	3.543683	1.831794	-1.628481
1	2.450691	1.748405	-1.559482
1	3.802428	2.888432	-1.472756
1	3.833366	1.579345	-2.657172
6	5.773418	1.064275	-0.745713
1	6.086795	2.117569	-0.750673
1	6.310456	0.576133	0.077845
1	6.132198	0.621667	-1.686642
6	3.649310	-1.220019	-3.397735
1	4.194707	-0.289979	-3.594648
1	3.820964	-1.883028	-4.257808
1	2.576997	-0.973698	-3.386439
6	3.469873	-3.286044	-1.989037
1	3.643894	-3.867961	-2.905928
1	3.882733	-3.863887	-1.152197
1	2.379815	-3.217051	-1.842197

3RE21_Pd-Ag

Number of imaginary frequencies : 1
The smallest frequency is : -65.7478 cm(-1)

Electronic energy :	-2903.8587663
Zero-point correction=	0.615935
Thermal correction to Energy=	0.666420
Thermal correction to Enthalpy=	0.667364
Thermal correction to Gibbs Free Energy=	0.533852
Sum of electronic and zero-point Energies=	-2903.242831
Sum of electronic and thermal Energies=	-2903.192346
Sum of electronic and thermal Enthalpies=	-2903.191402

Sum of electronic and thermal Free Energies= -2903.324914

.....
Cartesian Coordinates
.....

8	-3.858773	-2.566703	-1.490135
6	-2.645529	-2.355439	-1.955823
6	-2.047595	-3.522538	-2.662457
8	-2.055790	-1.289656	-1.796841
1	-2.803150	-4.251249	-2.961875
1	-1.334607	-4.008868	-1.983067
1	-1.481394	-3.176232	-3.532081
6	-1.147631	1.665148	2.846353
6	-0.765516	1.874060	4.170645
6	-0.238401	0.824143	4.912615
6	-0.087185	-0.435503	4.348714
6	-0.446441	-0.678025	3.017423
6	-0.995600	0.397527	2.325998
7	-0.224346	-1.970792	2.467263
6	0.945701	-2.747865	2.901760
46	-1.833880	0.104914	0.489311
35	-4.411493	0.129922	0.569055
6	0.148845	0.189078	0.323431
6	1.364759	0.378494	0.227686
14	3.210553	0.624229	0.091943
6	3.914319	-0.840818	1.081938
6	-1.055711	-2.518892	1.571212
8	-1.959475	-1.871071	0.976226
6	-0.953869	-3.965033	1.242122
8	2.012204	-2.511418	-2.432905
6	2.234464	-3.170532	-1.374456
6	3.464245	-4.049656	-1.353006
8	1.531444	-3.105046	-0.331187
6	3.649495	0.552687	-1.752912
6	3.581137	2.335830	0.842787
1	4.274299	-3.497601	-0.856785
1	3.796302	-4.305253	-2.362122
1	3.285372	-4.958510	-0.771270
1	-1.540441	2.473084	2.235003
1	0.309734	-1.253855	4.944633
1	0.056555	0.980543	5.946517
1	1.650473	-2.071615	3.383174
1	0.664516	-3.535198	3.609281
1	1.433664	-3.174063	2.016593
1	-0.857417	-4.586734	2.137023
1	-1.848160	-4.254238	0.685139
1	-0.062993	-4.103806	0.609523
1	3.393348	3.052814	0.025483
1	3.260261	-1.678921	0.776042
1	3.573757	-0.513327	-2.031825
1	-0.879001	2.862916	4.606410
47	0.357760	-1.124200	-1.663600
1	-4.144800	-1.773836	-0.981280
8	-1.076936	1.404214	-2.288318
16	-1.658640	2.486299	-1.505104
6	-0.313387	3.726063	-1.304899
8	-2.789342	3.229346	-2.024699
8	-1.862643	2.096969	-0.023701
9	0.722634	3.187028	-0.680289
9	0.069594	4.129577	-2.506007
9	-0.747252	4.763433	-0.608252
6	2.657952	2.703822	2.006340
1	1.599724	2.704045	1.714811
1	2.762063	2.006921	2.850973
1	2.895413	3.707116	2.388043
6	5.050497	2.482421	1.245879
1	5.256933	3.503328	1.597110
1	5.317584	1.804359	2.067697
1	5.740650	2.280817	0.416318
6	3.744785	-0.640090	2.587280
1	3.968533	-1.566996	3.136838

1	4.430636	0.125052	2.976008
1	2.726571	-0.323678	2.857597
6	2.667807	1.339417	-2.622325
1	1.632516	0.977850	-2.546011
1	2.651155	2.406588	-2.356293
1	2.955258	1.275886	-3.680944
6	5.071762	1.043821	-2.025864
1	5.336497	0.894690	-3.081807
1	5.160950	2.121218	-1.826596
1	5.834066	0.532639	-1.425169
6	5.357057	-1.217987	0.753324
1	5.664140	-2.110958	1.317589
1	5.500890	-1.442794	-0.311641
1	6.060991	-0.416706	1.019390

3RE22_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -60.1151 cm(-1)

Electronic energy : -1942.0258375
 Zero-point correction= 0.571651
 Thermal correction to Energy= 0.613932
 Thermal correction to Enthalpy= 0.614876
 Thermal correction to Gibbs Free Energy= 0.497516
 Sum of electronic and zero-point Energies= -1941.454186
 Sum of electronic and thermal Energies= -1941.411905
 Sum of electronic and thermal Enthalpies= -1941.410961
 Sum of electronic and thermal Free Energies= -1941.528322

 Cartesian Coordinates

6	2.552465	0.828109	2.594319
6	3.193633	1.783054	3.381825
6	3.068432	3.132975	3.080796
6	2.289296	3.527761	2.004668
6	1.625632	2.604078	1.186500
6	1.826063	1.262633	1.499992
7	0.759835	3.100008	0.175443
6	-0.556044	3.514776	0.648054
35	3.264719	-1.913197	-0.851471
6	-0.275194	0.236302	0.668512
6	-1.505144	0.244725	0.695502
14	-3.327898	0.127015	0.381875
6	-4.258955	1.338148	1.520871
6	1.341278	3.668987	-0.947322
8	2.541143	3.626059	-1.147282
6	0.389818	4.338919	-1.907084
8	0.060142	-3.149843	0.767479
6	0.741842	-2.765037	1.735080
6	0.828328	-3.649842	2.950418
8	1.424189	-1.681972	1.828509
6	-3.495989	0.452136	-1.485367
6	-3.874336	-1.647695	0.797436
1	2.639080	-0.227983	2.828549
1	2.165752	4.582350	1.762384
1	3.566792	3.880781	3.692097
1	-0.894063	2.808349	1.410882
1	-0.543943	4.527120	1.080598
1	-1.281161	3.485081	-0.170434
1	-0.047917	5.241845	-1.463431
1	0.953703	4.629572	-2.795933
1	-0.441458	3.684856	-2.198731
1	-4.976585	-1.624840	0.745216
1	-3.703528	1.307903	2.473733
1	-3.012810	-0.431793	-1.940304
1	3.789589	1.452413	4.228866
1	1.098426	-3.085007	3.844793

1	1.601042	-4.405675	2.770789
1	-0.122814	-4.168223	3.096446
46	1.540935	-0.367975	0.223769
47	-0.271511	-2.009597	-1.156171
8	0.222177	-0.431755	-2.671162
6	1.035518	0.499730	-2.507724
6	1.356102	1.383117	-3.685541
8	1.665737	0.817558	-1.439052
1	2.009937	2.211815	-3.406084
1	0.424786	1.752121	-4.127810
1	1.855583	0.769761	-4.443071
6	-3.386323	-2.712411	-0.180062
1	-3.623109	-2.484862	-1.227624
1	-2.297396	-2.857675	-0.083721
1	-3.833417	-3.690627	0.047326
6	-3.461138	-2.020420	2.220510
1	-3.812238	-1.298020	2.969330
1	-3.855675	-3.005878	2.505493
1	-2.365339	-2.072468	2.300807
6	-2.724246	1.673176	-1.982117
1	-1.678315	1.648311	-1.643776
1	-2.716971	1.711982	-3.081087
1	-3.176104	2.610973	-1.628199
6	-4.952702	0.483492	-1.942526
1	-5.511668	-0.411258	-1.635734
1	-5.480986	1.356147	-1.532994
1	-5.025756	0.552069	-3.036974
6	-5.696506	0.896580	1.797236
1	-5.752307	-0.088643	2.275582
1	-6.199146	1.610834	2.464495
1	-6.294086	0.849414	0.875293
6	-4.247404	2.778976	1.015282
1	-4.713188	3.454574	1.746576
1	-3.234935	3.154326	0.825131
1	-4.818861	2.877903	0.081840

3RE23_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -165.7617 cm(-1)

Electronic energy : -2903.8439184
 Zero-point correction= 0.613143
 Thermal correction to Energy= 0.664921
 Thermal correction to Enthalpy= 0.665865
 Thermal correction to Gibbs Free Energy= 0.527406
 Sum of electronic and zero-point Energies= -2903.230775
 Sum of electronic and thermal Energies= -2903.178997
 Sum of electronic and thermal Enthalpies= -2903.178053
 Sum of electronic and thermal Free Energies= -2903.316512

 Cartesian Coordinates

8	-3.202179	3.786051	0.265635
6	-2.224724	4.160703	-0.505972
6	-2.568235	5.301538	-1.404366
8	-1.107478	3.631470	-0.530100
1	-3.072451	6.093020	-0.843102
1	-3.271355	4.940565	-2.163852
1	-1.674499	5.685302	-1.897642
6	0.059148	-1.781404	2.011295
6	0.406107	-2.611411	3.078545
6	1.192746	-3.733480	2.854343
6	1.641788	-4.030615	1.572987
6	1.316561	-3.209898	0.488420
6	0.481524	-2.128357	0.747503
7	1.871189	-3.511357	-0.786507
6	3.287783	-3.873329	-0.837366

46	-0.501126	-1.218337	-0.824215
35	-0.744827	0.788328	-2.763480
6	1.266362	-0.460816	-0.516446
6	2.297572	0.156588	-0.247252
14	3.732573	1.104591	0.441414
6	5.230936	0.723469	-0.659235
6	1.109114	-3.517341	-1.902133
8	-0.042627	-3.038431	-1.934698
6	1.662318	-4.127714	-3.149055
8	-0.612728	1.215786	1.923773
6	-1.618125	1.581359	2.635373
6	-1.563857	1.110394	4.069271
8	-2.596506	2.225693	2.237777
6	3.148035	2.908595	0.501568
6	3.976469	0.411499	2.197029
1	-0.535223	0.915273	4.388088
1	-2.134189	0.174612	4.133758
1	-2.039318	1.838827	4.730976
1	-0.488580	-0.855733	2.178219
1	2.260524	-4.908495	1.398918
1	1.478283	-4.377165	3.682077
1	3.801708	-3.366607	-0.016024
1	3.445424	-4.954866	-0.750883
1	3.730223	-3.519459	-1.771171
1	2.193393	-5.064053	-2.955149
1	0.838775	-4.302146	-3.843179
1	2.359860	-3.426033	-3.623007
1	4.848142	0.932002	2.629351
1	5.432762	-0.345701	-0.469245
1	2.177935	2.837341	1.025930
1	0.075721	-2.350233	4.081264
47	-0.814444	1.393052	-0.203475
1	-2.917832	3.083417	0.934501
8	-4.919962	-1.214684	-1.234019
16	-3.682410	-0.921227	-0.534525
6	-3.976057	-1.426620	1.205760
8	-2.554477	-1.848049	-0.936094
8	-3.270477	0.480385	-0.401048
9	-4.982855	-0.735586	1.713066
9	-4.251596	-2.719185	1.282724
9	-2.882203	-1.181879	1.932544
6	4.950233	0.879738	-2.151995
1	5.812660	0.553452	-2.750627
1	4.078651	0.295217	-2.473783
1	4.752892	1.926137	-2.418741
6	6.466525	1.519951	-0.245712
1	6.686156	1.438118	0.827881
1	7.359598	1.179705	-0.788417
1	6.344050	2.587445	-0.476279
6	4.277658	-1.085657	2.164277
1	5.192718	-1.321284	1.604318
1	4.405994	-1.486020	3.180313
1	3.444521	-1.642460	1.706412
6	2.755971	0.687040	3.075861
1	2.585925	1.757703	3.245172
1	1.836224	0.285358	2.627416
1	2.871076	0.214160	4.062666
6	2.885787	3.505206	-0.878822
1	2.398004	4.485884	-0.792820
1	3.823438	3.663378	-1.430235
1	2.235024	2.871702	-1.498010
6	4.069820	3.812582	1.318102
1	5.043237	3.944528	0.826066
1	3.632796	4.814519	1.431592
1	4.264151	3.427993	2.327714

3RE24_Pd-Ag

Number of imaginary frequencies : 1
The smallest frequency is : -213.4120 cm(-1)

Electronic energy : -1942.0089026
Zero-point correction= 0.569724
Thermal correction to Energy= 0.612976
Thermal correction to Enthalpy= 0.613920
Thermal correction to Gibbs Free Energy= 0.493372
Sum of electronic and zero-point Energies= -1941.439178
Sum of electronic and thermal Energies= -1941.395927
Sum of electronic and thermal Enthalpies= -1941.394983
Sum of electronic and thermal Free Energies= -1941.515531

.....
Cartesian Coordinates
.....

6	0.952692	0.641605	2.418567
6	0.774189	1.266188	3.654193
6	0.508465	2.627840	3.715634
6	0.422849	3.379800	2.549944
6	0.593371	2.780596	1.299872
6	0.897798	1.424464	1.282267
7	0.432752	3.572284	0.128447
6	-0.710561	4.483274	0.091781
46	1.798416	0.608638	-0.364993
35	1.867211	-1.291743	-2.376127
6	-0.173963	0.647689	-0.512413
6	-1.398976	0.526816	-0.567560
14	-3.212478	0.161601	-0.441051
6	-3.629902	-0.850101	-1.990163
6	1.328537	3.526352	-0.881407
8	2.222155	2.657460	-0.960384
6	1.251724	4.562023	-1.956862
8	3.847315	0.376908	-0.132788
6	4.120708	-0.697984	0.526990
6	5.587033	-0.971387	0.705251
8	3.266565	-1.481732	0.970021
6	-3.348752	-0.826693	1.172292
6	-4.062365	1.857909	-0.350670
1	6.155797	-0.043955	0.812766
1	5.952085	-1.485162	-0.191799
1	5.749284	-1.623089	1.567142
1	1.117298	-0.431706	2.362873
1	0.218407	4.446997	2.599619
1	0.356679	3.112978	4.676267
1	-1.521036	4.038179	0.675391
1	-0.468436	5.469218	0.506673
1	-1.061777	4.607852	-0.934485
1	1.098080	5.568630	-1.557588
1	2.175292	4.527361	-2.536718
1	0.418923	4.325116	-2.630776
1	-3.493791	2.389263	0.433450
1	-3.225270	-0.262413	-2.831346
1	-2.524519	-1.555295	1.096120
1	0.824737	0.666184	4.558840
47	0.903886	-1.938907	-0.002879
8	-0.252851	-3.923431	0.432786
6	-0.697612	-3.407093	1.491393
6	-1.722580	-4.149822	2.298623
8	-0.328033	-2.253181	1.879751
1	-1.348037	-5.144555	2.560772
1	-2.620839	-4.293709	1.685924
1	-1.989128	-3.602276	3.206914
6	-4.653721	-1.593873	1.366225
1	-4.816667	-2.344031	0.581500
1	-4.651029	-2.127633	2.328393
1	-5.531416	-0.932376	1.374604
6	-3.043378	0.065463	2.373151
1	-2.948886	-0.530957	3.292051
1	-2.101519	0.620371	2.250964
1	-3.843390	0.801574	2.543258

6	-5.524521	1.814013	0.084068
1	-5.646817	1.366466	1.078671
1	-5.954276	2.825326	0.127073
1	-6.143109	1.234816	-0.614960
6	-3.895312	2.622090	-1.661592
1	-4.477776	2.158018	-2.469793
1	-4.246987	3.660261	-1.569987
1	-2.848458	2.652069	-1.994850
6	-5.125432	-1.052773	-2.224114
1	-5.610665	-1.560287	-1.378965
1	-5.654961	-0.105615	-2.386096
1	-5.299703	-1.676115	-3.112655
6	-2.886307	-2.185676	-1.954234
1	-3.050350	-2.753175	-2.880816
1	-1.801076	-2.055641	-1.841495
1	-3.228494	-2.821318	-1.124425

Monometallic Reductive Elimination (Pd)

3RE1_Pd

Number of imaginary frequencies : 1
The smallest frequency is : -340.9629 cm(-1)

Electronic energy : -2529.6525482
Zero-point correction= 0.560782
Thermal correction to Energy= 0.605390
Thermal correction to Enthalpy= 0.606334
Thermal correction to Gibbs Free Energy= 0.481681
Sum of electronic and zero-point Energies= -2529.091766
Sum of electronic and thermal Energies= -2529.047158
Sum of electronic and thermal Enthalpies= -2529.046214
Sum of electronic and thermal Free Energies= -2529.170867

Cartesian Coordinates

6	-0.167840	1.907786	-1.716423
6	-0.041538	3.232226	-2.122009
6	0.328488	4.211650	-1.209461
6	0.583987	3.867059	0.110336
6	0.473470	2.542737	0.540056
6	0.081398	1.572788	-0.390461
7	0.841309	2.247613	1.885017
6	2.022932	2.923563	2.425673
46	-0.778344	-0.171193	0.287215
35	-0.713773	-1.495952	-1.841226
6	1.160293	-0.117580	0.089032
6	2.378063	-0.286496	0.092269
14	4.203247	-0.426732	-0.169241
6	4.978211	-1.450221	1.237521
6	0.134990	1.396585	2.650921
8	-0.781990	0.672179	2.201946
6	0.440256	1.300133	4.108966
8	-1.301632	-2.149336	1.363729
6	-2.064292	-3.108497	1.281698
6	-1.864407	-4.339171	2.106132
8	-3.108363	-3.198804	0.499836
6	4.395280	-1.252390	-1.866422
6	4.857590	1.357150	-0.042055
1	-0.469229	1.146603	-2.428093
1	0.871786	4.633224	0.826526
1	0.414581	5.249763	-1.518551
1	2.682217	3.182313	1.593797
1	1.760949	3.835122	2.975419
1	2.569171	2.249208	3.089787
1	0.589740	2.279333	4.572766
1	-0.384855	0.780219	4.598304
1	1.350568	0.704737	4.254254
1	4.707717	1.592449	1.028153

1	5.238059	-0.707153	2.012250
1	5.476571	-1.381015	-2.043599
1	-0.245996	3.488152	-3.158175
1	-1.659079	-5.186733	1.443431
1	-2.780989	-4.573990	2.655832
1	-1.032509	-4.204709	2.798235
1	-3.301916	-2.396648	-0.052375
16	-3.888989	0.114087	-0.737921
6	-5.446779	0.728072	0.010875
9	-5.298304	1.983822	0.409978
9	-6.415747	0.675014	-0.892623
9	-5.789484	-0.016237	1.052764
8	-3.623483	1.022445	-1.843210
8	-2.957941	0.230288	0.433005
8	-4.179479	-1.292098	-1.068609
6	6.271160	-2.139013	0.798040
1	6.764738	-2.629685	1.648720
1	6.074678	-2.919869	0.051181
1	6.999605	-1.446033	0.356660
6	4.018500	-2.460005	1.864305
1	4.503425	-3.001439	2.689372
1	3.114496	-1.983478	2.262624
1	3.685965	-3.213168	1.137174
6	6.352800	1.457183	-0.336194
1	6.713720	2.489028	-0.218583
1	6.955176	0.827897	0.331641
1	6.581458	1.157755	-1.369179
6	4.070440	2.380469	-0.857593
1	4.280678	2.285123	-1.930429
1	2.983578	2.272145	-0.734344
1	4.342926	3.408639	-0.575179
6	3.809621	-0.397869	-2.988840
1	4.359947	0.539076	-3.136820
1	3.830436	-0.941971	-3.943593
1	2.758177	-0.141493	-2.788141
6	3.733173	-2.630937	-1.859807
1	3.834557	-3.117342	-2.840319
1	4.167588	-3.308430	-1.113821
1	2.657282	-2.551018	-1.646933

3RE2_Pd

Number of imaginary frequencies : 1

The smallest frequency is : -340.1697 cm(-1)

Electronic energy : -2529.6512386
 Zero-point correction= 0.561789
 Thermal correction to Energy= 0.605711
 Thermal correction to Enthalpy= 0.606655
 Thermal correction to Gibbs Free Energy= 0.486157
 Sum of electronic and zero-point Energies= -2529.089449
 Sum of electronic and thermal Energies= -2529.045528
 Sum of electronic and thermal Enthalpies= -2529.044584
 Sum of electronic and thermal Free Energies= -2529.165081

Cartesian Coordinates

6	0.447311	3.166555	-0.084497
6	0.944303	4.307304	0.537494
6	1.319757	4.266414	1.874364
6	1.219295	3.078583	2.585437
6	0.737459	1.917615	1.978179
6	0.334855	1.983375	0.637295
7	0.769188	0.710602	2.733949
6	1.971461	0.436559	3.525489
46	-0.952802	0.548048	-0.080153
35	-0.785039	1.065449	-2.521339
6	0.949086	0.164851	-0.173811

6	2.076303	-0.311519	-0.266404
14	3.792837	-0.973588	-0.432195
6	3.817379	-2.623334	0.510916
6	-0.243312	-0.173072	2.699578
8	-1.200541	-0.071999	1.896621
6	-0.255292	-1.324231	3.646491
8	-2.930066	1.599156	0.119821
6	-3.661187	2.098430	-0.742744
6	-3.811739	3.575129	-0.874540
8	-4.333185	1.409143	-1.616218
6	4.146396	-1.081756	-2.292488
6	4.958726	0.246378	0.462137
1	0.161576	3.196315	-1.131141
1	1.518616	3.041712	3.630471
1	1.696802	5.157424	2.369004
1	2.810320	0.976059	3.078663
1	1.857603	0.748024	4.570010
1	2.205526	-0.630037	3.489937
1	0.114421	-1.064836	4.641858
1	-1.278151	-1.698353	3.711005
1	0.367390	-2.130838	3.236418
1	4.996753	-0.125934	1.501995
1	3.689174	-2.307629	1.563059
1	5.190942	-1.421857	-2.395670
1	1.032358	5.227850	-0.033696
1	-4.764077	3.848406	-1.333147
1	-3.001639	3.927876	-1.526857
1	-3.691599	4.055015	0.098998
1	-4.196452	0.426155	-1.474774
16	-3.218516	-2.078532	-0.661812
6	-3.684691	-2.202983	1.109901
9	-3.848614	-1.002717	1.645303
9	-4.820380	-2.880057	1.227493
9	-2.735673	-2.846604	1.786265
8	-4.254777	-1.186399	-1.218976
8	-1.862077	-1.467110	-0.614615
8	-3.230870	-3.453644	-1.132049
6	6.381171	0.208112	-0.098610
1	6.417789	0.607062	-1.121152
1	7.061163	0.822452	0.508357
1	6.801727	-0.805630	-0.132804
6	4.434767	1.681452	0.496944
1	4.350354	2.107022	-0.512851
1	3.436031	1.754377	0.949924
1	5.110122	2.336144	1.067018
6	2.668755	-3.568350	0.168749
1	2.628735	-4.408575	0.876416
1	1.692103	-3.067256	0.187638
1	2.787511	-4.004191	-0.831149
6	5.168044	-3.326422	0.393604
1	5.995165	-2.709168	0.768390
1	5.179844	-4.265061	0.965438
1	5.396929	-3.587169	-0.649763
6	3.231099	-2.081562	-2.996917
1	3.404558	-2.069527	-4.082180
1	3.387533	-3.111666	-2.655143
1	2.170769	-1.836865	-2.837514
6	4.016121	0.294852	-2.945071
1	4.710450	1.034031	-2.525368
1	4.217691	0.234902	-4.023928
1	2.997212	0.692302	-2.828702

3RE3_Pd

Number of imaginary frequencies : 1
The smallest frequency is : -311.0936 cm(-1)

Electronic energy : -1796.8058345

Zero-point correction= 0.582334
 Thermal correction to Energy= 0.623414
 Thermal correction to Enthalpy= 0.624358
 Thermal correction to Gibbs Free Energy= 0.509247
 Sum of electronic and zero-point Energies= -1796.223501
 Sum of electronic and thermal Energies= -1796.182420
 Sum of electronic and thermal Enthalpies= -1796.181476
 Sum of electronic and thermal Free Energies= -1796.296588

.....
 Cartesian Coordinates

6	-0.757425	1.885998	-1.712826
6	-0.574724	3.192722	-2.151093
6	-0.157932	4.174322	-1.259754
6	0.095226	3.840964	0.063165
6	-0.070909	2.529762	0.517051
6	-0.524178	1.554590	-0.380554
7	0.311800	2.246423	1.861953
6	1.535880	2.877245	2.360392
46	-1.420097	-0.151033	0.337379
35	-1.488946	-1.477286	-1.788805
6	0.519044	-0.205972	0.114831
6	1.729709	-0.409475	0.099149
14	3.543698	-0.605261	-0.166790
6	4.307327	-1.611084	1.259177
6	-0.401724	1.425989	2.656323
8	-1.361589	0.738764	2.244412
6	-0.047823	1.327037	4.104269
8	-3.490767	0.930004	0.138782
6	-4.341750	0.790651	-0.744976
6	-4.868741	1.962147	-1.511329
8	-4.831631	-0.352116	-1.117343
6	3.722913	-1.469968	-1.847392
6	4.264898	1.159024	-0.106262
1	-1.083118	1.118734	-2.409552
1	0.426053	4.606980	0.760883
1	-0.026009	5.201472	-1.589528
1	2.181192	3.104170	1.508248
1	1.329102	3.802650	2.911088
1	2.074652	2.186418	3.013400
1	0.130488	2.304357	4.562340
1	-0.863123	0.818149	4.620598
1	0.858876	0.720026	4.221153
1	4.164554	1.429885	0.961063
1	4.567855	-0.856633	2.022912
1	4.804655	-1.583550	-2.034285
1	-0.764030	3.437217	-3.193505
1	-5.930850	1.841669	-1.739079
1	-4.328235	2.014588	-2.465183
1	-4.691823	2.889136	-0.962513
1	-4.456461	-1.109431	-0.534534
8	-2.195049	-1.849008	1.368403
6	-3.265838	-2.519405	1.189099
6	-3.363200	-3.746579	2.068795
8	-4.186213	-2.282622	0.391026
1	-4.366711	-4.176014	2.022407
1	-3.104054	-3.499385	3.102515
1	-2.637942	-4.490115	1.719949
6	5.597755	-2.317819	0.841310
1	6.082463	-2.796872	1.703806
1	5.398849	-3.110956	0.108104
1	6.334261	-1.639433	0.390967
6	3.335933	-2.602928	1.896082
1	2.428548	-2.114604	2.271070
1	3.009656	-3.369581	1.180373
1	3.807745	-3.129179	2.738544
6	5.749009	1.199913	-0.462310
1	6.145076	2.224262	-0.407341
1	6.359342	0.582649	0.209424
1	5.926021	0.844295	-1.487601

6	3.480021	2.185194	-0.920272
1	2.396098	2.110616	-0.756412
1	3.791000	3.212010	-0.674346
1	3.648977	2.056275	-1.996857
6	3.088945	-2.860772	-1.811590
1	3.187640	-3.359633	-2.786328
1	3.546283	-3.518335	-1.061782
1	2.014991	-2.803008	-1.585669
6	3.110027	-0.646929	-2.979560
1	3.649266	0.291217	-3.159464
1	3.119118	-1.213145	-3.921901
1	2.060130	-0.393622	-2.765421

3RE4_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -274.1787 cm(-1)

Electronic energy : -1796.804637
 Zero-point correction= 0.582536
 Thermal correction to Energy= 0.623757
 Thermal correction to Enthalpy= 0.624701
 Thermal correction to Gibbs Free Energy= 0.509152
 Sum of electronic and zero-point Energies= -1796.222101
 Sum of electronic and thermal Energies= -1796.180880
 Sum of electronic and thermal Enthalpies= -1796.179936
 Sum of electronic and thermal Free Energies= -1796.295485

 Cartesian Coordinates

6	-0.434089	1.759477	-2.175630
6	-0.154102	2.987906	-2.765255
6	-0.052855	4.129520	-1.979870
6	-0.214990	4.042720	-0.604358
6	-0.475802	2.815398	0.014152
6	-0.606788	1.691595	-0.802147
7	-0.543546	2.779915	1.436383
6	0.363076	3.657317	2.178990
46	-1.559186	0.014502	-0.090345
35	-4.031133	-0.092084	-0.858209
6	0.388225	0.116672	0.282989
6	1.591341	-0.055631	0.458581
14	3.392768	-0.451906	0.411914
6	3.811374	-1.286271	2.064314
6	-1.444942	2.024378	2.095483
8	-2.146713	1.146980	1.549238
6	-1.645263	2.240901	3.559906
8	-2.209960	-1.657752	1.604512
6	-2.845733	-2.687748	1.417613
6	-4.076546	-3.038519	2.185986
8	-1.056494	-0.985079	-1.787799
6	-0.474689	-2.143133	-1.759505
6	-0.012042	-2.572002	-3.130841
8	-2.527255	-3.581577	0.508065
8	-0.324802	-2.869155	-0.777992
6	3.529899	-1.629041	-1.075071
6	4.319078	1.204109	0.232981
1	0.411823	-1.733874	-3.691526
1	-0.876895	-2.944303	-3.691411
1	0.717777	-3.379992	-3.036593
1	-0.530359	0.857660	-2.772140
1	-0.140071	4.938724	0.007309
1	0.149406	5.095332	-2.435156
1	1.263754	3.813152	1.581776
1	-0.092545	4.629386	2.401683
1	0.664351	3.179065	3.112648
1	-1.678744	3.300405	3.828163
1	-2.576189	1.751789	3.850298

1	-0.827813	1.766851	4.117045
1	4.404949	1.577857	1.269327
1	3.348414	-0.621755	2.814640
1	2.731765	-2.366426	-0.877893
1	-0.026175	3.043630	-3.843222
1	-4.131016	-4.112598	2.381536
1	-4.944376	-2.763547	1.574148
1	-4.116972	-2.470506	3.116807
1	-1.688854	-3.281768	0.059978
6	3.140623	-2.653903	2.167608
1	2.064749	-2.608418	1.951286
1	3.585704	-3.369328	1.462005
1	3.258907	-3.081588	3.173366
6	5.303226	-1.373117	2.375555
1	5.785860	-0.387159	2.390092
1	5.472378	-1.830527	3.361120
1	5.840429	-1.992178	1.643387
6	5.730242	1.044822	-0.332359
1	6.270303	2.002503	-0.321138
1	6.339051	0.322325	0.226157
1	5.700289	0.710100	-1.378869
6	3.541412	2.242644	-0.575410
1	3.417861	1.931869	-1.621878
1	2.532007	2.410852	-0.176478
1	4.068254	3.207988	-0.587796
6	3.185648	-0.916993	-2.381686
1	3.949487	-0.171615	-2.647006
1	3.132175	-1.628165	-3.218996
1	2.219369	-0.395366	-2.320484
6	4.854628	-2.378420	-1.188364
1	5.079447	-2.965942	-0.289089
1	4.837689	-3.079376	-2.035407
1	5.698269	-1.695384	-1.356171

3RE5_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -221.0141 cm(-1)

Electronic energy : -2529.6440101
 Zero-point correction= 0.563109
 Thermal correction to Energy= 0.606055
 Thermal correction to Enthalpy= 0.606999
 Thermal correction to Gibbs Free Energy= 0.490754
 Sum of electronic and zero-point Energies= -2529.080902
 Sum of electronic and thermal Energies= -2529.037955
 Sum of electronic and thermal Enthalpies= -2529.037011
 Sum of electronic and thermal Free Energies= -2529.153257

 Cartesian Coordinates

6	1.005743	2.945819	1.382088
6	0.796135	4.323377	1.373518
6	0.526410	4.982933	0.179935
6	0.455455	4.273726	-1.012351
6	0.649264	2.890970	-1.027267
6	0.941607	2.265943	0.181091
7	0.477711	2.180338	-2.248668
6	-0.671445	2.527396	-3.090631
46	1.710586	0.371284	0.156956
35	4.227711	0.398813	0.699806
6	-0.266464	0.442846	-0.014750
6	-1.486804	0.333686	0.015654
14	-3.301003	0.100309	0.240380
6	-3.833764	-1.309670	-0.916100
6	1.290548	1.170240	-2.594284
8	2.145297	0.679296	-1.807561
6	1.215372	0.587554	-3.958923

8	1.340344	0.067689	2.183607
6	1.394329	-1.017370	2.801730
6	1.087733	-1.028977	4.256647
8	1.702001	-2.163191	2.301744
6	-3.452402	-0.381028	2.074287
6	-4.106900	1.760265	-0.237758
1	1.970759	-1.375971	4.803111
1	0.281486	-1.744585	4.446688
1	0.800317	-0.035878	4.601823
1	1.213838	2.413917	2.305807
1	0.242717	4.786884	-1.947866
1	0.370399	6.058084	0.171967
1	-1.428503	3.005139	-2.463991
1	-0.394370	3.204339	-3.905996
1	-1.113667	1.615620	-3.500831
1	1.016994	1.331465	-4.734009
1	2.150688	0.061902	-4.160132
1	0.420602	-0.170572	-3.954230
1	-4.166932	1.729206	-1.341338
1	-3.494324	-2.237403	-0.422012
1	-2.699661	-1.183345	2.174561
1	0.846324	4.873486	2.309585
1	1.852178	-2.163880	1.302210
16	1.065322	-2.752912	-1.295575
8	0.365584	-1.851014	-2.206658
8	1.885187	-2.022492	-0.255055
8	1.752116	-3.901115	-1.863743
6	-0.267158	-3.473593	-0.250652
9	-0.834232	-2.529500	0.497875
9	-1.200241	-4.026988	-1.012569
9	0.239099	-4.394794	0.560284
6	-3.037665	0.760259	3.000108
1	-2.997402	0.426902	4.047361
1	-2.047050	1.162684	2.742971
1	-3.757015	1.590716	2.957516
6	-4.807194	-0.957230	2.476362
1	-5.068941	-1.846306	1.889001
1	-4.808687	-1.256859	3.534333
1	-5.616748	-0.225014	2.351812
6	-3.255990	2.971156	0.149289
1	-3.698642	3.902673	-0.232957
1	-3.183953	3.076550	1.240527
1	-2.226487	2.905646	-0.228992
6	-5.523866	1.922288	0.313261
1	-5.514051	1.990483	1.410585
1	-5.988053	2.847610	-0.057020
1	-6.189390	1.093703	0.040967
6	-3.122983	-1.211817	-2.265303
1	-3.410062	-0.290205	-2.796085
1	-2.030843	-1.217755	-2.166019
1	-3.400877	-2.052888	-2.916229
6	-5.345353	-1.384325	-1.126920
1	-5.709303	-0.498832	-1.667598
1	-5.613163	-2.258628	-1.736624
1	-5.913617	-1.455044	-0.190688

3RE6_Pd

Number of imaginary frequencies : 1
The smallest frequency is : -271.6517 cm(-1)

Electronic energy : -2529.6402435
Zero-point correction= 0.563282
Thermal correction to Energy= 0.607042
Thermal correction to Enthalpy= 0.607987
Thermal correction to Gibbs Free Energy= 0.487978
Sum of electronic and zero-point Energies= -2529.076961
Sum of electronic and thermal Energies= -2529.033201

Sum of electronic and thermal Enthalpies= -2529.032257
 Sum of electronic and thermal Free Energies= -2529.152266

.....
 Cartesian Coordinates

6	-0.525843	-0.946130	2.631955
6	-0.177555	-1.634269	3.790689
6	0.404686	-2.893196	3.708498
6	0.658473	-3.465203	2.469460
6	0.336870	-2.787220	1.290451
6	-0.281416	-1.546289	1.408604
7	0.715602	-3.368145	0.045585
6	2.019181	-4.037462	-0.007555
46	-1.334489	-0.794536	-0.178675
35	-3.842380	-1.384275	0.029176
6	0.605945	-0.380025	-0.189361
6	1.774640	-0.023722	-0.306202
14	3.461841	0.735681	-0.328658
6	3.319682	2.288054	-1.412808
6	-0.048609	-3.290513	-1.054182
8	-1.066520	-2.559963	-1.155583
6	0.288072	-4.118021	-2.249056
8	-1.820078	0.092549	-2.394747
6	-2.765782	0.810108	-2.699220
6	-3.958945	0.321249	-3.444803
8	-2.834866	2.086029	-2.373174
6	3.759034	1.181893	1.491989
6	4.624315	-0.629273	-0.964726
1	-4.660492	-0.079988	-2.700958
1	-3.675892	-0.497801	-4.108983
1	-4.454608	1.122863	-3.996509
1	-0.984759	0.035195	2.685031
1	1.115851	-4.449677	2.408021
1	0.666104	-3.437933	4.611505
1	2.679683	-3.556492	0.717690
1	1.943319	-5.105872	0.223527
1	2.466399	-3.913854	-0.996191
1	0.620268	-5.124985	-1.983249
1	-0.595668	-4.172218	-2.886951
1	1.082247	-3.623730	-2.822378
1	4.398360	-1.484351	-0.302076
1	2.839536	3.023236	-0.741950
1	2.820102	1.692817	1.764616
1	-0.368838	-1.172849	4.755889
1	-2.034615	2.319719	-1.843452
16	-0.941225	2.276351	0.647359
8	0.172351	2.320108	1.577940
8	-1.794804	1.010251	0.726931
8	-0.714392	2.729370	-0.729288
6	-2.206480	3.425133	1.326537
9	-2.564745	3.041301	2.539404
9	-1.677868	4.637365	1.390355
9	-3.263425	3.449021	0.534881
6	2.400419	2.090324	-2.617873
1	1.397511	1.756333	-2.326375
1	2.289217	3.029800	-3.177788
1	2.809075	1.346182	-3.316425
6	4.670225	2.847767	-1.860375
1	4.542230	3.816406	-2.364005
1	5.375519	3.003051	-1.033188
1	5.155870	2.178434	-2.584846
6	3.879663	-0.062871	2.367561
1	3.938012	0.207542	3.431433
1	3.015447	-0.734077	2.254937
1	4.786496	-0.640411	2.135074
6	4.911344	2.152146	1.736562
1	4.777808	3.096159	1.193690
1	4.989820	2.403956	2.803930
1	5.881960	1.731850	1.437130
6	4.288210	-1.047766	-2.394431

1	4.533660	-0.253264	-3.112717
1	4.862535	-1.936304	-2.695584
1	3.221311	-1.279110	-2.521106
6	6.110456	-0.310277	-0.823283
1	6.391943	-0.088313	0.213639
1	6.730226	-1.156157	-1.154282
1	6.400062	0.555418	-1.433791

3RE7_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -275.5202 cm(-1)

Electronic energy : -1796.79997
 Zero-point correction= 0.583722
 Thermal correction to Energy= 0.624303
 Thermal correction to Enthalpy= 0.625248
 Thermal correction to Gibbs Free Energy= 0.511891
 Sum of electronic and zero-point Energies= -1796.216248
 Sum of electronic and thermal Energies= -1796.175667
 Sum of electronic and thermal Enthalpies= -1796.174722
 Sum of electronic and thermal Free Energies= -1796.288079

 Cartesian Coordinates

6	0.934463	1.624965	2.440437
6	0.853866	2.826646	3.133527
6	0.465046	3.980452	2.463598
6	0.123839	3.925242	1.119775
6	0.172761	2.718016	0.412909
6	0.619700	1.576520	1.087646
7	-0.294236	2.714647	-0.936811
6	-1.348222	3.672969	-1.284297
46	1.335333	-0.059355	0.050263
35	1.847304	-2.157175	-1.454215
6	-0.584308	-0.098829	0.363424
6	-1.789863	-0.319130	0.327524
14	-3.529899	-0.793678	-0.041559
6	-4.359822	0.782224	-0.712518
6	0.209634	1.913529	-1.895703
8	1.055841	1.013025	-1.694987
6	-0.231526	2.100632	-3.312421
8	3.468938	0.871803	-0.143975
6	4.535583	0.439841	-0.584027
6	5.467605	1.292087	-1.381014
8	1.464569	-1.174950	1.734466
6	2.519820	-1.855778	2.071374
6	2.258923	-2.684873	3.306682
8	4.958714	-0.779555	-0.411863
8	3.611687	-1.892588	1.517264
6	-3.449061	-2.076829	-1.443409
6	-4.337843	-1.533215	1.515743
1	1.869631	-3.656901	2.983635
1	1.515323	-2.223976	3.960756
1	3.197045	-2.848058	3.842537
1	1.240607	0.713351	2.945108
1	-0.176746	4.836479	0.609360
1	0.421030	4.933146	2.984994
1	-1.941983	3.883723	-0.393673
1	-0.934281	4.611217	-1.672225
1	-2.020301	3.243619	-2.029130
1	-0.243760	3.150857	-3.617557
1	0.445507	1.534402	-3.953470
1	-1.240473	1.688726	-3.444195
1	-5.111392	-2.225579	1.137993
1	-3.771968	0.993597	-1.624009
1	-4.496403	-2.308970	-1.706984
1	1.105192	2.857597	4.190720

1	5.472766	0.932984	-2.416245
1	6.488816	1.200318	-1.000194
1	5.145079	2.333894	-1.362180
1	4.316668	-1.263187	0.186566
6	-3.330217	-2.329054	2.345627
1	-2.577567	-1.658215	2.781585
1	-3.830082	-2.847244	3.176490
1	-2.784434	-3.080691	1.764610
6	-5.013261	-0.496493	2.410203
1	-4.284421	0.239221	2.781087
1	-5.813345	0.053706	1.900028
1	-5.459295	-0.975159	3.294044
6	-5.808608	0.549930	-1.134670
1	-6.252414	1.459621	-1.564605
1	-5.902372	-0.242997	-1.888113
1	-6.438525	0.263134	-0.280575
6	-4.228904	2.001205	0.196479
1	-3.198868	2.132882	0.559440
1	-4.525225	2.921345	-0.329856
1	-4.875338	1.922245	1.078891
6	-2.746770	-1.512546	-2.676644
1	-1.712631	-1.221693	-2.435395
1	-2.686664	-2.267313	-3.473353
1	-3.262734	-0.639249	-3.097975
6	-2.767562	-3.373999	-1.011198
1	-3.298891	-3.876272	-0.193185
1	-2.715456	-4.084278	-1.848515
1	-1.734445	-3.188824	-0.683005

3RE8_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -238.3013 cm(-1)

Electronic energy : -2529.6363641
 Zero-point correction= 0.562696
 Thermal correction to Energy= 0.606622
 Thermal correction to Enthalpy= 0.607567
 Thermal correction to Gibbs Free Energy= 0.487254
 Sum of electronic and zero-point Energies= -2529.073668
 Sum of electronic and thermal Energies= -2529.029742
 Sum of electronic and thermal Enthalpies= -2529.028797
 Sum of electronic and thermal Free Energies= -2529.149110

 Cartesian Coordinates

6	-1.002231	-0.562066	2.656303
6	-0.802213	-1.140236	3.905168
6	-0.273193	-2.423076	3.999629
6	0.064077	-3.127446	2.852673
6	-0.123691	-2.557588	1.590138
6	-0.667284	-1.275655	1.514090
7	0.307830	-3.298156	0.449846
6	1.534207	-4.089123	0.594986
46	-1.421399	-0.561511	-0.263199
35	-2.419913	0.167428	-2.577078
6	0.508538	-0.366968	-0.111331
6	1.717893	-0.192168	-0.193566
14	3.488393	0.220969	-0.516351
6	3.726173	0.014336	-2.387563
6	-0.332835	-3.259187	-0.726894
8	-1.263772	-2.454407	-0.998327
6	0.024994	-4.231898	-1.799744
8	-3.636975	-1.070582	0.343975
6	-4.612719	-0.324431	0.336792
6	-6.012016	-0.832379	0.389317
8	-4.542315	0.986085	0.262781
6	3.722094	2.028922	0.009644

6	4.517925	-1.066236	0.431180
1	-1.419931	0.437318	2.569210
1	0.470250	-4.132499	2.934893
1	-0.125572	-2.885375	4.972073
1	2.195923	-3.571202	1.295135
1	1.328497	-5.099479	0.966086
1	2.051021	-4.160138	-0.363413
1	0.209914	-5.236162	-1.409633
1	-0.790626	-4.254667	-2.524306
1	0.924587	-3.886046	-2.324859
1	4.278614	-2.013073	-0.085765
1	4.762877	0.312179	-2.620422
1	2.801386	2.518729	-0.352461
1	-1.063557	-0.583600	4.801531
1	-6.631351	-0.204214	1.034858
1	-6.027248	-1.870089	0.724938
1	-6.431493	-0.780409	-0.622289
1	-3.605122	1.271181	0.192181
16	-1.193685	2.683647	-0.105108
8	-1.742988	1.335545	0.454840
8	-2.310132	3.596917	-0.272388
8	-0.169012	2.556418	-1.117038
6	-0.316642	3.237475	1.413623
9	0.593183	2.340434	1.761753
9	0.282591	4.391332	1.169767
9	-1.176184	3.389821	2.411006
6	4.117821	-1.233406	1.894801
1	3.030214	-1.338359	2.020856
1	4.597867	-2.117601	2.339932
1	4.425423	-0.369774	2.497507
6	6.018374	-0.817949	0.295150
1	6.603221	-1.626160	0.757352
1	6.339642	-0.741582	-0.752668
1	6.312511	0.113759	0.799183
6	2.766271	0.930033	-3.146469
1	1.719835	0.680418	-2.919471
1	2.904467	1.989990	-2.897201
1	2.899052	0.830544	-4.232972
6	3.532037	-1.435764	-2.823473
1	2.533080	-1.798453	-2.533794
1	3.600994	-1.533932	-3.915963
1	4.277951	-2.114260	-2.388316
6	3.785501	2.206989	1.525296
1	3.688404	3.267448	1.798937
1	2.993292	1.660807	2.051971
1	4.749519	1.859979	1.924941
6	4.921163	2.695825	-0.661405
1	5.024947	3.738298	-0.328307
1	5.863009	2.185896	-0.411741
1	4.836147	2.713122	-1.754961

3RE9_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -280.6068 cm(-1)

Electronic energy : -2529.6251433
 Zero-point correction= 0.561918
 Thermal correction to Energy= 0.605505
 Thermal correction to Enthalpy= 0.606449
 Thermal correction to Gibbs Free Energy= 0.486686
 Sum of electronic and zero-point Energies= -2529.063226
 Sum of electronic and thermal Energies= -2529.019638
 Sum of electronic and thermal Enthalpies= -2529.018694
 Sum of electronic and thermal Free Energies= -2529.138457

 Cartesian Coordinates

6	0.726580	-1.263890	-1.977241
6	0.683075	-2.504290	-2.602220
6	0.290747	-3.624713	-1.879106
6	-0.073862	-3.508818	-0.544408
6	-0.056046	-2.264746	0.095044
6	0.365488	-1.154462	-0.640127
7	-0.517807	-2.190071	1.444312
6	-1.518304	-3.178908	1.862344
46	0.826126	0.637421	0.275012
35	1.091536	2.955185	1.502426
6	-1.066515	0.363568	-0.109217
6	-2.288342	0.307385	-0.176512
14	-4.098607	-0.026685	-0.292962
6	-4.721117	-0.432494	1.465264
6	-0.086234	-1.281055	2.332254
8	0.634475	-0.285026	2.058068
6	-0.428742	-1.427466	3.779087
8	0.803863	1.765666	-1.485896
6	1.561858	2.700497	-1.840501
6	0.959539	3.966536	-2.327428
8	2.846268	2.654297	-1.843895
6	-4.933833	1.511730	-1.018751
6	-4.215012	-1.613717	-1.336474
1	1.046792	-0.383713	-2.526369
1	-0.364366	-4.398946	0.006596
1	0.270303	-4.603342	-2.351114
1	-2.157299	-3.408592	1.006619
1	-1.051593	-4.101972	2.223845
1	-2.152562	-2.768793	2.648893
1	-0.312263	-2.457073	4.128538
1	0.224478	-0.765819	4.350069
1	-1.464837	-1.110760	3.955504
1	-3.730130	-2.360344	-0.678870
1	-4.579746	-1.524922	1.556914
1	-6.020015	1.319219	-1.015382
1	0.965380	-2.590042	-3.648142
1	1.621866	4.482462	-3.024763
1	0.807446	4.602173	-1.445011
1	-0.020015	3.775448	-2.770143
1	3.216039	1.734661	-1.636631
16	4.191112	-0.016065	-0.114748
8	5.498502	0.425067	0.338577
8	3.837350	0.290681	-1.527661
8	3.062386	0.273783	0.807609
6	4.293050	-1.846246	-0.108281
9	4.565046	-2.268482	1.118665
9	3.139021	-2.378181	-0.493928
9	5.248925	-2.255220	-0.928127
6	-3.913298	0.238787	2.574296
1	-4.026338	1.331202	2.552538
1	-4.245963	-0.098730	3.567395
1	-2.836270	0.040418	2.484360
6	-6.211945	-0.139605	1.634541
1	-6.831725	-0.612412	0.861231
1	-6.577969	-0.496343	2.607691
1	-6.413442	0.939475	1.595483
6	-3.419607	-1.583281	-2.638950
1	-3.335887	-2.590523	-3.071718
1	-3.904418	-0.951431	-3.394534
1	-2.400722	-1.198898	-2.495252
6	-5.655166	-2.060666	-1.575293
1	-5.692533	-3.001325	-2.143316
1	-6.202070	-2.227249	-0.638063
1	-6.217423	-1.316267	-2.157276
6	-4.489746	1.782559	-2.454363
1	-4.794084	0.988626	-3.146929
1	-4.921299	2.722340	-2.827608
1	-3.396319	1.881142	-2.521361
6	-4.650194	2.730889	-0.140426
1	-5.131862	3.630218	-0.549512

1	-5.011784	2.607848	0.888408
1	-3.571487	2.936202	-0.085392

3RE10_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -52.7971 cm(-1)

Electronic energy : -3262.4497059
 Zero-point correction= 0.541077
 Thermal correction to Energy= 0.587860
 Thermal correction to Enthalpy= 0.588804
 Thermal correction to Gibbs Free Energy= 0.462347
 Sum of electronic and zero-point Energies= -3261.908629
 Sum of electronic and thermal Energies= -3261.861846
 Sum of electronic and thermal Enthalpies= -3261.860902
 Sum of electronic and thermal Free Energies= -3261.987359

 Cartesian Coordinates

6	-0.655157	-0.483818	2.628707
6	-0.479272	-1.019384	3.900605
6	0.088621	-2.280083	4.048513
6	0.488868	-3.005136	2.935878
6	0.326715	-2.477393	1.650030
6	-0.260805	-1.220866	1.523965
7	0.797930	-3.246182	0.543615
6	2.030905	-4.021174	0.725606
46	-0.830182	-0.521706	-0.316716
35	-1.733593	0.164683	-2.662033
6	1.093645	-0.367456	-0.259876
6	2.312201	-0.256881	-0.275344
14	4.107750	0.123731	-0.519478
6	4.403316	-0.073139	-2.382636
6	0.190834	-3.240613	-0.647331
8	-0.737790	-2.442249	-0.961401
6	0.582959	-4.226931	-1.692235
6	4.369246	1.919468	0.037661
6	5.069384	-1.190552	0.459254
1	-1.089040	0.505165	2.505822
1	0.917856	-3.996086	3.062378
1	0.217321	-2.709776	5.038329
1	2.646284	-3.520501	1.476941
1	1.824813	-5.048626	1.044879
1	2.600459	-4.035791	-0.206271
1	0.797207	-5.216487	-1.281205
1	-0.223243	-4.288722	-2.425273
1	1.476587	-3.860119	-2.214583
1	4.820723	-2.133667	-0.059843
1	5.455409	0.196436	-2.577285
1	3.476928	2.441927	-0.346456
1	-0.787632	-0.445919	4.770812
16	-0.429580	2.727975	-0.143065
8	-1.155918	1.418631	0.311926
8	-1.443507	3.760436	-0.254388
8	0.571614	2.540616	-1.166540
6	0.490916	3.074961	1.415711
9	1.196290	2.013728	1.774534
9	1.307711	4.094932	1.214121
9	-0.362487	3.370809	2.383728
6	4.625464	-1.335374	1.913015
1	3.531394	-1.384966	2.014578
1	5.050395	-2.241421	2.369891
1	4.962549	-0.487812	2.522283
6	6.579063	-0.980317	0.363131
1	7.130845	-1.794486	0.854320
1	6.931309	-0.928310	-0.676120
1	6.880221	-0.046686	0.859439
6	3.497188	0.874133	-3.169031

1	2.436009	0.654332	-2.982970
1	3.657567	1.927995	-2.907552
1	3.667408	0.777045	-4.250419
6	4.186192	-1.515472	-2.833924
1	3.165685	-1.851481	-2.591346
1	4.300877	-1.611422	-3.922643
1	4.893186	-2.216211	-2.369956
6	4.393905	2.093649	1.555160
1	4.334091	3.157715	1.824963
1	3.562913	1.584516	2.057681
1	5.329965	1.707603	1.983657
6	5.609136	2.551507	-0.593402
1	5.734595	3.588596	-0.251618
1	6.525924	2.010928	-0.316316
1	5.559483	2.575892	-1.688857
16	-4.209658	0.076768	0.728988
8	-4.750155	0.080375	2.066205
8	-3.139094	-0.857775	0.381899
8	-3.854664	1.530782	0.253665
6	-5.605563	-0.262617	-0.423963
9	-6.065130	-1.465387	-0.130882
9	-6.546030	0.639451	-0.233406
9	-5.182036	-0.228433	-1.664608
1	-2.875452	1.628575	0.096211

Reaction 4

DiPhenylAcetylene

Number of imaginary frequencies : 0

Electronic energy : HF=-539.0412
 Zero-point correction= 0.190614
 Thermal correction to Energy= 0.201843
 Thermal correction to Enthalpy= 0.202787
 Thermal correction to Gibbs Free Energy= 0.150813
 Sum of electronic and zero-point Energies= -538.850586
 Sum of electronic and thermal Energies= -538.839357
 Sum of electronic and thermal Enthalpies= -538.838413
 Sum of electronic and thermal Free Energies= -538.890387

Cartesian Coordinates

6	0.607795	-0.000167	-0.000783
6	-0.607795	-0.000042	-0.000750
6	2.035756	-0.000061	-0.000431
6	2.745204	0.858019	0.854585
6	2.745980	-0.857996	-0.854926
6	4.133950	0.854680	0.851658
1	2.194295	1.522769	1.516662
6	4.134731	-0.854402	-0.850937
1	2.195708	-1.522865	-1.517412
6	4.831757	0.000193	0.000624
1	4.675269	1.522935	1.517524
1	4.676673	-1.522564	-1.516390
1	5.919286	0.000272	0.001036
6	-2.035756	-0.000025	-0.000415
6	-2.745287	-0.854802	0.857834
6	-2.745898	0.854719	-0.858172
6	-4.134033	-0.851360	0.854873
1	-2.194442	-1.517074	1.522442
6	-4.134649	0.851244	-0.854201
1	-2.195561	1.517016	-1.523175
6	-4.831757	-0.000055	0.000588

1	-4.675415	-1.517027	1.523273
1	-4.676527	1.516902	-1.522210
1	-5.919286	-0.000048	0.000980

Isatin

Number of imaginary frequencies : 0

Electronic energy : HF=-512.7566217
 Zero-point correction= 0.115354
 Thermal correction to Energy= 0.123366
 Thermal correction to Enthalpy= 0.124311
 Thermal correction to Gibbs Free Energy= 0.082347
 Sum of electronic and zero-point Energies= -512.641268
 Sum of electronic and thermal Energies= -512.633255
 Sum of electronic and thermal Enthalpies= -512.632311
 Sum of electronic and thermal Free Energies= -512.674275

Cartesian Coordinates

6	0.252977	0.578617	-0.000128
6	0.380819	-0.820776	-0.000173
6	1.625201	-1.425454	-0.000031
6	2.742966	-0.587620	0.000275
6	2.631024	0.805410	0.000440
6	1.373466	1.400345	0.000253
6	-1.172164	0.886944	-0.000725
6	-1.888225	-0.498991	0.000152
1	1.728890	-2.507259	-0.000068
1	3.732810	-1.038681	0.000430
1	3.527846	1.418969	0.000671
1	1.255481	2.481989	0.000279
1	-1.031654	-2.429901	-0.000282
8	-1.758264	1.947096	0.000076
8	-3.082909	-0.692279	-0.000048
7	-0.880054	-1.427786	-0.000232

[Ag(OAc)₂(DMF)₂]

Number of imaginary frequencies : 0

Electronic energy : HF=-1245.1325053
 Zero-point correction= 0.309617
 Thermal correction to Energy= 0.339383
 Thermal correction to Enthalpy= 0.340327
 Thermal correction to Gibbs Free Energy= 0.238335
 Sum of electronic and zero-point Energies= -1244.822888
 Sum of electronic and thermal Energies= -1244.793122
 Sum of electronic and thermal Enthalpies= -1244.792178
 Sum of electronic and thermal Free Energies= -1244.894170

Cartesian Coordinates

1	-1.419987	4.412744	-1.001080
6	-1.761005	3.878540	-0.108688
6	-1.147945	2.493683	-0.096543
1	-1.401678	4.442960	0.756918
1	-2.852341	3.837887	-0.101505
8	0.107564	2.457585	-0.039707
8	-1.940551	1.514531	-0.149447
47	-1.292791	-0.614706	-0.142160
47	1.287216	0.613364	-0.021567
1	2.273947	-4.012410	0.932867
6	1.783109	-3.867166	-0.035287
6	1.138151	-2.496996	-0.061812
1	2.560627	-3.922890	-0.803458

1	1.045951	-4.656445	-0.191261
8	1.930263	-1.516964	0.017495
8	-0.113972	-2.460264	-0.150014
8	-3.712569	-1.116663	-0.049905
8	3.706171	1.116540	0.012675
6	-4.439862	-0.132089	0.054572
1	-4.032112	0.896089	0.026791
7	-5.780774	-0.189112	0.212097
6	-6.470184	-1.459232	0.270503
1	-6.981742	-1.575077	1.234794
1	-7.217895	-1.527543	-0.530076
1	-5.735392	-2.257426	0.151102
6	-6.577590	1.007686	0.331568
1	-7.117424	1.023954	1.287796
1	-5.931139	1.889206	0.282990
1	-7.315534	1.070613	-0.479356
6	4.436592	0.131257	0.084841
1	4.025633	-0.896040	0.094245
7	5.784651	0.187592	0.159484
6	6.587043	-1.008698	0.242252
1	7.275700	-1.077876	-0.610462
1	7.183013	-1.017035	1.164679
1	5.939228	-1.890379	0.238845
6	6.478089	1.456936	0.158352
1	7.175429	1.511730	-0.687447
1	5.738913	2.255349	0.072739
1	7.048068	1.584620	1.087674

[Pd(OAc)₂] [SMD(DMF)/M06/6-31G//M06/6-31G** (Gas Phase)]**

Total Energy= -1750.604734

Number of imaginary frequencies : 0

Electronic energy : HF=-1750.5747527
 Zero-point correction= 0.315721
 Thermal correction to Energy= 0.349705
 Thermal correction to Enthalpy= 0.350649
 Thermal correction to Gibbs Free Energy= 0.246602
 Sum of electronic and zero-point Energies= -1750.259032
 Sum of electronic and thermal Energies= -1750.225048
 Sum of electronic and thermal Enthalpies= -1750.224104
 Sum of electronic and thermal Free Energies= -1750.328150

 Cartesian Coordinates

46	1.559037	0.928514	-0.001488
8	2.288923	0.035247	-1.687034
8	2.647809	-0.307202	1.230488
6	2.237849	-1.316722	1.863936
8	1.167662	-1.961746	1.678836
46	0.023733	-1.809013	-0.005073
6	2.293810	-1.213956	-1.872974
8	1.643990	-2.088612	-1.240602
8	1.121000	1.989958	1.685653
8	0.987212	2.468094	-1.238768
6	-0.097355	2.595324	-1.866543
8	-1.177725	1.970204	-1.674795
46	-1.584818	0.884530	0.004864
6	0.023813	2.584005	1.881424
8	-1.056834	2.431774	1.252415
8	-2.292781	-0.036952	1.684456
8	-2.637838	-0.371229	-1.237573
6	-2.258257	-1.285446	1.868666
6	-2.201320	-1.367910	-1.873886
8	-1.586272	-2.139520	1.230445
8	-1.115966	-1.986972	-1.689102
6	3.211147	-1.714141	-2.954887

1	4.199552	-1.887537	-2.516001
1	2.841563	-2.655565	-3.365126
1	3.317396	-0.959703	-3.737086
6	-0.122286	3.635851	-2.952546
1	-0.414387	4.592792	-2.507050
1	0.869108	3.748845	-3.395060
1	-0.863046	3.373594	-3.710443
6	0.023207	3.615209	2.976519
1	-0.981076	3.739542	3.385116
1	0.731778	3.332597	3.757816
1	0.350769	4.570525	2.552863
6	-3.146918	-1.821609	2.957425
1	-2.653970	-2.649810	3.470838
1	-3.413998	-1.029045	3.658558
1	-4.064063	-2.205104	2.497903
6	-3.092000	-1.901618	-2.962005
1	-3.830496	-2.570373	-2.507229
1	-3.626655	-1.083012	-3.447853
1	-2.508404	-2.473334	-3.685744
6	3.143996	-1.833103	2.947659
1	3.668480	-1.005122	3.428560
1	2.574299	-2.412786	3.676207
1	3.889791	-2.491572	2.489745

Conformational and Configurational Study of C-H Activation

Bimetallic C-H activation (Pd-Ag)

4CHI_Pd-Ag

Number of imaginary frequencies : 1
The smallest frequency is : -1620.8825 cm(-1)

Electronic energy : HF=-2548.6576134
Zero-point correction= 0.656742
Thermal correction to Energy= 0.706733
Thermal correction to Enthalpy= 0.707678
Thermal correction to Gibbs Free Energy= 0.570543
Sum of electronic and zero-point Energies= -2548.000872
Sum of electronic and thermal Energies= -2547.950880
Sum of electronic and thermal Enthalpies= -2547.949936
Sum of electronic and thermal Free Energies= -2548.087070

Cartesian Coordinates

8	-2.639340	1.715808	-2.223056
47	-2.756370	-0.023168	-0.827617
46	-0.138816	-1.289791	-1.190071
8	-5.496069	-1.614128	0.968052
6	-5.910618	-0.466969	0.460563
8	-5.315053	0.142641	-0.418136
6	-7.168790	0.028161	1.095510
1	-7.865663	-0.792798	1.284390
1	-7.636248	0.790660	0.470243
1	-6.916931	0.476059	2.065064
1	0.081679	1.007150	-2.086017
6	1.146561	0.201746	-2.117967
6	1.454773	-0.402882	-3.365016
1	0.635236	-0.857829	-3.923084
6	2.730893	-0.442136	-3.927746
1	2.892896	-0.936921	-4.881731
6	3.785588	0.177198	-3.265549
1	4.793256	0.184684	-3.676460
6	3.529644	0.820641	-2.059790
6	2.244378	0.828615	-1.494491
6	3.516705	2.099498	-0.048194
6	0.618530	0.652403	1.114023
6	1.131706	1.783255	0.566073

7	2.245783	1.598560	-0.307484
6	4.416864	1.591209	-1.202195
8	5.601300	1.829413	-1.291824
8	3.853961	2.779438	0.890816
6	1.491430	-0.562403	1.063302
6	0.731619	3.178257	0.810868
6	0.768339	4.134878	-0.210836
6	0.372217	3.583366	2.103985
6	0.415615	5.455319	0.048126
1	1.042916	3.827988	-1.217386
6	0.020412	4.901706	2.359433
1	0.381074	2.854391	2.912959
6	0.035774	5.842493	1.330489
1	0.436760	6.185278	-0.758878
1	-0.252901	5.200853	3.368983
1	-0.235857	6.876382	1.532079
6	-0.718111	0.517568	1.719304
6	-1.795556	1.338481	1.328275
6	-0.975842	-0.506208	2.642373
6	-3.068320	1.148681	1.863299
1	-1.629476	2.147197	0.617392
6	-2.247793	-0.692642	3.175785
1	-0.165343	-1.164605	2.952356
6	-3.299831	0.130744	2.790399
1	-3.884198	1.795799	1.545410
1	-2.413474	-1.488991	3.898225
1	-4.295432	-0.021184	3.201546
6	1.283852	-1.533397	0.165318
6	2.670378	-0.533086	1.970618
6	2.563639	0.031161	3.249502
6	3.931972	-0.962264	1.535494
6	3.677749	0.143084	4.073461
1	1.595060	0.382606	3.603731
6	5.046140	-0.845578	2.359343
1	4.045046	-1.370316	0.532550
6	4.923979	-0.293692	3.631706
1	3.571395	0.579372	5.064504
1	6.017548	-1.176410	1.997824
1	5.797045	-0.197921	4.273246
6	1.896286	-2.849098	0.027092
6	2.643709	-3.203500	-1.106333
6	1.715475	-3.794599	1.048879
6	3.215282	-4.466001	-1.201841
1	2.784627	-2.473007	-1.903049
6	2.286975	-5.056063	0.946868
1	1.118483	-3.523826	1.918973
6	3.036661	-5.395273	-0.177830
1	3.804190	-4.727263	-2.078273
1	2.144534	-5.780721	1.745502
1	3.481168	-6.384763	-0.258074
8	-1.116818	-2.998298	-0.281216
6	-2.320340	-3.022734	0.079289
8	-3.189429	-2.146242	-0.211061
6	-2.786133	-4.187999	0.908821
1	-1.977823	-4.895898	1.103335
1	-3.176633	-3.811549	1.862137
1	-3.610655	-4.699879	0.401186
1	-4.635073	-1.880561	0.534823
6	-1.669195	2.497279	-2.346251
6	-1.959034	3.955866	-2.585700
1	-1.136132	4.450093	-3.108964
1	-2.894443	4.081941	-3.137104
1	-2.078009	4.439504	-1.606704
8	-0.436758	2.189281	-2.259552

4CH2_Pd-Ag

Number of imaginary frequencies : 1

The smallest frequency is : -883.8676 cm(-1)

Electronic energy : HF=-2548.6362119
 Zero-point correction= 0.654824
 Thermal correction to Energy= 0.705242
 Thermal correction to Enthalpy= 0.706186
 Thermal correction to Gibbs Free Energy= 0.568161
 Sum of electronic and zero-point Energies= -2547.981388
 Sum of electronic and thermal Energies= -2547.930970
 Sum of electronic and thermal Enthalpies= -2547.930026
 Sum of electronic and thermal Free Energies= -2548.068051

.....
 Cartesian Coordinates

8	0.443034	1.644908	3.161082
6	1.497187	1.883049	2.468255
6	2.796795	1.975712	3.225673
1	3.150154	3.013414	3.223612
1	2.701413	1.634377	4.259749
1	3.556628	1.378263	2.703182
8	1.500363	2.039842	1.233634
47	2.317521	0.321340	-0.286103
46	-0.015196	-0.914872	1.010453
8	5.624151	0.237074	1.187988
6	5.576264	1.026260	0.133521
8	4.623130	1.083825	-0.636583
6	6.806195	1.856673	-0.028637
1	6.894296	2.541771	0.821907
1	6.762303	2.430696	-0.955291
1	7.696481	1.219973	-0.023483
1	-0.414748	1.052552	2.531593
6	-1.524290	0.193369	2.332378
6	-1.705725	-0.500040	3.552558
1	-0.817892	-0.660857	4.165890
6	-2.931781	-0.971836	4.031829
1	-2.983517	-1.504822	4.978447
6	-4.083413	-0.724453	3.297846
1	-5.065824	-1.047719	3.637429
6	-3.960411	-0.042108	2.091345
6	-2.708219	0.379090	1.609800
6	-4.230493	1.038468	-0.008099
6	-1.075808	0.471974	-1.189719
6	-1.914016	1.389242	-0.639499
7	-2.884200	0.992411	0.326660
6	-4.987595	0.335152	1.140008
8	-6.188780	0.163712	1.150453
8	-4.715061	1.495103	-1.018297
6	-1.141338	-0.967433	-0.799676
6	-1.953885	2.823352	-0.985877
6	-1.990257	3.769543	0.045463
6	-1.973919	3.264734	-2.313649
6	-2.008668	5.129049	-0.245447
1	-1.988912	3.431845	1.081794
6	-1.996478	4.623839	-2.601663
1	-1.988898	2.534275	-3.121149
6	-2.008062	5.560432	-1.569527
1	-2.023961	5.854353	0.565226
1	-2.017448	4.954052	-3.637986
1	-2.026496	6.623793	-1.797886
6	0.011640	0.842823	-2.130598
6	0.947546	1.847645	-1.823761
6	0.131910	0.160443	-3.346845
6	1.981572	2.143989	-2.716957
1	0.830780	2.421344	-0.905784
6	1.158037	0.465317	-4.234312
1	-0.597016	-0.607112	-3.603411
6	2.091543	1.450593	-3.919647
1	2.694313	2.926515	-2.466612
1	1.227171	-0.068831	-5.179369
1	2.895479	1.684493	-4.613469
6	0.039013	-1.743351	-0.752669

6	-2.439888	-1.709555	-0.815260
6	-2.693857	-2.749644	0.087830
6	-3.408425	-1.397037	-1.775745
6	-3.892589	-3.452936	0.037619
1	-1.952227	-2.982541	0.853047
6	-4.613141	-2.090988	-1.812702
1	-3.225257	-0.587689	-2.481235
6	-4.859023	-3.121668	-0.908806
1	-4.076267	-4.253769	0.750551
1	-5.363749	-1.823100	-2.553138
1	-5.802763	-3.661416	-0.939184
6	0.689105	-2.759744	-1.476759
6	1.899657	-3.299036	-0.977654
6	0.157784	-3.247836	-2.697146
6	2.559317	-4.288096	-1.683032
1	2.301410	-2.900633	-0.046122
6	0.815373	-4.250204	-3.381603
1	-0.780132	-2.842443	-3.071147
6	2.015140	-4.763257	-2.878335
1	3.493676	-4.697568	-1.309203
1	0.406486	-4.637321	-4.310852
1	2.532128	-5.547233	-3.426959
8	1.502143	-1.314741	2.586408
6	2.746567	-1.313218	2.437354
8	3.354891	-1.048905	1.351332
6	3.602025	-1.674578	3.625383
1	3.024368	-1.662895	4.552308
1	4.013258	-2.680060	3.477108
1	4.452134	-0.988425	3.709299
1	4.778289	-0.301981	1.262949

4CH3_Pd-Ag

Number of imaginary frequencies : 1

The smallest frequency is : -883.4249 cm(-1)

Electronic energy : HF=-2548.6362119
 Zero-point correction= 0.654822
 Thermal correction to Energy= 0.705241
 Thermal correction to Enthalpy= 0.706185
 Thermal correction to Gibbs Free Energy= 0.568156
 Sum of electronic and zero-point Energies= -2547.981390
 Sum of electronic and thermal Energies= -2547.930971
 Sum of electronic and thermal Enthalpies= -2547.930027
 Sum of electronic and thermal Free Energies= -2548.068056

Cartesian Coordinates

8	0.443063	1.644880	3.161109
6	1.497246	1.882991	2.468310
6	2.796820	1.975674	3.225778
1	3.150185	3.013374	3.223687
1	2.701390	1.634380	4.259864
1	3.556670	1.378197	2.703343
8	1.500466	2.039744	1.233687
47	2.317590	0.321221	-0.286039
46	-0.015266	-0.914926	1.010461
8	5.624135	0.236937	1.188153
6	5.576351	1.025939	0.133545
8	4.623279	1.083398	-0.636645
6	6.806327	1.856272	-0.028672
1	6.894432	2.541483	0.821779
1	6.762514	2.430161	-0.955412
1	7.696577	1.219522	-0.023387
1	-0.414703	1.052569	2.531639
6	-1.524296	0.193365	2.332410
6	-1.705683	-0.500153	3.552535
1	-0.817821	-0.661014	4.165816

6	-2.931715	-0.972029	4.031795
1	-2.983409	-1.505105	4.978365
6	-4.083369	-0.724629	3.297856
1	-5.065760	-1.047966	3.637432
6	-3.960414	-0.042190	2.091401
6	-2.708246	0.379090	1.609869
6	-4.230561	1.038442	-0.008008
6	-1.075904	0.472083	-1.189667
6	-1.914090	1.389334	-0.639395
7	-2.884268	0.992488	0.326766
6	-4.987622	0.335069	1.140090
8	-6.188803	0.163596	1.150544
8	-4.715157	1.495039	-1.018211
6	-1.141411	-0.967339	-0.799669
6	-1.953855	2.823453	-0.985766
6	-1.974021	3.264747	-2.313560
6	-1.989995	3.769719	0.045511
6	-1.996475	4.623829	-2.601685
1	-1.989151	2.534190	-3.120956
6	-2.008303	5.129204	-0.245501
1	-1.988555	3.432103	1.081864
6	-2.007825	5.560493	-1.569612
1	-2.017537	4.953966	-3.638029
1	-2.023411	5.854569	0.565122
1	-2.026176	6.623841	-1.798042
6	0.011527	0.842959	-2.130557
6	0.947537	1.847651	-1.823627
6	0.131723	0.160683	-3.346869
6	1.981614	2.143950	-2.716779
1	0.830828	2.421258	-0.905587
6	1.157900	0.465511	-4.234294
1	-0.597294	-0.606754	-3.603522
6	2.091527	1.450640	-3.919524
1	2.694444	2.926370	-2.466354
1	1.226987	-0.068567	-5.179395
1	2.895507	1.684498	-4.613308
6	0.038947	-1.743253	-0.752733
6	-2.439943	-1.709493	-0.815280
6	-2.693904	-2.749588	0.087806
6	-3.408473	-1.396999	-1.775780
6	-3.892615	-3.452913	0.037571
1	-1.952290	-2.982448	0.853050
6	-4.613169	-2.090984	-1.812762
1	-3.225312	-0.587650	-2.481270
6	-4.859040	-3.121672	-0.908873
1	-4.076289	-4.253749	0.750501
1	-5.363771	-1.823110	-2.553208
1	-5.802766	-3.661444	-0.939268
6	0.689062	-2.759524	-1.476974
6	1.899674	-3.298800	-0.978003
6	0.157724	-3.247465	-2.697413
6	2.559394	-4.287682	-1.683577
1	2.301419	-2.900516	-0.046416
6	0.815371	-4.249659	-3.382067
1	-0.780248	-2.842095	-3.071298
6	2.015208	-4.762686	-2.878940
1	3.493804	-4.697136	-1.309855
1	0.406476	-4.636663	-4.311359
1	2.532242	-5.546523	-3.427718
8	1.502029	-1.314819	2.586469
6	2.746463	-1.313266	2.437495
8	3.354846	-1.048968	1.351502
6	3.601856	-1.674586	3.625584
1	3.024163	-1.662806	4.552486
1	4.013031	-2.680104	3.477397
1	4.452005	-0.988481	3.709481
1	4.778261	-0.302100	1.263134

4CH4_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -883.5562 cm(-1)

Electronic energy : HF=-2548.6362118
 Zero-point correction= 0.654825
 Thermal correction to Energy= 0.705243
 Thermal correction to Enthalpy= 0.706187
 Thermal correction to Gibbs Free Energy= 0.568166
 Sum of electronic and zero-point Energies= -2547.981386
 Sum of electronic and thermal Energies= -2547.930968
 Sum of electronic and thermal Enthalpies= -2547.930024
 Sum of electronic and thermal Free Energies= -2548.068046

Cartesian Coordinates

8	0.443299	1.645040	3.160866
6	1.497463	1.883097	2.468025
6	2.797051	1.975804	3.225467
1	3.150325	3.013536	3.223477
1	2.701671	1.634409	4.259523
1	3.556935	1.378432	2.702963
8	1.500670	2.039787	1.233392
47	2.317456	0.320982	-0.286092
46	-0.015215	-0.914892	1.010530
8	5.624174	0.237083	1.187857
6	5.576147	1.026400	0.133491
8	4.622932	1.084027	-0.636502
6	6.805979	1.856968	-0.028634
1	6.893314	2.542804	0.821403
1	6.762453	2.430275	-0.955749
1	7.696460	1.220562	-0.022401
1	-0.414536	1.052736	2.531455
6	-1.524189	0.193628	2.332366
6	-1.705638	-0.499678	3.552603
1	-0.817796	-0.660535	4.165913
6	-2.931720	-0.971325	4.031959
1	-2.983458	-1.504258	4.978606
6	-4.083367	-0.723857	3.298029
1	-5.065792	-1.046998	3.637691
6	-3.960356	-0.041586	2.091486
6	-2.708137	0.379419	1.609845
6	-4.230402	1.038847	-0.008036
6	-1.075845	0.471853	-1.189747
6	-1.913914	1.389270	-0.639571
7	-2.884101	0.992685	0.326680
6	-4.987538	0.335741	1.140173
8	-6.188748	0.164475	1.150689
8	-4.714962	1.495402	-1.018274
6	-1.141470	-0.967502	-0.799529
6	-1.953603	2.823343	-0.986125
6	-1.989746	3.769660	0.045107
6	-1.973655	3.264570	-2.313947
6	-2.007968	5.129135	-0.245959
1	-1.988371	3.432066	1.081474
6	-1.996023	4.623646	-2.602117
1	-1.988828	2.534017	-3.121357
6	-2.007388	5.560361	-1.570089
1	-2.023092	5.854537	0.564631
1	-2.017009	4.953742	-3.638476
1	-2.025666	6.623698	-1.798574
6	0.011594	0.842528	-2.130712
6	0.947574	1.847307	-1.823978
6	0.131768	0.160067	-3.346924
6	1.981575	2.143552	-2.717231
1	0.830857	2.421057	-0.906027
6	1.157884	0.464826	-4.234444
1	-0.597223	-0.607443	-3.603437
6	2.091457	1.450073	-3.919879

1	2.694363	2.926061	-2.466974
1	1.226955	-0.069386	-5.179470
1	2.895377	1.683883	-4.613749
6	0.038834	-1.743492	-0.752548
6	-2.440067	-1.709534	-0.814996
6	-2.694102	-2.749533	0.088174
6	-3.408601	-1.396997	-1.775482
6	-3.892903	-3.452716	0.038044
1	-1.952464	-2.982468	0.853372
6	-4.613380	-2.090841	-1.812361
1	-3.225365	-0.587707	-2.481022
6	-4.859335	-3.121424	-0.908376
1	-4.076640	-4.253484	0.751034
1	-5.363986	-1.822927	-2.552789
1	-5.803127	-3.661084	-0.938685
6	0.688854	-2.759918	-1.476651
6	1.899439	-3.299216	-0.977634
6	0.157405	-3.248052	-2.696964
6	2.559020	-4.288309	-1.683041
1	2.301268	-2.900793	-0.046142
6	0.814910	-4.250457	-3.381445
1	-0.780545	-2.842665	-3.070887
6	2.014720	-4.763505	-2.878276
1	3.493405	-4.697785	-1.309282
1	0.405925	-4.637609	-4.310636
1	2.531642	-5.547516	-3.426912
8	1.502209	-1.314812	2.586416
6	2.746645	-1.313214	2.437393
8	3.354986	-1.049103	1.351325
6	3.602088	-1.674273	3.625527
1	3.024418	-1.662330	4.552441
1	4.013289	-2.679809	3.477529
1	4.452223	-0.988133	3.709269
1	4.778340	-0.302006	1.262852

4CH5_Pd-Ag

Number of imaginary frequencies : 1
The smallest frequency is : -883.9191 cm(-1)

Electronic energy : HF=-2548.6362119
Zero-point correction= 0.654825
Thermal correction to Energy= 0.705242
Thermal correction to Enthalpy= 0.706186
Thermal correction to Gibbs Free Energy= 0.568164
Sum of electronic and zero-point Energies= -2547.981387
Sum of electronic and thermal Energies= -2547.930970
Sum of electronic and thermal Enthalpies= -2547.930025
Sum of electronic and thermal Free Energies= -2548.068048

Cartesian Coordinates

8	0.443187	1.645141	3.160872
6	1.497299	1.883301	2.467989
6	2.796925	1.976117	3.225357
1	3.150379	3.013785	3.222936
1	2.701550	1.635122	4.259546
1	3.556694	1.378433	2.703042
8	1.500434	2.039986	1.233354
47	2.317506	0.321195	-0.286160
46	-0.015226	-0.914844	1.010534
8	5.624197	0.237170	1.187942
6	5.576263	1.026276	0.133416
8	4.623130	1.083722	-0.636696
6	6.806146	1.856752	-0.028796
1	6.894234	2.541879	0.821726
1	6.762202	2.430740	-0.955469
1	7.696467	1.220100	-0.023643

1	-0.414638	1.052750	2.531462
6	-1.524230	0.193622	2.332366
6	-1.705671	-0.499677	3.552607
1	-0.817833	-0.660475	4.165937
6	-2.931739	-0.971384	4.031938
1	-2.983480	-1.504291	4.978601
6	-4.083373	-0.724014	3.297956
1	-5.065792	-1.047207	3.637584
6	-3.960363	-0.041777	2.091394
6	-2.708161	0.379320	1.609788
6	-4.230435	1.038657	-0.008125
6	-1.075791	0.471883	-1.189752
6	-1.913941	1.389248	-0.639604
7	-2.884135	0.992553	0.326603
6	-4.987549	0.335471	1.140054
8	-6.188744	0.164098	1.150537
8	-4.715008	1.495236	-1.018345
6	-1.141401	-0.967488	-0.799581
6	-1.953734	2.823331	-0.986113
6	-1.990152	3.769621	0.045135
6	-1.973675	3.264597	-2.313928
6	-2.008527	5.129100	-0.245899
1	-1.988907	3.432026	1.081498
6	-1.996205	4.623676	-2.602066
1	-1.988607	2.534064	-3.121359
6	-2.007840	5.560363	-1.570017
1	-2.023861	5.854479	0.564708
1	-2.017114	4.953793	-3.638420
1	-2.026251	6.623704	-1.798475
6	0.011680	0.842583	-2.130665
6	0.947616	1.847417	-1.823950
6	0.131933	0.160047	-3.346828
6	1.981646	2.143625	-2.717184
1	0.830853	2.421236	-0.906048
6	1.158068	0.464783	-4.234331
1	-0.597021	-0.607514	-3.603296
6	2.091598	1.450075	-3.919788
1	2.694410	2.926163	-2.466937
1	1.227188	-0.069485	-5.179322
1	2.895539	1.683867	-4.613640
6	0.038904	-1.743474	-0.752523
6	-2.439986	-1.709547	-0.815100
6	-2.693968	-2.749599	0.088031
6	-3.408537	-1.397028	-1.775570
6	-3.892724	-3.452852	0.037872
1	-1.952318	-2.982509	0.853225
6	-4.613279	-2.090938	-1.812472
1	-3.225356	-0.587720	-2.481101
6	-4.859174	-3.121579	-0.908536
1	-4.076410	-4.253657	0.750834
1	-5.363897	-1.823045	-2.552895
1	-5.802933	-3.661294	-0.938870
6	0.688917	-2.759999	-1.476500
6	1.899436	-3.299309	-0.977335
6	0.157562	-3.248203	-2.696828
6	2.559032	-4.288497	-1.682593
1	2.301219	-2.900820	-0.045853
6	0.815087	-4.250695	-3.381165
1	-0.780326	-2.842795	-3.070882
6	2.014822	-4.763766	-2.877838
1	3.493367	-4.697982	-1.308717
1	0.406174	-4.637898	-4.310366
1	2.531763	-5.547835	-3.426373
8	1.502169	-1.314505	2.586477
6	2.746596	-1.313000	2.437445
8	3.354943	-1.048812	1.351406
6	3.602034	-1.674212	3.625534
1	3.024334	-1.662532	4.552431
1	4.013377	-2.679658	3.477325
1	4.452071	-0.987970	3.709441

1 4.778357 -0.301912 1.262947

4CH6_Pd-Ag

Number of imaginary frequencies : 1

The smallest frequency is : -884.1211 cm(-1)

Electronic energy : HF=-2548.6362119
Zero-point correction= 0.654819
Thermal correction to Energy= 0.705240
Thermal correction to Enthalpy= 0.706184
Thermal correction to Gibbs Free Energy= 0.568141
Sum of electronic and zero-point Energies= -2547.981393
Sum of electronic and thermal Energies= -2547.930972
Sum of electronic and thermal Enthalpies= -2547.930028
Sum of electronic and thermal Free Energies= -2548.068071

Cartesian Coordinates

8	0.442784	1.644124	3.161527
6	1.496947	1.882490	2.468802
6	2.796559	1.974846	3.226249
1	3.149798	3.012592	3.224790
1	2.701213	1.632912	4.260131
1	3.556462	1.377778	2.703414
8	1.500119	2.039737	1.234233
47	2.317549	0.321928	-0.285724
46	-0.015262	-0.915380	1.010381
8	5.624130	0.236918	1.187989
6	5.576297	1.026396	0.133736
8	4.623261	1.084038	-0.636482
6	6.806089	1.857103	-0.027956
1	6.893117	2.542832	0.822202
1	6.762747	2.430544	-0.954997
1	7.696635	1.220791	-0.021574
1	-0.414956	1.051915	2.531819
6	-1.524467	0.192751	2.332346
6	-1.705986	-0.500909	3.552370
1	-0.818196	-0.661880	4.165728
6	-2.932086	-0.972726	4.031515
1	-2.983873	-1.505924	4.978011
6	-4.083693	-0.725032	3.297604
1	-5.066141	-1.048247	3.637131
6	-3.960619	-0.042410	2.091265
6	-2.708380	0.378723	1.609792
6	-4.230633	1.038903	-0.007814
6	-1.075819	0.472019	-1.189567
6	-1.914063	1.389223	-0.639285
7	-2.884308	0.992376	0.326792
6	-4.987785	0.335342	1.140103
8	-6.189006	0.164161	1.150581
8	-4.715215	1.496049	-1.017774
6	-1.141303	-0.967467	-0.799809
6	-1.953833	2.823355	-0.985620
6	-1.989935	3.769579	0.045693
6	-1.974048	3.264685	-2.313405
6	-2.008241	5.129077	-0.245272
1	-1.988469	3.431913	1.082032
6	-1.996496	4.623778	-2.601475
1	-1.989288	2.534179	-3.120858
6	-2.007795	5.560408	-1.569369
1	-2.023325	5.854415	0.565375
1	-2.017602	4.953956	-3.637805
1	-2.026143	6.623764	-1.797763
6	0.011673	0.843044	-2.130319
6	0.947449	1.847941	-1.823344
6	0.132111	0.160762	-3.346604
6	1.981531	2.144436	-2.716427

1	0.830485	2.421642	-0.905390
6	1.158298	0.465773	-4.233954
1	-0.596743	-0.606820	-3.603296
6	2.091692	1.451105	-3.919139
1	2.694165	2.927027	-2.465978
1	1.227564	-0.068313	-5.179037
1	2.895678	1.685114	-4.612865
6	0.039061	-1.743373	-0.752954
6	-2.439842	-1.709595	-0.815531
6	-2.693765	-2.750067	0.087130
6	-3.408478	-1.396568	-1.775738
6	-3.892564	-3.453238	0.036747
1	-1.952048	-2.983399	0.852128
6	-4.613295	-2.090342	-1.812809
1	-3.225268	-0.586945	-2.480895
6	-4.859128	-3.121422	-0.909358
1	-4.076209	-4.254393	0.749325
1	-5.364008	-1.821989	-2.552972
1	-5.802930	-3.661055	-0.939822
6	0.689236	-2.759536	-1.477288
6	1.899866	-3.298797	-0.978342
6	0.157913	-3.247446	-2.697748
6	2.559617	-4.287628	-1.683958
1	2.301623	-2.900523	-0.046756
6	0.815586	-4.249599	-3.382436
1	-0.780082	-2.842108	-3.071613
6	2.015442	-4.762608	-2.879333
1	3.494044	-4.697062	-1.310257
1	0.406695	-4.636585	-4.311738
1	2.532499	-5.546409	-3.428143
8	1.502374	-1.315205	2.586052
6	2.746771	-1.313769	2.436809
8	3.354951	-1.049334	1.350728
6	3.602378	-1.675394	3.624652
1	3.024869	-1.663742	4.551669
1	4.013435	-2.680920	3.476190
1	4.452605	-0.989381	3.708516
1	4.778309	-0.302241	1.262669

4CH7_Pd-Ag

Number of imaginary frequencies : 1
The smallest frequency is : -920.2282 cm(-1)

Electronic energy : HF=-2548.636141
Zero-point correction= 0.655426
Thermal correction to Energy= 0.705777
Thermal correction to Enthalpy= 0.706721
Thermal correction to Gibbs Free Energy= 0.568535
Sum of electronic and zero-point Energies= -2547.980715
Sum of electronic and thermal Energies= -2547.930364
Sum of electronic and thermal Enthalpies= -2547.929420
Sum of electronic and thermal Free Energies= -2548.067606

Cartesian Coordinates

8	0.452272	1.724876	3.108838
6	1.491266	1.955280	2.391728
6	2.804753	2.067852	3.122612
1	3.171050	3.099499	3.066984
1	2.724248	1.773496	4.172296
1	3.548415	1.437876	2.615597
8	1.470069	2.087041	1.153916
47	2.330291	0.320884	-0.300815
46	-0.030020	-0.883575	1.028067
8	5.638275	0.224430	1.189268
6	5.599025	1.007504	0.129696
8	4.647027	1.069151	-0.641381

6	6.836939	1.825223	-0.035878
1	6.930673	2.514400	0.810729
1	6.799666	2.394292	-0.965877
1	7.721075	1.180081	-0.025914
1	-0.414299	1.114190	2.499712
6	-1.528973	0.268694	2.324655
6	-1.726162	-0.381589	3.565675
1	-0.842674	-0.544585	4.184852
6	-2.963104	-0.807536	4.059119
1	-3.027794	-1.309267	5.021876
6	-4.109026	-0.553357	3.318172
1	-5.099069	-0.840845	3.667434
6	-3.970182	0.088747	2.091620
6	-2.707712	0.461378	1.596106
6	-4.212709	1.105701	-0.042723
6	-1.071512	0.426838	-1.206159
6	-1.888771	1.378592	-0.684614
7	-2.867764	1.037145	0.293924
6	-4.987763	0.461564	1.128115
8	-6.192743	0.319767	1.141954
8	-4.686001	1.539121	-1.068337
6	-1.166952	-0.998835	-0.772867
6	-1.890739	2.803190	-1.072199
6	-1.858226	3.775471	-0.065742
6	-1.938109	3.208561	-2.410331
6	-1.840824	5.126798	-0.391788
1	-1.823502	3.459761	0.977068
6	-1.924201	4.560109	-2.733581
1	-2.001686	2.456610	-3.195791
6	-1.871010	5.522528	-1.726915
1	-1.801960	5.873326	0.398576
1	-1.966457	4.864750	-3.777078
1	-1.861892	6.579608	-1.983294
6	0.019368	0.744826	-2.162525
6	0.971299	1.747947	-1.900266
6	0.126534	0.008928	-3.348065
6	2.009760	1.986453	-2.806094
1	0.863847	2.367060	-1.010774
6	1.155902	0.257943	-4.249195
1	-0.615449	-0.757661	-3.567759
6	2.106757	1.239207	-3.977484
1	2.735581	2.767564	-2.590880
1	1.213994	-0.317505	-5.170382
1	2.913385	1.429237	-4.681460
6	-0.001064	-1.792032	-0.695735
6	-2.478753	-1.715379	-0.761268
6	-3.449622	-1.408462	-1.720954
6	-2.740358	-2.733621	0.164483
6	-4.663717	-2.086810	-1.736202
1	-3.260607	-0.616753	-2.444753
6	-3.948396	-3.422023	0.135616
1	-1.995159	-2.963808	0.926926
6	-4.916849	-3.096458	-0.810850
1	-5.415680	-1.823557	-2.476911
1	-4.137397	-4.206603	0.865039
1	-5.867480	-3.624643	-0.824815
6	0.637689	-2.845606	-1.375469
6	1.841382	-3.375215	-0.850353
6	0.105128	-3.380267	-2.575757
6	2.492829	-4.400684	-1.509732
1	2.246300	-2.940881	0.063290
6	0.754251	-4.418514	-3.213626
1	-0.826769	-2.981200	-2.971084
6	1.946865	-4.922110	-2.684549
1	3.422250	-4.802557	-1.115871
1	0.343973	-4.840870	-4.126795
1	2.457513	-5.733744	-3.197795
8	1.491677	-1.242972	2.607342
6	2.735551	-1.255131	2.457487
8	3.345530	-1.019674	1.365274

6	3.590563	-1.593744	3.652287
1	3.009955	-1.577723	4.577227
1	4.015698	-2.595121	3.516361
1	4.431176	-0.895207	3.730910
1	4.785075	-0.302029	1.268436

4CH8_Pd-Ag

Number of imaginary frequencies : 1

The smallest frequency is : -883.9569 cm(-1)

Electronic energy : HF=-2548.636212
 Zero-point correction= 0.654819
 Thermal correction to Energy= 0.705240
 Thermal correction to Enthalpy= 0.706184
 Thermal correction to Gibbs Free Energy= 0.568150
 Sum of electronic and zero-point Energies= -2547.981393
 Sum of electronic and thermal Energies= -2547.930972
 Sum of electronic and thermal Enthalpies= -2547.930028
 Sum of electronic and thermal Free Energies= -2548.068062

Cartesian Coordinates

8	0.442908	1.644142	3.161473
6	1.497058	1.882601	2.468751
6	2.796606	1.975346	3.226261
1	3.149956	3.013051	3.224122
1	2.701166	1.634090	4.260357
1	3.556487	1.377872	2.703868
8	1.500282	2.039636	1.234162
47	2.317380	0.321449	-0.285930
46	-0.015227	-0.915257	1.010386
8	5.624005	0.237211	1.188184
6	5.576208	1.025997	0.133420
8	4.623172	1.083206	-0.636838
6	6.806092	1.856455	-0.028868
1	6.893895	2.542002	0.821347
1	6.762363	2.430008	-0.955821
1	7.696453	1.219866	-0.023158
1	-0.414850	1.051949	2.531804
6	-1.524428	0.192837	2.332371
6	-1.705902	-0.500842	3.552394
1	-0.818090	-0.661775	4.165726
6	-2.931961	-0.972802	4.031498
1	-2.983716	-1.506026	4.977981
6	-4.083568	-0.725290	3.297522
1	-5.065981	-1.048684	3.636980
6	-3.960539	-0.042643	2.091194
6	-2.708335	0.378678	1.609785
6	-4.230535	1.038116	-0.008167
6	-1.075698	0.472209	-1.189617
6	-1.914018	1.389287	-0.639258
7	-2.884273	0.992169	0.326715
6	-4.987674	0.334643	1.139813
8	-6.188854	0.163158	1.150156
8	-4.715050	1.494784	-1.018377
6	-1.141174	-0.967277	-0.799895
6	-1.953953	2.823460	-0.985370
6	-1.990327	3.769495	0.046111
6	-1.974038	3.265035	-2.313076
6	-2.008797	5.129043	-0.244606
1	-1.988942	3.431644	1.082391
6	-1.996658	4.624179	-2.600898
1	-1.989011	2.534679	-3.120669
6	-2.008247	5.560619	-1.568623
1	-2.024091	5.854230	0.566172
1	-2.017669	4.954543	-3.637171
1	-2.026727	6.624013	-1.796825

6	0.011807	0.843350	-2.130315
6	0.947544	1.848251	-1.823204
6	0.132307	0.161190	-3.346667
6	1.981634	2.144881	-2.716229
1	0.830564	2.421789	-0.905156
6	1.158497	0.466354	-4.233961
1	-0.596493	-0.606405	-3.603460
6	2.091840	1.451696	-3.919019
1	2.694256	2.927443	-2.465664
1	1.227812	-0.067624	-5.179102
1	2.895832	1.685812	-4.612701
6	0.039157	-1.743216	-0.752980
6	-2.439751	-1.709338	-0.815629
6	-3.408066	-1.396650	-1.776282
6	-2.693949	-2.749483	0.087317
6	-4.612863	-2.090433	-1.813503
1	-3.224626	-0.587198	-2.481581
6	-3.892737	-3.452665	0.036794
1	-1.952500	-2.982468	0.852683
6	-4.858975	-3.121205	-0.909769
1	-5.363349	-1.822299	-2.553976
1	-4.076632	-4.253557	0.749604
1	-5.802766	-3.660851	-0.940350
6	0.689356	-2.759389	-1.477276
6	1.899905	-3.298724	-0.978215
6	0.158156	-3.247202	-2.697826
6	2.559708	-4.287530	-1.683814
1	2.301535	-2.900539	-0.046536
6	0.815883	-4.249326	-3.382506
1	-0.779769	-2.841786	-3.071783
6	2.015662	-4.762406	-2.879292
1	3.494073	-4.697026	-1.310025
1	0.407096	-4.636235	-4.311885
1	2.532766	-5.546177	-3.428098
8	1.502001	-1.315393	2.586395
6	2.746442	-1.313429	2.437493
8	3.354803	-1.048641	1.351612
6	3.601849	-1.674897	3.625528
1	3.024306	-1.662546	4.552517
1	4.012329	-2.680733	3.477558
1	4.452447	-0.989313	3.709100
1	4.778152	-0.301865	1.263229

4CH9_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -884.1927 cm(-1)

Electronic energy : HF=-2548.6362119
 Zero-point correction= 0.654822
 Thermal correction to Energy= 0.705241
 Thermal correction to Enthalpy= 0.706186
 Thermal correction to Gibbs Free Energy= 0.568151
 Sum of electronic and zero-point Energies= -2547.981390
 Sum of electronic and thermal Energies= -2547.930971
 Sum of electronic and thermal Enthalpies= -2547.930026
 Sum of electronic and thermal Free Energies= -2548.068061

 Cartesian Coordinates

8	0.443052	1.644740	3.161177
6	1.497183	1.882895	2.468329
6	2.796813	1.975539	3.225711
1	3.150172	3.013242	3.223663
1	2.701460	1.634181	4.259782
1	3.556634	1.378105	2.703186
8	1.500321	2.039716	1.233710
47	2.317471	0.321328	-0.286088

46	-0.015215	-0.914974	1.010435
8	5.624125	0.237051	1.187985
6	5.576188	1.026468	0.133693
8	4.623005	1.084229	-0.636332
6	6.806109	1.856920	-0.028340
1	6.893887	2.542237	0.822065
1	6.762413	2.430742	-0.955128
1	7.696457	1.220315	-0.022776
1	-0.414772	1.052425	2.531645
6	-1.524301	0.193280	2.332427
6	-1.705730	-0.500146	3.552598
1	-0.817894	-0.660964	4.165925
6	-2.931786	-0.971927	4.031883
1	-2.983514	-1.504924	4.978495
6	-4.083425	-0.724517	3.297922
1	-5.065836	-1.047764	3.637525
6	-3.960430	-0.042168	2.091423
6	-2.708239	0.379021	1.609866
6	-4.230536	1.038475	-0.007985
6	-1.075867	0.471968	-1.189693
6	-1.914062	1.389215	-0.639422
7	-2.884236	0.992366	0.326737
6	-4.987626	0.335153	1.140121
8	-6.188818	0.163767	1.150599
8	-4.715119	1.495132	-1.018168
6	-1.141328	-0.967463	-0.799717
6	-1.953914	2.823332	-0.985787
6	-1.990191	3.769543	0.045535
6	-1.974009	3.264693	-2.313565
6	-2.008570	5.129044	-0.245404
1	-1.988804	3.431870	1.081873
6	-1.996537	4.623791	-2.601609
1	-1.989069	2.534214	-3.121043
6	-2.008025	5.560404	-1.569490
1	-2.023789	5.854365	0.565257
1	-2.017555	4.953984	-3.637937
1	-2.026432	6.623762	-1.797867
6	0.011552	0.842879	-2.130580
6	0.947458	1.847682	-1.823696
6	0.131782	0.160595	-3.346885
6	1.981459	2.144099	-2.716895
1	0.830680	2.421332	-0.905690
6	1.157890	0.465534	-4.234352
1	-0.597172	-0.606917	-3.603499
6	2.091407	1.450784	-3.919634
1	2.694196	2.926618	-2.466516
1	1.227001	-0.068539	-5.179454
1	2.895327	1.684734	-4.613457
6	0.039076	-1.743306	-0.752752
6	-2.439833	-1.709650	-0.815359
6	-2.693688	-2.749956	0.087517
6	-3.408473	-1.396942	-1.775677
6	-3.892431	-3.453229	0.037297
1	-1.951945	-2.983091	0.852549
6	-4.613210	-2.090862	-1.812626
1	-3.225376	-0.587425	-2.480994
6	-4.858998	-3.121722	-0.908911
1	-4.076023	-4.254222	0.750069
1	-5.363907	-1.822793	-2.552906
1	-5.802756	-3.661437	-0.939272
6	0.689253	-2.759596	-1.476909
6	1.899831	-3.298846	-0.977823
6	0.157981	-3.247634	-2.697339
6	2.559570	-4.287807	-1.683267
1	2.301542	-2.900483	-0.046254
6	0.815648	-4.249905	-3.381861
1	-0.779961	-2.842280	-3.071318
6	2.015443	-4.762914	-2.878614
1	3.493950	-4.697246	-1.309455
1	0.406799	-4.636984	-4.311142

1	2.532488	-5.546819	-3.427287
8	1.502185	-1.314924	2.586332
6	2.746603	-1.313351	2.437243
8	3.354890	-1.049026	1.351201
6	3.602101	-1.674713	3.625246
1	3.024519	-1.662804	4.552215
1	4.013108	-2.680301	3.477068
1	4.452361	-0.988729	3.709002
1	4.778258	-0.302004	1.262882

4CH10 Pd-Ag

Number of imaginary frequencies : 1

The smallest frequency is : -899.9062 cm(-1)

Electronic energy : HF=-2548.6361412
 Zero-point correction= 0.654741
 Thermal correction to Energy= 0.705128
 Thermal correction to Enthalpy= 0.706072
 Thermal correction to Gibbs Free Energy= 0.568180
 Sum of electronic and zero-point Energies= -2547.981400
 Sum of electronic and thermal Energies= -2547.931013
 Sum of electronic and thermal Enthalpies= -2547.930069
 Sum of electronic and thermal Free Energies= -2548.067961

Cartesian Coordinates

8	0.399532	1.621450	3.201945
6	1.450026	1.878335	2.510524
6	2.751384	1.969183	3.264971
1	3.106982	3.006008	3.262992
1	2.659219	1.624778	4.298262
1	3.507720	1.370918	2.738511
8	1.447892	2.051710	1.278070
47	2.309841	0.374295	-0.260061
46	-0.012852	-0.917624	1.007110
8	5.703465	0.078750	1.072552
6	5.614148	0.997333	0.132197
8	4.605348	1.200555	-0.535203
6	6.876290	1.775898	-0.041052
1	7.118774	2.294153	0.892998
1	6.772420	2.503269	-0.847366
1	7.707084	1.096154	-0.256864
1	-0.449061	1.031161	2.558305
6	-1.543636	0.159175	2.336482
6	-1.723492	-0.555142	3.544805
1	-0.838315	-0.709379	4.163713
6	-2.945331	-1.053992	4.007487
1	-2.995354	-1.602060	4.945542
6	-4.095350	-0.813229	3.268898
1	-5.075098	-1.156003	3.596902
6	-3.974177	-0.111089	2.073559
6	-2.725227	0.335969	1.607414
6	-4.246035	0.994601	-0.012506
6	-1.078714	0.482230	-1.180590
6	-1.930791	1.383301	-0.624786
7	-2.901502	0.964051	0.331290
6	-5.000541	0.266012	1.121281
8	-6.199699	0.080628	1.122876
8	-4.730062	1.456114	-1.020730
6	-1.131630	-0.962637	-0.809382
6	-1.987202	2.819832	-0.957733
6	-2.041263	3.756640	0.081295
6	-2.005893	3.272248	-2.281794
6	-2.075316	5.118216	-0.198539
1	-2.040903	3.410128	1.114745
6	-2.044069	4.633233	-2.558797
1	-2.007591	2.548406	-3.095370

6	-2.073045	5.560833	-1.518913
1	-2.104061	5.836466	0.618034
1	-2.063723	4.971813	-3.592434
1	-2.103469	6.625805	-1.738301
6	0.010645	0.877482	-2.109268
6	0.932146	1.889851	-1.783255
6	0.148029	0.212121	-3.333050
6	1.970250	2.208458	-2.664366
1	0.799826	2.452876	-0.860746
6	1.177572	0.539521	-4.208566
1	-0.570607	-0.559505	-3.605779
6	2.097833	1.530740	-3.874272
1	2.671473	2.996401	-2.398674
1	1.259977	0.018247	-5.159741
1	2.904879	1.781874	-4.558381
6	0.055578	-1.727428	-0.763905
6	-2.422088	-1.717987	-0.843050
6	-2.673715	-2.767208	0.049985
6	-3.384896	-1.408108	-1.810230
6	-3.864616	-3.482394	-0.016522
1	-1.937834	-2.996317	0.821916
6	-4.581724	-2.114457	-1.863816
1	-3.203793	-0.590740	-2.507003
6	-4.825286	-3.154448	-0.969939
1	-4.047003	-4.289950	0.689112
1	-5.328080	-1.849014	-2.609417
1	-5.763102	-3.703566	-1.013224
6	0.718895	-2.728111	-1.498104
6	1.931571	-3.264043	-1.000928
6	0.197772	-3.202820	-2.728084
6	2.603273	-4.236622	-1.717892
1	2.326340	-2.874434	-0.062725
6	0.867577	-4.188762	-3.424413
1	-0.742167	-2.800329	-3.100173
6	2.069425	-4.698613	-2.922944
1	3.539522	-4.643286	-1.345661
1	0.466604	-4.565495	-4.361355
1	2.596007	-5.469685	-3.480647
8	1.519043	-1.310187	2.573792
6	2.761521	-1.314615	2.407882
8	3.355483	-1.050689	1.314033
6	3.631594	-1.683413	3.582804
1	3.070652	-1.654505	4.519620
1	4.020113	-2.698007	3.435170
1	4.495970	-1.012972	3.645291
1	4.828795	-0.405931	1.173471

4CH11_Pd-Ag

Number of imaginary frequencies : 1

The smallest frequency is : -873.4309 cm(-1)

Electronic energy : HF=-2548.6360479
 Zero-point correction= 0.654689
 Thermal correction to Energy= 0.705230
 Thermal correction to Enthalpy= 0.706174
 Thermal correction to Gibbs Free Energy= 0.567136
 Sum of electronic and zero-point Energies= -2547.981359
 Sum of electronic and thermal Energies= -2547.930818
 Sum of electronic and thermal Enthalpies= -2547.929874
 Sum of electronic and thermal Free Energies= -2548.068911

Cartesian Coordinates

8	0.485598	1.729260	3.107682
6	1.535957	1.948611	2.402805
6	2.841980	2.045456	3.148781
1	3.210094	3.077395	3.114320

1	2.749895	1.734494	4.192674
1	3.589464	1.422576	2.638373
8	1.530925	2.083921	1.165739
47	2.341842	0.324291	-0.313437
46	-0.016290	-0.875251	1.018754
8	5.653400	0.222203	1.156436
6	5.609553	1.011897	0.101894
8	4.654650	1.078246	-0.665007
6	6.854871	1.816065	-0.073912
1	7.073891	2.371434	0.843766
1	6.751093	2.506974	-0.911696
1	7.701307	1.144684	-0.254476
1	-0.380917	1.129954	2.498175
6	-1.503517	0.281064	2.332271
6	-1.682686	-0.355613	3.583427
1	-0.792334	-0.495966	4.198169
6	-2.908785	-0.795794	4.090949
1	-2.958418	-1.285141	5.060972
6	-4.062889	-0.578292	3.350826
1	-5.044610	-0.886975	3.705631
6	-3.943032	0.052780	2.117077
6	-2.691244	0.447644	1.611629
6	-4.215426	1.016993	-0.038356
6	-1.067432	0.437669	-1.201647
6	-1.900891	1.373781	-0.674896
7	-2.870449	0.999795	0.301766
6	-4.969813	0.362412	1.140430
8	-6.168370	0.175151	1.154433
8	-4.700978	1.426867	-1.067834
6	-1.159300	-0.991013	-0.780968
6	-1.936072	2.799971	-1.050678
6	-1.993760	3.765846	-0.038346
6	-1.931998	3.217074	-2.386891
6	-2.010820	5.119629	-0.354425
1	-2.011167	3.448219	1.004151
6	-1.953234	4.570626	-2.699986
1	-1.928242	2.472406	-3.181369
6	-1.987245	5.526333	-1.686070
1	-2.043530	5.859638	0.442324
1	-1.956018	4.881509	-3.742489
1	-2.004939	6.585149	-1.934617
6	0.022739	0.769511	-2.152689
6	0.965128	1.779344	-1.883812
6	0.134706	0.042140	-3.343178
6	1.999036	2.035265	-2.790035
1	0.852797	2.389576	-0.988940
6	1.159261	0.308803	-4.244704
1	-0.601886	-0.729181	-3.564923
6	2.100316	1.298113	-3.967522
1	2.718340	2.821100	-2.570102
1	1.221590	-0.258464	-5.170675
1	2.903441	1.501709	-4.671733
6	-0.002382	-1.792700	-0.701885
6	-2.479459	-1.694950	-0.775300
6	-3.385857	-1.465211	-1.816370
6	-2.820341	-2.600038	0.235941
6	-4.619731	-2.105453	-1.827330
1	-3.127317	-0.761875	-2.607598
6	-4.053616	-3.243957	0.219094
1	-2.121587	-2.764895	1.057230
6	-4.959095	-2.992752	-0.807852
1	-5.322256	-1.905686	-2.633458
1	-4.312400	-3.931458	1.021571
1	-5.929006	-3.484842	-0.813728
6	0.626117	-2.855112	-1.377904
6	1.816963	-3.405166	-0.845053
6	0.094895	-3.376985	-2.584092
6	2.456601	-4.439384	-1.502254
1	2.221700	-2.979499	0.072572
6	0.732213	-4.423529	-3.220466

1	-0.826896	-2.960751	-2.985387
6	1.911707	-4.948385	-2.683127
1	3.376170	-4.857550	-1.102272
1	0.322796	-4.835880	-4.138583
1	2.413505	-5.766511	-3.194788
8	1.516151	-1.243077	2.585439
6	2.759199	-1.265140	2.429213
8	3.365784	-1.031544	1.334873
6	3.616654	-1.614503	3.619296
1	3.041170	-1.591524	4.547310
1	4.028325	-2.621179	3.481128
1	4.466511	-0.926762	3.693387
1	4.802442	-0.307949	1.234183

4CH12_Pd-Ag

Number of imaginary frequencies : 1
The smallest frequency is : -887.0301 cm(-1)

Electronic energy : HF=-2548.6361996
Zero-point correction= 0.654926
Thermal correction to Energy= 0.705271
Thermal correction to Enthalpy= 0.706215
Thermal correction to Gibbs Free Energy= 0.568626
Sum of electronic and zero-point Energies= -2547.981274
Sum of electronic and thermal Energies= -2547.930929
Sum of electronic and thermal Enthalpies= -2547.929984
Sum of electronic and thermal Free Energies= -2548.067573

Cartesian Coordinates

8	0.443810	1.644396	3.161716
6	1.497161	1.883308	2.467987
6	2.797647	1.975530	3.223971
1	3.151727	3.012976	3.220988
1	2.703201	1.634682	4.258292
1	3.556522	1.377302	2.700930
8	1.498919	2.040967	1.233456
47	2.317688	0.323734	-0.285957
46	-0.015117	-0.914557	1.010297
8	5.626214	0.235263	1.186732
6	5.576940	1.031717	0.137792
8	4.621467	1.097401	-0.628629
6	6.817242	1.844594	-0.033384
1	7.035041	2.393102	0.888711
1	6.707991	2.542241	-0.864859
1	7.667051	1.179517	-0.221410
1	-0.414496	1.052411	2.532011
6	-1.524093	0.193956	2.332713
6	-1.705870	-0.498899	3.553158
1	-0.818212	-0.659726	4.166751
6	-2.932126	-0.969912	4.032652
1	-2.984091	-1.502494	4.979484
6	-4.083666	-0.722136	3.298664
1	-5.066245	-1.044719	3.638404
6	-3.960357	-0.040201	2.091976
6	-2.707976	0.380153	1.610139
6	-4.230185	1.040020	-0.007659
6	-1.075896	0.471531	-1.189590
6	-1.913676	1.389375	-0.639616
7	-2.883839	0.993291	0.326865
6	-4.987475	0.337355	1.140694
8	-6.188746	0.166526	1.151360
8	-4.714684	1.496704	-1.017864
6	-1.142372	-0.967730	-0.799299
6	-1.953189	2.823329	-0.986694
6	-1.989418	3.770039	0.044171
6	-1.973078	3.264076	-2.314691

6	-2.007476	5.129410	-0.247389
1	-1.988188	3.432835	1.080658
6	-1.995267	4.623046	-2.603357
1	-1.988220	2.533247	-3.121852
6	-2.006662	5.560149	-1.571677
1	-2.022644	5.855112	0.562931
1	-2.016099	4.952760	-3.639842
1	-2.024803	6.623401	-1.800565
6	0.011771	0.841537	-2.130536
6	0.947406	1.846919	-1.824616
6	0.132393	0.157954	-3.346086
6	1.981399	2.142708	-2.718064
1	0.830269	2.421729	-0.907373
6	1.158490	0.462253	-4.233781
1	-0.596260	-0.610104	-3.601930
6	2.091656	1.448147	-3.920063
1	2.693764	2.925831	-2.468486
1	1.227847	-0.072828	-5.178293
1	2.895536	1.681631	-4.614088
6	0.037384	-1.744409	-0.752156
6	-2.441416	-1.708955	-0.814307
6	-3.409848	-1.396339	-1.774866
6	-2.695813	-2.748545	0.089224
6	-4.614917	-2.089697	-1.811439
1	-3.226306	-0.587387	-2.480716
6	-3.894901	-3.451260	0.039389
1	-1.954215	-2.981496	0.854454
6	-4.861232	-3.119892	-0.907103
1	-5.365452	-1.821744	-2.551924
1	-4.078926	-4.251719	0.752652
1	-5.805240	-3.659187	-0.937197
6	0.686330	-2.762100	-1.475473
6	1.896401	-3.302272	-0.976189
6	0.154038	-3.250920	-2.695141
6	2.554551	-4.293038	-1.680593
1	2.299086	-2.903201	-0.045355
6	0.810106	-4.254968	-3.378610
1	-0.783456	-2.844765	-3.069379
6	2.009351	-4.768991	-2.875112
1	3.488527	-4.703224	-1.306586
1	0.400409	-4.642658	-4.307263
1	2.525171	-5.554285	-3.422950
8	1.504390	-1.314200	2.584169
6	2.748627	-1.313763	2.433621
8	3.355968	-1.050125	1.346842
6	3.605142	-1.675553	3.620759
1	3.028483	-1.663145	4.548295
1	4.015400	-2.681403	3.472304
1	4.455888	-0.990051	3.703556
1	4.780435	-0.304169	1.259130

4CH13_Pd-Ag

Number of imaginary frequencies : 1

The smallest frequency is : -924.5646 cm(-1)

Electronic energy :	HF=-2548.6361248
Zero-point correction=	0.655515
Thermal correction to Energy=	0.705809
Thermal correction to Enthalpy=	0.706753
Thermal correction to Gibbs Free Energy=	0.568893
Sum of electronic and zero-point Energies=	-2547.980610
Sum of electronic and thermal Energies=	-2547.930316
Sum of electronic and thermal Enthalpies=	-2547.929372
Sum of electronic and thermal Free Energies=	-2548.067232

Cartesian Coordinates

8	0.454519	1.723750	3.109571
6	1.492740	1.954577	2.391545
6	2.806985	2.066579	3.121182
1	3.174169	3.097847	3.064546
1	2.727135	1.772861	4.171095
1	3.549680	1.435570	2.614017
8	1.470240	2.086939	1.153799
47	2.330648	0.321487	-0.301124
46	-0.029496	-0.883756	1.027883
8	5.640885	0.223580	1.186973
6	5.599299	1.013638	0.132622
8	4.645113	1.081687	-0.635060
6	6.845842	1.816201	-0.041778
1	6.743930	2.507183	-0.879740
1	7.691680	1.143790	-0.221266
1	7.064407	2.371407	0.876111
1	-0.412751	1.113389	2.500314
6	-1.527557	0.268947	2.325383
6	-1.724943	-0.381519	3.566268
1	-0.841421	-0.545533	4.185145
6	-2.962136	-0.806326	4.060048
1	-3.026991	-1.308301	5.022664
6	-4.108068	-0.550579	3.319667
1	-5.098301	-0.837034	3.669240
6	-3.969010	0.091816	2.093294
6	-2.706350	0.463177	1.597300
6	-4.211438	1.109931	-0.040501
6	-1.071298	0.427045	-1.205315
6	-1.887479	1.379760	-0.683743
7	-2.866337	1.039665	0.295406
6	-4.986613	0.466133	1.130422
8	-6.191724	0.325519	1.144701
8	-4.684821	1.544269	-1.065676
6	-1.168366	-0.998484	-0.772116
6	-1.888714	2.804057	-1.072465
6	-1.855629	3.777315	-0.066982
6	-1.936177	3.208174	-2.410995
6	-1.837566	5.128318	-0.394361
1	-1.821063	3.462640	0.976140
6	-1.921588	4.559381	-2.735579
1	-2.000411	2.455530	-3.195739
6	-1.867693	5.522758	-1.729867
1	-1.798231	5.875594	0.395271
1	-1.963887	4.863019	-3.779366
1	-1.858044	6.579583	-1.987275
6	0.019609	0.743586	-2.162120
6	0.972062	1.746572	-1.901101
6	0.126147	0.006456	-3.346968
6	2.010335	1.983738	-2.807512
1	0.865071	2.366784	-1.012306
6	1.155340	0.254152	-4.248657
1	-0.616287	-0.759981	-3.565676
6	2.106676	1.235283	-3.978185
1	2.736482	2.764826	-2.593362
1	1.212908	-0.322220	-5.169297
1	2.913152	1.424307	-4.682606
6	-0.003650	-1.793280	-0.695376
6	-2.481075	-1.713221	-0.760038
6	-2.743327	-2.731781	0.165166
6	-3.452039	-1.404543	-1.719057
6	-3.952186	-3.418760	0.136455
1	-1.997890	-2.963494	0.926917
6	-4.666970	-2.081396	-1.734070
1	-3.262307	-0.612763	-2.442581
6	-4.920785	-3.091345	-0.809234
1	-4.141727	-4.203648	0.865405
1	-5.419022	-1.816728	-2.474184
1	-5.872058	-3.618378	-0.823027
6	0.632353	-2.848890	-1.374548
6	1.834995	-3.381024	-0.849641

6	0.097571	-3.383494	-2.573854
6	2.483243	-4.409035	-1.508228
1	2.241638	-2.946652	0.063207
6	0.743484	-4.424225	-3.210935
1	-0.833520	-2.982428	-2.969067
6	1.935060	-4.930420	-2.682033
1	3.411856	-4.812914	-1.114511
1	0.331479	-4.846558	-4.123338
1	2.443235	-5.743994	-3.194662
8	1.494906	-1.243311	2.604417
6	2.738646	-1.256524	2.453417
8	3.347959	-1.021756	1.360672
6	3.594319	-1.595466	3.647661
1	3.014339	-1.578905	4.572986
1	4.018796	-2.597111	3.511667
1	4.435374	-0.897380	3.725579
1	4.788362	-0.304166	1.263912

MonoMetallic C-H activation

4CHI_Pd

Number of imaginary frequencies : 1
The smallest frequency is : -876.6078 cm(-1)

Electronic energy : HF=-1945.4219986
Zero-point correction= 0.539180
Thermal correction to Energy= 0.576557
Thermal correction to Enthalpy= 0.577501
Thermal correction to Gibbs Free Energy= 0.468611
Sum of electronic and zero-point Energies= -1944.882819
Sum of electronic and thermal Energies= -1944.845442
Sum of electronic and thermal Enthalpies= -1944.844498
Sum of electronic and thermal Free Energies= -1944.953387

Cartesian Coordinates

46	0.835299	0.088066	1.425065
8	1.113443	1.422589	3.163402
6	0.065025	2.002259	3.530631
8	-1.103929	1.748180	3.067700
6	0.139843	3.069413	4.579007
1	-0.505279	2.803026	5.422555
1	-0.240511	4.010302	4.167082
1	1.164705	3.210414	4.926787
1	-1.084326	0.698892	2.463354
6	-1.183024	-0.677009	2.077133
6	-1.222388	-1.474443	3.240655
1	-0.732308	-1.084336	4.135994
6	-1.851192	-2.719599	3.324700
1	-1.832057	-3.281790	4.255131
6	-2.505552	-3.227146	2.208219
1	-3.013043	-4.189732	2.226803
6	-2.503707	-2.469685	1.042254
6	-1.845180	-1.229343	0.978472
6	-2.699925	-1.548580	-1.145472
6	-0.051838	0.660572	-0.945982
6	-1.404382	0.508336	-0.861452
7	-1.952813	-0.700457	-0.343509
6	-3.067587	-2.765966	-0.263115
8	-3.685943	-3.728156	-0.665769
8	-2.988701	-1.383289	-2.308104
6	0.876967	-0.466285	-0.643816
6	-2.405345	1.521556	-1.242729
6	-2.300596	2.255433	-2.431287
6	-3.506113	1.745315	-0.405483
6	-3.259923	3.205156	-2.758924
1	-1.468273	2.065724	-3.106684

6	-4.461613	2.700605	-0.732987
1	-3.603030	1.172498	0.516380
6	-4.340894	3.435240	-1.909816
1	-3.169827	3.761601	-3.689407
1	-5.303772	2.871677	-0.065967
1	-5.090857	4.179122	-2.169182
6	0.578031	1.973046	-1.243164
6	0.282014	3.102599	-0.471561
6	1.509669	2.082519	-2.280517
6	0.897107	4.319418	-0.742101
1	-0.429480	3.015129	0.349468
6	2.119918	3.302684	-2.553443
1	1.745582	1.205807	-2.883938
6	1.815174	4.423288	-1.785108
1	0.662660	5.189343	-0.132394
1	2.835418	3.378180	-3.369296
1	2.296332	5.376018	-1.994924
6	2.112236	-0.207963	-0.029168
6	0.603466	-1.841802	-1.152691
6	0.720230	-2.956538	-0.315718
6	0.262047	-2.031454	-2.496665
6	0.483367	-4.235898	-0.808343
1	0.972014	-2.807641	0.734996
6	0.036398	-3.312159	-2.988678
1	0.166696	-1.168962	-3.155566
6	0.142077	-4.417093	-2.145958
1	0.560903	-5.092280	-0.142055
1	-0.231314	-3.447014	-4.034375
1	-0.044769	-5.416721	-2.531821
6	3.477173	-0.460742	-0.295555
6	4.423688	-0.348018	0.746739
6	3.916231	-0.792406	-1.599160
6	5.764644	-0.575312	0.497034
1	4.072906	-0.078090	1.741247
6	5.258870	-1.017237	-1.839152
1	3.185689	-0.875652	-2.401395
6	6.179415	-0.909975	-0.793454
1	6.493791	-0.490706	1.298250
1	5.598530	-1.276680	-2.838361
1	7.234583	-1.087268	-0.989019

4CH2_Pd

Number of imaginary frequencies : 1
The smallest frequency is : -876.2901 cm(-1)

Electronic energy : HF=-1945.4219986
Zero-point correction= 0.539182
Thermal correction to Energy= 0.576558
Thermal correction to Enthalpy= 0.577502
Thermal correction to Gibbs Free Energy= 0.468622
Sum of electronic and zero-point Energies= -1944.882817
Sum of electronic and thermal Energies= -1944.845441
Sum of electronic and thermal Enthalpies= -1944.844497
Sum of electronic and thermal Free Energies= -1944.953377

Cartesian Coordinates

46	0.835285	0.088224	1.424856
8	1.113924	1.422860	3.163028
6	0.065611	2.002696	3.530299
8	-1.103439	1.748610	3.067607
6	0.140684	3.070032	4.578470
1	-0.504444	2.803917	5.422098
1	-0.239501	4.010917	4.166387
1	1.165587	3.210897	4.926192
1	-1.084003	0.699251	2.463405

6	-1.182891	-0.676689	2.077279
6	-1.222232	-1.474081	3.240830
1	-0.731965	-1.084032	4.136092
6	-1.851235	-2.719127	3.324984
1	-1.832066	-3.281302	4.255424
6	-2.505829	-3.226593	2.208602
1	-3.013490	-4.189088	2.227286
6	-2.504004	-2.469169	1.042615
6	-1.845256	-1.228950	0.978707
6	-2.700154	-1.548193	-1.145172
6	-0.051694	0.660526	-0.945987
6	-1.404280	0.508536	-0.861373
7	-1.952910	-0.700108	-0.343285
6	-3.068090	-2.765397	-0.262679
8	-3.686865	-3.727391	-0.665158
8	-2.988870	-1.382980	-2.307831
6	0.876931	-0.466535	-0.643937
6	-2.405161	1.521829	-1.242699
6	-2.300417	2.255562	-2.431342
6	-3.505842	1.745818	-0.405398
6	-3.259623	3.205399	-2.759000
1	-1.468206	2.065612	-3.106791
6	-4.461226	2.701220	-0.732919
1	-3.602791	1.173087	0.516515
6	-4.340485	3.435736	-1.909821
1	-3.169527	3.761724	-3.689554
1	-5.303311	2.872473	-0.065853
1	-5.090349	4.179715	-2.169191
6	0.578496	1.972838	-1.243245
6	0.282668	3.102613	-0.471887
6	1.510309	2.081907	-2.280491
6	0.898035	4.319249	-0.742625
1	-0.428781	3.015454	0.349210
6	2.120828	3.301893	-2.553619
1	1.746193	1.205024	-2.883677
6	1.816209	4.422730	-1.785578
1	0.663734	5.189335	-0.133091
1	2.836449	3.377059	-3.369396
1	2.297576	5.375320	-1.995547
6	2.112226	-0.208397	-0.029293
6	0.603000	-1.842012	-1.152667
6	0.719239	-2.956681	-0.315538
6	0.261520	-2.031680	-2.496620
6	0.481756	-4.235995	-0.807987
1	0.971113	-2.807759	0.735150
6	0.035334	-3.312349	-2.988476
1	0.166540	-1.169216	-3.155616
6	0.140448	-4.417214	-2.145596
1	0.558813	-5.092315	-0.141564
1	-0.232403	-3.447223	-4.034165
1	-0.046871	-5.416807	-2.531320
6	3.477123	-0.461481	-0.295624
6	4.423665	-0.348602	0.746626
6	3.916108	-0.793657	-1.599120
6	5.764581	-0.576209	0.496984
1	4.072942	-0.078284	1.741050
6	5.258703	-1.018843	-1.839040
1	3.185549	-0.877002	-2.401331
6	6.179280	-0.911395	-0.793389
1	6.493751	-0.491455	1.298163
1	5.598304	-1.278701	-2.838162
1	7.234412	-1.088957	-0.988904

4CH3_Pd

Number of imaginary frequencies : 1

The smallest frequency is : -876.6919 cm(-1)

Electronic energy : HF=-1945.4219991
 Zero-point correction= 0.539185
 Thermal correction to Energy= 0.576561
 Thermal correction to Enthalpy= 0.577505
 Thermal correction to Gibbs Free Energy= 0.468626
 Sum of electronic and zero-point Energies= -1944.882814
 Sum of electronic and thermal Energies= -1944.845438
 Sum of electronic and thermal Enthalpies= -1944.844494
 Sum of electronic and thermal Free Energies= -1944.953373

 Cartesian Coordinates

46	0.835216	0.088320	1.425073
8	1.113025	1.423187	3.163172
6	0.064467	2.002674	3.530301
8	-1.104430	1.748222	3.067438
6	0.139099	3.070131	4.578377
1	1.163814	3.210865	4.926715
1	-0.506684	2.804384	5.421609
1	-0.240552	4.011016	4.165794
1	-1.084557	0.698842	2.463241
6	-1.182954	-0.677104	2.077161
6	-1.222217	-1.474472	3.240732
1	-0.732216	-1.084236	4.136058
6	-1.850837	-2.719717	3.324835
1	-1.831634	-3.281851	4.255299
6	-2.505102	-3.227429	2.208372
1	-3.012448	-4.190090	2.227011
6	-2.503349	-2.470039	1.042360
6	-1.845004	-1.229603	0.978521
6	-2.699645	-1.549086	-1.145424
6	-0.051912	0.660505	-0.946013
6	-1.404432	0.508049	-0.861478
7	-1.952678	-0.700809	-0.343490
6	-3.067154	-2.766477	-0.263007
8	-3.685341	-3.728788	-0.665630
8	-2.988407	-1.383907	-2.308076
6	0.877072	-0.466187	-0.643774
6	-2.405564	1.521095	-1.242787
6	-2.301048	2.254793	-2.431466
6	-3.506228	1.744878	-0.405412
6	-3.260497	3.204391	-2.759110
1	-1.468852	2.064966	-3.106971
6	-4.461853	2.700041	-0.732919
1	-3.602947	1.172179	0.516548
6	-4.341357	3.434517	-1.909873
1	-3.170589	3.760697	-3.689694
1	-5.303931	2.871144	-0.065805
1	-5.091417	4.178300	-2.169239
6	0.577751	1.973051	-1.243314
6	0.281559	3.102670	-0.471870
6	1.509439	2.082513	-2.280627
6	0.896503	4.319534	-0.742550
1	-0.429922	3.015232	0.349174
6	2.119530	3.302725	-2.553697
1	1.745579	1.205753	-2.883891
6	1.814595	4.423395	-1.785539
1	0.661928	5.189504	-0.132957
1	2.835068	3.378199	-3.369518
1	2.295632	5.376162	-1.995460
6	2.112264	-0.207633	-0.029079
6	0.603814	-1.841763	-1.152611
6	0.720724	-2.956458	-0.315605
6	0.262513	-2.031503	-2.496603
6	0.484122	-4.235871	-0.808219
1	0.972427	-2.807495	0.735119
6	0.037104	-3.312256	-2.988599
1	0.167072	-1.169040	-3.155531
6	0.142931	-4.417153	-2.145848
1	0.561778	-5.092225	-0.141911

1	-0.230519	-3.447184	-4.034309
1	-0.043713	-5.416821	-2.531703
6	3.477250	-0.460313	-0.295333
6	4.423662	-0.347365	0.747029
6	3.916456	-0.792083	-1.598859
6	5.764662	-0.574560	0.497473
1	4.072765	-0.077340	1.741471
6	5.259140	-1.016815	-1.838703
1	3.185995	-0.875489	-2.401151
6	6.179581	-0.909340	-0.792936
1	6.493731	-0.489784	1.298743
1	5.598913	-1.276344	-2.837851
1	7.234784	-1.086555	-0.988386

4CH4_Pd

Number of imaginary frequencies : 1
The smallest frequency is : -117.1717 cm(-1)

Electronic energy : HF=-1945.4276799
Zero-point correction= 0.543542
Thermal correction to Energy= 0.580790
Thermal correction to Enthalpy= 0.581734
Thermal correction to Gibbs Free Energy= 0.472431
Sum of electronic and zero-point Energies= -1944.884138
Sum of electronic and thermal Energies= -1944.846890
Sum of electronic and thermal Enthalpies= -1944.845946
Sum of electronic and thermal Free Energies= -1944.955249

Cartesian Coordinates

46	0.833590	0.182287	1.402175
8	1.019981	1.441286	3.246800
6	0.013369	1.928521	3.767775
8	-1.208519	1.630423	3.386883
6	0.103394	2.896273	4.894022
1	0.781818	3.709329	4.620621
1	0.539917	2.384221	5.758348
1	-0.873835	3.297199	5.166352
1	-1.149238	0.894760	2.714283
6	-0.861178	-0.948307	1.963095
6	-0.917128	-1.702623	3.151693
1	-0.306024	-1.380265	3.998398
6	-1.694792	-2.855138	3.312849
1	-1.680309	-3.393307	4.257887
6	-2.465789	-3.315565	2.252509
1	-3.067468	-4.219219	2.326606
6	-2.456589	-2.584073	1.070167
6	-1.683378	-1.416201	0.940164
6	-2.714162	-1.671902	-1.113946
6	-0.076500	0.676447	-0.946389
6	-1.405426	0.377654	-0.885986
7	-1.859873	-0.868749	-0.374172
6	-3.127720	-2.841691	-0.191419
8	-3.858443	-3.746074	-0.537464
8	-3.065592	-1.499785	-2.258968
6	0.973984	-0.342060	-0.661203
6	-2.486182	1.309311	-1.268191
6	-2.462982	2.004290	-2.482874
6	-3.569085	1.499424	-0.400579
6	-3.485248	2.886497	-2.809481
1	-1.640843	1.838882	-3.177490
6	-4.588815	2.386590	-0.727032
1	-3.600336	0.954926	0.543648
6	-4.549227	3.084768	-1.931458
1	-3.456975	3.415580	-3.759659
1	-5.416555	2.534303	-0.036725
1	-5.349206	3.775249	-2.189203

6	0.401105	2.052599	-1.243143
6	0.006306	3.142476	-0.459890
6	1.285725	2.265889	-2.305819
6	0.475302	4.420293	-0.743454
1	-0.672014	2.979577	0.378306
6	1.746518	3.546168	-2.594590
1	1.596716	1.421603	-2.921311
6	1.343565	4.626448	-1.813610
1	0.164928	5.258989	-0.123928
1	2.423012	3.700104	-3.432414
1	1.707304	5.627101	-2.036157
6	2.186955	0.058148	-0.062865
6	0.817631	-1.728173	-1.190840
6	1.081916	-2.845407	-0.393230
6	0.433771	-1.919734	-2.523429
6	0.949753	-4.129673	-0.911601
1	1.363826	-2.697671	0.649659
6	0.308301	-3.203799	-3.041369
1	0.215696	-1.053378	-3.148228
6	0.561737	-4.312456	-2.236259
1	1.145406	-4.990363	-0.275732
1	0.004559	-3.339646	-4.077201
1	0.453097	-5.316309	-2.640868
6	3.548420	-0.238553	-0.349102
6	4.521461	-0.053244	0.656101
6	3.961293	-0.670165	-1.630395
6	5.856990	-0.309595	0.397621
1	4.195619	0.294108	1.635313
6	5.299626	-0.911547	-1.886008
1	3.213192	-0.817774	-2.407310
6	6.245314	-0.735664	-0.873192
1	6.601927	-0.172849	1.177276
1	5.615482	-1.242396	-2.872278
1	7.295451	-0.930853	-1.078887

4CH5_Pd

Number of imaginary frequencies : 1
The smallest frequency is : -878.4995 cm(-1)

Electronic energy : HF=-1945.421998
Zero-point correction= 0.539180
Thermal correction to Energy= 0.576557
Thermal correction to Enthalpy= 0.577501
Thermal correction to Gibbs Free Energy= 0.468620
Sum of electronic and zero-point Energies= -1944.882818
Sum of electronic and thermal Energies= -1944.845441
Sum of electronic and thermal Enthalpies= -1944.844497
Sum of electronic and thermal Free Energies= -1944.953378

Cartesian Coordinates

46	0.835356	0.088015	1.424942
8	1.113665	1.422352	3.163362
6	0.065188	2.001703	3.530983
8	-1.103809	1.747453	3.068325
6	0.140103	3.068643	4.579583
1	-0.504738	2.801942	5.423244
1	-0.240527	4.009552	4.167968
1	1.165030	3.209788	4.927127
1	-1.084182	0.698162	2.463583
6	-1.182839	-0.677453	2.077155
6	-1.221986	-1.475130	3.240515
1	-0.731868	-1.085142	4.135884
6	-1.850630	-2.720378	3.324353
1	-1.831338	-3.282761	4.254665
6	-2.505058	-3.227760	2.207835
1	-3.012434	-4.190410	2.226266

6	-2.503426	-2.470051	1.042032
6	-1.845049	-1.229619	0.978442
6	-2.700057	-1.548459	-1.145453
6	-0.051925	0.660676	-0.945811
6	-1.404462	0.508390	-0.861192
7	-1.952887	-0.700460	-0.343406
6	-3.067457	-2.766093	-0.263326
8	-3.685748	-3.728266	-0.666120
8	-2.989014	-1.382921	-2.308004
6	0.876975	-0.466202	-0.643999
6	-2.405385	1.521709	-1.242302
6	-2.300746	2.255410	-2.430972
6	-3.505935	1.745741	-0.404856
6	-3.259946	3.205288	-2.758519
1	-1.468576	2.065420	-3.106475
6	-4.461326	2.701172	-0.732278
1	-3.602794	1.173001	0.517063
6	-4.340699	3.435663	-1.909210
1	-3.169938	3.761619	-3.689078
1	-5.303339	2.872456	-0.065129
1	-5.090574	4.179658	-2.168505
6	0.577788	1.973232	-1.242962
6	1.509214	2.082895	-2.280484
6	0.281863	3.102676	-0.471158
6	2.119265	3.303155	-2.553438
1	1.745155	1.206279	-2.884032
6	0.896766	4.319584	-0.741719
1	-0.429415	3.015051	0.350041
6	1.814573	4.423658	-1.784939
1	2.834585	3.378792	-3.369435
1	0.662384	5.189421	-0.131862
1	2.295569	5.376462	-1.994785
6	2.112239	-0.207963	-0.029355
6	0.603428	-1.841654	-1.153017
6	0.720091	-2.956457	-0.316121
6	0.261965	-2.031165	-2.497000
6	0.483090	-4.235758	-0.808831
1	0.971870	-2.807647	0.734608
6	0.036166	-3.311814	-2.989093
1	0.166622	-1.168603	-3.155812
6	0.141753	-4.416819	-2.146453
1	0.560525	-5.092193	-0.142602
1	-0.231585	-3.446570	-4.034793
1	-0.045217	-5.416398	-2.532382
6	3.477192	-0.460621	-0.295769
6	4.423663	-0.348278	0.746606
6	3.916298	-0.791849	-1.599466
6	5.764621	-0.575524	0.496883
1	4.072850	-0.078706	1.741200
6	5.258946	-1.016615	-1.839481
1	3.185780	-0.874828	-2.401751
6	6.179446	-0.909739	-0.793706
1	6.493733	-0.491226	1.298163
1	5.598636	-1.275721	-2.838767
1	7.234619	-1.086987	-0.989285

4CH6_Pd

Number of imaginary frequencies : 1
The smallest frequency is : -876.6530 cm(-1)

Electronic energy :	HF=-1945.4219994
Zero-point correction=	0.539188
Thermal correction to Energy=	0.576562
Thermal correction to Enthalpy=	0.577507
Thermal correction to Gibbs Free Energy=	0.468646
Sum of electronic and zero-point Energies=	-1944.882811
Sum of electronic and thermal Energies=	-1944.845437

Sum of electronic and thermal Enthalpies= -1944.844493
 Sum of electronic and thermal Free Energies= -1944.953354

.....
 Cartesian Coordinates

46	0.834957	0.088151	1.425144
8	1.112892	1.422977	3.163263
6	0.064436	2.002791	3.530161
8	-1.104446	1.748667	3.067065
6	0.139166	3.070215	4.578267
1	1.163897	3.210808	4.926609
1	-0.506619	2.804460	5.421500
1	-0.240419	4.011165	4.165773
1	-1.084767	0.699209	2.463020
6	-1.183455	-0.676778	2.077074
6	-1.223113	-1.474010	3.240724
1	-0.733197	-1.083788	4.136103
6	-1.852017	-2.719112	3.324839
1	-1.833126	-3.281143	4.255373
6	-2.506150	-3.226822	2.208299
1	-3.013692	-4.189381	2.226942
6	-2.504001	-2.469569	1.042199
6	-1.845410	-1.229263	0.978371
6	-2.699761	-1.548747	-1.145691
6	-0.051669	0.660378	-0.946091
6	-1.404221	0.508171	-0.861686
7	-1.952739	-0.700569	-0.343708
6	-3.067616	-2.766018	-0.263249
8	-3.685849	-3.728278	-0.665923
8	-2.988335	-1.383581	-2.308392
6	0.877080	-0.466465	-0.643673
6	-2.405130	1.521428	-1.243029
6	-2.300597	2.254893	-2.431844
6	-3.505558	1.745691	-0.405474
6	-3.259812	3.204740	-2.759463
1	-1.468591	2.064683	-3.107477
6	-4.460948	2.701096	-0.732962
1	-3.602241	1.173195	0.516618
6	-4.340440	3.435339	-1.910061
1	-3.169902	3.760873	-3.690150
1	-5.302845	2.872578	-0.065716
1	-5.090313	4.179319	-2.169406
6	0.578275	1.972779	-1.243444
6	1.510118	2.081963	-2.280649
6	0.282208	3.102532	-0.472147
6	2.120472	3.302034	-2.553764
1	1.746202	1.205100	-2.883784
6	0.897423	4.319250	-0.742865
1	-0.429388	3.015317	0.348820
6	1.815659	4.422838	-1.785753
1	2.836131	3.377288	-3.369500
1	0.662944	5.189321	-0.133378
1	2.296908	5.375491	-1.995706
6	2.112200	-0.208075	-0.028775
6	0.603684	-1.842011	-1.152513
6	0.720270	-2.956698	-0.315452
6	0.262574	-2.031737	-2.496556
6	0.483567	-4.236091	-0.808073
1	0.971795	-2.807743	0.735315
6	0.037039	-3.312469	-2.988549
1	0.167377	-1.169280	-3.155526
6	0.142568	-4.417358	-2.145753
1	0.560991	-5.092439	-0.141730
1	-0.230435	-3.447387	-4.034299
1	-0.044155	-5.417009	-2.531614
6	3.477204	-0.460797	-0.294874
6	4.423510	-0.347949	0.747594
6	3.916530	-0.792495	-1.598379
6	5.764528	-0.575169	0.498157
1	4.072521	-0.077975	1.742017

6	5.259229	-1.017260	-1.838102
1	3.186138	-0.875808	-2.400746
6	6.179565	-0.909881	-0.792233
1	6.493520	-0.490469	1.299503
1	5.599098	-1.276735	-2.837232
1	7.234782	-1.087119	-0.987585

4CH7_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -128.7707 cm(-1)

Electronic energy : HF=-1945.4276671
 Zero-point correction= 0.543454
 Thermal correction to Energy= 0.580746
 Thermal correction to Enthalpy= 0.581690
 Thermal correction to Gibbs Free Energy= 0.471961
 Sum of electronic and zero-point Energies= -1944.884213
 Sum of electronic and thermal Energies= -1944.846921
 Sum of electronic and thermal Enthalpies= -1944.845977
 Sum of electronic and thermal Free Energies= -1944.955706

 Cartesian Coordinates

46	0.816709	0.165902	1.419566
8	1.015827	1.422323	3.266289
6	0.015427	1.934699	3.774807
8	-1.208287	1.675717	3.371723
6	0.115330	2.893422	4.908034
1	-0.856519	3.308755	5.177995
1	0.807280	3.697655	4.642162
1	0.540423	2.370044	5.771118
1	-1.160472	0.940047	2.698073
6	-0.915110	-0.918693	1.963066
6	-1.005700	-1.664775	3.154793
1	-0.400401	-1.351516	4.009048
6	-1.809926	-2.799728	3.310369
1	-1.821456	-3.332509	4.258507
6	-2.573189	-3.250650	2.240500
1	-3.194026	-4.141671	2.309664
6	-2.530862	-2.526165	1.054631
6	-1.732757	-1.374289	0.930943
6	-2.738232	-1.619919	-1.137083
6	-0.055967	0.673414	-0.942295
6	-1.391852	0.404323	-0.900230
7	-1.879176	-0.829860	-0.388782
6	-3.186808	-2.777656	-0.215898
8	-3.927632	-3.670981	-0.569277
8	-3.069733	-1.446964	-2.287942
6	0.966542	-0.366705	-0.638618
6	-2.447073	1.355474	-1.304824
6	-2.392833	2.039665	-2.524584
6	-3.537815	1.573516	-0.453994
6	-3.393701	2.938213	-2.872684
1	-1.564759	1.851757	-3.206401
6	-4.536059	2.476741	-0.802010
1	-3.591337	1.037927	0.494330
6	-4.466153	3.163470	-2.011719
1	-3.342239	3.458506	-3.826777
1	-5.370722	2.646077	-0.125117
1	-5.249212	3.866521	-2.286897
6	0.464790	2.034140	-1.235391
6	1.396633	2.210062	-2.264373
6	0.075155	3.142097	-0.475196
6	1.910236	3.472152	-2.543142
1	1.709159	1.348767	-2.855801
6	0.596921	4.401543	-0.748767
1	-0.635856	3.006767	0.340596

6	1.512645	4.570843	-1.785341
1	2.625318	3.597269	-3.353289
1	0.292144	5.254481	-0.146123
1	1.919347	5.556978	-1.998251
6	2.182403	0.010990	-0.030818
6	0.791703	-1.750470	-1.167692
6	1.030564	-2.870162	-0.365352
6	0.418561	-1.938956	-2.503697
6	0.884150	-4.153317	-0.882449
1	1.303274	-2.724284	0.680238
6	0.279821	-3.222057	-3.020657
1	0.218970	-1.070798	-3.132156
6	0.507919	-4.332865	-2.210884
1	1.059664	-5.015467	-0.242729
1	-0.015069	-3.355401	-4.059363
1	0.388740	-5.335763	-2.614902
6	3.538252	-0.300926	-0.323636
6	4.516850	-0.165650	0.683940
6	3.939107	-0.696240	-1.620534
6	5.845976	-0.441719	0.412902
1	4.200914	0.156712	1.674863
6	5.271617	-0.955174	-1.888590
1	3.184973	-0.796768	-2.399583
6	6.222415	-0.833875	-0.872524
1	6.595701	-0.345045	1.193976
1	5.578590	-1.257145	-2.886826
1	7.267889	-1.043790	-1.087283

Conformational and Configurational Study of Reductive Elimination

Bimetallic Reductive Elimination (RE)

4RE1_Pd-Ag

Number of imaginary frequencies : 1

The smallest frequency is : -209.7998 cm(-1)

Electronic energy : HF=-2548.6912912
 Zero-point correction= 0.661877
 Thermal correction to Energy= 0.711593
 Thermal correction to Enthalpy= 0.712537
 Thermal correction to Gibbs Free Energy= 0.575944
 Sum of electronic and zero-point Energies= -2548.029414
 Sum of electronic and thermal Energies= -2547.979698
 Sum of electronic and thermal Enthalpies= -2547.978754
 Sum of electronic and thermal Free Energies= -2548.115347

Cartesian Coordinates

6	-1.292037	3.368265	4.208387
6	-1.725083	2.045774	4.229743
6	-1.550697	1.235463	3.114020
6	-0.944368	1.724792	1.944116
6	-0.487100	3.052374	1.949954
6	-0.670027	3.863342	3.064092
6	-0.850161	0.826102	0.767743
6	-0.923036	1.205525	-0.541262
6	-1.073335	2.600851	-1.003363
6	-2.250789	3.317774	-0.747587
6	-2.380381	4.636620	-1.165436
6	-1.341200	5.261097	-1.852982
6	-0.176720	4.551235	-2.134552
6	-0.049166	3.227955	-1.722560
46	-0.427379	-0.220039	-1.929702
6	-2.395516	0.182819	-1.627880
6	-3.275764	-0.384707	-0.713647
6	-4.668166	-0.281926	-0.881704
6	-5.229265	0.363283	-1.976419
6	-4.369027	0.927992	-2.909941

6	-2.987560	0.857062	-2.714966
6	-5.309152	-0.890126	0.272931
6	-4.147797	-1.383571	1.167653
7	-2.978430	-1.056852	0.498846
8	-4.243005	-1.934266	2.240221
6	-1.704427	-1.506117	0.949216
6	-1.612827	-2.960748	1.204430
6	-2.072829	-3.860452	0.236817
6	-1.971082	-5.231392	0.447289
6	-1.423552	-5.717161	1.632455
6	-0.979682	-4.826127	2.606988
6	-1.075977	-3.455652	2.396407
8	-6.480968	-1.015068	0.556739
8	0.678404	-1.609174	-3.213427
6	1.929961	-1.599511	-3.167926
6	2.682477	-2.680775	-3.896780
6	-0.684461	-0.635371	1.064856
6	0.696668	-1.088860	1.397184
6	1.362321	-0.651482	2.551272
6	2.663155	-1.067933	2.817311
6	3.331611	-1.912336	1.932211
6	2.684821	-2.352070	0.781169
6	1.376988	-1.946227	0.514844
8	2.623611	-0.746351	-2.523233
1	-2.503720	-3.477773	-0.689184
1	-0.743736	-2.757030	3.163327
1	-2.322960	-5.922773	-0.315341
1	-0.566740	-5.201049	3.541002
1	-1.349290	-6.789465	1.799436
1	0.852502	0.008358	3.251561
1	0.865442	-2.303064	-0.379128
1	3.159830	-0.727964	3.723594
1	3.193916	-3.009547	0.077615
1	4.352215	-2.227537	2.141664
1	2.044352	-3.192221	-4.620324
1	3.564729	-2.272242	-4.399296
1	3.033733	-3.417046	-3.162245
1	-6.310602	0.429157	-2.073704
1	-2.339480	1.368558	-3.425811
1	-4.760753	1.450342	-3.779096
1	-3.063946	2.831011	-0.208539
1	0.860413	2.668391	-1.950081
1	-3.297884	5.181610	-0.952769
1	0.635396	5.027641	-2.679801
1	-1.442589	6.294978	-2.175580
1	-1.896607	0.202739	3.143807
1	0.041593	3.447568	1.087838
1	-2.204707	1.639976	5.117943
1	-0.306260	4.888717	3.042294
1	-1.428895	4.005838	5.078870
8	4.581381	0.305465	-0.362617
6	5.241498	-0.703429	-0.632261
8	4.954638	-1.472986	-1.648050
6	6.440648	-1.124603	0.144229
1	6.470760	-2.212866	0.247840
1	7.340727	-0.820921	-0.403472
1	6.450978	-0.646703	1.126604
47	1.995015	0.525337	-0.607911
8	2.469447	2.188281	1.028056
6	3.217847	2.140599	2.000276
8	4.400191	1.558224	1.979546
6	2.896318	2.768709	3.313949
1	3.456550	3.706340	3.408861
1	1.826898	2.985563	3.378696
1	3.206023	2.117636	4.136926
1	4.543592	1.133324	1.091342
1	4.092890	-1.155949	-2.078202

4RE2_Pd-Ag

Number of imaginary frequencies : 1
The smallest frequency is : -239.7621 cm(-1)

Electronic energy : HF=-2548.6821676
Zero-point correction= 0.660706
Thermal correction to Energy= 0.711012
Thermal correction to Enthalpy= 0.711956
Thermal correction to Gibbs Free Energy= 0.571711
Sum of electronic and zero-point Energies= -2548.021462
Sum of electronic and thermal Energies= -2547.971156
Sum of electronic and thermal Enthalpies= -2547.970212
Sum of electronic and thermal Free Energies= -2548.110456

Cartesian Coordinates

6 3.384524 -3.688324 3.826523
6 4.131331 -2.902089 2.952531
6 3.496972 -2.024495 2.082763
6 2.094414 -1.917763 2.045238
6 1.359099 -2.701626 2.950476
6 1.997258 -3.575866 3.823345
6 1.479503 -0.992211 1.067996
6 0.297108 -1.168255 0.409593
6 -0.709907 -2.200108 0.754169
6 -0.669251 -3.497966 0.240209
6 -1.677806 -4.411008 0.542492
6 -2.751098 -4.045573 1.349589
6 -2.797363 -2.762251 1.892842
6 -1.782769 -1.842510 1.601289
46 -0.493548 0.537881 -0.418092
6 0.361946 -1.021767 -1.492336
6 1.676249 -1.210304 -1.941337
6 1.983077 -2.030951 -3.038900
6 0.997258 -2.661681 -3.788431
6 -0.321854 -2.465538 -3.403413
6 -0.612264 -1.690124 -2.279904
6 3.429342 -2.136079 -3.139599
6 3.978685 -1.274729 -1.979689
7 2.871877 -0.747562 -1.332394
8 5.140461 -1.093944 -1.696498
6 2.976207 0.321252 -0.397351
6 3.828443 1.448719 -0.830830
6 3.668969 1.986096 -2.112529
6 4.440014 3.068862 -2.522097
6 5.387337 3.616504 -1.660212
6 5.564907 3.072574 -0.389495
6 4.793313 1.992651 0.022129
8 4.128118 -2.749650 -3.917441
8 -1.491833 2.248446 -1.596017
6 -2.733352 2.185623 -1.821852
6 -3.432321 3.425081 -2.315161
6 2.249124 0.252479 0.736540
6 2.089144 1.394534 1.671650
6 2.098266 1.192913 3.057893
6 1.916723 2.257710 3.935924
6 1.713392 3.544471 3.447593
6 1.679110 3.756324 2.070416
6 1.858338 2.693923 1.193491
8 -3.447033 1.155728 -1.640369
1 2.924947 1.556753 -2.785000
1 4.934072 1.560138 1.012253
1 4.300414 3.487046 -3.516724
1 6.314212 3.487307 0.281391
1 5.991739 4.462466 -1.980124
1 2.259122 0.194400 3.459221
1 1.804371 2.868840 0.119686
1 1.936917 2.076752 5.008535
1 1.497602 4.753592 1.674446
1 1.569923 4.375946 4.134439

1	-2.722654	4.208445	-2.590252
1	-4.073245	3.187391	-3.170246
1	-4.084281	3.802988	-1.517342
1	1.270697	-3.293245	-4.630656
1	-1.657387	-1.627925	-1.977110
1	-1.135055	-2.935685	-3.950958
1	0.163247	-3.791461	-0.399002
1	-1.757869	-0.873658	2.106782
1	-1.625734	-5.418853	0.136236
1	-3.607032	-2.472557	2.559943
1	-3.538657	-4.761356	1.571449
1	4.095863	-1.409659	1.411174
1	0.277535	-2.611378	2.995882
1	5.217280	-2.969481	2.948335
1	1.400715	-4.166174	4.516061
1	3.879361	-4.372101	4.512507
8	-1.475632	1.765917	1.417225
6	-1.513021	2.984140	1.559376
8	-1.350560	3.839890	0.566408
6	-1.793553	3.642942	2.867648
1	-1.235494	4.578528	2.961848
1	-2.862112	3.885999	2.913486
1	-1.552338	2.968284	3.691822
47	-3.114490	-0.578623	-0.059635
8	-5.502619	-0.549029	0.119493
6	-6.332467	0.212466	-0.373441
8	-6.040121	1.165715	-1.229079
6	-7.787847	0.134556	-0.056535
1	-8.349508	-0.096446	-0.968096
1	-7.976896	-0.633276	0.694745
1	-8.143050	1.105339	0.304041
1	-5.055170	1.184604	-1.425668
1	-1.257727	3.333969	-0.282622

4RE3_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -243.7585 cm(-1)

Electronic energy : HF=-2548.6818743
 Zero-point correction= 0.660611
 Thermal correction to Energy= 0.710768
 Thermal correction to Enthalpy= 0.711712
 Thermal correction to Gibbs Free Energy= 0.572682
 Sum of electronic and zero-point Energies= -2548.021263
 Sum of electronic and thermal Energies= -2547.971107
 Sum of electronic and thermal Enthalpies= -2547.970162
 Sum of electronic and thermal Free Energies= -2548.109192

 Cartesian Coordinates

6	3.343242	-3.919723	3.640502
6	4.088340	-3.168030	2.735249
6	3.462891	-2.241223	1.911580
6	2.069639	-2.047919	1.953420
6	1.337405	-2.800592	2.887332
6	1.967020	-3.724721	3.713738
6	1.462258	-1.066469	1.027430
6	0.233670	-1.149047	0.437051
6	-0.818010	-2.120679	0.822344
6	-0.896964	-3.401716	0.273164
6	-1.945484	-4.254830	0.612759
6	-2.940899	-3.843870	1.494479
6	-2.865806	-2.578171	2.074797
6	-1.810168	-1.718507	1.745626
46	-0.475692	0.639246	-0.294379
6	0.179500	-0.956159	-1.453739
6	1.444007	-1.232776	-1.991182

6	1.618003	-2.043356	-3.124632
6	0.540605	-2.572498	-3.824929
6	-0.733235	-2.280675	-3.355543
6	-0.892496	-1.517109	-2.198211
6	3.043251	-2.254523	-3.318854
6	3.727212	-1.466261	-2.178552
7	2.705755	-0.877451	-1.449256
8	4.914736	-1.375414	-1.969131
6	2.946584	0.167768	-0.512004
6	3.837541	1.240599	-1.002608
6	3.601545	1.810038	-2.258718
6	4.414982	2.834020	-2.731341
6	5.481765	3.289572	-1.960164
6	5.732798	2.714058	-0.715995
6	4.917897	1.693655	-0.240227
8	3.644773	-2.898129	-4.151776
8	-1.411578	2.421798	-1.418622
6	-2.655681	2.393343	-1.648001
6	-3.251192	3.598396	-2.325041
6	2.294440	0.129965	0.667743
6	2.281587	1.262919	1.627177
6	2.139826	2.586432	1.181756
6	2.103400	3.643601	2.082170
6	2.189811	3.403018	3.452370
6	2.303190	2.094312	3.910116
6	2.345963	1.034879	3.008141
8	-3.416081	1.429147	-1.351631
1	2.765795	1.450917	-2.861141
1	5.116625	1.235611	0.728179
1	4.216974	3.277110	-3.705034
1	6.574687	3.055618	-0.117517
1	6.121428	4.087531	-2.330791
1	2.040550	2.786035	0.115823
1	2.441949	0.019037	3.385886
1	1.989701	4.660344	1.711002
1	2.362093	1.891660	4.977462
1	2.157354	4.230670	4.157911
1	-2.783481	3.733818	-3.306027
1	-4.333293	3.511218	-2.449736
1	-3.025364	4.495474	-1.737057
1	0.710343	-3.199884	-4.696927
1	-1.910351	-1.368815	-1.835770
1	-1.613129	-2.664568	-3.866036
1	-0.126625	-3.731042	-0.423920
1	-1.684762	-0.770406	2.275985
1	-1.987424	-5.250542	0.176552
1	-3.610426	-2.256638	2.800292
1	-3.761330	-4.511477	1.745520
1	4.060429	-1.654952	1.213908
1	0.266824	-2.646637	2.990891
1	5.166303	-3.301276	2.670573
1	1.374046	-4.288311	4.431284
1	3.831908	-4.641296	4.291299
8	-1.215784	1.903509	1.617297
6	-1.171139	3.122165	1.750959
8	-1.035732	3.962678	0.741121
6	-1.304126	3.804255	3.070389
1	-0.611528	4.648147	3.140282
1	-2.321662	4.203164	3.160904
1	-1.125966	3.097785	3.883350
47	-3.121383	-0.342687	0.195048
8	-5.508631	-0.494191	0.077204
6	-6.327271	0.119478	-0.604516
8	-6.017141	1.098913	-1.423591
6	-7.787067	-0.185421	-0.581954
1	-8.114231	-0.482610	-1.584072
1	-8.001415	-0.985584	0.127506
1	-8.350248	0.713899	-0.312079
1	-5.028944	1.272779	-1.420978
1	-1.049779	3.450625	-0.110035

4RE4_Pd-Ag

Number of imaginary frequencies : 1
The smallest frequency is : -243.8766 cm(-1)

Electronic energy : HF=-2548.6818366
Zero-point correction= 0.660110
Thermal correction to Energy= 0.710496
Thermal correction to Enthalpy= 0.711440
Thermal correction to Gibbs Free Energy= 0.571607
Sum of electronic and zero-point Energies= -2548.021727
Sum of electronic and thermal Energies= -2547.971341
Sum of electronic and thermal Enthalpies= -2547.970396
Sum of electronic and thermal Free Energies= -2548.110230

Cartesian Coordinates

6	3.385388	-3.937074	3.608954
6	2.003051	-3.781780	3.655729
6	1.365840	-2.854806	2.838512
6	2.096551	-2.059001	1.939522
6	3.495382	-2.212745	1.924906
6	4.128564	-3.142343	2.739660
6	1.481313	-1.074897	1.022307
6	0.262767	-1.169532	0.413088
6	-0.779680	-2.162606	0.766006
6	-0.840135	-3.433010	0.190296
6	-1.881933	-4.304005	0.504703
6	-2.888657	-3.922365	1.386642
6	-2.831979	-2.667849	1.993063
6	-1.783493	-1.790711	1.689583
46	-0.465975	0.617810	-0.302686
6	0.238124	-0.942181	-1.477540
6	1.516252	-1.186339	-1.997634
6	1.724476	-1.974101	-3.140922
6	0.668325	-2.509188	-3.868774
6	-0.618505	-2.247357	-3.416890
6	-0.811845	-1.507059	-2.249415
6	3.156720	-2.152784	-3.315214
6	3.806547	-1.367538	-2.152216
7	2.761449	-0.814193	-1.428987
8	4.988542	-1.253388	-1.923651
6	2.961055	0.221345	-0.471599
6	3.821571	1.332372	-0.930272
6	3.587495	1.912418	-2.182044
6	4.364262	2.979699	-2.619402
6	5.392952	3.468506	-1.817435
6	5.644320	2.881590	-0.578762
6	4.865849	1.817698	-0.138147
8	3.784373	-2.770764	-4.148213
8	-1.388628	2.399996	-1.433639
6	-2.630900	2.363047	-1.671708
6	-3.239422	3.569025	-2.334981
6	2.289099	0.147576	0.695158
6	2.214812	1.267653	1.667532
6	2.016333	2.587759	1.233595
6	1.905110	3.629879	2.145339
6	1.974925	3.376805	3.514159
6	2.149255	2.070335	3.959455
6	2.264623	1.025871	3.046514
8	-3.390885	1.401663	-1.364020
1	2.780978	1.528627	-2.808535
1	5.065682	1.350769	0.825672
1	4.166975	3.430988	-3.589485
1	6.457603	3.249214	0.043318
1	6.002998	4.301530	-2.159729
1	1.928757	2.795225	0.167897

1	2.403557	0.010814	3.413393
1	1.745157	4.644062	1.784509
1	2.197504	1.857886	5.025425
1	1.882765	4.192217	4.228606
1	-2.568050	3.966818	-3.100684
1	-4.217005	3.347771	-2.771194
1	-3.369963	4.352162	-1.576976
1	0.863700	-3.117589	-4.748879
1	-1.837919	-1.381612	-1.902247
1	-1.482437	-2.636810	-3.950007
1	-0.059797	-3.741221	-0.505140
1	-1.671746	-0.853495	2.241443
1	-1.909109	-5.291294	0.048659
1	-3.585187	-2.369702	2.719694
1	-3.703005	-4.604351	1.618027
1	0.289491	-2.733801	2.922742
1	4.092096	-1.593438	1.255658
1	1.410164	-4.379894	4.344882
1	5.210986	-3.244053	2.695825
1	3.879789	-4.661493	4.252213
8	-1.324191	1.818588	1.606270
6	-1.326952	3.035209	1.765991
8	-1.165801	3.900899	0.781833
6	-1.562091	3.682199	3.089082
1	-0.986288	4.607011	3.182887
1	-2.624665	3.944413	3.162496
1	-1.317272	2.992113	3.899030
47	-3.098797	-0.393420	0.162001
8	-5.485469	-0.533087	0.049445
6	-6.306434	0.106460	-0.605199
8	-5.996837	1.103134	-1.403112
6	-7.768764	-0.185310	-0.572115
1	-8.104954	-0.477352	-1.572850
1	-7.984635	-0.986615	0.135621
1	-8.323006	0.717539	-0.296018
1	-5.006516	1.265452	-1.412668
1	-1.108370	3.407383	-0.077608

4RE5_Pd-Ag

Number of imaginary frequencies : 1

The smallest frequency is : -239.8338 cm(-1)

Electronic energy :	HF=-2548.6822306
Zero-point correction=	0.661349
Thermal correction to Energy=	0.711356
Thermal correction to Enthalpy=	0.712300
Thermal correction to Gibbs Free Energy=	0.573559
Sum of electronic and zero-point Energies=	-2548.020882
Sum of electronic and thermal Energies=	-2547.970875
Sum of electronic and thermal Enthalpies=	-2547.969931
Sum of electronic and thermal Free Energies=	-2548.108672

Cartesian Coordinates

6	3.397528	-3.687473	3.822035
6	2.009519	-3.584930	3.812477
6	1.369379	-2.710812	2.941000
6	2.103426	-1.916796	2.043522
6	3.506561	-2.013625	2.087629
6	4.142947	-2.891257	2.955925
6	1.486300	-0.991515	1.067653
6	0.306984	-1.171050	0.404733
6	-0.696764	-2.208459	0.741954
6	-0.650715	-3.503674	0.221803
6	-1.656738	-4.421649	0.517763
6	-2.732830	-4.063802	1.324485
6	-2.784392	-2.783380	1.874071

6	-1.772302	-1.858857	1.589065
46	-0.486864	0.537191	-0.415767
6	0.376600	-1.014179	-1.495366
6	1.693151	-1.193850	-1.941823
6	2.006981	-2.007451	-3.042573
6	1.026203	-2.638808	-3.798272
6	-0.294950	-2.450678	-3.416180
6	-0.592299	-1.682664	-2.289425
6	3.454013	-2.105862	-3.139075
6	3.995963	-1.247705	-1.973278
7	2.884847	-0.728375	-1.327009
8	5.156121	-1.063346	-1.685782
6	2.980170	0.337270	-0.387362
6	3.828012	1.471324	-0.811772
6	3.678361	2.009038	-2.094589
6	4.447242	3.096546	-2.495459
6	5.382567	3.649045	-1.623607
6	5.550022	3.105494	-0.351413
6	4.780551	2.020759	0.051533
8	4.157887	-2.712952	-3.917411
8	-1.488458	2.246379	-1.593116
6	-2.727384	2.175875	-1.830562
6	-3.426161	3.406139	-2.346982
6	2.248717	0.259449	0.743090
6	2.072416	1.398189	1.679362
6	1.819403	2.693391	1.200991
6	1.618625	3.751955	2.077807
6	1.653099	3.539780	3.455063
6	1.880831	2.257061	3.943393
6	2.084407	1.196173	3.065340
8	-3.439175	1.145519	-1.643973
1	2.943912	1.575858	-2.775076
1	4.914519	1.587987	1.042475
1	4.315296	3.514619	-3.491180
1	6.290076	3.523953	0.327390
1	5.985483	4.498549	-1.936886
1	1.762415	2.866051	0.126977
1	2.263247	0.200416	3.466158
1	1.419638	4.746276	1.682672
1	1.902644	2.076273	5.016012
1	1.492060	4.367970	4.141988
1	-4.043152	3.157189	-3.216433
1	-4.102069	3.782640	-1.568746
1	-2.717398	4.194587	-2.609582
1	1.304828	-3.264867	-4.642908
1	-1.638536	-1.626591	-1.989149
1	-1.104341	-2.921544	-3.968743
1	0.184091	-3.791491	-0.416955
1	-1.751346	-0.892951	2.100223
1	-1.600339	-5.427340	0.106763
1	-3.596184	-2.499782	2.541212
1	-3.518376	-4.783348	1.541244
1	0.286937	-2.629163	2.981301
1	4.104456	-1.391223	1.422156
1	1.413744	-4.183285	4.498941
1	5.229357	-2.950874	2.956677
1	3.893880	-4.371354	4.506819
8	-1.476296	1.745170	1.425828
6	-1.576413	2.959467	1.569302
8	-1.428738	3.825820	0.583383
6	-1.925917	3.594424	2.872344
1	-1.469655	4.582891	2.971990
1	-3.014212	3.726749	2.910246
1	-1.628896	2.946928	3.700118
47	-3.104625	-0.590187	-0.066084
8	-5.493091	-0.560257	0.115414
6	-6.324538	0.196248	-0.382384
8	-6.034253	1.144772	-1.244006
6	-7.779708	0.117806	-0.064538
1	-8.342504	-0.111905	-0.975672

1	-7.968110	-0.650471	0.686445
1	-8.134196	1.088344	0.297524
1	-5.048936	1.166883	-1.437952
1	-1.294305	3.328061	-0.264534

4RE6_Pd-Ag

Number of imaginary frequencies : 1
 The smallest frequency is : -243.7028 cm(-1)

Electronic energy : HF=-2548.6818392
 Zero-point correction= 0.660065
 Thermal correction to Energy= 0.710471
 Thermal correction to Enthalpy= 0.711415
 Thermal correction to Gibbs Free Energy= 0.571534
 Sum of electronic and zero-point Energies= -2548.021775
 Sum of electronic and thermal Energies= -2547.971368
 Sum of electronic and thermal Enthalpies= -2547.970424
 Sum of electronic and thermal Free Energies= -2548.110305

 Cartesian Coordinates

6	3.374815	-3.930649	3.618953
6	4.118531	-3.148401	2.738846
6	3.487345	-2.219953	1.921300
6	2.089935	-2.054959	1.944130
6	1.358813	-2.838209	2.853656
6	1.994053	-3.764129	3.673635
6	1.476797	-1.072069	1.024012
6	0.255036	-1.163419	0.420795
6	-0.790208	-2.150086	0.783670
6	-0.856489	-3.423756	0.215935
6	-1.900637	-4.289148	0.537841
6	-2.904071	-3.898392	1.419566
6	-2.841562	-2.640454	2.018231
6	-1.790519	-1.768855	1.707195
46	-0.468577	0.624098	-0.298972
6	0.220943	-0.946174	-1.470451
6	1.495012	-1.200041	-1.996017
6	1.692980	-1.995251	-3.136097
6	0.630400	-2.529492	-3.855074
6	-0.652584	-2.258847	-3.397676
6	-0.835643	-1.510747	-2.233579
6	3.123239	-2.183140	-3.316822
6	3.783382	-1.395904	-2.161247
7	2.745262	-0.832211	-1.435932
8	4.967144	-1.287908	-1.938970
6	2.957044	0.206307	-0.484484
6	3.825512	1.306921	-0.953191
6	3.589140	1.883795	-2.205954
6	4.376136	2.938715	-2.654753
6	5.417351	3.418071	-1.863304
6	5.670232	2.834635	-0.623274
6	4.881478	1.783233	-0.171158
8	3.743074	-2.809134	-4.149707
8	-1.395589	2.411491	-1.419916
6	-2.638535	2.375914	-1.655824
6	-3.237059	3.577938	-2.335734
6	2.291684	0.142835	0.686601
6	2.235243	1.267444	1.654723
6	2.047936	2.587778	1.216754
6	1.955970	3.635088	2.124748
6	2.034595	3.387148	3.494011
6	2.197491	2.080662	3.943564
6	2.293538	1.031011	3.034350
8	-3.395133	1.407702	-1.363269
1	2.772988	1.506989	-2.824182
1	5.082434	1.318915	0.793719

1	4.177272	3.387549	-3.625646
1	6.492972	3.194815	-0.009317
1	6.035770	4.241011	-2.214845
1	1.953948	2.791384	0.150900
1	2.424426	0.016199	3.404754
1	1.803856	4.649318	1.760655
1	2.252103	1.872289	5.010034
1	1.957659	4.206686	4.205535
1	-2.769199	3.711926	-3.316884
1	-4.318814	3.487378	-2.461168
1	-3.013928	4.477336	-1.750353
1	0.818125	-3.144064	-4.732532
1	-1.859261	-1.378540	-1.881613
1	-1.521385	-2.647355	-3.923502
1	-0.079167	-3.738476	-0.480017
1	-1.674521	-0.828359	2.252594
1	-1.932469	-5.279028	0.087750
1	-3.592178	-2.335014	2.744509
1	-3.720536	-4.575850	1.656737
1	4.084231	-1.610244	1.243444
1	0.283984	-2.707862	2.943662
1	5.199809	-3.259052	2.688779
1	1.401163	-4.352324	4.371254
1	3.867714	-4.654040	4.264519
8	-1.297738	1.838943	1.613703
6	-1.285515	3.055952	1.770110
8	-1.125351	3.917179	0.782009
6	-1.499700	3.708439	3.094146
1	-0.917436	4.630032	3.178476
1	-2.559709	3.977352	3.179845
1	-1.249985	3.019032	3.903213
47	-3.104962	-0.380127	0.170955
8	-5.492250	-0.518223	0.056504
6	-6.310971	0.110680	-0.611129
8	-5.998663	1.096703	-1.421342
6	-7.773012	-0.182572	-0.580940
1	-8.106892	-0.478010	-1.581403
1	-7.989910	-0.981254	0.129423
1	-8.328431	0.720875	-0.308988
1	-5.008699	1.261184	-1.425163
1	-1.087728	3.420621	-0.077287

Monometallic Reductive Elimination

4RE1_Pd

Number of imaginary frequencies : 1

The smallest frequency is : -240.2635 cm(-1)

Electronic energy : HF=-2174.4554941
 Zero-point correction= 0.607791
 Thermal correction to Energy= 0.650947
 Thermal correction to Enthalpy= 0.651891
 Thermal correction to Gibbs Free Energy= 0.530143
 Sum of electronic and zero-point Energies= -2173.847703
 Sum of electronic and thermal Energies= -2173.804547
 Sum of electronic and thermal Enthalpies= -2173.803603
 Sum of electronic and thermal Free Energies= -2173.925351

Cartesian Coordinates

6	-3.724301	1.006096	4.218874
6	-2.448286	0.488367	4.429172
6	-1.612441	0.228004	3.349638
6	-2.040557	0.466233	2.034680
6	-3.324726	0.993676	1.838217

6	-4.157050	1.258906	2.919501
6	-1.106420	0.206543	0.913580
6	-1.432469	-0.396553	-0.270615
6	-2.785211	-0.924282	-0.564677
6	-3.337048	-1.934837	0.234297
6	-4.596545	-2.450167	-0.046439
6	-5.323420	-1.969307	-1.134290
6	-4.775516	-0.980880	-1.947045
6	-3.510453	-0.469667	-1.670355
46	-0.107721	0.087769	-1.784182
6	-0.212481	-1.762310	-0.889718
6	0.523519	-2.272825	0.183900
6	0.707426	-3.650671	0.375688
6	0.203994	-4.586565	-0.520564
6	-0.513335	-4.116496	-1.614586
6	-0.733582	-2.747007	-1.768990
6	1.401014	-3.838849	1.641436
6	1.628378	-2.410594	2.194168
7	1.088404	-1.543945	1.256945
8	2.168629	-2.112871	3.234120
6	1.325119	-0.137957	1.292621
6	2.745782	0.248950	1.436277
6	3.706675	-0.343955	0.608364
6	5.045079	0.020662	0.711042
6	5.439838	0.974643	1.646307
6	4.490220	1.558366	2.481612
6	3.151855	1.196532	2.379940
8	1.747559	-4.848049	2.215325
8	1.818975	0.327411	-3.115069
6	2.713228	-0.508455	-3.088445
6	4.079515	-0.292028	-3.632728
6	0.295849	0.708517	1.101109
6	0.494439	2.176808	0.949458
6	-0.161844	3.093068	1.780360
6	-0.013313	4.462356	1.579836
6	0.782457	4.939541	0.542730
6	1.443406	4.036633	-0.288340
6	1.304025	2.668780	-0.083902
8	2.554588	-1.713194	-2.550604
1	3.397821	-1.091998	-0.124528
1	2.412205	1.641293	3.043912
1	5.783704	-0.443548	0.060964
1	4.795518	2.292713	3.223844
1	6.487043	1.257031	1.728396
1	-0.783744	2.734936	2.598808
1	1.815413	1.965294	-0.741322
1	-0.524128	5.159502	2.240646
1	2.070632	4.398428	-1.100793
1	0.892681	6.010323	0.384805
1	4.788706	-0.246302	-2.797787
1	4.375186	-1.133609	-4.266140
1	4.122211	0.641044	-4.195457
1	1.647666	-1.757558	-2.177331
1	0.359511	-5.648794	-0.346104
1	-1.361430	-2.416189	-2.595674
1	-0.932423	-4.810817	-2.338424
1	-2.761153	-2.316687	1.077939
1	-3.073248	0.287056	-2.322568
1	-5.011689	-3.234289	0.583307
1	-5.331041	-0.609916	-2.805792
1	-6.309297	-2.373201	-1.353807
1	-0.610124	-0.164895	3.521872
1	-3.670443	1.209980	0.828651
1	-2.099954	0.288821	5.440408
1	-5.146506	1.676900	2.745985
1	-4.374841	1.219212	5.064125
8	-0.577925	2.152727	-2.748180
6	-1.305581	2.988902	-2.226110
8	-1.971556	2.768661	-1.101569
6	-1.538068	4.350003	-2.780070

1	-2.611657	4.529632	-2.896136
1	-1.158203	5.094688	-2.071329
1	-1.032724	4.463328	-3.739738
1	-1.716518	1.881284	-0.764738

4RE2_Pd

Number of imaginary frequencies : 1
 The smallest frequency is : -239.7870 cm(-1)

Electronic energy : HF=-2174.4554056
 Zero-point correction= 0.608468
 Thermal correction to Energy= 0.651261
 Thermal correction to Enthalpy= 0.652205
 Thermal correction to Gibbs Free Energy= 0.532244
 Sum of electronic and zero-point Energies= -2173.846937
 Sum of electronic and thermal Energies= -2173.804145
 Sum of electronic and thermal Enthalpies= -2173.803201
 Sum of electronic and thermal Free Energies= -2173.923162

 Cartesian Coordinates

6	-3.778406	0.996019	4.196892
6	-2.485738	0.525769	4.415685
6	-1.638978	0.280626	3.341150
6	-2.070228	0.487196	2.021224
6	-3.371305	0.970020	1.817205
6	-4.215004	1.218832	2.893360
6	-1.125763	0.234187	0.907942
6	-1.436853	-0.357929	-0.286498
6	-2.789541	-0.864953	-0.614003
6	-3.366141	-1.883613	0.156497
6	-4.626977	-2.377732	-0.154102
6	-5.330720	-1.866677	-1.243597
6	-4.757811	-0.870092	-2.028539
6	-3.490826	-0.380622	-1.722296
46	-0.062281	0.105269	-1.762329
6	-0.229249	-1.745353	-0.880738
6	0.475642	-2.269459	0.207046
6	0.629361	-3.649857	0.403924
6	0.125850	-4.576970	-0.501858
6	-0.561156	-4.094069	-1.609399
6	-0.753344	-2.720234	-1.768605
6	1.295881	-3.848600	1.682709
6	1.540466	-2.423329	2.237007
7	1.031813	-1.549063	1.289401
8	2.069096	-2.133449	3.285103
6	1.293301	-0.147605	1.323630
6	2.719843	0.212329	1.476715
6	3.139294	1.145240	2.428748
6	4.483459	1.483088	2.535916
6	5.424106	0.890384	1.696747
6	5.015103	-0.048228	0.751896
6	3.671264	-0.390083	0.644731
8	1.612199	-4.862748	2.265254
8	1.926825	0.305730	-3.011870
6	2.733050	-0.612993	-3.084222
6	4.095876	-0.489290	-3.666158
6	0.281527	0.715920	1.114453
6	0.509696	2.179606	0.961106
6	-0.160636	3.111869	1.762238
6	0.025402	4.477322	1.566055
6	0.873716	4.934729	0.562238
6	1.546254	4.015763	-0.241451
6	1.368339	2.651798	-0.041738
8	2.462530	-1.840343	-2.654511
1	2.404664	1.598217	3.092996
1	3.348208	-1.123919	-0.097065

1	4.800278	2.206034	3.284508
1	5.746755	-0.515972	0.096717
1	6.475741	1.154703	1.782470
1	-0.823496	2.769297	2.554715
1	1.889150	1.936028	-0.677933
1	-0.497438	5.186715	2.204042
1	2.212144	4.362383	-1.029369
1	1.014387	6.002493	0.408041
1	4.839188	-0.883849	-2.966107
1	4.155370	-1.094763	-4.577382
1	4.316282	0.551878	-3.903853
1	1.552649	-1.834975	-2.285976
1	0.257903	-5.641882	-0.324642
1	-1.359948	-2.378613	-2.606759
1	-0.979545	-4.780889	-2.340753
1	-2.808605	-2.287859	1.002068
1	-3.033245	0.382198	-2.352852
1	-5.061889	-3.168802	0.453218
1	-5.294678	-0.475645	-2.888707
1	-6.317906	-2.253599	-1.486559
1	-0.624746	-0.075929	3.522512
1	-3.724498	1.161850	0.805641
1	-2.132359	0.351041	5.429760
1	-5.217538	1.600676	2.711788
1	-4.438681	1.196181	5.037726
8	-0.460816	2.171743	-2.747009
6	-1.182543	3.032311	-2.257607
8	-1.885902	2.844716	-1.149954
6	-1.365239	4.390007	-2.838415
1	-2.428661	4.585387	-3.010058
1	-1.007185	5.138823	-2.122895
1	-0.811976	4.479568	-3.773898
1	-1.665370	1.957122	-0.791501

4RE3_Pd

Number of imaginary frequencies : 1

The smallest frequency is : -240.3197 cm(-1)

Electronic energy : HF=-2174.4554942
 Zero-point correction= 0.607794
 Thermal correction to Energy= 0.650949
 Thermal correction to Enthalpy= 0.651893
 Thermal correction to Gibbs Free Energy= 0.530145
 Sum of electronic and zero-point Energies= -2173.847700
 Sum of electronic and thermal Energies= -2173.804545
 Sum of electronic and thermal Enthalpies= -2173.803601
 Sum of electronic and thermal Free Energies= -2173.925350

Cartesian Coordinates

6	-3.723295	1.005027	4.219983
6	-2.447065	0.487659	4.429855
6	-1.611499	0.227535	3.350047
6	-2.040109	0.465654	2.035222
6	-3.324477	0.992789	1.839197
6	-4.156528	1.257750	2.920754
6	-1.106291	0.206213	0.913816
6	-1.432657	-0.396429	-0.270536
6	-2.785501	-0.923948	-0.564514
6	-3.337319	-1.934651	0.234283
6	-4.596951	-2.449713	-0.046338
6	-5.323976	-1.968439	-1.133906
6	-4.776082	-0.979884	-1.946510
6	-3.510886	-0.468935	-1.669932
46	-0.108137	0.088475	-1.784126
6	-0.212972	-1.761914	-0.890279
6	0.523262	-2.272963	0.182940

6	0.707238	-3.650899	0.373994
6	0.203647	-4.586355	-0.522630
6	-0.513937	-4.115745	-1.616253
6	-0.734258	-2.746187	-1.769920
6	1.401091	-3.839705	1.639506
6	1.628507	-2.411727	2.192932
7	1.088336	-1.544612	1.256249
8	2.168905	-2.114512	3.232952
6	1.325245	-0.138678	1.292389
6	2.745932	0.248058	1.436151
6	3.706777	-0.344798	0.608154
6	5.045221	0.019624	0.710963
6	5.440055	0.973350	1.646461
6	4.490476	1.557025	2.481846
6	3.152068	1.195386	2.380032
8	1.747795	-4.849187	2.212803
8	1.818825	0.329129	-3.114454
6	2.713015	-0.506822	-3.088483
6	4.079368	-0.289998	-3.632442
6	0.296077	0.707972	1.101170
6	0.494909	2.176260	0.949800
6	-0.161141	3.092453	1.780960
6	-0.012356	4.461761	1.580764
6	0.783424	4.939036	0.543709
6	1.444070	4.036196	-0.287675
6	1.304438	2.668315	-0.083568
8	2.554193	-1.712052	-2.551789
1	3.397819	-1.092673	-0.124869
1	2.412403	1.640077	3.044035
1	5.783816	-0.444548	0.060822
1	4.795841	2.291166	3.224253
1	6.487294	1.255578	1.728667
1	-0.783054	2.734238	2.599362
1	1.815454	1.964909	-0.741370
1	-0.522976	5.158848	2.241788
1	2.071246	4.398064	-1.100134
1	0.893866	6.009833	0.386042
1	4.788531	-0.245100	-2.797438
1	4.375010	-1.131007	-4.266622
1	4.122185	0.643588	-4.194309
1	1.647270	-1.756597	-2.178546
1	0.359236	-5.648668	-0.348754
1	-1.362274	-2.414976	-2.596316
1	-0.933168	-4.809714	-2.340346
1	-2.761309	-2.316811	1.077705
1	-3.073687	0.287890	-2.322029
1	-5.012086	-3.233947	0.583275
1	-5.331718	-0.608609	-2.805051
1	-6.309964	-2.372115	-1.353327
1	-0.609029	-0.165120	3.521965
1	-3.670523	1.209116	0.829751
1	-2.098327	0.288229	5.440974
1	-5.146145	1.675499	2.747565
1	-4.373618	1.217951	5.065450
8	-0.578426	2.153665	-2.747593
6	-1.305967	2.989697	-2.225136
8	-1.971716	2.769132	-1.100521
6	-1.538580	4.350954	-2.778663
1	-2.612221	4.530973	-2.893598
1	-1.157762	5.095410	-2.070186
1	-1.034137	4.464308	-3.738802
1	-1.716471	1.881719	-0.763946

4RE4_Pd

Number of imaginary frequencies : 1

The smallest frequency is : -239.7855 cm(-1)

Electronic energy : HF=-2174.4555244
 Zero-point correction= 0.608293
 Thermal correction to Energy= 0.651278
 Thermal correction to Enthalpy= 0.652222
 Thermal correction to Gibbs Free Energy= 0.531333
 Sum of electronic and zero-point Energies= -2173.847231
 Sum of electronic and thermal Energies= -2173.804247
 Sum of electronic and thermal Enthalpies= -2173.803302
 Sum of electronic and thermal Free Energies= -2173.924191

 Cartesian Coordinates

6	-3.903363	1.041980	4.071097
6	-2.633797	0.534113	4.337535
6	-1.758133	0.260464	3.293461
6	-2.139235	0.474979	1.960557
6	-3.417183	0.991189	1.706953
6	-4.289595	1.270713	2.752839
6	-1.157771	0.208466	0.882352
6	-1.421361	-0.441205	-0.291861
6	-2.743843	-1.025784	-0.611777
6	-3.291434	-2.027254	0.201724
6	-4.524975	-2.589806	-0.102601
6	-5.230139	-2.166489	-1.228041
6	-4.685867	-1.187354	-2.054482
6	-3.446375	-0.629597	-1.754133
46	-0.032336	0.011973	-1.763671
6	-0.123893	-1.802397	-0.819129
6	0.594740	-2.235998	0.297928
6	0.827097	-3.594830	0.554802
6	0.388236	-4.588210	-0.313821
6	-0.314345	-4.194772	-1.446332
6	-0.582991	-2.841486	-1.667388
6	1.494308	-3.699003	1.844272
6	1.650095	-2.239220	2.338044
7	1.100674	-1.437692	1.350307
8	2.151238	-1.875343	3.376646
6	1.277330	-0.021713	1.331183
6	2.681759	0.429231	1.443764
6	3.655002	-0.169432	0.633905
6	4.976716	0.259626	0.685869
6	5.344718	1.281866	1.557792
6	4.385149	1.868904	2.379194
6	3.062091	1.445418	2.324576
8	1.866729	-4.667042	2.470451
8	2.039045	0.228377	-2.880447
6	2.886243	-0.655264	-2.855731
6	4.308615	-0.455066	-3.243287
6	0.215993	0.773091	1.098617
6	0.344764	2.246066	0.913423
6	1.100982	2.752440	-0.151402
6	1.158402	4.119849	-0.396146
6	0.473687	5.008457	0.430494
6	-0.264598	4.517570	1.503488
6	-0.334933	3.147918	1.741760
8	2.610774	-1.905742	-2.502758
1	3.366915	-0.975360	-0.044629
1	2.315764	1.896456	2.976229
1	5.722791	-0.207093	0.046113
1	4.670189	2.657081	3.072664
1	6.379225	1.614846	1.602015
1	1.624820	2.059442	-0.810091
1	-0.914823	2.779282	2.586035
1	1.736519	4.490399	-1.240703
1	-0.793590	5.203883	2.161304
1	0.518560	6.078677	0.240259
1	4.589828	0.590898	-3.108877
1	4.970186	-1.110524	-2.671297
1	4.420754	-0.710256	-4.303809
1	1.661688	-1.949589	-2.258653

1	0.581236	-5.634699	-0.088999
1	-1.196470	-2.571786	-2.526741
1	-0.685775	-4.934750	-2.150672
1	-2.733024	-2.364875	1.075509
1	-3.011750	0.122694	-2.413315
1	-4.937073	-3.365836	0.539092
1	-5.224359	-0.860029	-2.941361
1	-6.195848	-2.607385	-1.465226
1	-0.759936	-0.121733	3.507497
1	-3.725557	1.188791	0.681644
1	-2.322470	0.353006	5.364187
1	-5.274139	1.680120	2.536434
1	-4.586049	1.265066	4.887972
8	-0.451553	2.022359	-2.849498
6	-1.270363	2.834568	-2.434967
8	-2.066289	2.596100	-1.401581
6	-1.483414	4.178417	-3.036061
1	-2.512311	4.261745	-3.402255
1	-1.346281	4.947814	-2.268490
1	-0.784546	4.341584	-3.857251
1	-1.821202	1.722868	-1.021165

4RE5_Pd

Number of imaginary frequencies : 1
The smallest frequency is : -239.3467 cm(-1)

Electronic energy : HF=-2174.4554461
Zero-point correction= 0.608900
Thermal correction to Energy= 0.651634
Thermal correction to Enthalpy= 0.652578
Thermal correction to Gibbs Free Energy= 0.532738
Sum of electronic and zero-point Energies= -2173.846546
Sum of electronic and thermal Energies= -2173.803812
Sum of electronic and thermal Enthalpies= -2173.802868
Sum of electronic and thermal Free Energies= -2173.922708

Cartesian Coordinates

6	-3.910700	0.837138	4.126207
6	-2.624073	0.360546	4.366556
6	-1.745487	0.156147	3.309137
6	-2.139473	0.408985	1.986268
6	-3.434143	0.897289	1.760177
6	-4.309355	1.107464	2.819542
6	-1.161818	0.195624	0.893445
6	-1.430927	-0.393186	-0.311599
6	-2.763150	-0.934819	-0.665059
6	-3.321024	-1.983103	0.078796
6	-4.566795	-2.501119	-0.253814
6	-5.273541	-1.984493	-1.338696
6	-4.719559	-0.956492	-2.096460
6	-3.467860	-0.443267	-1.768219
46	-0.020501	0.083786	-1.755901
6	-0.159584	-1.759361	-0.877903
6	0.550552	-2.246377	0.222437
6	0.756108	-3.617564	0.430919
6	0.295457	-4.570630	-0.471575
6	-0.400152	-4.123501	-1.588110
6	-0.640801	-2.757794	-1.761595
6	1.423368	-3.779772	1.714319
6	1.609326	-2.341558	2.258425
7	1.071958	-1.495370	1.301766
8	2.121548	-2.024556	3.306946
6	1.271037	-0.082499	1.333291
6	2.682504	0.341813	1.458593
6	3.651150	-0.264214	0.648383
6	4.978457	0.146174	0.707259

6	5.358526	1.154953	1.589551
6	4.404671	1.746360	2.414484
6	3.075709	1.343251	2.350951
8	1.777164	-4.776010	2.306082
8	2.084560	0.291870	-2.811965
6	2.895355	-0.625429	-2.830241
6	4.333920	-0.453929	-3.169365
6	0.219840	0.734086	1.128938
6	0.364644	2.210820	0.994175
6	1.138208	2.748783	-0.042636
6	1.212035	4.123687	-0.235324
6	0.526370	4.988121	0.615772
6	-0.231586	4.465191	1.659277
6	-0.318944	3.088393	1.844823
8	2.562481	-1.885179	-2.573488
1	3.357584	-1.064464	-0.034205
1	2.334455	1.799615	3.004589
1	5.718283	-0.325037	0.063235
1	4.698730	2.522627	3.117550
1	6.397321	1.473398	1.639536
1	1.663542	2.076238	-0.720988
1	-0.913264	2.695085	2.667422
1	1.804779	4.519713	-1.057955
1	-0.762873	5.131779	2.335300
1	0.585366	6.064195	0.467128
1	4.953478	-1.200027	-2.665932
1	4.455080	-0.591043	-4.250561
1	4.659203	0.556047	-2.912250
1	1.605902	-1.908516	-2.357575
1	0.467214	-5.628184	-0.284661
1	-1.249683	-2.445127	-2.609581
1	-0.787412	-4.831178	-2.316754
1	-2.761133	-2.390275	0.921487
1	-3.027187	0.351401	-2.370953
1	-4.987709	-3.314804	0.333157
1	-5.259949	-0.554898	-2.951076
1	-6.248879	-2.390074	-1.598449
1	-0.735899	-0.204624	3.506051
1	-3.755967	1.124766	0.745246
1	-2.301632	0.148151	5.383750
1	-5.306960	1.494723	2.622973
1	-4.596839	1.004404	4.953431
8	-0.368877	2.124393	-2.798329
6	-1.165323	2.956131	-2.378934
8	-1.964117	2.735128	-1.344274
6	-1.347876	4.305477	-2.977269
1	-0.633066	4.461453	-3.786040
1	-2.368759	4.403286	-3.362294
1	-1.215429	5.070706	-2.204972
1	-1.741391	1.854983	-0.966893

4RE6_Pd

Number of imaginary frequencies : 1

The smallest frequency is : -239.5398 cm(-1)

Electronic energy : HF=-2174.4552537
 Zero-point correction= 0.607616
 Thermal correction to Energy= 0.650902
 Thermal correction to Enthalpy= 0.651846
 Thermal correction to Gibbs Free Energy= 0.529558
 Sum of electronic and zero-point Energies= -2173.847637
 Sum of electronic and thermal Energies= -2173.804352
 Sum of electronic and thermal Enthalpies= -2173.803408
 Sum of electronic and thermal Free Energies= -2173.925696

Cartesian Coordinates

6	-3.910864	0.841600	4.124261
6	-2.625592	0.361452	4.364791
6	-1.747107	0.155604	3.307622
6	-2.139656	0.410479	1.984607
6	-3.433249	0.901715	1.758349
6	-4.308282	1.113507	2.817562
6	-1.160616	0.196572	0.893117
6	-1.427357	-0.394737	-0.311609
6	-2.764413	-0.926066	-0.666025
6	-3.326230	-1.976080	0.072091
6	-4.576678	-2.483437	-0.259489
6	-5.283968	-1.954176	-1.337920
6	-4.726106	-0.924254	-2.090120
6	-3.469853	-0.421546	-1.762772
46	-0.030023	0.082333	-1.770758
6	-0.174336	-1.756662	-0.879816
6	0.538855	-2.249331	0.216878
6	0.743612	-3.621952	0.419303
6	0.280478	-4.570689	-0.485924
6	-0.416292	-4.118354	-1.600174
6	-0.655710	-2.752591	-1.768016
6	1.412408	-3.790283	1.701227
6	1.600491	-2.354709	2.250862
7	1.062906	-1.503817	1.298141
8	2.114166	-2.041717	3.299780
6	1.268117	-0.091876	1.334886
6	2.681394	0.323597	1.469195
6	3.644491	-0.268550	0.642889
6	4.975922	0.126378	0.716551
6	5.363577	1.108439	1.625505
6	4.413288	1.688389	2.462662
6	3.080779	1.298611	2.387124
8	1.765878	-4.789440	2.288144
8	2.000244	0.231976	-2.990930
6	2.873587	-0.619991	-2.897524
6	4.302241	-0.396750	-3.243802
6	0.221390	0.730185	1.132461
6	0.374655	2.206315	1.006086
6	1.171667	2.744577	-0.012549
6	1.257763	4.119604	-0.197601
6	0.561062	4.984121	0.644310
6	-0.220054	4.461280	1.670495
6	-0.320171	3.084259	1.847257
8	2.634498	-1.847692	-2.445705
1	3.342000	-1.041565	-0.066704
1	2.341934	1.744127	3.051128
1	5.713072	-0.336669	0.063019
1	4.713300	2.444085	3.185338
1	6.405305	1.415250	1.686175
1	1.706462	2.071443	-0.682356
1	-0.933445	2.690933	2.655775
1	1.868370	4.515846	-1.006899
1	-0.760374	5.128025	2.339163
1	0.629157	6.060428	0.501526
1	4.708427	-1.249714	-3.794115
1	4.413696	0.521641	-3.821411
1	4.872259	-0.302942	-2.310237
1	1.691603	-1.890282	-2.178998
1	0.451394	-5.629145	-0.303447
1	-1.264456	-2.435874	-2.614441
1	-0.804308	-4.822922	-2.331390
1	-2.766259	-2.392463	0.910250
1	-3.026664	0.375236	-2.360879
1	-5.000966	-3.298370	0.323305
1	-5.267149	-0.512459	-2.939446
1	-6.263020	-2.351244	-1.596870
1	-0.738533	-0.207855	3.504895
1	-3.754366	1.130669	0.743566
1	-2.304104	0.147475	5.381960
1	-5.304853	1.503329	2.620804

1	-4.596871	1.010221	4.951319
8	-0.345772	2.142170	-2.772507
6	-1.132848	2.979930	-2.347143
8	-1.944354	2.754924	-1.323678
6	-1.299520	4.332336	-2.944491
1	-2.218873	4.347093	-3.541506
1	-1.402757	5.091700	-2.164117
1	-0.452374	4.563421	-3.592016
1	-1.735430	1.866739	-0.957025

4RE7_Pd

Number of imaginary frequencies : 1
The smallest frequency is : -226.6925 cm(-1)

Electronic energy : HF=-1945.4114426
Zero-point correction= 0.544708
Thermal correction to Energy= 0.582339
Thermal correction to Enthalpy= 0.583283
Thermal correction to Gibbs Free Energy= 0.471788
Sum of electronic and zero-point Energies= -1944.866735
Sum of electronic and thermal Energies= -1944.829104
Sum of electronic and thermal Enthalpies= -1944.828160
Sum of electronic and thermal Free Energies= -1944.939654

Cartesian Coordinates

6	-3.514392	3.942234	2.115257
6	-2.366262	3.436953	2.718101
6	-1.592005	2.488573	2.060964
6	-1.961714	2.016319	0.792846
6	-3.115758	2.537829	0.194317
6	-3.883374	3.490649	0.851051
6	-1.101229	1.016751	0.121214
6	-1.540478	-0.029890	-0.624449
6	-2.951177	-0.393980	-0.842539
6	-3.463814	-0.490077	-2.139935
6	-4.789388	-0.853465	-2.353196
6	-5.616239	-1.141250	-1.271853
6	-5.110164	-1.067908	0.023945
6	-3.788065	-0.701331	0.237735
46	-0.038835	-0.759076	-1.812248
6	-0.657324	-1.833641	-0.177123
6	-0.151879	-1.735379	1.119407
6	-0.378374	-2.738316	2.074328
6	-1.088136	-3.890718	1.767232
6	-1.588277	-4.024940	0.477638
6	-1.391433	-3.005627	-0.457360
6	0.188708	-2.293501	3.345213
6	0.790370	-0.894633	3.050119
7	0.553725	-0.655188	1.695776
8	1.343886	-0.152892	3.821234
6	1.145316	0.445879	1.011434
6	2.613099	0.548909	1.160462
6	3.406505	-0.586240	0.957890
6	4.791029	-0.505665	1.060480
6	5.398168	0.706455	1.376233
6	4.612714	1.834348	1.597132
6	3.229852	1.756384	1.493966
8	0.211954	-2.834842	4.424928
8	1.856771	-1.374423	-2.888395
6	2.617869	-2.138529	-2.305713
6	4.074598	-2.227495	-2.603162
6	0.378383	1.234988	0.231808
6	0.944863	2.287123	-0.655183
6	0.452859	3.597120	-0.638476
6	0.962044	4.554262	-1.510273
6	1.959612	4.220642	-2.419486

6	2.451756	2.918829	-2.449431
6	1.950615	1.962900	-1.575614
8	2.237185	-2.937500	-1.321487
1	2.932978	-1.538323	0.711628
1	2.612967	2.633518	1.679656
1	5.396857	-1.396487	0.904667
1	5.080082	2.779638	1.862815
1	6.480307	0.769396	1.463173
1	-0.327829	3.872944	0.067083
1	2.339801	0.945604	-1.599587
1	0.571936	5.569047	-1.476584
1	3.229563	2.643978	-3.158305
1	2.351070	4.969925	-3.103650
1	4.605045	-1.643632	-1.839695
1	4.427563	-3.259198	-2.538571
1	4.283249	-1.799635	-3.584085
1	1.287035	-2.765445	-1.130889
1	-1.247103	-4.642985	2.536518
1	-1.857317	-3.101415	-1.437386
1	-2.158629	-4.905826	0.194582
1	-2.807187	-0.270295	-2.981738
1	-3.383592	-0.651476	1.248629
1	-5.176767	-0.915051	-3.367843
1	-5.748293	-1.303287	0.872754
1	-6.651795	-1.429249	-1.437928
1	-0.684972	2.105865	2.529380
1	-3.400864	2.200241	-0.799644
1	-2.067994	3.784317	3.704676
1	-4.771972	3.890340	0.367509
1	-4.115421	4.691185	2.625717

-----End of Supplementary Information, Part-B-----