Computational and Experimental Studies on Cu/Au-catalyzed Stereoselective Synthesis of 1,3-disubstituted Allenes

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1 Computational Methods

The geometries of the stationary points were computed with the meta-hybrid M06-2X[1] density functional, which is known to provide superior performance at a moderate cost.[2] All main group atoms have been described with the 6-31+G(d,p) basis set, and the LANL2DZ ECP was used to describe the Cu, Ag and Au atoms. To benchmark these results we performed DLPNO-CCSD(T) single-point energy calculations on DFT-optimized geometries, using the triple-ζ quality basis set Def2-TZVPP and its associated ECP. To account solvation effects all density functional calculations (geometry optimizations and first and second derivatives) included a dielectric continuum (PCM) surrounding the molecular system with parameters for 1,4-dioxane, as implemented in the Gaussian 09 package.[3–5] Coupled cluster (CC) calculations also included implicit solvation via the COSMO formulation.[6,7] All calculations were performed with the Gaussian09 electronic structure package,[8] and the CC energy refinement was performed with the Orca 3 package.[9] The nature of the stationary points was established obtaining the second derivatives of the energy with respect to the displacement of the atoms (Hessian). Due to the functional dependence on the kinetic energy density, an ultrafine pruned grid (99, 590) was used for all computations. For the topological analysis of the electron density of intermediate (**3**) with the different transition-metals, atoms in molecules (AIM) theory was used.[10]. The electron density ρ, and its associated Laplacian $\nabla^2\rho$, at the BCP was used to define the nature of the chemical bonds. A large value for ρ and a negative value for $\nabla^2\rho$ denotes a shared interaction, whereas a small value for ρ and a positive value for $\nabla^2\rho$ denotes a closed-shell interaction. Natural Bond Orbital (NBO) theory[11–14] was employed to analyze the bonding structure of intermediate (**3**).

2 Figures related to the computational study of the reaction mechanism

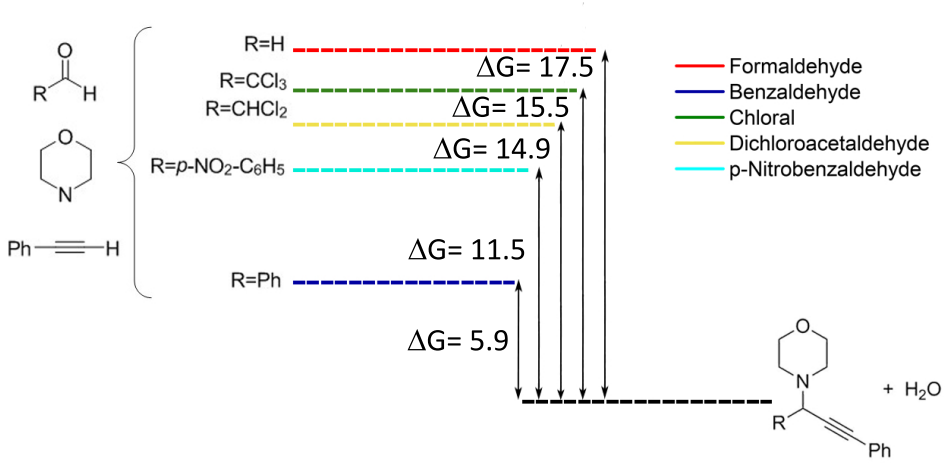

Figure S22 Relative Gibbs free energies (in kcal/mol at the M06-2X/6-31+G(d,p) level) computed for the synthesis of the model Mannich base (propargylamine) with phenylacetylene, morpholine and different aldehydes.

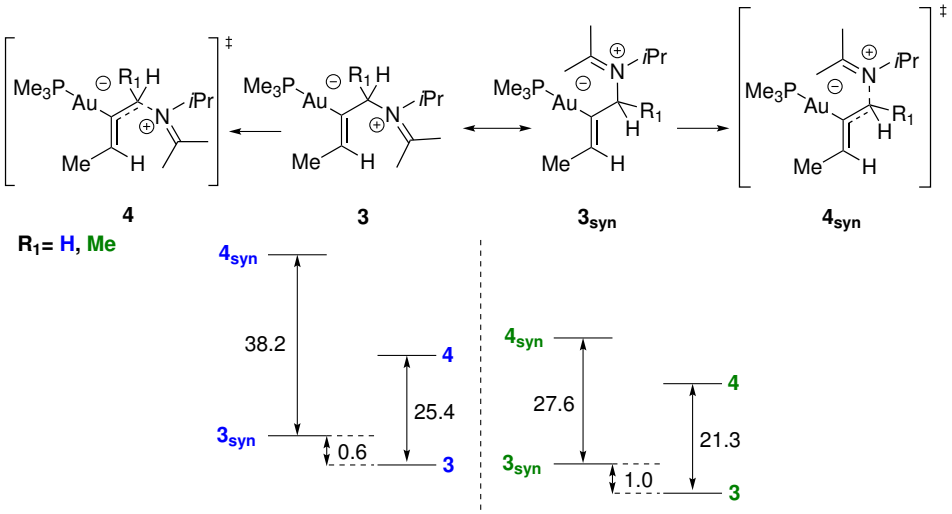

Figure S23 Structures (top) and barriers (bottom, in kcal/mol) of the species involved in the syn- (3syn and 4syn) and anti-(3 and 4) elimination of the imine fragment for the reaction with both formaldehyde (blue) and acetaldehyde (green).

3 Computational Section: Cartesian coordinates

3.1 Reaction with formaldehyde

3.1.1 Non-catalyzed reaction

1
SCF Energy: -446.996957662
Num. Imaginary Frequencies: 0

C	-4.318600	-1.068486	-1.132298
C	-3.573842	-1.664151	-3.651699
C	-3.178622	-1.965707	-5.029373
H	-3.792869	-1.400984	-5.736530
H	-3.302270	-3.029583	-5.247089
N	-5.540025	-0.302777	-0.956020
H	-3.492642	-0.504487	-0.681456
H	-4.403028	-1.995114	-0.554157
C	-5.558770	1.005728	-1.620031
C	-6.144550	1.018690	-3.040310
C	-6.271192	2.033511	-0.737071
H	-4.505763	1.307432	-1.694339
H	-5.628898	0.306355	-3.688489
H	-6.044257	2.018534	-3.474702
H	-7.212233	0.771317	-3.026686
H	-6.220681	3.029926	-1.187385
H	-7.330179	1.780550	-0.614004
H	-5.811699	2.068212	0.253976
C	-6.793390	-1.065866	-0.939064
C	-6.939172	-2.114517	-2.051262
C	-6.999529	-1.710175	0.434590
H	-7.593797	-0.328823	-1.071436
H	-6.796246	-1.678147	-3.042539
H	-6.205171	-2.919034	-1.931687
H	-7.936325	-2.564290	-2.007545
H	-7.962968	-2.228109	0.479595
H	-6.218009	-2.448970	0.644605
H	-6.968218	-0.948780	1.218146
H	-2.132534	-1.700721	-5.202552
C	-3.922945	-1.409821	-2.521167

2
SCF Energy: -446.929171017
Num. Imaginary Frequencies: 1
Imaginary Frequency: -515.7919

C	-3.002491	-1.968352	-2.254103
C	-1.675645	-1.271935	-2.308365
C	-1.192060	-0.142338	-1.887160
C	0.210113	0.281560	-2.206296
N	1.065659	-0.885401	-2.609466
C	1.891429	-1.451037	-1.514520
C	2.913681	-0.424677	-1.022509
C	0.592523	-1.700101	-3.570275
C	0.099474	-1.053353	-4.844872
C	1.118868	-3.106753	-3.720590
C	1.053107	-2.011079	-0.365697
H	-3.391689	-2.157965	-3.260551
H	-3.724626	-1.352099	-1.714663
H	0.209041	1.018537	-3.014369
H	0.707879	0.745846	-1.356256
H	2.465412	-2.262712	-1.965006
H	3.666855	-0.938040	-0.418408
H	3.416497	0.057776	-1.864913
H	2.463166	0.346760	-0.392568
H	0.354052	-2.776984	-0.712627
H	1.715380	-2.450244	0.386366
H	0.462940	-1.220268	0.107221
H	-0.490209	-0.158051	-4.650590
H	-0.520216	-1.754707	-5.406934
H	0.962410	-0.780668	-5.466536
H	0.507362	-3.637113	-4.452250
H	1.098276	-3.672530	-2.788201
H	2.150785	-3.094722	-4.097240
H	-0.860072	-1.936415	-2.915304
H	-2.923737	-2.935869	-1.746437

3
SCF Energy: -446.933951045
Num. Imaginary Frequencies: 0

C	-2.894733	-3.240489	-3.541502
C	-3.415367	-2.906468	-4.919556
C	-3.919561	-3.800455	-5.776117
C	-4.387482	-3.369930	-7.134547
N	-4.465657	-1.866909	-7.387984
C	-3.398618	-1.144559	-7.511249
C	-3.450660	0.359753	-7.589941
C	-5.816864	-1.261269	-7.254019
C	-6.476749	-1.658036	-5.935330
C	-6.655125	-1.629741	-8.477614
C	-2.047756	-1.774207	-7.678780
H	-1.842486	-2.949627	-3.422382
H	-2.978069	-4.315621	-3.363573
H	-3.748646	-3.776526	-7.924366
H	-5.396088	-3.732078	-7.338716
H	-5.687238	-0.179607	-7.245658
H	-7.613720	-1.107380	-8.424347
H	-6.150169	-1.333710	-9.401535
H	-6.858566	-2.702795	-8.519309
H	-5.862448	-1.358525	-5.084202
H	-7.444669	-1.153002	-5.873243
H	-6.641296	-2.735965	-5.863818
H	-2.003937	-2.796171	-7.311476
H	-1.310157	-1.177221	-7.138274
H	-1.777937	-1.740579	-8.742543
H	-2.450182	0.747282	-7.779761
H	-3.809760	0.791903	-6.651380
H	-4.108319	0.697731	-8.395976
H	-3.339697	-1.818490	-5.146982
H	-3.457776	-2.716490	-2.757570

4
SCF Energy: -446.931166093
Num. Imaginary Frequencies: 1
Imaginary Frequency: -393.3431

C	-2.909292	-3.395153	-3.497131
C	-3.414513	-3.085466	-4.884732
C	-3.868779	-3.970890	-5.764634
C	-4.349928	-3.752124	-7.090254
N	-4.519524	-2.094641	-7.556009
C	-3.473012	-1.342382	-7.560599
C	-3.519155	0.151898	-7.357533
C	-5.880127	-1.536708	-7.416113
C	-6.390757	-1.663732	-5.982399
C	-6.814965	-2.202957	-8.426850
C	-2.132653	-1.975858	-7.825855
H	-1.873029	-3.060770	-3.360785
H	-2.951663	-4.471476	-3.313667
H	-3.700195	-4.132413	-7.880677
H	-5.371957	-4.085381	-7.264112
H	-5.829484	-0.476989	-7.681047
H	-7.766220	-1.664065	-8.440667
H	-6.386942	-2.173153	-9.432366
H	-7.027879	-3.243176	-8.168394
H	-5.726816	-1.155372	-5.278347
H	-7.386805	-1.217073	-5.915210
H	-6.454473	-2.711874	-5.676987
H	-2.154561	-2.535711	-8.765258
H	-1.895292	-2.675782	-7.018493
H	-1.350389	-1.219406	-7.884976
H	-2.548648	0.502803	-7.004821
H	-4.278920	0.452563	-6.635253
H	-3.727544	0.656000	-8.309151
H	-3.383811	-2.002729	-5.137670
H	-3.509110	-2.890232	-2.729336

5
SCF Energy: -155.902157265
Num. Imaginary Frequencies: 0

C	-1.538830	1.320011	0.947504
C	-2.512430	1.415156	0.077466
C	-3.482586	1.512490	-0.795987
C	-3.336037	2.118984	-2.168788
H	-3.586086	1.385378	-2.941347
H	-2.314895	2.466309	-2.335793
H	-4.017264	2.966991	-2.288608
H	-4.463695	1.130622	-0.515831
H	-0.895306	0.445169	0.976549
H	-1.347612	2.112860	1.665224

6
SCF Energy: -291.075921311
Num. Imaginary Frequencies: 0

N	-0.030672	-0.157823	-0.077543
C	1.112667	0.337708	0.179803
C	1.444599	1.676975	0.813682
H	0.667932	2.045939	1.480440
H	2.378393	1.595716	1.376523
H	1.603351	2.422710	0.026097
C	2.329664	-0.470600	-0.201587
H	3.002416	0.127100	-0.827308
H	2.892452	-0.752165	0.695509
H	2.031390	-1.370218	-0.739741
C	-1.301383	0.513761	0.222408
H	-2.052915	-0.099537	-0.288125
C	-1.443101	1.926070	-0.358099
H	-2.499729	2.211120	-0.358106
H	-0.897943	2.681177	0.212223
H	-1.086933	1.950790	-1.392522
C	-1.635418	0.447403	1.715676
H	-2.656046	0.803995	1.885453
H	-1.566659	-0.583588	2.072857
H	-0.959123	1.061474	2.316850

3.1.2 CuBr-catalyzed reaction

1_CuBr
SCF Energy: -656.400487310
Num. Imaginary Frequencies: 0

C	-3.073827	-2.068971	-3.724209
C	-1.945256	-2.202461	-2.793589
Cu	-2.540892	-2.632561	-0.718886
Br	-3.816571	-3.055210	1.198756
C	-0.919624	-2.270089	-2.128932
C	0.448173	-2.342670	-1.516493
N	1.527427	-1.900511	-2.361439
C	1.792756	-0.456801	-2.399162
C	0.555354	0.424689	-2.617827
C	1.737505	-2.669678	-3.593836
C	3.235114	-2.855953	-3.848105
C	1.045858	-2.103947	-4.842942
C	2.548126	-0.024140	-1.140374
H	-2.686537	-1.834239	-4.720111
H	-3.645155	-2.997507	-3.783281
H	0.447858	-1.757323	-0.591736
H	0.618400	-3.385275	-1.224377
H	1.310072	-3.661123	-3.395553
H	2.465476	-0.302743	-3.249928
H	3.460609	-0.614109	-1.024389
H	2.814902	1.035587	-1.196693
H	1.935439	-0.160082	-0.242298
H	0.005427	0.137998	-3.517996
H	-0.130961	0.360287	-1.765759
H	0.859274	1.471136	-2.716452
H	-0.030294	-1.989252	-4.691686
H	1.462442	-1.127751	-5.114539
H	1.201818	-2.776670	-5.691652
H	3.724007	-1.895972	-4.046347
H	3.715181	-3.310750	-2.978290
H	3.399875	-3.496503	-4.719761
H	-3.743107	-1.264001	-3.413743

2_CuBr
SCF Energy: -656.366387713
Num. Imaginary Frequencies: 1
Imaginary Frequency: -700.0722

C	-3.375317	-2.877336	-3.012087
C	-3.747802	-2.838652	-4.448342
C	-4.237931	-3.464811	-5.456424
C	-4.305345	-2.864561	-6.857052
N	-4.223325	-1.403049	-6.807535
C	-3.217914	-0.917959	-5.989508
C	-3.276789	0.533629	-5.551547
Cu	-4.923926	-5.331151	-5.101543
Br	-5.745852	-7.503341	-4.681026
C	-5.532700	-0.706764	-6.825181
C	-6.409913	-1.033544	-5.614616
C	-6.268217	-0.974003	-8.138651
C	-1.811531	-1.368832	-6.357130
H	-2.305193	-2.694675	-2.880442
H	-3.608783	-3.866351	-2.609341
H	-3.484529	-3.279641	-7.448131
H	-5.228878	-3.144296	-7.360609
H	-5.296460	0.358997	-6.816697
H	-7.092842	-0.262795	-8.234921
H	-5.597545	-0.844582	-8.991944
H	-6.702142	-1.976841	-8.179681
H	-5.906854	-0.805696	-4.669912
H	-7.332685	-0.448623	-5.664585
H	-6.678640	-2.094728	-5.599688
H	-1.753683	-2.440032	-6.549741
H	-1.120701	-1.131995	-5.544933
H	-1.490991	-0.830142	-7.255275
H	-2.442543	0.731259	-4.876186
H	-4.202264	0.787062	-5.033157
H	-3.167397	1.190498	-6.421865
H	-3.413864	-1.586918	-4.885709
H	-3.928990	-2.128182	-2.439808

3_CuBr
SCF Energy: -656.395932206
Num. Imaginary Frequencies: 0

C	-2.889224	-2.992396	-3.302390
C	-2.973293	-2.719259	-4.780699
C	-3.463037	-3.574929	-5.688499
C	-3.494173	-3.214517	-7.155764
N	-3.075895	-1.818491	-7.514381
C	-1.830202	-1.480367	-7.558300
C	-1.395182	-0.089952	-7.927667
Cu	-4.167106	-5.403308	-5.259764
Br	-5.001774	-7.590549	-4.827688
C	-4.177981	-0.850677	-7.785038
C	-5.240395	-0.898003	-6.689574
C	-4.745640	-1.117060	-9.178120
C	-0.736777	-2.458864	-7.268141
H	-1.855624	-2.927982	-2.941686
H	-3.270678	-3.991582	-3.072656
H	-2.862185	-3.891049	-7.738565
H	-4.503439	-3.327312	-7.554621
H	-3.732292	0.143302	-7.766509
H	-5.505805	-0.365380	-9.403224
H	-3.965753	-1.061292	-9.942792
H	-5.218695	-2.100993	-9.233990
H	-4.806946	-0.705319	-5.706955
H	-5.978574	-0.121989	-6.907303
H	-5.759045	-1.858716	-6.651112
H	-1.072814	-3.356506	-6.756029
H	0.012796	-1.958235	-6.649317
H	-0.247012	-2.717946	-8.215005
H	-0.319120	-0.081583	-8.098419
H	-1.612609	0.603402	-7.107945
H	-1.896429	0.272946	-8.827101
H	-2.595578	-1.723782	-5.063708
H	-3.473478	-2.262913	-2.728587

4_CuBr
SCF Energy: -656.369646392
Num. Imaginary Frequencies: 1
Imaginary Frequency: -342.1706

C	-3.353792	-2.015980	-2.384812
C	-1.915539	-1.582216	-2.400791
C	-1.434484	-0.438173	-1.937557
Cu	-2.609099	1.030145	-1.087850
Br	-4.074964	2.631879	-0.163703
C	-0.246315	0.240941	-1.773139
N	1.352717	-0.873768	-2.535344
C	2.194731	-1.528990	-1.528168
C	2.900819	-0.469015	-0.684900
C	1.323796	-1.277278	-3.747147
C	0.453239	-0.593770	-4.764327
C	2.145110	-2.436838	-4.273918
C	1.333102	-2.465195	-0.679407
H	-3.718542	-2.198860	-3.401118
H	-3.990271	-1.256089	-1.923003
H	-0.021558	1.103932	-2.395303
H	0.195231	0.280977	-0.780031
H	2.969316	-2.124929	-2.024769
H	3.597642	-0.952774	0.004902
H	3.464432	0.220145	-1.319168
H	2.192155	0.112737	-0.088853
H	0.866614	-3.237864	-1.297756
H	1.950633	-2.953414	0.079388
H	0.535508	-1.914057	-0.171960
H	-0.098719	0.248834	-4.353583
H	-0.258326	-1.314825	-5.179698
H	1.080175	-0.248709	-5.593695
H	1.848639	-2.674223	-5.296264
H	2.015823	-3.330169	-3.657458
H	3.209845	-2.182979	-4.279175
H	-1.199385	-2.288545	-2.839178
H	-3.472189	-2.950454	-1.826267

5_CuBr
SCF Energy: -365.303404440
Num. Imaginary Frequencies: 0

C	-3.214778	-5.575515	-3.551196
C	-3.297503	-4.311270	-3.143136
C	-3.402205	-3.105784	-2.647712
Cu	-2.753755	-4.436889	-5.352740
Br	-2.213620	-3.563342	-7.457963
C	-3.208365	-1.810957	-3.389722
H	-2.289552	-6.137946	-3.436481
H	-4.103494	-6.115457	-3.873741
H	-3.655404	-3.049165	-1.588826
H	-2.966545	-1.971572	-4.443408
H	-4.118555	-1.208323	-3.329968
H	-2.398475	-1.237128	-2.931312

3.1.3 AgBr-catalyzed reaction

1_AgBr
SCF Energy: -605.875463799
Num. Imaginary Frequencies: 0

C	-3.082790	-2.077211	-3.743261
C	-1.940701	-2.195897	-2.828417
Ag	-2.665380	-2.700240	-0.505519
Br	-4.058988	-3.170230	1.605067
C	-0.913845	-2.251403	-2.168475
C	0.445477	-2.318271	-1.542422
N	1.537763	-1.889366	-2.379605
C	1.813376	-0.447906	-2.422861
C	0.583500	0.440990	-2.653417
C	1.750427	-2.665372	-3.607252
C	3.248257	-2.865495	-3.849539
C	1.072740	-2.099434	-4.864017
C	2.564093	-0.014299	-1.161546
H	-2.713388	-1.838059	-4.744897
H	-3.643818	-3.012460	-3.796396
H	0.439326	-1.721350	-0.624825
H	0.612608	-3.357302	-1.234622
H	1.313093	-3.652372	-3.408056
H	2.492483	-0.302295	-3.270048
H	3.472194	-0.609435	-1.037786
H	2.837710	1.043574	-1.220359
H	1.945448	-0.143201	-0.266452
H	0.036911	0.153106	-3.555160
H	-0.108347	0.384907	-1.805174
H	0.894663	1.485034	-2.755196
H	-0.003579	-1.975489	-4.720832
H	1.499405	-1.127851	-5.136618
H	1.229784	-2.776955	-5.708754
H	3.746809	-1.910385	-4.047381
H	3.717839	-3.321115	-2.974422
H	3.414320	-3.510537	-4.717666
H	-3.758517	-1.280275	-3.425720

2_AgBr
SCF Energy: -605.841038967
Num. Imaginary Frequencies: 1
Imaginary Frequency: -721.5291

C	-3.353492	-2.852436	-3.005605
C	-3.727031	-2.810604	-4.442358
C	-4.219005	-3.442516	-5.445303
C	-4.292841	-2.852759	-6.848046
N	-4.215113	-1.388678	-6.806655
C	-3.208941	-0.893276	-5.998577
C	-3.275573	0.557451	-5.560731
Ag	-5.003146	-5.484087	-5.082631
Br	-5.961182	-7.852424	-4.669934
C	-5.527810	-0.698459	-6.825816
C	-6.404275	-1.029273	-5.615968
C	-6.260485	-0.969912	-8.140077
C	-1.801984	-1.339451	-6.367802
H	-2.283474	-2.668531	-2.874493
H	-3.586153	-3.841501	-2.603210
H	-3.473493	-3.267385	-7.441559
H	-5.218066	-3.135107	-7.347008
H	-5.296981	0.368415	-6.817448
H	-7.089623	-0.264026	-8.236742
H	-5.589976	-0.835780	-8.992747
H	-6.687871	-1.975539	-8.182095
H	-5.903711	-0.796909	-4.671110
H	-7.330990	-0.450854	-5.668094
H	-6.665860	-2.092403	-5.599736
H	-1.740558	-2.410985	-6.557529
H	-1.109976	-1.097326	-5.558211
H	-1.485671	-0.802274	-7.268496
H	-2.439435	0.760939	-4.889483
H	-4.200255	0.804528	-5.037818
H	-3.174998	1.215603	-6.431324
H	-3.397472	-1.569094	-4.884711
H	-3.906106	-2.103402	-2.431952

3_AgBr
SCF Energy: -605.869995877
Num. Imaginary Frequencies: 0

C	-2.873379	-2.960427	-3.298854
C	-2.962666	-2.698446	-4.778369
C	-3.452349	-3.553017	-5.684874
C	-3.487824	-3.201328	-7.152830
N	-3.070191	-1.805305	-7.516939
C	-1.824661	-1.466432	-7.563373
C	-1.391498	-0.076287	-7.935797
Ag	-4.227747	-5.544473	-5.235935
Br	-5.155750	-7.942343	-4.793401
C	-4.173589	-0.839113	-7.789042
C	-5.234664	-0.884183	-6.692181
C	-4.742585	-1.110114	-9.180677
C	-0.729364	-2.442446	-7.272232
H	-1.838648	-2.889109	-2.942954
H	-3.250844	-3.958691	-3.059732
H	-2.856889	-3.880194	-7.733755
H	-4.498200	-3.315286	-7.547980
H	-3.728704	0.155266	-7.773984
H	-5.503896	-0.359966	-9.406947
H	-3.963719	-1.055514	-9.946447
H	-5.214639	-2.094730	-9.233371
H	-4.800637	-0.687247	-5.710641
H	-5.974207	-0.110009	-6.911699
H	-5.752292	-1.845382	-6.649831
H	-1.063619	-3.344809	-6.767388
H	0.014192	-1.942070	-6.645829
H	-0.232433	-2.693329	-8.217495
H	-0.315162	-0.066166	-8.104618
H	-1.612034	0.619091	-7.118648
H	-1.891910	0.282793	-8.837259
H	-2.586239	-1.704573	-5.068673
H	-3.457811	-2.227462	-2.729794

4_AgBr
SCF Energy: -605.845581084
Num. Imaginary Frequencies: 1
Imaginary Frequency: -335.1878

C	-3.320858	-2.043016	-2.417101
C	-1.889482	-1.587230	-2.421589
C	-1.419775	-0.440469	-1.954938
Ag	-2.742534	1.133761	-0.987277
Br	-4.331735	2.862336	0.105266
C	-0.224811	0.233452	-1.796938
N	1.356631	-0.884179	-2.545887
C	2.195551	-1.533083	-1.531446
C	2.909342	-0.467923	-0.701059
C	1.330452	-1.295535	-3.755351
C	0.467023	-0.615289	-4.780525
C	2.149549	-2.461580	-4.270630
C	1.331532	-2.456752	-0.671694
H	-3.670734	-2.242153	-3.435610
H	-3.974690	-1.288902	-1.970659
H	-0.004081	1.096435	-2.420400
H	0.212883	0.281170	-0.802704
H	2.966123	-2.137816	-2.023281
H	3.605151	-0.948595	-0.008132
H	3.475452	0.211116	-1.343961
H	2.205955	0.124289	-0.109150
H	0.859193	-3.232697	-1.281364
H	1.949527	-2.940974	0.089248
H	0.538505	-1.897436	-0.166158
H	-0.084445	0.231259	-4.377256
H	-0.244259	-1.336573	-5.195810
H	1.099846	-0.276849	-5.608168
H	1.855103	-2.705787	-5.291933
H	2.015343	-3.349616	-3.647597
H	3.215110	-2.211268	-4.274865
H	-1.163387	-2.285944	-2.856663
H	-3.431135	-2.973676	-1.850422

5_AgBr
SCF Energy: -314.780874967
Num. Imaginary Frequencies: 0

C	-3.234983	-5.572157	-3.473847
C	-3.317412	-4.310372	-3.068019
C	-3.420090	-3.101776	-2.581827
Ag	-2.698186	-4.449090	-5.571692
Br	-2.083351	-3.581879	-7.912450
C	-3.226580	-1.809872	-3.328410
H	-2.309310	-6.133563	-3.362069
H	-4.122989	-6.111661	-3.797398
H	-3.671642	-3.037484	-1.522922
H	-2.998920	-1.976258	-4.384343
H	-4.131417	-1.200042	-3.260713
H	-2.407372	-1.239194	-2.882518

3.1.4 AuBr-catalyzed reaction

1_AuBr
SCF Energy: -595.508338544
Num. Imaginary Frequencies: 0

C	-2.924655	-1.809679	-3.726141
C	-1.927007	-2.105931	-2.688179
Au	-2.606372	-2.955389	-0.711543
Br	-4.017126	-3.860126	1.176603
C	-0.914607	-2.246201	-1.992002
C	0.481414	-2.296649	-1.438131
N	1.518520	-1.878963	-2.342143
C	1.768611	-0.437570	-2.459383
C	0.516964	0.420613	-2.689841
C	1.716281	-2.711813	-3.533874
C	3.210847	-2.885682	-3.814409
C	0.984576	-2.227711	-4.793931
C	2.552736	0.066678	-1.245511
H	-2.417416	-1.356190	-4.583247
H	-3.427368	-2.721395	-4.054362
H	0.506121	-1.678531	-0.535066
H	0.668258	-3.326644	-1.115009
H	1.312017	-3.697926	-3.271607
H	2.416668	-0.321086	-3.334843
H	3.472698	-0.510180	-1.122642
H	2.809544	1.123595	-1.365133
H	1.964484	-0.025336	-0.325903
H	-0.051088	0.083131	-3.561358
H	-0.147019	0.392589	-1.818534
H	0.806810	1.463343	-2.850632
H	-0.091110	-2.136437	-4.623967
H	1.367509	-1.255272	-5.122487
H	1.139593	-2.937527	-5.611969
H	3.676681	-1.930767	-4.080837
H	3.720211	-3.280249	-2.931959
H	3.366670	-3.573495	-4.650917
H	-3.674572	-1.109793	-3.352670

2_AuBr
SCF Energy: -595.484641198
Num. Imaginary Frequencies: 1
Imaginary Frequency: -636.3557

C	-3.379233	-2.823318	-2.991788
C	-3.767175	-2.883171	-4.413377
C	-4.241948	-3.460028	-5.449761
C	-4.289668	-2.852880	-6.857523
N	-4.213157	-1.401112	-6.816586
C	-3.209527	-0.924637	-5.955274
C	-3.259100	0.547541	-5.576067
Au	-4.974761	-5.377780	-5.171984
Br	-5.904833	-7.737969	-4.894973
C	-5.526489	-0.714068	-6.815464
C	-6.383097	-1.030042	-5.586049
C	-6.287514	-0.998135	-8.110751
C	-1.801694	-1.364119	-6.345651
H	-2.309316	-2.626871	-2.884206
H	-3.599795	-3.793533	-2.537758
H	-3.455849	-3.277952	-7.422784
H	-5.203284	-3.153625	-7.366148
H	-5.295838	0.353067	-6.823059
H	-7.115355	-0.289787	-8.200544
H	-5.633166	-0.878891	-8.978078
H	-6.720937	-2.002058	-8.130722
H	-5.863084	-0.796790	-4.651274
H	-7.304774	-0.442267	-5.621430
H	-6.656921	-2.090132	-5.559267
H	-1.730415	-2.439717	-6.510775
H	-1.097806	-1.098015	-5.553538
H	-1.506370	-0.845607	-7.263384
H	-2.425636	0.766151	-4.905761
H	-4.183733	0.828486	-5.069957
H	-3.143172	1.167290	-6.471742
H	-3.406859	-1.525854	-4.909111
H	-3.941043	-2.052231	-2.458482

3_AuBr
SCF Energy: -595.528417203
Num. Imaginary Frequencies: 0

C	-2.890687	-2.957142	-3.286374
C	-2.977622	-2.701271	-4.764764
C	-3.452292	-3.557406	-5.678997
C	-3.491189	-3.204772	-7.152224
N	-3.072745	-1.814106	-7.500953
C	-1.825091	-1.483977	-7.563705
C	-1.389879	-0.098396	-7.947111
Au	-4.160783	-5.422803	-5.315795
Br	-5.067703	-7.818298	-4.883465
C	-4.175447	-0.844917	-7.774315
C	-5.238755	-0.890345	-6.679785
C	-4.742398	-1.113685	-9.167212
C	-0.732060	-2.461295	-7.272743
H	-1.856811	-2.873740	-2.931544
H	-3.260592	-3.956003	-3.043439
H	-2.864811	-3.888197	-7.731331
H	-4.504328	-3.321155	-7.538183
H	-3.726615	0.147541	-7.756818
H	-5.499922	-0.360006	-9.394151
H	-3.962501	-1.062346	-9.932111
H	-5.219260	-2.095875	-9.220836
H	-4.809527	-0.687545	-5.697384
H	-5.979967	-0.119332	-6.904333
H	-5.754157	-1.852678	-6.635728
H	-1.064621	-3.368076	-6.774751
H	0.008376	-1.962207	-6.641206
H	-0.230575	-2.705151	-8.217337
H	-0.315546	-0.093864	-8.128001
H	-1.598342	0.600110	-7.129221
H	-1.899634	0.260024	-8.843436
H	-2.616653	-1.710755	-5.068739
H	-3.481823	-2.223633	-2.725556

4_AuBr
SCF Energy: -595.488902344
Num. Imaginary Frequencies: 1
Imaginary Frequency: -365.4481

C	-3.555452	-2.041679	-2.217075
C	-2.113014	-1.635739	-2.263767
C	-1.606037	-0.472529	-1.887234
Au	-2.572513	1.212653	-1.104784
Br	-4.019971	3.107138	-0.181584
C	-0.389933	0.189377	-1.797349
N	1.207417	-1.150071	-2.548416
C	2.076759	-1.746272	-1.531771
C	2.962274	-0.658769	-0.923135
C	1.424615	-1.305785	-3.795788
C	0.478172	-0.717478	-4.806775
C	2.598660	-2.071045	-4.373336
C	1.209826	-2.437920	-0.480747
H	-3.917096	-2.300608	-3.217504
H	-4.178052	-1.236945	-1.819690
H	-0.103691	0.927830	-2.541237
H	0.119536	0.257943	-0.840759
H	2.723247	-2.508336	-1.984197
H	3.616244	-1.090356	-0.160633
H	3.584892	-0.186120	-1.688323
H	2.356087	0.119255	-0.448848
H	0.577442	-3.201671	-0.941354
H	1.846184	-2.919315	0.266952
H	0.558880	-1.724757	0.033871
H	-0.432665	-0.334943	-4.347441
H	0.207453	-1.487097	-5.536955
H	0.979407	0.083725	-5.361063
H	2.683769	-1.874694	-5.443068
H	2.454780	-3.148330	-4.238671
H	3.538948	-1.793591	-3.891743
H	-1.393065	-2.366239	-2.644879
H	-3.686758	-2.927154	-1.586750

5_AuBr
SCF Energy: -304.414762453
Num. Imaginary Frequencies: 0

C	-3.207441	-5.582558	-3.563836
C	-3.268515	-4.262415	-3.258684
C	-3.399963	-3.094804	-2.678299
Au	-2.728463	-4.477304	-5.427474
Br	-2.137804	-3.767071	-7.779708
C	-3.229249	-1.742198	-3.306517
H	-2.308551	-6.155582	-3.348328
H	-4.114657	-6.134713	-3.798263
H	-3.662372	-3.133476	-1.620461
H	-2.983638	-1.817955	-4.367537
H	-4.149961	-1.162257	-3.198655
H	-2.431639	-1.193017	-2.798446

3.1.5 AuCl-catalyzed reaction

1_AuCl
SCF Energy: -597.290746153
Num. Imaginary Frequencies: 0

C	-2.914152	-1.777253	-3.707823
C	-1.928220	-2.095125	-2.664625
Au	-2.594544	-2.988772	-0.729680
Cl	-3.946862	-3.905618	1.034570
C	-0.915411	-2.244706	-1.968254
C	0.484890	-2.291415	-1.423727
N	1.515469	-1.878133	-2.336590
C	1.763925	-0.437567	-2.464901
C	0.510700	0.417613	-2.697984
C	1.708727	-2.719615	-3.522966
C	3.202154	-2.895538	-3.808169
C	0.971992	-2.244738	-4.783531
C	2.551182	0.076521	-1.257198
H	-2.398330	-1.299352	-4.546262
H	-3.407650	-2.682897	-4.065499
H	0.514096	-1.668172	-0.524245
H	0.674523	-3.319369	-1.096023
H	1.305494	-3.703786	-3.252031
H	2.409268	-0.326986	-3.343122
H	3.471695	-0.499016	-1.132325
H	2.807283	1.132514	-1.386009
H	1.965564	-0.008241	-0.335221
H	-0.059045	0.073218	-3.565741
H	-0.150784	0.395083	-1.824632
H	0.798755	1.459486	-2.867296
H	-0.103024	-2.152513	-4.609944
H	1.353515	-1.274733	-5.120828
H	1.123749	-2.960540	-5.596935
H	3.666915	-1.942558	-4.083266
H	3.715007	-3.283791	-2.924939
H	3.354644	-3.589364	-4.640302
H	-3.672654	-1.091231	-3.326130

2_AuCl
SCF Energy: -597.267370698
Num. Imaginary Frequencies: 1
Imaginary Frequency: -601.8448

C	-3.382782	-2.828796	-2.992302
C	-3.771878	-2.894706	-4.412550
C	-4.244646	-3.465965	-5.452642
C	-4.288190	-2.855073	-6.859940
N	-4.213268	-1.404271	-6.817241
C	-3.210574	-0.928985	-5.951365
C	-3.259991	0.544577	-5.576131
Au	-4.977346	-5.370902	-5.178381
Cl	-5.872529	-7.614581	-4.913416
C	-5.527403	-0.719031	-6.814107
C	-6.381953	-1.036047	-5.583418
C	-6.290260	-1.003775	-8.108138
C	-1.802225	-1.366965	-6.342735
H	-2.312962	-2.631053	-2.886332
H	-3.601501	-3.798248	-2.535638
H	-3.451948	-3.279336	-7.422212
H	-5.199734	-3.157198	-7.371327
H	-5.298099	0.348409	-6.822007
H	-7.119610	-0.296952	-8.196044
H	-5.637678	-0.882811	-8.976562
H	-6.721913	-2.008474	-8.127936
H	-5.860677	-0.802421	-4.649387
H	-7.304191	-0.449049	-5.617074
H	-6.654868	-2.096390	-5.556387
H	-1.729058	-2.442859	-6.505373
H	-1.097901	-1.097958	-5.551952
H	-1.508662	-0.850120	-7.261916
H	-2.427290	0.764674	-4.905326
H	-4.185050	0.827239	-5.071717
H	-3.142855	1.161807	-6.473325
H	-3.408865	-1.525266	-4.909653
H	-3.945639	-2.057528	-2.460736

3_AuCl
SCF Energy: -597.312090535
Num. Imaginary Frequencies: 0

C	-2.895003	-2.960732	-3.286059
C	-2.984139	-2.704599	-4.764298
C	-3.455341	-3.563096	-5.678542
C	-3.496252	-3.207731	-7.151589
N	-3.075756	-1.817715	-7.499257
C	-1.827453	-1.490207	-7.562097
C	-1.389400	-0.105433	-7.945124
Au	-4.149374	-5.425082	-5.321289
Cl	-4.993419	-7.706160	-4.911649
C	-4.176558	-0.846542	-7.772911
C	-5.240477	-0.890172	-6.678890
C	-4.743396	-1.114330	-9.166053
C	-0.736342	-2.469674	-7.271204
H	-1.860925	-2.875186	-2.932210
H	-3.262313	-3.960415	-3.042862
H	-2.872274	-3.891594	-7.732697
H	-4.510412	-3.322028	-7.535493
H	-3.725950	0.145122	-7.755205
H	-5.499364	-0.359235	-9.393477
H	-3.963002	-1.064608	-9.930558
H	-5.222048	-2.095644	-9.219749
H	-4.811592	-0.687003	-5.696429
H	-5.980830	-0.118602	-6.904387
H	-5.756763	-1.851993	-6.634345
H	-1.070755	-3.376998	-6.775469
H	0.003604	-1.972668	-6.637403
H	-0.233507	-2.712116	-8.215445
H	-0.314970	-0.102903	-8.125454
H	-1.596991	0.593336	-7.127236
H	-1.898030	0.254101	-8.841660
H	-2.627824	-1.712635	-5.068259
H	-3.487102	-2.228760	-2.724250

4_AuCl
SCF Energy: -597.271898157
Num. Imaginary Frequencies: 1
Imaginary Frequency: -370.4829

C	-3.550373	-2.043816	-2.220781
C	-2.109501	-1.632254	-2.264409
C	-1.609010	-0.467108	-1.884687
Au	-2.562744	1.208183	-1.104535
Cl	-3.932401	3.015689	-0.221827
C	-0.393241	0.198138	-1.792275
N	1.203349	-1.143449	-2.545861
C	2.072332	-1.741370	-1.529916
C	2.959575	-0.655180	-0.921471
C	1.417841	-1.302006	-3.793361
C	0.472442	-0.711102	-4.803823
C	2.587526	-2.073306	-4.371848
C	1.205100	-2.432134	-0.478524
H	-3.909608	-2.302051	-3.222262
H	-4.176735	-1.242404	-1.822748
H	-0.105383	0.935866	-2.536120
H	0.117536	0.263388	-0.836264
H	2.717685	-2.504140	-1.982718
H	3.613459	-1.087802	-0.159478
H	3.582310	-0.183134	-1.686931
H	2.354671	0.123511	-0.446621
H	0.571846	-3.195386	-0.938758
H	1.841317	-2.914026	0.268978
H	0.554968	-1.718393	0.036337
H	-0.434719	-0.320980	-4.343660
H	0.194749	-1.481495	-5.530594
H	0.977497	0.084787	-5.362274
H	2.669759	-1.881466	-5.442617
H	2.440927	-3.149598	-4.232360
H	3.530292	-1.796823	-3.894516
H	-1.385725	-2.358596	-2.645669
H	-3.679396	-2.931067	-1.592459

5_AuCl
SCF Energy: -306.197184188
Num. Imaginary Frequencies: 0

C	-3.202731	-5.577640	-3.588145
C	-3.261791	-4.253753	-3.286892
C	-3.395591	-3.093135	-2.692157
Au	-2.729392	-4.472409	-5.429138
Cl	-2.162340	-3.823602	-7.675271
C	-3.229044	-1.733842	-3.306092
H	-2.306022	-6.151878	-3.366881
H	-4.111821	-6.130097	-3.814372
H	-3.656067	-3.144383	-1.634471
H	-2.991586	-1.797677	-4.369611
H	-4.148506	-1.154571	-3.184936
H	-2.427360	-1.190362	-2.798241

3.1.6 $AuPMe_3$-catalyzed reaction

1_AuPMe3
SCF Energy: -1043.19818559
Num. Imaginary Frequencies: 0

C	-0.164868	0.200514	-0.070099
H	0.080948	0.300599	0.988737
H	0.746898	-0.058817	-0.616772
C	-0.689030	1.459061	-0.614780
C	-0.982890	2.500031	-1.197818
C	-1.078449	3.736105	-2.052362
H	-1.180216	4.595319	-1.379913
H	-2.005109	3.674944	-2.632140
P	-4.681413	2.427723	1.574328
C	-4.739733	3.935132	2.594029
H	-5.679346	3.961190	3.153296
H	-3.899753	3.942191	3.291390
H	-4.675850	4.815575	1.951675
C	-4.934000	1.046130	2.734268
H	-5.864610	1.200521	3.287449
H	-4.098518	0.996906	3.435613
H	-4.991572	0.106386	2.181105
C	-6.184259	2.482967	0.547851
H	-7.064440	2.561867	1.191993
H	-6.142225	3.347567	-0.117745
H	-6.253270	1.574524	-0.053492
N	0.032512	3.946034	-2.935592
C	1.332712	4.200601	-2.300685
H	1.098474	4.573935	-1.295096
C	2.073887	5.312839	-3.045363
H	1.451768	6.208401	-3.112478
H	3.003982	5.565212	-2.527932
H	2.336486	5.000745	-4.061542
C	2.230576	2.965195	-2.145167
H	1.731798	2.168472	-1.587092
H	3.144495	3.234904	-1.608073
H	2.527553	2.569137	-3.122218
C	0.017100	3.235196	-4.220946
H	1.022111	3.361166	-4.636826
C	-0.260889	1.729188	-4.123078
H	-1.281601	1.538058	-3.771940
H	0.434037	1.231508	-3.440981
H	-0.161944	1.269043	-5.110414
C	-0.960537	3.905587	-5.188144
H	-1.993602	3.824955	-4.831464
H	-0.717762	4.965013	-5.299179
H	-0.916660	3.427321	-6.170933
H	-0.884520	-0.610699	-0.196246
Au	-2.746907	2.211537	0.339811

2_AuPMe3
SCF Energy: -1043.17997431
Num. Imaginary Frequencies: 1
Imaginary Frequency: -564.6153

C	-0.083123	-1.302451	0.609095
C	0.046529	-0.599730	1.897169
C	0.670353	-0.029229	2.849002
C	0.038760	0.512253	4.145394
H	-0.547313	-2.282614	0.744095
H	0.917097	-1.449113	0.190612
H	0.547892	1.419902	4.463790
H	0.207785	-0.240504	4.920218
Au	2.774856	0.158154	2.581475
P	5.072955	0.432588	2.366621
C	5.905998	0.825064	3.941339
H	5.735500	0.018387	4.657356
H	5.498427	1.751998	4.350268
H	6.980389	0.942525	3.774836
C	5.552765	1.783850	1.238575
H	5.128444	2.725085	1.594248
H	5.167335	1.579175	0.237520
H	6.642470	1.868430	1.198927
C	5.946927	-1.037761	1.732842
H	5.771391	-1.883817	2.400536
H	7.020313	-0.837063	1.674356
H	5.569866	-1.287877	0.739045
N	-1.372709	0.783188	3.973311
C	-1.144091	2.592333	2.233944
H	-2.789526	2.222656	3.567356
H	-1.487557	3.600677	1.987228
C	-1.699527	2.179997	3.600013
H	-0.048540	2.599580	2.242720
H	-1.468275	1.915178	1.437108
C	-2.067420	-0.262414	3.332298
H	-1.413649	-0.485213	2.337555
H	-2.456630	-2.378608	3.480389
C	-2.017987	-1.586035	4.090813
H	-1.000961	-1.885243	4.347754
C	-3.469366	0.047451	2.828759
H	-3.878991	-0.847685	2.357299
H	-3.494143	0.856073	2.096983
H	-4.118109	0.311089	3.670651
C	-1.264117	3.153220	4.695280
H	-1.740242	4.121513	4.521258
H	-0.183486	3.324503	4.700143
H	-1.568928	2.790129	5.679906
H	-2.601511	-1.493520	5.011990
H	-0.676385	-0.720717	-0.100445

3_AuPMe3
SCF Energy: -1043.22872981
Num. Imaginary Frequencies: 0

C	0.058394	0.074187	0.052448
C	0.045323	0.071128	1.555151
C	1.120515	0.039947	2.352937
C	0.985521	0.030959	3.861880
H	-0.503601	-0.777550	-0.346500
H	1.079531	0.025118	-0.334770
H	-0.962210	0.107663	1.987243
H	1.380502	-0.898265	4.282240
H	1.578619	0.835932	4.298393
Au	3.079609	-0.012889	1.678407
P	5.312824	-0.069987	0.892552
C	6.194926	1.530541	0.956586
C	5.482130	-0.591443	-0.851761
H	6.534808	-0.590650	-1.148736
H	4.923989	0.094482	-1.493164
H	5.070680	-1.595941	-0.974249
H	7.214441	1.418579	0.576651
H	5.660433	2.265796	0.350985
H	7.419976	-1.196619	1.364024
H	6.014561	-2.226354	1.746290
C	6.416593	-1.212202	1.798775
H	6.471218	-0.912424	2.847784
H	6.229987	1.887688	1.988168
N	-0.395312	0.206378	4.399254
C	-1.226418	-0.782586	4.461292
C	-0.871175	-2.143600	3.956852
H	-1.736482	-2.546434	3.423713
H	-0.008513	-2.160268	3.295836
H	-0.700931	-2.796667	4.821712
C	-2.595109	-0.629459	5.058096
H	-3.240881	-0.067809	4.373896
H	-3.038238	-1.613678	5.205489
H	-2.571554	-0.106048	6.015785
C	-0.744798	1.576916	4.884047
H	-1.829176	1.600469	4.983243
C	-0.110118	1.798609	6.255385
H	0.981613	1.803410	6.194970
H	-0.417193	1.026545	6.966137
H	-0.428340	2.769351	6.642083
C	-0.353527	2.644106	3.865661
H	-0.822137	2.464488	2.896752
H	0.727584	2.707576	3.720080
H	-0.698985	3.608351	4.246183
H	-0.415703	0.980592	-0.340608

4_AuPMe3
SCF Energy: -1043.18033600
Num. Imaginary Frequencies: 1
Imaginary Frequency: -318.0962

C	6.517049	-0.867140	1.980708
P	5.260466	0.033195	1.012880
C	5.340232	-0.688770	-0.660142
Au	3.112952	-0.038181	1.930856
C	1.000383	-0.267863	2.522858
C	1.240181	0.486506	3.639845
N	-0.749909	0.644757	4.784322
C	-1.433736	1.936106	4.667310
C	-1.737343	2.205226	3.192762
C	0.101922	-0.927609	1.813755
C	0.314359	-1.646333	0.514802
C	5.926000	1.721559	0.832711
C	-1.390562	-0.408163	5.117869
C	-2.870909	-0.447800	5.443036
C	-0.676261	-1.727853	5.220346
C	-0.562791	3.030012	5.279828
H	0.059374	-2.705564	0.616604
H	1.351581	-1.570018	0.178470
H	-0.909146	-0.941998	2.231922
H	1.702090	0.054735	4.523246
H	1.260666	1.570713	3.570143
H	6.922377	1.683279	0.383566
H	5.987963	2.196463	1.814129
H	5.262685	2.310817	0.196423
H	7.490590	-0.794230	1.487710
H	6.584194	-0.436111	2.981817
H	6.360647	-0.621677	-1.047489
H	4.663555	-0.147918	-1.325417
H	5.035069	-1.736814	-0.622032
H	6.230831	-1.917370	2.066953
H	-1.118181	-2.443050	4.518084
H	0.389500	-1.639262	5.015231
H	-0.817775	-2.140373	6.224922
H	-3.467523	0.026535	4.659492
H	-3.205855	-1.479399	5.557964
H	-3.071142	0.079517	6.381184
H	-2.380745	1.917492	5.220240
H	0.367868	3.161145	4.718817
H	-0.309345	2.791410	6.315933
H	-1.097252	3.983628	5.265233
H	-2.389253	1.430224	2.778351
H	-0.814298	2.220997	2.603494
H	-2.233872	3.172639	3.079277
H	-0.334778	-1.231161	-0.262077

5-AuPMe3
SCF Energy: -752.101390978
Num. Imaginary Frequencies: 0

C	-0.266740	0.062316	0.127354
H	-0.263050	0.079055	1.220189
H	0.760342	-0.051650	-0.227171
C	-0.902018	1.318866	-0.398602
H	-1.928418	1.531234	-0.096594
C	-0.368870	2.209519	-1.189990
C	0.057442	3.190425	-1.993793
H	0.452856	4.113549	-1.573616
H	-0.181415	3.174109	-3.055848
Au	1.979733	1.841608	-1.967413
P	4.037506	0.812871	-2.182935
C	4.237528	-0.598198	-1.048818
H	3.460883	-1.340215	-1.245588
H	4.149113	-0.255039	-0.015777
H	5.220859	-1.053273	-1.198183
C	5.432727	1.928349	-1.829859
H	5.350766	2.304431	-0.808082
H	5.413418	2.772705	-2.521805
C	4.345467	0.147431	-3.849436
H	3.574467	-0.583239	-4.101994
H	4.319744	0.958175	-4.580482
H	5.326645	-0.335090	-3.874729
H	6.375472	1.386306	-1.944027
H	-0.848438	-0.807250	-0.189205

1b
SCF Energy: -486.290433068
Num. Imaginary Frequencies: 0

C	-3.331556	-2.131563	-5.064744
C	-3.656871	-1.758745	-3.686126
C	-3.957256	-1.442601	-2.556916
C	-4.270643	-1.044887	-1.156433
N	-5.533474	-0.337828	-0.951488
C	-6.808890	-1.070068	-1.031508
C	-7.208205	-1.688269	0.314951
C	-5.558260	1.015274	-1.532082
C	-6.335681	1.971247	-0.623478
C	-6.070476	1.107151	-2.978203
C	-6.931343	-2.096028	-2.166767
H	-4.023234	-1.654415	-5.764938
H	-3.401249	-3.213480	-5.203359
H	-3.496930	-0.318992	-0.874964
C	-4.081553	-2.242164	-0.216528
H	-4.513788	1.350670	-1.535266
H	-5.512723	0.438863	-3.638608
H	-5.958314	2.131721	-3.347197
H	-7.134283	0.851109	-3.039589
H	-6.273561	2.995548	-1.004519
H	-7.396723	1.702752	-0.574910
H	-5.930654	1.945852	0.391454
H	-7.562087	-0.300566	-1.232497
H	-6.726314	-1.644354	-3.140226
H	-6.240017	-2.933845	-2.038110
H	-7.948552	-2.501387	-2.177000
H	-8.253890	-2.012431	0.279827
H	-6.600629	-2.560333	0.567977
H	-7.097783	-0.948525	1.112640
H	-2.317025	-1.819030	-5.324901
H	-3.047663	-2.589556	-0.285548
H	-4.289865	-1.936722	0.811904
H	-4.731255	-3.078831	-0.480096

3.2 Reaction with acetaldehyde

3.2.1 Non-catalyzed reaction

1a
SCF Energy: -486.294704496
Num. Imaginary Frequencies: 0

C	-3.119274	-1.740799	-5.064717
C	-3.535479	-1.531384	-3.676148
C	-3.903458	-1.354580	-2.536582
C	-4.332521	-1.103751	-1.137493
N	-5.548533	-0.306166	-1.007772
C	-6.805830	-1.055469	-0.914388
C	-6.970061	-1.638556	0.492079
C	-5.578387	0.958566	-1.753141
C	-6.179921	2.062333	-0.879428
C	-6.278222	0.908231	-3.120091
C	-6.998329	-2.147036	-1.978443
H	-3.801726	-1.231226	-5.750974
H	-3.118768	-2.804781	-5.314740
C	-3.180044	-0.490984	-0.328964
H	-4.548301	-2.080062	-0.688793
H	-4.530826	1.220394	-1.942087
H	-5.831471	0.147671	-3.764748
H	-6.184308	1.879191	-3.616910
H	-7.347962	0.696031	-3.013972
H	-6.164225	3.025209	-1.400252
H	-7.222802	1.836818	-0.628749
H	-5.618966	2.153532	0.054515
H	-7.604349	-0.316546	-1.048191
H	-6.887344	-1.750273	-2.989965
H	-6.267534	-2.953710	-1.853593
H	-7.996158	-2.587633	-1.884863
H	-7.933936	-2.148064	0.591591
H	-6.185547	-2.371943	0.710790
H	-6.909146	-0.842887	1.239123
H	-2.112858	-1.349804	-5.234233
H	-2.289087	-1.121392	-0.393463
H	-2.920140	0.502014	-0.705720
H	-3.488108	-0.399081	0.715645

2a
SCF Energy: -486.217570799
Num. Imaginary Frequencies: 1
Imaginary Frequency: -546.3395

C	-2.959544	-2.071727	-2.201715
C	-1.657218	-1.331946	-2.266655
C	-1.196230	-0.200982	-1.825872
C	0.182731	0.293148	-2.197930
N	1.063291	-0.878747	-2.545810
C	0.612875	-1.659305	-3.554802
C	1.145390	-3.059449	-3.768050
C	1.850833	-1.538018	-1.467116
C	0.991080	-2.056134	-0.314052
C	3.044323	-0.703591	-0.984521
C	0.122445	-0.967283	-4.812041
H	-3.362121	-2.251995	-3.204538
H	-3.690457	-1.491880	-1.634484
H	0.079868	0.858329	-3.129203
C	0.782999	1.267894	-1.192436
H	2.306965	-2.400355	-1.949061
H	3.783147	-1.388224	-0.557085
H	3.513745	-0.176793	-1.819750
H	2.784407	0.019881	-0.212647
H	0.243874	-2.772070	-0.667176
H	1.639399	-2.550993	0.415846
H	0.451502	-1.248635	0.186725
H	-0.684700	-0.262621	-4.614822
H	-0.250164	-1.709971	-5.518889
H	0.954382	-0.428722	-5.284070
H	0.563154	-3.536936	-4.556983
H	1.074133	-3.687075	-2.878668
H	2.193555	-3.037163	-4.096291
H	-0.833713	-1.953084	-2.915725
H	-2.839249	-3.047512	-1.718241
H	1.775361	1.610154	-1.497375
H	0.111993	2.128515	-1.159059
H	0.827575	0.857859	-0.182160

2b
SCF Energy: -486.223924612
Num. Imaginary Frequencies: 1
Imaginary Frequency: -513.8597

C	-2.729227	-2.918144	-3.735984
C	-3.349907	-2.897853	-5.100539
C	-3.935490	-3.754827	-5.879373
C	-4.426097	-3.437748	-7.247472
N	-4.419559	-1.933603	-7.501784
C	-5.773607	-1.325637	-7.444602
C	-6.661355	-1.879876	-8.560618
C	-3.364257	-1.196221	-7.105991
C	-1.985948	-1.633756	-7.551299
C	-3.511413	0.287153	-6.855610
C	-6.425067	-1.455661	-6.067371
H	-1.670075	-2.641176	-3.780036
H	-2.807605	-3.918209	-3.304753
C	-3.757125	-4.233521	-8.369943
H	-5.487136	-3.689395	-7.295053
H	-5.637218	-0.266830	-7.670050
H	-7.565438	-1.268404	-8.630313
H	-6.141944	-1.838215	-9.521825
H	-6.978263	-2.910363	-8.379216
H	-5.790748	-1.032974	-5.283228
H	-7.384873	-0.930678	-6.065179
H	-6.604914	-2.504390	-5.812561
H	-1.795358	-2.677239	-7.310178
H	-1.225356	-1.026258	-7.056747
H	-1.890821	-1.497731	-8.636528
H	-2.597568	0.659214	-6.390290
H	-4.347700	0.532035	-6.199852
H	-3.643688	0.827801	-7.803014
H	-3.248159	-1.801517	-5.614522
H	-3.224473	-2.209472	-3.063579
H	-4.131221	-3.902958	-9.344005
H	-2.670241	-4.147304	-8.362919
H	-4.007050	-5.288545	-8.233832

3b
SCF Energy: -486.228848283
Num. Imaginary Frequencies: 0

C	-2.797558	-3.262044	-3.562418
C	-3.355742	-2.907214	-4.920357
C	-3.741415	-3.794036	-5.841190
C	-4.330875	-3.378264	-7.146480
N	-4.411759	-1.846179	-7.412783
C	-5.790234	-1.285689	-7.389688
C	-6.631684	-1.892723	-8.512016
C	-3.376171	-1.068624	-7.410295
C	-1.976673	-1.603778	-7.469051
C	-3.503733	0.434803	-7.441733
C	-6.411472	-1.456243	-6.004568
H	-1.781814	-2.867950	-3.423625
H	-2.765002	-4.348300	-3.446807
C	-3.769462	-4.073708	-8.389421
H	-5.388591	-3.646968	-7.106047
H	-5.708326	-0.219393	-7.595778
H	-7.587219	-1.363554	-8.556068
H	-6.132307	-1.779355	-9.478251
H	-6.844432	-2.952027	-8.350212
H	-5.799506	-0.969961	-5.240496
H	-7.404933	-0.999619	-6.004447
H	-6.511005	-2.509545	-5.730437
H	-1.903164	-2.636172	-7.144163
H	-1.337001	-0.990907	-6.830294
H	-1.611594	-1.498437	-8.499673
H	-2.512008	0.883891	-7.402211
H	-4.081774	0.805596	-6.591041
H	-3.993028	0.773178	-8.360659
H	-3.403980	-1.806026	-5.085148
H	-3.410734	-2.846721	-2.751841
H	-4.257166	-3.710964	-9.301356
H	-2.689987	-3.953376	-8.495735
H	-3.968551	-5.141995	-8.283979

3a
SCF Energy: -486.222438159
Num. Imaginary Frequencies: 0

C	-3.003122	-2.880905	-3.379361
C	-3.494440	-2.716103	-4.798335
C	-3.929412	-3.715639	-5.573006
C	-4.340707	-3.471709	-6.994320
N	-4.515737	-1.977735	-7.338418
C	-5.790697	-1.253742	-7.026004
C	-6.500223	-0.895723	-8.331677
C	-3.458221	-1.278647	-7.624682
C	-2.130664	-1.941013	-7.880896
C	-3.433150	0.217144	-7.776601
C	-6.738833	-1.970945	-6.064124
H	-1.968135	-2.532113	-3.266455
H	-3.045922	-3.933392	-3.087832
H	-3.510142	-3.769332	-7.636329
C	-5.532447	-4.310120	-7.465271
H	-5.480940	-0.343427	-6.508964
H	-7.388687	-0.298195	-8.109088
H	-5.860040	-0.326180	-9.010562
H	-6.822805	-1.804855	-8.846487
H	-6.198679	-2.495844	-5.274061
H	-7.366665	-1.202984	-5.603795
H	-7.399107	-2.666258	-6.583396
H	-1.864461	-2.594120	-7.046591
H	-1.360018	-1.178589	-7.996625
H	-2.161563	-2.536513	-8.799874
H	-3.030592	0.440924	-8.770705
H	-2.723671	0.630131	-7.052182
H	-4.385548	0.726512	-7.669974
H	-3.461803	-1.655182	-5.138613
H	-3.609809	-2.301881	-2.670601
H	-5.975317	-3.922690	-8.389965
H	-5.153246	-5.314152	-7.667141
H	-6.297921	-4.410443	-6.698578

4a
SCF Energy: -486.220928365
Num. Imaginary Frequencies: 1
Imaginary Frequency: -362.8458

C	-2.989560	-3.198748	-3.460644
C	-3.494877	-2.985901	-4.866732
C	-3.951349	-3.932624	-5.680733
C	-4.354121	-3.790617	-7.058208
N	-4.564708	-2.152340	-7.519612
C	-5.878030	-1.484058	-7.314942
C	-6.908481	-1.908432	-8.367581
C	-3.491039	-1.430577	-7.580859
C	-2.169647	-2.079520	-7.905065
C	-3.465377	0.066160	-7.370078
C	-6.400972	-1.634254	-5.888055
H	-1.952210	-2.857498	-3.350368
H	-3.034536	-4.258706	-3.199272
H	-3.527992	-4.056509	-7.721193
C	-5.576508	-4.573511	-7.510050
H	-5.708740	-0.421757	-7.494670
H	-7.681005	-1.135601	-8.417175
H	-6.447998	-1.992339	-9.356041
H	-7.398066	-2.851162	-8.125702
H	-5.711863	-1.193965	-5.163729
H	-7.364659	-1.120891	-5.816597
H	-6.538570	-2.681198	-5.610624
H	-2.253968	-2.739083	-8.772077
H	-1.834037	-2.674480	-7.049039
H	-1.418616	-1.318792	-8.117517
H	-2.449493	0.376453	-7.124298
H	-4.123868	0.390223	-6.563605
H	-3.758164	0.589258	-8.288759
H	-3.458787	-1.920982	-5.186700
H	-3.586147	-2.638179	-2.729371
H	-5.827118	-4.366697	-8.553601
H	-5.322506	-5.631131	-7.418425
H	-6.446776	-4.396169	-6.874776

4b
SCF Energy: -486.227694561
Num. Imaginary Frequencies: 1
Imaginary Frequency: -325.0915

C	-2.794546	-3.380850	-3.515205
C	-3.326542	-3.079923	-4.894914
C	-3.789339	-3.969890	-5.765964
C	-4.343284	-3.734052	-7.070147
N	-4.460695	-2.087085	-7.510226
C	-5.842193	-1.556094	-7.453800
C	-6.722894	-2.264372	-8.484658
C	-3.447268	-1.287602	-7.458351
C	-2.056877	-1.829947	-7.645564
C	-3.595451	0.209871	-7.321340
C	-6.404547	-1.634290	-6.034923
H	-1.753560	-3.051647	-3.403172
H	-2.839400	-4.455105	-3.320814
C	-3.714006	-4.465825	-8.251226
H	-5.413261	-3.946121	-7.062438
H	-5.800335	-0.506271	-7.752452
H	-7.682881	-1.744385	-8.545159
H	-6.256851	-2.240091	-9.473538
H	-6.926351	-3.305087	-8.221213
H	-5.765661	-1.096771	-5.328843
H	-7.402715	-1.187811	-6.017100
H	-6.478861	-2.668802	-5.689110
H	-1.890901	-2.041441	-8.708849
H	-1.922610	-2.751498	-7.079995
H	-1.314235	-1.101685	-7.319876
H	-2.638771	0.652428	-7.045635
H	-4.333170	0.483506	-6.564680
H	-3.906001	0.652897	-8.275221
H	-3.299283	-1.995474	-5.150339
H	-3.375258	-2.864535	-2.740306
H	-4.078171	-4.063650	-9.202480
H	-2.623978	-4.417633	-8.233995
H	-3.995567	-5.519122	-8.186534

5a
SCF Energy: -195.200332125
Num. Imaginary Frequencies: 0

C	-1.670343	1.223058	0.974810
C	-2.579947	1.347767	0.039708
C	-3.486239	1.471192	-0.898763
C	-3.290936	2.241689	-2.180521
H	-3.421996	1.586976	-3.047839
H	-2.292629	2.681168	-2.223721
H	-4.029660	3.045188	-2.263040
H	-4.451880	0.987956	-0.750020
C	-0.650330	0.113591	1.033056
H	-1.642824	1.967540	1.770469
H	0.365050	0.521715	1.010160
H	-0.752956	-0.455343	1.962540
H	-0.769482	-0.571016	0.191189

5b
SCF Energy: -195.200328878
Num. Imaginary Frequencies: 0

C	-1.692223	1.303721	1.008000
C	-2.608358	1.451614	0.082712
C	-3.522485	1.603703	-0.843867
C	-3.244908	2.071749	-2.250480
H	-3.560208	1.316076	-2.976906
H	-2.180880	2.269193	-2.393542
H	-3.802454	2.987935	-2.469147
H	-4.557861	1.377131	-0.589330
H	-1.199716	0.335318	1.096110
C	-1.265975	2.383886	1.970407
H	-0.196813	2.593591	1.865650
H	-1.820840	3.306944	1.792392
H	-1.437207	2.067783	3.004274

3.2.2 CuBr-catalyzed reaction

1a_CuBr
SCF Energy: -695.699402842
Num. Imaginary Frequencies: 0

C	-3.046290	-2.040947	-3.769614
C	-1.933707	-2.183573	-2.820676
C	-0.922208	-2.224465	-2.132067
C	0.427653	-2.233332	-1.475425
N	1.492550	-1.864124	-2.384830
C	1.614759	-2.645301	-3.622872
C	1.000130	-1.995718	-4.871575
Cu	-2.508786	-3.064126	-0.886026
Br	-3.751369	-4.023681	0.854182
C	1.840525	-0.439280	-2.443385
C	2.638112	-0.035346	-1.200782
C	0.651632	0.508146	-2.660059
C	3.082065	-3.004376	-3.867995
H	-2.674746	-1.576131	-4.687544
H	-3.475075	-3.013377	-4.019695
H	0.394723	-1.472969	-0.687637
C	0.687733	-3.581996	-0.790199
H	1.070795	-3.580357	-3.446967
H	2.511875	-0.334974	-3.302743
H	3.516297	-0.676557	-1.090987
H	2.965451	1.006185	-1.275178
H	2.033948	-0.124156	-0.290891
H	0.078194	0.241684	-3.551394
H	-0.029290	0.491803	-1.801469
H	1.009476	1.535797	-2.774735
H	-0.057026	-1.761782	-4.724423
H	1.524277	-1.072962	-5.142253
H	1.081926	-2.681354	-5.720281
H	3.684101	-2.101666	-4.020533
H	3.488405	-3.542660	-3.007883
H	3.186250	-3.628917	-4.760589
H	-3.833248	-1.407755	-3.354784
H	1.663119	-3.540025	-0.300727
H	-0.078225	-3.792340	-0.035304
H	0.689059	-4.404427	-1.509851

1b_CuBr
SCF Energy: -695.695568072
Num. Imaginary Frequencies: 0

C	-3.069223	-1.794826	-3.699822
C	-1.962335	-2.058316	-2.770596
C	-0.938477	-2.215701	-2.118042
C	0.423652	-2.367246	-1.492716
N	1.507800	-1.879254	-2.322436
C	1.781225	-2.696974	-3.517240
C	1.066610	-2.245552	-4.800214
Cu	-2.581674	-2.736261	-0.773905
Br	-3.875266	-3.395903	1.066125
C	1.737246	-0.432361	-2.480237
C	2.598036	0.151481	-1.352735
C	0.485186	0.422136	-2.720630
C	3.289605	-2.807600	-3.751060
H	-2.655594	-1.451714	-4.653001
H	-3.655409	-2.698299	-3.879199
C	0.421773	-1.812086	-0.063402
H	0.581461	-3.448770	-1.403404
H	1.415902	-3.702476	-3.275587
H	2.345460	-0.347457	-3.386446
H	3.462203	-0.492689	-1.169276
H	2.957655	1.144639	-1.640802
H	2.044328	0.261704	-0.417595
H	-0.082825	0.069202	-3.585698
H	-0.184275	0.423367	-1.855036
H	0.786443	1.457769	-2.905958
H	-0.015378	-2.185559	-4.658550
H	1.427328	-1.266572	-5.134023
H	1.264871	-2.959957	-5.604918
H	3.726536	-1.836981	-4.009241
H	3.787597	-3.178620	-2.851936
H	3.497039	-3.492280	-4.578997
H	-3.731124	-1.019248	-3.309049
H	1.421754	-1.916958	0.362527
H	0.123483	-0.762766	-0.025752
H	-0.279890	-2.383346	0.553892

2a_CuBr
SCF Energy: -695.655987928
Num. Imaginary Frequencies: 1
Imaginary Frequency: -684.9038

C	-3.379333	-2.822246	-2.995453
C	-3.754749	-2.809720	-4.431883
C	-4.258779	-3.457000	-5.420372
Cu	-5.044918	-5.274647	-5.010413
Br	-6.005820	-7.380476	-4.544135
C	-4.287704	-2.900224	-6.853858
N	-4.275797	-1.427082	-6.803305
C	-5.570337	-0.695095	-6.743998
C	-6.352366	-0.720649	-8.063123
C	-3.236237	-0.928992	-6.027593
C	-1.831288	-1.373010	-6.421706
C	-3.269312	0.525368	-5.585546
C	-6.441102	-1.074205	-5.543652
H	-2.304735	-2.661398	-2.871248
H	-3.634114	-3.795103	-2.567297
H	-3.337024	-3.203592	-7.300482
C	-5.368047	-3.538454	-7.718603
H	-5.282576	0.348123	-6.626746
H	-7.012610	0.151320	-8.081062
H	-5.674073	-0.649870	-8.917486
H	-6.979521	-1.603773	-8.180897
H	-5.917602	-0.909791	-4.596853
H	-7.345320	-0.458385	-5.550147
H	-6.742486	-2.124868	-5.572575
H	-1.720019	-2.454695	-6.480216
H	-1.114160	-1.007037	-5.684423
H	-1.581038	-0.936130	-7.394545
H	-2.393533	0.719056	-4.964468
H	-4.155310	0.778463	-5.002145
H	-3.215751	1.188207	-6.456668
H	-3.400521	-1.584869	-4.904261
H	-3.912360	-2.045754	-2.439989
H	-5.358019	-3.130164	-8.731147
H	-5.144820	-4.606969	-7.778745
H	-6.367845	-3.438830	-7.292915

2b_CuBr
SCF Energy: -695.660830302
Num. Imaginary Frequencies: 1
Imaginary Frequency: -702.1118

C	-2.739877	-2.922322	-3.864339
C	-3.399250	-3.052996	-5.187878
C	-3.986797	-3.823341	-6.030005
C	-4.460963	-3.410111	-7.411503
C	-3.765871	-4.179239	-8.539214
N	-4.429918	-1.936478	-7.550243
C	-3.361975	-1.277875	-6.962101
C	-3.500967	0.207565	-6.674234
C	-5.773180	-1.308708	-7.467589
C	-6.450516	-1.515816	-6.110594
C	-6.656950	-1.770152	-8.627107
C	-1.978389	-1.633946	-7.490104
H	-1.695163	-2.618970	-3.977073
H	-2.765963	-3.888688	-3.354288
H	-5.515401	-3.684249	-7.478051
H	-5.612041	-0.240778	-7.622054
H	-7.552123	-1.143295	-8.662829
H	-6.126503	-1.670030	-9.577699
H	-6.992254	-2.805698	-8.520930
H	-5.826320	-1.155623	-5.287008
H	-7.400164	-0.974007	-6.085747
H	-6.660441	-2.574619	-5.927992
H	-1.777255	-2.701412	-7.435151
H	-1.216547	-1.116486	-6.902367
H	-1.898322	-1.308700	-8.532875
H	-2.609667	0.545678	-6.143273
H	-4.371716	0.449534	-6.064448
H	-3.561665	0.766141	-7.615372
H	-3.313988	-1.823806	-5.776730
H	-3.250510	-2.184772	-3.239812
H	-4.129794	-3.818381	-9.504908
H	-2.680158	-4.089465	-8.517262
H	-4.016221	-5.239864	-8.444029
Cu	-4.309789	-5.726616	-5.420867
Br	-4.709823	-7.944012	-4.719684

3a_CuBr
SCF Energy: -695.685370360
Num. Imaginary Frequencies: 0

C	-2.981508	-2.852189	-3.289551
C	-2.975266	-2.683011	-4.785590
C	-3.545598	-3.530598	-5.654294
Cu	-4.503887	-5.205261	-5.095314
Br	-5.667664	-7.200147	-4.513719
C	-3.429609	-3.289877	-7.149675
N	-3.081573	-1.864396	-7.517731
C	-4.162279	-0.826818	-7.612238
C	-4.807791	-0.816973	-9.000319
C	-1.841145	-1.520923	-7.664271
C	-0.717931	-2.486591	-7.419233
C	-1.432602	-0.138786	-8.091143
C	-5.181394	-0.911404	-6.476545
H	-1.962788	-2.870066	-2.884306
H	-3.479590	-3.784516	-3.007574
H	-2.576555	-3.871437	-7.507366
C	-4.605589	-3.808306	-7.980661
H	-3.649736	0.124319	-7.475305
H	-5.339938	0.129699	-9.124970
H	-4.057305	-0.894065	-9.792711
H	-5.528693	-1.625304	-9.123592
H	-4.713582	-0.730011	-5.508842
H	-5.925379	-0.130782	-6.660183
H	-5.694686	-1.870520	-6.420152
H	-0.928750	-3.161208	-6.589246
H	0.188204	-1.921267	-7.198008
H	-0.527092	-3.073738	-8.325754
H	-0.435586	-0.187254	-8.529692
H	-1.374045	0.517456	-7.214417
H	-2.113603	0.306587	-8.815987
H	-2.469851	-1.760551	-5.115712
H	-3.505473	-2.023112	-2.797708
H	-4.446420	-3.641016	-9.050064
H	-4.654280	-4.886709	-7.810435
H	-5.570735	-3.395465	-7.686062

3b_CuBr
SCF Energy: -695.691059689
Num. Imaginary Frequencies: 0

C	-2.869252	-3.010501	-3.290872
C	-3.015353	-2.706739	-4.758490
C	-3.362116	-3.602919	-5.693243
Cu	-3.765943	-5.531330	-5.297804
Br	-4.249787	-7.835356	-4.939916
C	-3.542751	-3.198398	-7.142181
N	-3.051399	-1.809136	-7.508224
C	-4.119284	-0.848687	-7.915746
C	-4.793601	-1.322953	-9.201547
C	-1.808690	-1.460842	-7.443094
C	-0.720757	-2.387572	-7.002683
C	-1.351490	-0.077203	-7.822759
C	-5.093736	-0.621340	-6.761746
H	-1.852048	-2.801930	-2.937275
H	-3.092296	-4.062496	-3.089858
C	-3.035560	-4.210207	-8.176979
H	-4.621281	-3.129425	-7.300523
H	-3.630545	0.100266	-8.127013
H	-5.503356	-0.557438	-9.524264
H	-4.059652	-1.467986	-9.999226
H	-5.348261	-2.253830	-9.060497
H	-4.573486	-0.239409	-5.880289
H	-5.832887	0.119358	-7.077249
H	-5.624280	-1.533059	-6.477061
H	-1.070709	-3.323096	-6.581296
H	-0.127595	-1.863446	-6.246434
H	-0.059446	-2.565817	-7.859421
H	-0.265094	-0.026104	-7.763125
H	-1.766996	0.669812	-7.139324
H	-1.655118	0.180023	-8.840567
H	-2.797303	-1.657343	-5.011133
H	-3.548138	-2.395698	-2.687895
H	-3.192740	-3.843142	-9.196318
H	-1.981167	-4.461070	-8.049795
H	-3.606551	-5.133602	-8.052250

4a_CuBr
SCF Energy: -695.663767168
Num. Imaginary Frequencies: 1
Imaginary Frequency: -301.0221

C	-3.371534	-2.213072	-2.025754
C	-1.955850	-1.710908	-2.051771
C	-1.555638	-0.471003	-1.788323
C	-0.332110	0.196962	-1.802636
Cu	-2.870185	1.050484	-1.390537
Br	-4.396626	2.803307	-0.960988
N	1.167476	-1.117533	-2.460116
C	1.363346	-1.161207	-3.724245
C	2.524899	-1.873087	-4.384379
C	2.019947	-1.915278	-1.556513
C	1.158038	-2.607078	-0.502945
C	3.133619	-1.074092	-0.928463
C	0.408629	-0.501703	-4.687705
H	-3.662503	-2.614885	-3.002535
H	-4.069941	-1.414066	-1.760915
H	-0.141628	0.813684	-2.680968
C	0.279452	0.786002	-0.555220
H	2.491852	-2.709286	-2.145523
H	3.866380	-1.738735	-0.462459
H	3.648289	-0.468863	-1.680931
H	2.747267	-0.411066	-0.152028
H	0.453318	-3.300824	-0.966973
H	1.803383	-3.175423	0.173082
H	0.586287	-1.889883	0.088773
H	-0.598493	-0.416120	-4.279861
H	0.363679	-1.097161	-5.603208
H	0.779812	0.490220	-4.970868
H	2.713644	-1.424590	-5.361501
H	2.271462	-2.926564	-4.550233
H	3.440920	-1.826855	-3.794882
H	-1.187015	-2.448020	-2.311440
H	-3.485953	-3.024182	-1.298370
H	1.327467	1.033202	-0.724807
H	-0.242160	1.722270	-0.331987
H	0.173187	0.132207	0.311246

4b_CuBr
SCF Energy: -695.669085436
Num. Imaginary Frequencies: 1
Imaginary Frequency: -305.3754

C	-3.596504	-1.905823	-2.310099
C	-2.167428	-1.444591	-2.348670
C	-1.702170	-0.284226	-1.899851
C	-0.461218	0.327749	-1.774800
C	-0.095516	1.591422	-2.521475
Cu	-2.893319	1.135806	-1.015732
Br	-4.283587	2.766031	-0.020430
N	1.051979	-0.970077	-2.476682
C	1.256073	-1.234548	-3.708834
C	2.420368	-2.057888	-4.222698
C	1.915152	-1.505591	-1.418608
C	1.056379	-2.249786	-0.395278
C	2.726224	-0.369546	-0.794310
C	0.316273	-0.722820	-4.764503
H	-3.974200	-2.101688	-3.319539
H	-4.240762	-1.156259	-1.841866
H	-0.012822	0.264075	-0.784115
H	2.618254	-2.231017	-1.842535
H	3.389035	-0.768386	-0.021786
H	3.338021	0.132209	-1.549999
H	2.078140	0.378169	-0.327484
H	0.482090	-3.043705	-0.880278
H	1.701268	-2.701219	0.363632
H	0.351026	-1.584712	0.110485
H	-0.607671	-0.335825	-4.340319
H	0.077593	-1.537761	-5.455222
H	0.812896	0.058864	-5.351240
H	2.478197	-1.981945	-5.309187
H	2.288367	-3.113516	-3.963720
H	3.369826	-1.722050	-3.799463
H	-1.445233	-2.139608	-2.795018
H	-3.689012	-2.840022	-1.745618
H	0.979812	1.623479	-2.711432
H	-0.641851	1.680880	-3.461578
H	-0.347607	2.456254	-1.899377

5a_CuBr
SCF Energy: -404.603201985
Num. Imaginary Frequencies: 0

C	-3.271165	-5.547958	-3.518293
Cu	-2.634767	-4.403625	-5.295700
Br	-1.938403	-3.681454	-7.413880
C	-3.323508	-4.263843	-3.165507
C	-3.425137	-3.047175	-2.689147
C	-3.191691	-1.763740	-3.438924
H	-2.335852	-6.086746	-3.350608
C	-4.468893	-6.359511	-3.961499
H	-3.704965	-2.967440	-1.638120
H	-2.928774	-1.938701	-4.485570
H	-4.090906	-1.142389	-3.406473
H	-2.381743	-1.198382	-2.969550
H	-4.244595	-6.940713	-4.859582
H	-4.731462	-7.067014	-3.168756
H	-5.329275	-5.717692	-4.156512

5b_CuBr
SCF Energy: -404.603184167
Num. Imaginary Frequencies: 0

C	-3.175885	-5.548549	-3.499061
Cu	-2.897862	-4.398870	-5.361477
Br	-2.513884	-3.683847	-7.560009
C	-3.260800	-4.264210	-3.153207
C	-3.361480	-3.048343	-2.674608
C	-3.191554	-1.762599	-3.437397
C	-1.928098	-6.390472	-3.345287
H	-4.095622	-6.063658	-3.785658
H	-3.596482	-2.971037	-1.612495
H	-2.944060	-1.934805	-4.488284
H	-4.113175	-1.175693	-3.391524
H	-2.395109	-1.163374	-2.987538
H	-1.721431	-6.964729	-4.251976
H	-1.061967	-5.770462	-3.109570
H	-2.080472	-7.105330	-2.530613

3.2.3 AgBr-catalyzed reaction

1a_AgBr
SCF Energy: -645.189658773
Num. Imaginary Frequencies: 0

C	0.018851	3.132373	-0.703007
C	-0.348290	1.803883	-0.198065
C	-0.762422	0.727826	0.204768
C	-1.451420	-0.494684	0.728077
C	-1.290904	-0.570712	2.252577
Ag	1.677270	0.332926	0.007726
Br	4.120940	-0.643219	0.037158
N	-2.841399	-0.590573	0.316721
C	-3.692787	0.577480	0.588483
C	-3.894928	1.539298	-0.592313
C	-3.093393	-1.330761	-0.927534
C	-2.991752	-2.837713	-0.677385
C	-2.213862	-0.919253	-2.117664
C	-5.043775	0.116092	1.140187
H	-0.887203	3.730462	-0.834412
H	0.675719	3.648862	-0.000239
H	-3.188329	1.142381	1.380842
H	-4.134796	-1.119538	-1.193555
H	-3.677483	-3.136594	0.119866
H	-3.240413	-3.395558	-1.585511
H	-1.976449	-3.125512	-0.381743
H	-2.278966	0.152507	-2.318775
H	-1.161228	-1.167206	-1.936786
H	-2.528799	-1.459729	-3.015522
H	-2.942675	1.902452	-0.985731
H	-4.446885	1.059835	-1.407937
H	-4.479698	2.403303	-0.262288
H	-5.577446	-0.493524	0.402231
H	-4.900414	-0.486308	2.041312
H	-5.677067	0.974542	1.384807
H	0.527252	3.056869	-1.666325
H	-1.738161	-1.502450	2.606363
H	-0.232061	-0.552588	2.527443
H	-1.786473	0.268371	2.747298
H	-0.935113	-1.364425	0.309244

1b_AgBr
SCF Energy: -645.170029370
Num. Imaginary Frequencies: 0

C	-3.072146	-1.764914	-3.706038
C	-1.955007	-2.024435	-2.788484
C	-0.931868	-2.181262	-2.138579
C	0.424763	-2.337220	-1.508501
N	1.518837	-1.866270	-2.338208
C	1.794763	-2.701513	-3.520109
C	1.086969	-2.267208	-4.812659
Ag	-2.743266	-2.825821	-0.581002
Br	-4.168652	-3.613254	1.411410
C	1.756291	-0.422963	-2.515423
C	2.611823	0.174346	-1.390840
C	0.510788	0.435280	-2.775143
C	3.303914	-2.820253	-3.745600
H	-2.671672	-1.411362	-4.661084
H	-3.651978	-2.672025	-3.888600
C	0.431165	-1.768214	-0.084292
H	0.576705	-3.418777	-1.407760
H	1.425824	-3.702509	-3.265408
H	2.370789	-0.354082	-3.418746
H	3.469810	-0.472310	-1.188136
H	2.980858	1.159836	-1.693055
H	2.050171	0.305274	-0.463035
H	-0.056934	0.071421	-3.635774
H	-0.160969	0.454708	-1.911447
H	0.819370	1.465815	-2.976437
H	0.004559	-2.202720	-4.675832
H	1.451635	-1.293970	-5.158898
H	1.287145	-2.993591	-5.606151
H	3.745058	-1.855467	-4.018091
H	3.796911	-3.177658	-2.838216
H	3.512934	-3.519257	-4.561089
H	-3.738740	-0.997848	-3.306304
H	1.436919	-1.856418	0.331580
H	0.119612	-0.722324	-0.052600
H	-0.253638	-2.344861	0.546604

2a_AgBr
SCF Energy: -645.130529213
Num. Imaginary Frequencies: 1
Imaginary Frequency: -706.6384

C	-3.390807	-2.794125	-2.985578
C	-3.760980	-2.778742	-4.424500
C	-4.273360	-3.428434	-5.407059
C	-4.295808	-2.884961	-6.843680
C	-5.377622	-3.513825	-7.713385
Ag	-5.159797	-5.411982	-4.941871
Br	-6.219276	-7.706679	-4.379499
N	-4.272069	-1.409797	-6.802682
C	-3.226283	-0.912695	-6.038223
C	-3.247541	0.542879	-5.601380
C	-5.561166	-0.667520	-6.745502
C	-6.434937	-1.036876	-5.544482
C	-6.343659	-0.690157	-8.064448
C	-1.826277	-1.373170	-6.429379
H	-2.314884	-2.644770	-2.858071
H	-3.658658	-3.761792	-2.554194
H	-3.346328	-3.196838	-7.286878
H	-5.265503	0.373666	-6.630746
H	-6.997569	0.186529	-8.083741
H	-5.665354	-0.625894	-8.919302
H	-6.977284	-1.568946	-8.180094
H	-5.911237	-0.871806	-4.597988
H	-7.335654	-0.416023	-5.554553
H	-6.742219	-2.086087	-5.569543
H	-1.724139	-2.456361	-6.475223
H	-1.104666	-1.004569	-5.697911
H	-1.573956	-0.950069	-7.407897
H	-2.368130	0.732796	-4.984353
H	-4.129561	0.804229	-5.015581
H	-3.192706	1.202801	-6.474828
H	-3.394655	-1.570028	-4.901815
H	-3.915326	-2.008797	-2.434274
H	-5.363204	-3.099509	-8.723432
H	-5.159112	-4.582658	-7.780057
H	-6.377648	-3.411041	-7.288599

3a_AgBr
SCF Energy: -645.157745076
Num. Imaginary Frequencies: 0

C	-2.910899	-2.736967	-3.282870
C	-3.009282	-2.590304	-4.777866
C	-3.491964	-3.515731	-5.617758
Ag	-4.196182	-5.486273	-4.969279
Br	-5.010000	-7.865696	-4.273152
C	-3.510427	-3.288049	-7.116926
N	-3.137421	-1.874155	-7.525037
C	-4.167387	-0.782413	-7.636678
C	-4.588909	-0.590729	-9.093839
C	-1.883512	-1.574354	-7.660575
C	-0.796934	-2.587462	-7.439144
C	-1.401345	-0.199480	-8.023165
C	-5.381646	-0.943422	-6.718062
H	-1.876599	-2.617660	-2.938917
H	-3.266911	-3.720679	-2.963954
H	-2.712315	-3.895681	-7.549739
C	-4.785938	-3.773728	-7.810706
H	-3.646079	0.111396	-7.291683
H	-5.195966	0.315754	-9.166664
H	-3.732731	-0.488885	-9.765559
H	-5.198149	-1.429550	-9.435939
H	-5.124644	-1.414925	-5.769144
H	-5.765591	0.059221	-6.513093
H	-6.183749	-1.507440	-7.193606
H	-1.007406	-3.229606	-6.583416
H	0.145981	-2.065834	-7.272784
H	-0.679424	-3.208039	-8.335581
H	-0.481379	-0.297816	-8.602122
H	-1.142199	0.329604	-7.097174
H	-2.108754	0.403177	-8.586353
H	-2.653161	-1.611964	-5.140796
H	-3.507298	-1.973389	-2.768997
H	-4.810002	-3.490084	-8.866338
H	-4.774155	-4.865068	-7.762030
H	-5.695361	-3.444756	-7.311373

2b_AgBr
SCF Energy: -645.135497966
Num. Imaginary Frequencies: 1
Imaginary Frequency: -723.3267

C	0.672272	2.779286	-1.126653
C	1.001488	1.484206	-0.477805
C	0.554918	0.401842	0.047475
C	1.405712	-0.679797	0.683558
C	1.112986	-0.883312	2.173464
N	2.836556	-0.471040	0.355930
C	3.289886	0.836233	0.336692
C	4.569362	1.147656	-0.420198
C	3.346500	-1.407578	-0.677578
C	2.650031	-1.245144	-2.030840
C	3.292417	-2.849890	-0.172338
C	3.193098	1.604047	1.647931
H	1.047546	3.618212	-0.533657
H	-0.412962	2.874912	-1.212235
H	1.135609	-1.620786	0.200762
H	4.405234	-1.172290	-0.795518
H	3.856055	-3.488098	-0.858292
H	3.743621	-2.926154	0.820445
H	2.274348	-3.246631	-0.125144
H	2.717148	-0.217132	-2.399910
H	3.114954	-1.907035	-2.766852
H	1.588413	-1.504700	-1.966006
H	2.183524	1.605461	2.052487
H	3.494528	2.642077	1.489212
H	3.870159	1.149990	2.379577
H	4.731142	2.226645	-0.404328
H	4.545238	0.823166	-1.460756
H	5.423430	0.674385	0.078133
H	2.352022	1.443355	-0.361901
H	1.108126	2.841139	-2.127220
H	1.784071	-1.646887	2.575765
H	1.223460	0.026818	2.762531
H	0.081231	-1.230224	2.282893
Ag	-1.645908	0.095056	0.003301
Br	-4.208489	-0.264626	-0.062254

3b_AgBr
SCF Energy: -645.164856037
Num. Imaginary Frequencies: 0

C	-2.881079	-2.969339	-3.292134
C	-3.025570	-2.683679	-4.763165
C	-3.364098	-3.582588	-5.696416
Ag	-3.790223	-5.683429	-5.247951
Br	-4.295252	-8.202228	-4.788639
C	-3.542310	-3.186629	-7.147354
N	-3.046345	-1.798185	-7.513254
C	-4.110364	-0.835864	-7.927030
C	-4.782427	-1.312073	-9.213317
C	-1.802921	-1.453075	-7.443454
C	-0.719186	-2.382911	-6.999364
C	-1.340751	-0.070500	-7.820638
C	-5.087906	-0.601473	-6.777102
H	-1.864858	-2.752404	-2.940936
H	-3.101394	-4.018724	-3.075919
C	-3.033798	-4.196557	-8.183827
H	-4.620458	-3.115019	-7.307284
H	-3.617630	0.110555	-8.140317
H	-5.487967	-0.544739	-9.540848
H	-5.341546	-2.240099	-9.070992
H	-4.570645	-0.213591	-5.896504
H	-5.826376	0.136998	-7.099263
H	-5.619182	-1.511574	-6.488351
H	-1.072217	-3.320658	-6.585485
H	-0.131263	-1.863291	-6.235916
H	-0.051657	-2.557072	-7.852091
H	-0.254795	-0.020845	-7.752487
H	-1.760706	0.677829	-7.141400
H	-1.635875	0.186041	-8.841186
H	-2.811987	-1.635467	-5.024218
H	-3.562252	-2.347381	-2.699290
H	-3.164028	-3.812968	-9.200830
H	-1.986846	-4.468058	-8.038688
H	-3.624037	-5.110333	-8.083969

4a_AgBr
SCF Energy: -645.138854689
Num. Imaginary Frequencies: 1
Imaginary Frequency: -300.7788

C	-3.333410	-2.249171	-2.014287
C	-1.926468	-1.723294	-2.042829
C	-1.536427	-0.481303	-1.776779
C	-0.308096	0.183147	-1.802468
Ag	-3.020058	1.158042	-1.357694
Br	-4.729017	3.061217	-0.928413
N	1.169741	-1.119324	-2.463700
C	1.358030	-1.161300	-3.729360
C	2.516263	-1.872514	-4.395390
C	2.027384	-1.920382	-1.566334
C	1.175117	-2.612659	-0.505216
C	3.151529	-1.085342	-0.948251
C	0.398711	-0.501354	-4.687688
H	-3.620205	-2.651727	-2.992057
H	-4.045031	-1.463718	-1.744147
H	-0.132291	0.805921	-2.679566
C	0.318003	0.773028	-0.561293
H	2.489748	-2.714892	-2.161859
H	3.891169	-1.755326	-0.501207
H	3.654516	-0.472907	-1.702785
H	2.778745	-0.430140	-0.158751
H	0.466935	-3.307353	-0.962258
H	1.828169	-3.180360	0.163898
H	0.608514	-1.896900	0.092899
H	-0.607208	-0.418444	-4.276287
H	0.352144	-1.095096	-5.604158
H	0.767444	0.491741	-4.969905
H	2.700297	-1.422860	-5.372840
H	2.261473	-2.925655	-4.561362
H	3.434995	-1.827232	-3.810143
H	-1.150205	-2.449803	-2.311186
H	-3.431687	-3.065578	-1.290372
H	1.365468	1.014721	-0.742243
H	-0.196197	1.711327	-0.333463
H	0.219147	0.120922	0.307382

4b_AgBr
SCF Energy: -645.144357215
Num. Imaginary Frequencies: 1
Imaginary Frequency: -303.7987

C	-3.425920	-2.041462	-2.392539
C	-2.000821	-1.567856	-2.424947
C	-1.536272	-0.410183	-1.969992
Ag	-2.868232	1.101530	-0.953793
Br	-4.414437	2.823901	0.215356
C	-0.284968	0.188740	-1.856190
C	0.084832	1.451577	-2.604776
N	1.193392	-1.111785	-2.563314
C	2.053548	-1.661687	-1.509410
C	2.886527	-0.539555	-0.888897
C	1.382693	-1.383730	-3.796433
C	0.447608	-0.856283	-4.848247
C	2.526204	-2.232828	-4.314659
C	1.190908	-2.396126	-0.482236
H	-3.794808	-2.246982	-3.403347
H	-4.080669	-1.295558	-1.933381
H	0.164820	0.126532	-0.866185
H	2.742597	-2.396605	-1.939428
H	3.548581	-0.950744	-0.122280
H	3.500716	-0.046134	-1.648086
H	2.254211	0.217424	-0.415592
H	0.599894	-3.178710	-0.965558
H	1.835525	-2.861210	0.268595
H	0.500957	-1.722515	0.033301
H	-0.466767	-0.450484	-4.421394
H	0.190196	-1.668193	-5.535750
H	0.957142	-0.085934	-5.438903
H	2.576001	-2.165008	-5.402025
H	2.375588	-3.283902	-4.047482
H	3.485640	-1.912845	-3.901816
H	-1.275879	-2.258702	-2.874014
H	-3.513622	-2.973241	-1.823151
H	1.156309	1.468289	-2.817697
H	-0.479146	1.552949	-3.533276
H	-0.141286	2.317349	-1.975082

5a_AgBr
SCF Energy: -354.079692884
Num. Imaginary Frequencies: 0

C	-3.292616	-5.552534	-3.457081
Ag	-2.561973	-4.399211	-5.522637
Br	-1.782418	-3.639094	-7.853463
C	-3.334482	-4.270219	-3.107256
C	-3.425080	-3.052148	-2.634164
C	-3.215785	-1.765102	-3.384282
H	-2.354552	-6.092279	-3.312065
C	-4.502887	-6.362350	-3.867714
H	-3.678729	-2.971574	-1.576385
H	-2.987742	-1.934838	-4.439859
H	-4.113132	-1.143384	-3.320137
H	-2.391145	-1.200774	-2.939766
H	-4.293791	-6.972015	-4.750068
H	-4.768839	-7.044092	-3.053662
H	-5.357370	-5.715926	-4.073836

5b_AgBr
SCF Energy: -354.079647088
Num. Imaginary Frequencies: 0

C	-3.194533	-5.562204	-3.454445
Ag	-2.878022	-4.379107	-5.609700
Br	-2.521409	-3.626111	-8.044030
C	-3.279758	-4.282151	-3.104741
C	-3.379039	-3.066505	-2.627226
C	-3.167377	-1.777547	-3.373490
C	-1.958237	-6.413162	-3.265528
H	-4.107697	-6.068509	-3.774098
H	-3.649338	-2.989558	-1.573380
H	-2.840597	-1.946947	-4.402878
H	-4.094965	-1.198453	-3.396521
H	-2.411826	-1.170562	-2.867210
H	-1.742274	-7.006059	-4.157714
H	-1.090010	-5.796698	-3.027582
H	-2.127921	-7.111787	-2.440183

3.2.4 AuCl-catalyzed reaction

1a_AuCl
SCF Energy: -636.588835861
Num. Imaginary Frequencies: 0

C	-2.884015	-2.004806	-3.811400
C	-1.903781	-2.224297	-2.736641
C	-0.903367	-2.306211	-2.011048
C	0.483609	-2.289343	-1.425708
N	1.486383	-1.870211	-2.378822
C	1.618369	-2.654117	-3.612563
C	0.950576	-2.037534	-4.849781
Au	-2.625555	-2.941603	-0.749013
Cl	-4.029906	-3.687497	1.055974
C	1.776446	-0.433441	-2.447982
C	2.602878	0.004159	-1.235747
C	0.543567	0.465303	-2.621526
C	3.094594	-2.951073	-3.886900
H	-2.370764	-1.600326	-4.688567
H	-3.371323	-2.941610	-4.088276
H	0.463052	-1.542607	-0.624339
C	0.817436	-3.638204	-0.775027
H	1.118429	-3.610217	-3.421646
H	2.411464	-0.303241	-3.331082
H	3.508343	-0.602923	-1.157563
H	2.887866	1.056946	-1.324388
H	2.036737	-0.103842	-0.303890
H	-0.046073	0.178775	-3.496427
H	-0.108705	0.416566	-1.742216
H	0.854769	1.507314	-2.742336
H	-0.111140	-1.847070	-4.677333
H	1.427498	-1.094129	-5.135762
H	1.039186	-2.722725	-5.698050
H	3.653608	-2.023678	-4.054335
H	3.541053	-3.467635	-3.033371
H	3.207659	-3.574370	-4.779287
H	-3.648772	-1.293490	-3.493752
H	1.820713	-3.575165	-0.348149
H	0.102285	-3.871208	0.019029
H	0.793325	-4.453831	-1.501761

1b_AuCl
SCF Energy: -636.585395683
Num. Imaginary Frequencies: 0

C	-2.898499	-1.542711	-3.669916
C	-1.941918	-1.972300	-2.638902
C	-0.935018	-2.190597	-1.951368
C	0.460019	-2.302430	-1.385847
N	1.495038	-1.852997	-2.293243
C	1.737754	-2.740438	-3.443616
C	0.978401	-2.372112	-4.727199
Au	-2.645869	-3.088909	-0.847972
Cl	-4.026886	-4.224771	0.761275
C	1.713140	-0.418208	-2.540834
C	2.611727	0.234079	-1.482311
C	0.448335	0.416135	-2.784226
C	3.238962	-2.854729	-3.719641
H	-2.355652	-0.997590	-4.448353
H	-3.395440	-2.403477	-4.121586
C	0.513710	-1.666389	0.007675
H	0.629529	-3.376096	-1.243543
H	1.388946	-3.731663	-3.129979
H	2.286952	-0.384016	-3.472430
H	3.483479	-0.397339	-1.290751
H	2.958448	1.207615	-1.843789
H	2.091234	0.401476	-0.536724
H	-0.144004	0.010789	-3.609692
H	-0.190688	0.462950	-1.897179
H	0.734230	1.440916	-3.040503
H	-0.099893	-2.322327	-4.556129
H	1.312589	-1.408028	-5.125829
H	1.163563	-3.127310	-5.496947
H	3.658261	-1.899573	-4.053700
H	3.769090	-3.163644	-2.815401
H	3.426001	-3.589802	-4.508229
H	-3.657306	-0.883939	-3.243362
H	1.532671	-1.738921	0.393340
H	0.206612	-0.619094	-0.003894
H	-0.159386	-2.206509	0.679041

2a_AuCl
SCF Energy: -636.556454463
Num. Imaginary Frequencies: 1
Imaginary Frequency: -618.8045

C	-3.380781	-2.785287	-2.990898
C	-3.782233	-2.877199	-4.407851
C	-4.281279	-3.466932	-5.427010
Au	-5.076620	-5.325969	-5.006352
Cl	-6.030890	-7.513034	-4.537205
C	-4.282251	-2.892935	-6.865760
N	-4.272200	-1.430138	-6.813396
C	-5.569546	-0.708102	-6.735238
C	-6.362434	-0.717177	-8.048384
C	-3.232395	-0.948491	-5.986245
C	-1.825941	-1.366921	-6.416623
C	-3.263538	0.520477	-5.581216
C	-6.434973	-1.106135	-5.535993
H	-2.305599	-2.609978	-2.899266
H	-3.617650	-3.735400	-2.504327
H	-3.318089	-3.201048	-7.278675
C	-5.336235	-3.529801	-7.763705
H	-5.286867	0.335110	-6.605658
H	-7.032325	0.147703	-8.045463
H	-5.691019	-0.623593	-8.905948
H	-6.981454	-1.604529	-8.178171
H	-5.908891	-0.950874	-4.588522
H	-7.341897	-0.494317	-5.528877
H	-6.733903	-2.157808	-5.577471
H	-1.695769	-2.447117	-6.477810
H	-1.098277	-0.990578	-5.694455
H	-1.604419	-0.926351	-7.394032
H	-2.388443	0.728132	-4.963081
H	-4.149539	0.788778	-5.004051
H	-3.208381	1.160477	-6.468422
H	-3.391608	-1.548503	-4.936183
H	-3.919056	-1.985006	-2.476519
H	-5.309577	-3.083937	-8.759831
H	-5.097755	-4.591965	-7.853326
H	-6.344550	-3.455729	-7.353791

3a_AuCl
SCF Energy: -636.599015102
Num. Imaginary Frequencies: 0

C	-2.977583	-2.694979	-3.264072
C	-3.114973	-2.558431	-4.754746
C	-3.480014	-3.531989	-5.601964
Au	-3.852790	-5.449117	-5.070661
Cl	-4.264540	-7.800727	-4.447868
C	-3.570486	-3.293577	-7.103515
N	-3.164183	-1.892079	-7.506534
C	-4.158683	-0.768823	-7.637997
C	-4.517803	-0.542069	-9.107025
C	-1.900552	-1.639601	-7.651896
C	-0.851059	-2.690506	-7.432265
C	-1.365274	-0.286116	-8.013140
C	-5.413431	-0.911262	-6.773593
H	-1.958572	-2.454724	-2.938806
H	-3.211626	-3.712197	-2.942030
H	-2.817725	-3.923407	-7.580979
C	-4.904608	-3.737116	-7.715320
H	-3.624976	0.103011	-7.256352
H	-5.112128	0.372301	-9.185457
H	-3.635428	-0.436531	-9.742842
H	-5.121238	-1.366724	-9.491316
H	-5.209756	-1.397548	-5.818648
H	-5.780927	0.098188	-6.572337
H	-6.205891	-1.451459	-7.290957
H	-1.072295	-3.315785	-6.566451
H	0.115034	-2.205613	-7.290658
H	-0.776230	-3.327223	-8.321994
H	-0.490948	-0.421916	-8.653055
H	-1.011689	0.190477	-7.089718
H	-2.065999	0.379701	-8.507289
H	-2.892782	-1.551109	-5.129098
H	-3.650336	-2.003440	-2.743290
H	-5.028442	-3.369363	-8.737077
H	-4.887101	-4.827957	-7.752724
H	-5.760859	-3.454602	-7.106200

2b_AuCl
SCF Energy: -636.561509627
Num. Imaginary Frequencies: 1
Imaginary Frequency: -608.0828

C	-2.751969	-2.881215	-3.860229
C	-3.408067	-3.115395	-5.160040
C	-3.992770	-3.831685	-6.041667
Au	-4.378752	-5.771710	-5.445436
Cl	-4.881623	-8.057616	-4.790419
C	-4.449288	-3.401876	-7.435245
N	-4.425049	-1.939260	-7.566756
C	-5.769307	-1.320721	-7.454486
C	-6.678135	-1.783074	-8.594278
C	-3.725324	-4.168249	-8.548674
C	-3.351319	-1.286959	-6.927578
C	-1.969837	-1.627560	-7.482573
C	-3.493545	0.212088	-6.694857
C	-6.420567	-1.532402	-6.084416
H	-1.717364	-2.555570	-3.996855
H	-2.747472	-3.822620	-3.304081
H	-5.496889	-3.697937	-7.510818
H	-5.617240	-0.251787	-7.611094
H	-7.571657	-1.153124	-8.615585
H	-6.165464	-1.689432	-9.555231
H	-7.016588	-2.816603	-8.477236
H	-5.783747	-1.168428	-5.271574
H	-7.372769	-0.996299	-6.039056
H	-6.621789	-2.592844	-5.898693
H	-1.744355	-2.689743	-7.408773
H	-1.205601	-1.084357	-6.921033
H	-1.915978	-1.323922	-8.532851
H	-2.604562	0.569789	-6.172254
H	-4.365635	0.475420	-6.095414
H	-3.552078	0.735749	-7.655343
H	-3.324364	-1.771270	-5.812448
H	-3.289838	-2.132036	-3.274220
H	-4.068607	-3.794744	-9.516775
H	-2.640733	-4.077065	-8.501859
H	-3.978198	-5.229081	-8.467515

3b_AuCl
SCF Energy: -636.606204345
Num. Imaginary Frequencies: 0

C	-2.883703	-2.966178	-3.280326
C	-3.010405	-2.702212	-4.754813
C	-3.364713	-3.599592	-5.686112
Au	-3.847111	-5.526789	-5.294390
Cl	-4.437159	-7.875693	-4.818198
C	-3.523428	-3.206701	-7.148724
N	-3.047988	-1.812786	-7.483615
C	-4.127899	-0.853195	-7.866506
C	-4.752540	-1.276395	-9.194500
C	-1.802692	-1.466913	-7.459893
C	-0.706169	-2.388024	-7.030711
C	-1.355412	-0.089903	-7.870528
C	-5.143690	-0.705260	-6.735344
H	-1.867232	-2.755130	-2.927270
H	-3.121783	-4.006431	-3.046996
C	-2.979842	-4.202289	-8.182756
H	-4.599390	-3.157180	-7.326443
H	-3.652612	0.115655	-8.005675
H	-5.477646	-0.517552	-9.498073
H	-3.993685	-1.360056	-9.977748
H	-5.280600	-2.230111	-9.114488
H	-4.661405	-0.374625	-5.813099
H	-5.874301	0.050445	-7.034522
H	-5.682201	-1.632477	-6.526831
H	-1.047237	-3.300142	-6.553469
H	-0.071810	-1.837643	-6.328606
H	-0.087415	-2.615226	-7.907341
H	-0.267035	-0.059086	-7.901972
H	-1.695471	0.656274	-7.144961
H	-1.740974	0.185357	-8.854855
H	-2.777760	-1.669542	-5.040255
H	-3.560609	-2.320756	-2.708374
H	-3.064673	-3.789153	-9.193030
H	-1.944328	-4.491217	-7.999473
H	-3.583033	-5.110283	-8.127855

4a_AuCl
SCF Energy: -636.571639735
Num. Imaginary Frequencies: 1
Imaginary Frequency: -343.1136

C	-3.440641	-2.053548	-2.318770
C	-2.033298	-1.542194	-2.398339
C	-1.588870	-0.373672	-1.952183
C	-0.359080	0.291410	-1.877897
Au	-2.649891	1.084912	-0.926632
Cl	-4.063526	2.665175	0.275231
N	1.164551	-1.181145	-2.587839
C	1.411846	-1.434215	-3.813942
C	2.597132	-2.241973	-4.303832
C	2.007830	-1.713641	-1.513347
C	1.119472	-2.345676	-0.441761
C	2.890942	-0.595933	-0.956818
C	0.490786	-0.925777	-4.888411
H	-3.830288	-2.276055	-3.317744
H	-4.099695	-1.324041	-1.842854
C	0.019354	1.467227	-2.744127
H	0.159626	0.237568	-0.923551
H	2.660337	-2.503688	-1.903801
H	3.536394	-0.987574	-0.166077
H	3.523296	-0.170775	-1.742180
H	2.288949	0.212269	-0.530034
H	0.493304	-3.130610	-0.874238
H	1.743766	-2.789904	0.338428
H	0.459499	-1.611386	0.029112
H	-0.436812	-0.532012	-4.476132
H	0.256944	-1.743719	-5.577797
H	0.994297	-0.148249	-5.474696
H	2.714696	-2.114772	-5.380964
H	2.440748	-3.307746	-4.105988
H	3.525187	-1.940200	-3.813373
H	-1.289935	-2.196511	-2.862768
H	-3.480100	-2.984490	-1.743193
H	1.059863	1.366923	-3.062613
H	-0.631883	1.551081	-3.614953
H	-0.060806	2.387851	-2.159469

4b_AuCl
SCF Energy: -636.571640258
Num. Imaginary Frequencies: 1
Imaginary Frequency: -343.1064

C	-3.452680	-2.046058	-2.314792
C	-2.046036	-1.532647	-2.393443
C	-1.603662	-0.363315	-1.947372
Au	-2.667590	1.094158	-0.923236
Cl	-4.084620	2.672842	0.276692
C	-0.374920	0.303585	-1.872319
C	0.002590	1.479638	-2.738630
N	1.151394	-1.167002	-2.580761
C	1.994734	-1.697966	-1.505560
C	2.875817	-0.578823	-0.948706
C	1.400187	-1.419649	-3.806654
C	0.479043	-0.913063	-4.881923
C	2.587367	-2.225221	-4.295541
C	1.106564	-2.331020	-0.434424
H	-3.841210	-2.269528	-3.313985
H	-4.113199	-1.317357	-1.839672
H	0.143117	0.250761	-0.917554
H	2.648653	-2.487163	-1.895372
H	3.521265	-0.969295	-0.157384
H	3.508118	-0.152953	-1.733724
H	2.272326	0.228613	-0.522588
H	0.481838	-3.116976	-0.867126
H	1.730961	-2.774132	0.346319
H	0.445196	-1.597559	0.035785
H	-0.449607	-0.520967	-4.470446
H	0.247269	-1.731562	-5.571354
H	0.981563	-0.134708	-5.467961
H	2.706000	-2.097234	-5.372464
H	2.432408	-3.291356	-4.098503
H	3.514365	-1.922276	-3.803818
H	-1.301328	-2.186022	-2.857045
H	-3.491204	-2.976838	-1.738888
H	1.043596	1.380846	-3.055951
H	-0.647852	1.562092	-3.610186
H	-0.079662	2.400406	-2.154490

5a_AuCl
SCF Energy: -345.496997984
Num. Imaginary Frequencies: 0

C	-3.242230	-5.550391	-3.584254
Au	-2.618155	-4.444699	-5.410687
Cl	-1.887801	-3.917703	-7.644420
C	-3.265950	-4.211609	-3.332107
C	-3.416131	-3.050042	-2.736548
C	-3.225424	-1.691311	-3.343967
H	-2.333844	-6.097176	-3.328253
C	-4.481170	-6.371815	-3.857418
H	-3.705666	-3.096842	-1.686066
H	-2.967251	-1.757191	-4.402735
H	-4.140972	-1.102075	-3.240395
H	-2.428543	-1.154191	-2.821391
H	-4.295429	-7.120948	-4.629649
H	-4.755526	-6.897860	-2.936824
H	-5.315658	-5.739355	-4.162681

5b_AuCl
SCF Energy: -345.496961774
Num. Imaginary Frequencies: 0

C	-3.168689	-5.557347	-3.604869
Au	-2.866790	-4.431674	-5.498493
Cl	-2.483329	-3.881920	-7.811841
C	-3.232232	-4.220122	-3.350278
C	-3.341974	-3.066394	-2.730945
C	-3.204675	-1.697967	-3.330964
C	-1.959517	-6.410024	-3.295452
H	-4.105888	-6.080768	-3.798051
H	-3.562631	-3.128345	-1.664598
H	-2.953818	-1.745933	-4.392363
H	-4.139899	-1.142121	-3.216787
H	-2.423954	-1.136864	-2.809669
H	-1.791478	-7.154479	-4.076174
H	-1.063297	-5.798933	-3.181764
H	-2.144832	-6.942469	-2.356476

3.2.5 AuPMe$_3$-catalyzed reaction

1a_AuPMe3
SCF Energy: -1082.49663650
Num. Imaginary Frequencies: 0

C	0.031424	0.541206	0.180819
C	-0.578000	1.726895	-0.435520
C	-0.942558	2.720435	-1.060856
C	-1.114633	3.935662	-1.934731
H	1.028331	0.397941	-0.246198
H	0.133510	0.667805	1.260241
H	-0.563153	-0.352206	-0.019833
H	-2.040999	3.784985	-2.499264
C	-1.302570	5.191637	-1.073165
H	-1.463238	6.043909	-1.736505
H	-0.424698	5.388376	-0.453408
H	-2.169254	5.082268	-0.412227
N	-0.046225	4.076574	-2.893415
C	1.329106	4.120830	-2.376659
H	1.246014	4.354242	-1.308766
C	2.098333	5.264362	-3.040833
H	2.183724	5.101174	-4.120582
H	3.111339	5.338487	-2.634295
H	1.580644	6.213374	-2.880218
C	2.107097	2.802339	-2.493170
H	2.285569	2.533499	-3.539416
H	3.082757	2.906197	-2.009802
H	1.576135	1.975360	-2.014706
C	-0.261830	3.475729	-4.216341
H	0.704978	3.535840	-4.726886
C	-1.250294	4.315096	-5.028976
H	-2.249034	4.309746	-4.577170
H	-0.907253	5.350864	-5.088606
H	-1.349589	3.916049	-6.042642
C	-0.687507	2.001262	-4.188360
H	-0.753819	1.611811	-5.208306
H	-1.675897	1.883513	-3.728491
H	0.022167	1.384994	-3.630876
Au	-2.755440	2.270649	0.389295
P	-4.749301	2.321746	1.539714
C	-5.060037	3.920784	2.354789
H	-5.086420	4.716344	1.607071
H	-4.259162	4.130102	3.066875
H	-6.017498	3.886718	2.882115
H	-7.110018	2.050037	1.097127
C	-6.203215	2.016332	0.486795
H	-6.261590	2.777726	-0.293592
H	-6.116233	1.033822	0.018539
C	-4.839068	1.069494	2.859429
H	-4.734151	0.073298	2.424904
H	-4.033629	1.231918	3.578312
H	-5.803232	1.143601	3.370072

1b_AuPMe3
SCF Energy: -1082.49295512
Num. Imaginary Frequencies: 0

C	-4.698073	3.877433	2.669969
P	-4.676659	2.393219	1.615271
Au	-2.769057	2.184304	0.340029
C	-1.031375	2.500887	-1.241486
C	-1.113161	3.770233	-2.059529
N	-0.004790	3.934337	-2.970211
C	0.079015	3.147632	-4.214223
C	-0.718253	3.775467	-5.364237
C	-0.755133	1.441731	-0.681851
C	-0.227773	0.164520	-0.183925
C	-4.933032	0.990380	2.748511
C	-6.192738	2.490964	0.610653
C	1.284564	4.261674	-2.334331
C	2.193235	3.056796	-2.049608
C	2.028425	5.318007	-3.154158
C	-0.225672	1.650319	-4.076530
H	0.004344	0.221475	0.881231
H	0.692836	-0.064662	-0.729206
H	-1.031363	4.586871	-1.332341
C	-2.494618	3.899261	-2.710880
H	-5.628439	3.904250	3.244301
H	-3.847885	3.854847	3.354512
H	-4.629409	4.771837	2.047581
H	-5.851753	1.147043	3.320654
H	-4.086863	0.912457	3.434210
H	-5.014639	0.064149	2.176032
H	-7.063869	2.574314	1.266454
H	-6.144907	3.365150	-0.042232
H	-6.284594	1.593395	-0.004112
H	1.030617	4.718605	-1.369975
H	1.393972	6.192818	-3.315481
H	2.937184	5.631751	-2.632319
H	2.329406	4.927805	-4.131944
H	1.686760	2.303566	-1.440304
H	3.085596	3.385108	-1.508821
H	2.528862	2.582372	-2.977764
H	1.129216	3.219751	-4.512561
H	-1.267083	1.465028	-3.794966
H	0.419011	1.176974	-3.330403
H	-0.053017	1.157747	-5.037940
H	-1.795183	3.622295	-5.262422
H	-0.523294	4.850019	-5.412583
H	-0.411476	3.323527	-6.312587
H	-0.939992	-0.645705	-0.351852
H	-2.520488	4.810271	-3.311769
H	-2.735357	3.044268	-3.344723
H	-3.261439	3.969910	-1.932662

2b_AuPMe3
SCF Energy: -1082.47399372
Num. Imaginary Frequencies: 1
Imaginary Frequency: -577.4330

C	-2.850649	-2.705513	-3.773188
C	-3.448850	-3.003945	-5.086357
C	-3.980902	-3.745499	-5.973725
Au	-4.312171	-5.758386	-5.334189
P	-4.717716	-7.964145	-4.725489
C	-4.397372	-3.369189	-7.398585
N	-4.393278	-1.916182	-7.573564
C	-5.750328	-1.314506	-7.546900
C	-6.605015	-1.841047	-8.700247
C	-3.615944	-4.157297	-8.457067
C	-3.354890	-1.217615	-6.919737
C	-1.947151	-1.557567	-7.406387
C	-3.530680	0.288324	-6.766425
C	-6.453397	-1.473381	-6.196032
H	-1.814622	-2.375274	-3.883371
H	-2.861433	-3.617447	-3.168958
H	-5.436448	-3.687548	-7.503413
H	-5.604876	-0.252176	-7.745258
H	-7.500093	-1.220270	-8.792112
H	-6.052567	-1.791164	-9.642092
H	-6.943576	-2.870056	-8.545721
H	-5.850508	-1.072316	-5.374923
H	-7.408827	-0.941877	-6.209387
H	-6.658447	-2.527028	-5.977382
H	-1.703182	-2.610064	-7.272271
H	-1.215456	-0.971769	-6.844847
H	-1.858093	-1.303722	-8.467226
H	-2.669096	0.686724	-6.227972
H	-4.429737	0.565656	-6.215212
H	-3.558311	0.763710	-7.752800
H	-3.366425	-1.651786	-5.790070
H	-3.417795	-1.933527	-3.248020
H	-3.931136	-3.826299	-9.449446
H	-2.536186	-4.038788	-8.375646
H	-3.849776	-5.221425	-8.351080
C	-3.226288	-8.886668	-4.222654
C	-5.874064	-8.152582	-3.327368
C	-5.448285	-8.958939	-6.068506
H	-6.029819	-9.214184	-3.115877
H	-5.463284	-7.662042	-2.442469
H	-6.829926	-7.687031	-3.576247
H	-3.495885	-9.911461	-3.951785
H	-2.511623	-8.904995	-5.048249
H	-2.762091	-8.394740	-3.365333
H	-5.610933	-9.984879	-5.726724
H	-6.402166	-8.521811	-6.371239
H	-4.774132	-8.964767	-6.927599

2a_AuPMe3
SCF Energy: -1082.46942798
Num. Imaginary Frequencies: 1
Imaginary Frequency: -581.7684

C	5.976986	0.833782	3.836068
P	5.080394	0.437442	2.297563
C	5.922407	-1.041056	1.639705
Au	2.791491	0.181132	2.600761
C	0.689379	-0.009858	2.921946
C	0.023423	0.501408	4.230165
N	-1.371164	0.836062	3.971773
C	-2.058262	-0.232180	3.345843
C	-3.435831	0.054352	2.759947
C	0.082497	-0.591255	1.964191
C	-0.016316	-1.296977	0.673663
C	5.528481	1.778574	1.144760
C	-1.712954	2.207245	3.508521
C	-1.579270	3.282822	4.593417
C	-1.019659	2.611153	2.204519
C	-2.064525	-1.538454	4.141550
H	-0.452668	-2.290409	0.804858
H	0.990272	-1.414235	0.261537
C	0.857976	1.559009	4.942639
H	0.025375	-0.372667	4.886438
H	5.835672	0.029233	4.560872
H	5.586700	1.762063	4.258805
H	7.043657	0.950545	3.625121
H	5.128220	2.725826	1.512196
H	5.102401	1.573676	0.160382
H	6.616723	1.850759	1.062999
H	5.768827	-1.882619	2.318363
H	6.993643	-0.845562	1.539182
H	5.506537	-1.295004	0.662492
H	-2.782121	2.161864	3.311728
H	-1.374496	3.599600	1.899042
H	0.067513	2.661076	2.320069
H	-1.236276	1.904210	1.397048
H	-1.369380	-0.495931	2.382615
H	-2.585848	-2.308530	3.569582
H	-1.066193	-1.916217	4.362344
H	-3.829385	-0.869989	2.333893
H	-3.420698	0.804670	1.968246
H	-4.123408	0.380267	3.547594
H	-2.231252	4.118045	4.322673
H	-0.569862	3.681815	4.692682
H	-1.907647	2.898952	5.562601
H	-2.601760	-1.383256	5.082433
H	-0.622120	-0.733461	-0.040116
H	0.350850	1.904849	5.844755
H	1.801782	1.093474	5.239556
H	1.093302	2.413691	4.305845

3a_AuPMe3
SCF Energy: -1082.51725166
Num. Imaginary Frequencies: 0

C	-2.704972	-2.872602	-3.306071
C	-2.737877	-2.691513	-4.797579
C	-3.148490	-3.596157	-5.698122
C	-3.073962	-3.290506	-7.188805
C	-4.131163	-3.974128	-8.060152
Au	-3.802940	-5.492528	-5.154872
P	-4.541454	-7.638597	-4.489755
N	-2.994950	-1.816791	-7.494314
C	-1.841972	-1.253229	-7.680762
C	-1.707661	0.183261	-8.094831
C	-4.250185	-0.988611	-7.547232
C	-5.235763	-1.302780	-6.422783
C	-4.896193	-1.035564	-8.934793
C	-0.552011	-1.993902	-7.484848
H	-1.698730	-2.693641	-2.911446
H	-3.013334	-3.881758	-3.020737
H	-2.127650	-3.695043	-7.554068
H	-3.913351	0.030974	-7.365385
H	-5.570568	-0.180589	-9.027357
H	-4.150278	-0.969249	-9.731998
H	-5.484329	-1.941646	-9.082917
H	-4.811005	-1.083293	-5.443272
H	-6.104545	-0.657063	-6.578181
H	-5.576257	-2.337995	-6.416680
H	-0.605243	-2.725716	-6.678935
H	0.232975	-1.271536	-7.257652
H	-0.270197	-2.497662	-8.417619
H	-0.742982	0.318749	-8.584661
H	-1.712423	0.821128	-7.202195
H	-2.495902	0.517762	-8.767872
H	-2.407545	-1.696638	-5.121383
H	-3.372152	-2.156734	-2.811619
H	-4.006547	-3.704810	-9.112329
H	-3.971140	-5.050703	-7.967299
H	-5.155984	-3.769989	-7.749148
C	-6.012728	-7.634012	-3.403757
C	-5.015218	-8.753368	-5.859744
C	-3.306402	-8.605407	-3.550161
H	-6.294161	-8.657165	-3.138559
H	-5.793050	-7.070623	-2.494075
H	-6.845280	-7.150923	-3.920039
H	-3.719568	-9.576175	-3.262013
H	-2.417928	-8.757557	-4.167116
H	-3.016828	-8.053261	-2.653379
H	-5.344425	-9.719893	-5.467555
H	-5.826250	-8.300982	-6.434895
H	-4.158431	-8.903586	-6.520520

3b_AuPMe3
SCF Energy: -1082.52289077
Num. Imaginary Frequencies: 0

C	6.255856	1.367178	0.901548
P	5.308992	-0.196721	0.863969
C	6.384780	-1.377476	1.754743
Au	3.096860	-0.045025	1.688047
C	1.141028	0.096640	2.377632
C	0.995399	0.181452	3.888512
N	-0.425652	0.208529	4.397291
C	-0.848205	1.507493	5.008514
C	-0.720091	2.645707	3.998352
C	0.083906	0.191858	1.559324
C	0.120596	0.177185	0.056601
C	5.422357	-0.732719	-0.880474
C	-1.221338	-0.810165	4.343473
C	-2.598653	-0.772496	4.946486
C	-0.849883	-2.102871	3.692047
C	-0.075901	1.751287	6.303320
H	-0.482225	-0.646082	-0.343069
H	1.142486	0.068224	-0.316176
H	-0.928091	0.287789	1.969712
C	1.823148	-0.829006	4.694697
H	1.378590	1.164199	4.170260
H	6.468251	-0.781706	-1.196538
H	4.884909	-0.024017	-1.514649
H	4.962640	-1.717425	-0.991024
H	7.262172	1.212408	0.501875
H	5.739209	2.120915	0.303147
H	7.380888	-1.399446	1.303753
H	5.945312	-2.376426	1.711345
H	6.468072	-1.077914	2.802036
H	6.325722	1.727031	1.930427
H	-1.688589	-2.404018	3.056548
H	0.050527	-2.058433	3.089354
H	-0.756980	-2.865808	4.474452
H	-3.249395	-0.100231	4.378112
H	-3.033563	-1.770538	4.913654
H	-2.577756	-0.434602	5.985118
H	-1.903526	1.408642	5.252942
H	0.992509	1.898536	6.124349
H	-0.203797	0.920696	7.003228
H	-0.462245	2.658172	6.774081
H	-1.307267	2.444444	3.099985
H	0.314168	2.833233	3.700390
H	-1.105631	3.555378	4.465021
H	-0.297290	1.104266	-0.351552
H	1.596622	-0.748318	5.762123
H	1.674115	-1.861130	4.375219
H	2.879827	-0.591667	4.552033

4a_AuPMe3
SCF Energy: -1082.47768421
Num. Imaginary Frequencies: 1
Imaginary Frequency: -287.7329

C	6.447010	-1.430985	1.831255
P	5.460868	-0.229241	0.876454
C	6.451028	1.303349	0.895547
C	5.552414	-0.817180	-0.848303
Au	3.273296	0.023517	1.652601
C	1.183470	0.119439	2.221056
C	0.217932	-0.497194	1.551372
C	0.357407	-1.309249	0.298677
C	1.326215	0.885822	3.368975
C	1.576311	2.365784	3.339383
N	-0.743744	0.732529	4.402911
C	-1.782061	1.778041	4.342453
C	-1.825041	2.391172	2.945909
C	-0.946037	-0.311112	5.114210
C	-2.165003	-0.550040	5.980274
C	0.048002	-1.445443	5.130432
C	-1.553218	2.837565	5.422113
H	-0.011378	-2.327515	0.458142
H	1.398248	-1.364656	-0.030921
H	-0.788471	-0.397980	1.967371
H	1.668891	0.382857	4.271920
H	7.456597	1.100576	0.516018
H	6.518511	1.683792	1.916886
H	5.971300	2.057857	0.268546
H	7.448616	-1.516403	1.400951
H	6.523912	-1.099506	2.868999
H	6.598520	-0.912037	-1.153082
H	5.046157	-0.106684	-1.505258
H	5.060076	-1.788450	-0.932818
H	5.957139	-2.406523	1.808493
H	-0.489468	-2.395687	5.192827
H	0.675757	-1.463533	4.240211
H	0.675466	-1.377169	6.026775
H	-2.942235	-1.045063	5.386009
H	-1.903605	-1.224017	6.798574
H	-2.584047	0.363613	6.399899
H	-2.760298	1.313997	4.517564
H	-0.619634	3.380463	5.252532
H	-1.509269	2.391562	6.419507
H	-2.369451	3.564934	5.405475
H	-1.962872	1.620589	2.183087
H	-0.909143	2.940780	2.719944
H	-2.662792	3.090784	2.879915
H	-0.240076	-0.875216	-0.509325
H	1.055571	2.841624	4.171091
H	2.645813	2.548519	3.487912
H	1.270109	2.810230	2.392286

4b_AuPMe3
SCF Energy: -1082.48207905
Num. Imaginary Frequencies: 1
Imaginary Frequency: -289.7803

C	6.604921	-0.786604	1.906477
P	5.313072	0.083209	0.955792
C	5.920968	1.795960	0.799563
C	5.420767	-0.608503	-0.728830
Au	3.172511	-0.094108	1.871798
C	1.232223	0.330941	3.699076
C	1.115540	-0.381263	2.520845
C	0.196399	-1.011721	1.803036
C	0.376701	-1.678888	0.472556
N	-0.960039	0.509240	4.495245
C	-1.564369	-0.407176	5.146733
C	-0.988228	-1.796000	5.190497
C	-1.522188	1.858603	4.388653
C	-0.766984	2.799463	5.328256
C	-1.450799	2.315147	2.932282
C	-2.863995	-0.219089	5.902911
H	0.109654	-2.738562	0.533808
H	1.408005	-1.600958	0.118527
H	-0.805581	-1.038641	2.242032
C	1.883341	-0.194264	4.948430
H	1.170765	1.415426	3.623763
H	6.917102	1.798943	0.348223
H	5.968784	2.258949	1.787411
H	5.236336	2.371061	0.172934
H	7.574075	-0.674414	1.412115
H	6.660721	-0.368119	2.913686
H	6.438636	-0.500806	-1.113669
H	4.726626	-0.080008	-1.385997
H	5.150533	-1.666613	-0.708158
H	6.354638	-1.847032	1.979139
H	-1.771287	-2.521162	4.945813
H	-0.162575	-1.913727	4.489581
H	-0.646089	-2.028212	6.205700
H	-3.704816	-0.148543	5.204658
H	-3.043581	-1.073524	6.556999
H	-2.853318	0.688670	6.510134
H	-2.579274	1.856015	4.680458
H	0.295511	2.849285	5.067353
H	-0.845966	2.463303	6.366377
H	-1.177872	3.810213	5.259811
H	-1.979473	1.613798	2.281220
H	-0.416256	2.387062	2.582036
H	-1.912942	3.300530	2.828105
H	-0.282104	-1.224965	-0.274551
H	1.280743	0.092895	5.813663
H	2.000512	-1.278218	4.919457
H	2.868275	0.268003	5.070107

5a_AuPMe3
SCF Energy: -791.400767936
Num. Imaginary Frequencies: 0

C	4.272813	-0.626748	-1.058741
P	4.041745	0.781548	-2.190434
C	4.316945	0.117450	-3.863724
Au	1.978482	1.791071	-1.926489
C	0.072223	3.220701	-1.945540
C	-0.299049	2.177891	-1.187968
C	-0.852959	1.274210	-0.418630
C	-0.227687	0.029205	0.143091
C	5.439721	1.903500	-1.869154
H	-0.304906	0.034262	1.233550
H	0.825475	-0.059281	-0.134350
H	-1.897944	1.462508	-0.168122
C	0.509113	4.556978	-1.388694
H	-0.135052	3.168207	-3.016420
H	3.490600	-1.369009	-1.230869
H	4.212867	-0.279932	-0.024872
H	5.251379	-1.082957	-1.233357
H	5.379362	2.279469	-0.845867
H	5.400819	2.747478	-2.560661
H	3.544296	-0.616784	-4.100412
H	4.270768	0.928711	-4.593296
H	5.299924	-0.359819	-3.911621
H	6.382190	1.365918	-2.004610
H	-0.762023	-0.852912	-0.220179
H	1.363573	4.957940	-1.938380
H	-0.317952	5.264726	-1.503224
H	0.760499	4.482614	-0.329985

5b_AuPMe3
SCF Energy: -791.400779800
Num. Imaginary Frequencies: 0

C	4.309856	-0.558969	-0.965139
P	4.052350	0.805603	-2.143645
C	4.343233	0.089145	-3.792339
Au	1.972870	1.788570	-1.912586
C	0.036953	3.175713	-1.999982
C	-0.313941	2.153901	-1.204922
C	-0.854527	1.253677	-0.422056
C	-0.251809	-0.038672	0.050926
C	5.430461	1.962154	-1.861689
H	-0.179667	-0.039022	1.141982
H	0.744997	-0.200028	-0.367016
H	-1.862652	1.488357	-0.077522
H	0.468971	4.060254	-1.527421
C	-0.361164	3.292040	-3.453966
H	3.548305	-1.326209	-1.119827
H	4.232446	-0.181799	0.056686
H	5.301161	-0.994665	-1.118999
H	5.365940	2.369643	-0.850778
H	5.376332	2.782501	-2.580126
H	3.589829	-0.672983	-4.001483
H	4.277031	0.871654	-4.551053
H	5.338018	-0.364309	-3.822413
H	6.381181	1.435407	-1.981948
H	-0.893849	-0.875492	-0.236566
H	0.470825	3.645241	-4.067320
H	-0.721928	2.339459	-3.843890
H	-1.165439	4.030176	-3.533001

3_syn_formaldehyde
SCF Energy: -1043.22794562
Num. Imaginary Frequencies: 0

C	0.045305	3.759546	-0.294428
C	-1.107995	2.819919	-0.492633
C	-1.058006	1.479972	-0.469567
C	-2.344186	0.753318	-0.803781
N	-2.611627	-0.427249	0.072806
C	-2.784481	-1.738966	-0.620833
C	-2.687938	-0.307547	1.359123
C	-1.474676	-2.196616	-1.254381
C	-3.938292	-1.647676	-1.619549
C	-2.803188	-1.500613	2.262911
C	-2.672224	1.028630	2.025976
Au	0.673074	0.394977	-0.143239
P	2.700321	-0.796357	0.173971
C	3.411345	-0.712173	1.856638
C	4.063137	-0.223501	-0.901969
C	2.598376	-2.590761	-0.170870
H	0.969684	3.213328	-0.087353
H	0.202584	4.376868	-1.185683
H	-0.148382	4.446537	0.536904
H	-2.070564	3.312982	-0.676505
H	-2.285422	0.355399	-1.817064
H	-3.228170	1.403554	-0.762313
H	-3.029272	1.834442	1.388614
H	-3.273423	0.970661	2.935261
H	-1.640254	1.265877	2.311619
H	-0.689806	-2.311625	-0.501190
H	-2.129123	-2.307351	1.971780
H	-2.569969	-1.198178	3.283508
H	-3.829919	-1.883606	2.255563
H	-4.162057	-2.655676	-1.976177
H	-4.838423	-1.245733	-1.147192
H	-3.692201	-1.036642	-2.490549
H	-3.075507	-2.456021	0.144317
H	-1.639681	-3.162204	-1.739057
H	-1.121111	-1.491029	-2.012140
H	3.599521	0.331578	2.118106
H	4.349737	-1.272057	1.903883
H	2.703440	-1.129613	2.576227
H	1.888542	-3.056308	0.517109
H	3.577968	-3.062023	-0.050194
H	2.247107	-2.744867	-1.194113
H	4.968016	-0.808421	-0.714805
H	4.265676	0.831150	-0.702420
H	3.771659	-0.329346	-1.949244

3.3 Allene isomerization

4_syn_formaldehyde
SCF Energy: -1043.16152352
Num. Imaginary Frequencies: 1
Imaginary Frequency: -261.6382

C	1.054301	3.683216	0.576178
C	-0.255860	3.379058	-0.074809
C	-0.740209	2.155660	-0.365829
C	-1.986949	1.722506	-0.757800
N	-2.535139	-0.317029	0.338696
C	-3.082676	-1.353157	-0.542650
C	-2.019898	-1.805511	-1.545699
C	-4.324736	-0.802061	-1.240236
C	-2.094843	-0.605329	1.501359
C	-1.614423	0.484672	2.420118
C	-2.021598	-2.008202	2.069573
Au	0.611102	0.458078	-0.266521
P	2.188564	-1.234398	-0.032180
C	3.799816	-0.833975	-0.787544
C	2.560851	-1.586295	1.720282
C	1.747744	-2.860753	-0.733330
H	1.484723	2.796249	1.049630
H	1.772758	4.067071	-0.157065
H	0.921373	4.468710	1.326760
H	-0.826490	4.249566	-0.405868
H	-2.903862	2.043870	-0.270371
H	-2.113411	1.135506	-1.662477
H	-1.689764	-0.972737	-2.175948
H	-1.141199	-2.207267	-1.031405
H	-2.425249	-2.583449	-2.198442
H	-1.804001	1.477937	2.016589
H	-0.538966	0.373406	2.609865
H	-2.120422	0.381274	3.385925
H	-1.383325	-2.020770	2.954906
H	-1.630817	-2.722865	1.340882
H	-3.017200	-2.350291	2.372079
H	-3.391658	-2.224077	0.049220
H	-4.073886	0.037929	-1.895125
H	-5.059433	-0.458540	-0.507629
H	-4.786444	-1.580379	-1.853449
H	2.951903	-0.686408	2.199976
H	3.299275	-2.389136	1.796701
H	1.643996	-1.887532	2.233137
H	2.583644	-3.554578	-0.603727
H	1.521436	-2.758081	-1.796841
H	3.672186	-0.699143	-1.863759
H	4.184141	0.094431	-0.359742
H	4.512447	-1.642993	-0.604184
H	0.869537	-3.259630	-0.220333

TS_iso_allene_AuPMe3
SCF Energy: -1174.67664281
Num. Imaginary Frequencies: 1
Imaginary Frequency: -385.5342

C	1.734760	-2.527322	0.957354
C	1.751773	-2.246606	-0.420064
C	2.880607	-2.608356	-1.174353
C	3.955413	-3.252980	-0.572371
C	3.923527	-3.536709	0.793305
C	2.811997	-3.168872	1.555668
C	0.637191	-1.589386	-1.113294
Au	0.432383	0.711814	-0.284003
P	0.842225	2.884614	0.336945
C	2.599176	3.344010	0.196990
C	-0.652926	-1.415118	-0.665718
C	-1.577130	-1.620425	0.348149
C	-2.986609	-1.366004	0.201036
C	-3.851755	-1.623891	1.285378
C	-5.215912	-1.394815	1.169972
C	-5.743642	-0.903402	-0.026461
C	-4.897635	-0.642379	-1.110584
C	-3.534697	-0.869043	-1.002875
C	-0.066893	4.097365	-0.672131
C	0.373681	3.235701	2.061817
H	-1.242095	-1.999533	1.315760
H	0.816216	-1.359886	-2.166074
H	2.902434	-2.391564	-2.238742
H	4.817022	-3.535841	-1.167765
H	4.761484	-4.040167	1.263697
H	2.788237	-3.382500	2.619112
H	0.885933	-2.231483	1.565369
H	-2.878600	-0.670919	-1.846110
H	-5.310158	-0.264639	-2.040299
H	-6.810177	-0.726169	-0.116692
H	-5.871540	-1.600496	2.009441
H	-3.439868	-2.010801	2.213217
H	2.734509	4.383542	0.508447
H	3.201511	2.691446	0.832300
H	2.924439	3.228589	-0.838989
H	0.593683	4.281283	2.295268
H	-0.693897	3.049350	2.195618
H	0.935888	2.585920	2.735340
H	0.155422	5.108516	-0.319638
H	0.231790	4.001983	-1.717998
H	-1.139440	3.910267	-0.590093

allene_Ph_Ph_AuPMe3
SCF Energy: -1174.74582619
Num. Imaginary Frequencies: 0

C	0.774051	0.856597	-1.002008
C	1.218531	-0.267511	-0.413699
C	1.938537	-1.234266	0.115393
C	3.415275	-1.271884	0.077710
Au	-1.138984	-0.407083	-0.243926
P	-3.294662	-1.069718	0.249617
C	-4.441103	-0.836549	-1.146250
C	-4.028827	-0.154226	1.641717
C	-3.420523	-2.830210	0.697124
H	0.586519	0.833171	-2.078224
C	0.649137	2.175672	-0.338883
H	1.442715	-2.066998	0.610981
H	-3.064779	-3.445934	-0.131220
H	-2.807557	-3.030178	1.578366
H	-4.462802	-3.079676	0.914299
H	-3.440366	-0.324411	2.545550
H	-4.032504	0.914021	1.416266
H	-5.054917	-0.496246	1.803698
H	-4.103101	-1.424413	-2.002066
H	-4.468417	0.218460	-1.426544
H	-5.443238	-1.161388	-0.852406
C	4.070948	-2.393874	0.596070
C	5.462275	-2.466033	0.579359
C	6.207627	-1.416270	0.047071
C	5.558163	-0.291525	-0.467909
C	4.170577	-0.217222	-0.452845
H	3.489304	-3.212448	1.010854
H	5.961789	-3.340927	0.982072
H	7.291167	-1.470471	0.033821
H	6.136551	0.529009	-0.879506
H	3.670511	0.662178	-0.850102
C	0.136201	3.250900	-1.072633
C	0.032177	4.510691	-0.486780
C	0.437881	4.699548	0.833076
C	0.951546	3.627523	1.568395
C	1.056655	2.369375	0.988180
H	-0.173142	3.101184	-2.103740
H	-0.360952	5.342729	-1.061227
H	0.360127	5.680840	1.289403
H	1.274752	3.777454	2.593096
H	1.463253	1.534962	1.554031

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