

Supporting information for: Governing Effects in the Mechanism of the Gold–Catalyzed Cycloisomerization of Allenic Hydroxylamine Derivatives

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Naked Au(I) vs AuCl mechanism

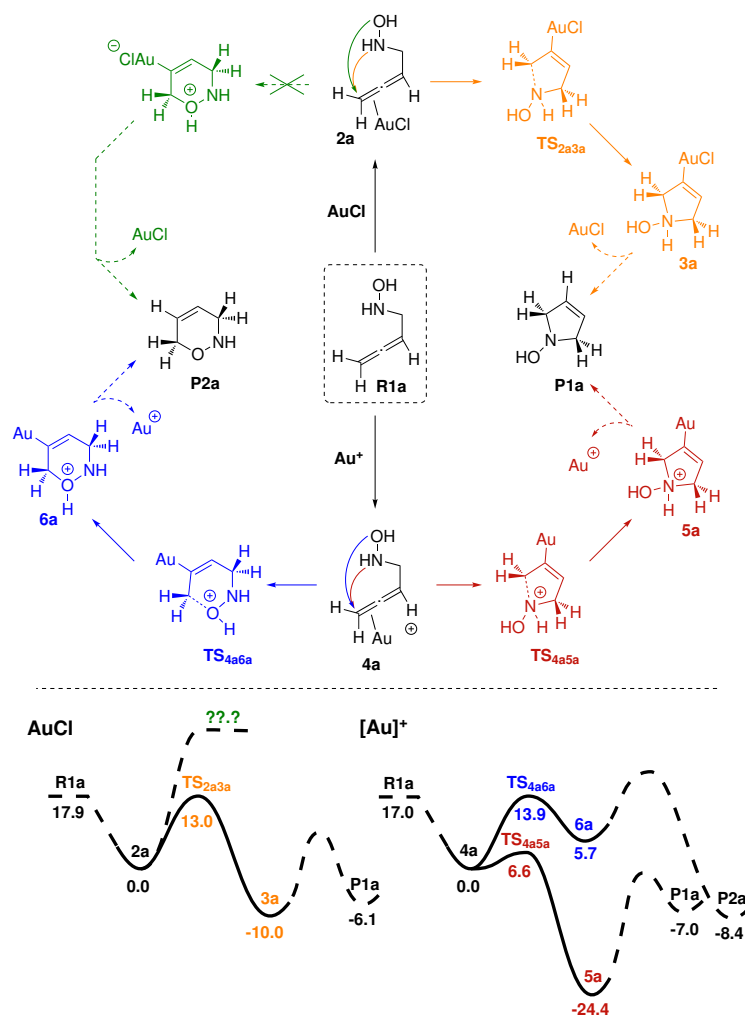


Figure S1: Reaction profiles considered for the transformation of *N*-hydroxy- α -aminoallene **R1a** into *N*-hydroxypyrraline **P1a** and dihydrooxazine **P2a** with AuCl and Au⁺.

Reaction 1

2a
SCF Energy: -881.875495377
ZPE-corrected Energy: -881.760560
 ΔU : -881.751455
 ΔH : -881.750511
 ΔG : -881.797678
Num. Imaginary Frequencies: 0

C	-1.073206	0.269223	-0.016645
C	-1.811115	1.393588	-0.017258
C	-3.294768	1.128270	-0.080832
N	-3.345323	-0.314122	0.339435
C	-2.011737	-0.912279	-0.066253
O	-4.382083	-1.052888	-0.200132
H	-3.398700	-0.358137	1.367428
H	-1.788288	-1.740704	0.619035
H	-1.429523	2.415976	-0.010711
H	-3.712167	1.162663	-1.101462
H	-3.927187	1.720847	0.595803
H	-5.216481	-0.648857	0.111299
H	-2.155921	-1.308183	-1.085141
Au	0.922861	0.030836	-0.005747
Cl	3.314183	-0.254736	0.015808

3a
 SCF Energy: -881.851602019
 ZPE-corrected Energy: -881.741881
 ΔU : -881.731218
 ΔH : -881.730273
 ΔG : -881.781706
 Num. Imaginary Frequencies: 0

C	0.367008	2.286137	-0.207217
Au	0.868866	0.154881	-0.020142
Cl	2.020092	-1.893567	0.052695
C	-0.786060	1.618537	0.056775
C	-2.038592	1.307041	0.302188
C	-2.586253	-0.066447	0.568050
N	-3.627046	-0.349523	-0.411499
O	-4.126676	-1.639370	-0.150455
H	0.630733	2.552873	-1.238475
H	0.919119	2.782732	0.600772
H	-2.759977	2.135316	0.299027
H	-1.778585	-0.823364	0.566937
H	-3.060663	-0.078653	1.563347
H	-3.191642	-0.417313	-1.334371
H	-5.074849	-1.506561	0.003555

4a
 SCF Energy: -1107.87691958
 ZPE-corrected Energy: -1107.63526
 ΔU : -1107.61545
 ΔH : -1107.61450
 ΔG : -1107.68575
 Num. Imaginary Frequencies: 0

C	2.769982	-1.783979	0.065872
Au	0.617909	-0.764073	-0.010350
C	3.086504	-0.499933	-0.126821
C	3.528913	0.717503	-0.325562
C	2.693865	1.970484	-0.449645
N	1.470530	1.847587	0.335002
O	0.599738	2.904063	0.034083
H	-0.154543	2.474721	-0.414275
H	1.694114	1.952112	1.327055
H	3.296971	2.850174	-0.165167
H	2.395716	2.101956	-1.502903
H	4.616533	0.819664	-0.436128
H	2.790038	-2.221710	1.072473
H	2.657388	-2.464197	-0.789165
P	-1.579914	-0.151116	-0.073137
O	-1.607048	1.254298	-0.877825
C	-2.846439	1.914036	-1.185964
H	-3.382637	1.346015	-1.960807
H	-3.463172	2.013271	-0.279041
H	-2.587018	2.908893	-1.568877
O	-2.287989	0.185903	1.327932
C	-1.592358	0.986617	2.290485
H	-0.802152	0.388873	2.773087
H	-1.149937	1.874825	1.808454
H	-2.332781	1.298745	3.037088
O	-2.654089	-1.102132	-0.749987
C	-4.024128	-1.251706	-0.342455
H	-4.071506	-1.539879	0.716363
H	-4.580342	-0.316662	-0.504248
H	-4.439419	-2.046607	-0.973338

5a
 SCF Energy: -1107.89652573
 ZPE-corrected Energy: -1107.65075
 ΔU : -1107.63289
 ΔH : -1107.63194
 ΔG : -1107.69959
 Num. Imaginary Frequencies: 1
 Imaginary Frequency: -48.3733

C	-3.158891	0.934384	0.118846
C	-2.245636	-0.249178	-0.071891
C	-2.999711	-1.355095	-0.184366
C	-4.478895	-1.080919	-0.075191
N	-4.519447	0.405280	-0.302925
Au	-0.186833	-0.099415	-0.074602
O	-5.513561	1.079148	0.382084
H	-4.623745	0.588007	-1.312216
H	-2.939412	1.823094	-0.487767
H	-2.635244	-2.377047	-0.304453
H	-4.885194	-1.248239	0.936300
H	-5.121872	-1.575812	-0.816957
H	-6.370365	0.715877	0.081450
H	-3.269016	1.231423	1.174679
P	2.135916	0.052077	-0.078050
O	2.795733	-1.414528	-0.046635
C	4.206376	-1.621608	-0.134227
H	4.547422	-1.451670	-1.167633
H	4.742996	-0.952146	0.557626
H	4.394918	-2.665850	0.146316
O	2.863306	0.850654	1.125070
C	2.560506	0.531009	2.481430
H	1.472720	0.579552	2.659329
H	2.932233	-0.475309	2.732936
H	3.067139	1.278213	3.105284
O	2.761857	0.821833	-1.333642
C	3.954541	1.611922	-1.322385
H	3.858988	2.432481	-0.597570
H	4.833557	0.998102	-1.073652
H	4.063608	2.015047	-2.337174

6a

SCF Energy: -1107.84962633

ZPE-corrected Energy: -1107.60429

ΔU : -1107.58661

ΔH : -1107.58566

ΔG : -1107.65254

Num. Imaginary Frequencies: 1

Imaginary Frequency: -34.3667

O	-4.468032	1.129333	-0.067832
N	-5.046070	-0.110912	0.477642
C	-4.534809	-1.171500	-0.392946
C	-3.029706	-1.141451	-0.419779
C	-2.305567	-0.061463	-0.091643
C	-2.990223	1.202615	0.278658
Au	-0.227130	-0.008358	-0.063774
H	-4.962825	-1.112784	-1.411040
H	-2.544079	-2.072260	-0.728344
H	-2.948044	1.431637	1.354631
H	-2.670431	2.065594	-0.320573
H	-4.945782	1.890656	0.334595
H	-6.043318	0.027459	0.283481
H	-4.899900	-2.100404	0.074519
P	2.097700	0.035027	-0.069238
O	2.683469	-1.331084	-0.683343
C	4.081042	-1.531519	-0.900765
H	4.414764	-0.939709	-1.767687
H	4.658634	-1.252235	-0.004567
H	4.222757	-2.599535	-1.110108
O	2.882693	0.222593	1.331662
C	2.563270	-0.604328	2.448546
H	1.488917	-0.534066	2.688788
H	2.829755	-1.653382	2.242020
H	3.153160	-0.234483	3.296774
O	2.744480	1.237247	-0.904865
C	3.965258	1.914548	-0.592566
H	3.909778	2.353216	0.413586
H	4.824371	1.228933	-0.650814
H	4.076050	2.706523	-1.344073

AuCl

SCF Energy: -595.686706393

ZPE-corrected Energy: -595.686003

ΔU : -595.683233

ΔH : -595.682289

ΔG : -595.711120

Num. Imaginary Frequencies: 0

Au	0.000000	0.000000	0.430055
Cl	0.000000	0.000000	-1.907115
Au	0.000000	0.000000	0.413874
Cl	0.000000	0.000000	-1.923296

Au
 SCF Energy: -135.405079526
 ZPE-corrected Energy: -135.405080
 ΔU : -135.403663
 ΔH : -135.402719
 ΔG : -135.422550
 Num. Imaginary Frequencies: 0

Au	0.000000	0.000000	0.000000
Au	0.000000	0.000000	0.000000
Au	0.000000	0.000000	0.000000
Au	0.000000	0.000000	0.000000

complexA
 SCF Energy: -821.712392234
 ZPE-corrected Energy: -821.580225
 ΔU : -821.568371
 ΔH : -821.567426
 ΔG : -821.620745
 Num. Imaginary Frequencies: 0

Au	-1.385607	-0.087328	0.041355
P	0.837560	-0.064589	0.019782
O	1.359494	0.351184	1.466064
C	2.754532	0.295761	1.805074
H	3.079612	-0.753910	1.865715
H	3.354189	0.843710	1.061447
H	2.854531	0.773843	2.786833
O	1.546620	0.912117	-1.026287
C	1.257033	2.313523	-1.075995
H	0.179910	2.476673	-1.244382
H	1.572148	2.800984	-0.140697
H	1.828323	2.717493	-1.920191
O	1.483924	-1.460618	-0.358484
C	2.664176	-1.652765	-1.156972
H	2.517553	-1.214593	-2.153355
H	3.539300	-1.198855	-0.669250
H	2.799222	-2.738149	-1.232905

P1a
 SCF Energy: -286.161163626
 ZPE-corrected Energy: -286.051494
 ΔU : -286.045922
 ΔH : -286.044978
 ΔG : -286.080318
 Num. Imaginary Frequencies: 0

C	-0.078865	-1.186120	0.013129
C	-1.491337	-0.667119	0.030560
C	-1.491336	0.667120	0.030567
C	-0.078862	1.186121	0.013128
N	0.686940	-0.000001	-0.384975
O	1.944464	-0.000006	0.234292
H	0.083695	-2.019314	-0.691893
H	-2.371328	1.312407	0.067163
H	0.235396	1.530840	1.020683
H	0.083697	2.019312	-0.691898
H	2.582590	0.000032	-0.495707
H	0.235388	-1.530836	1.020687
H	-2.371330	-1.312404	0.067151

P2a
 SCF Energy: -286.166210953
 ZPE-corrected Energy: -286.054452
 ΔU : -286.049457
 ΔH : -286.048513
 ΔG : -286.082586
 Num. Imaginary Frequencies: 0

N	-0.729325	-1.001081	-0.411567
C	-1.416667	0.177918	0.105353
C	-0.465888	1.344545	0.048246
C	0.847643	1.141589	-0.072241
C	1.405353	-0.257730	-0.075580
O	0.443588	-1.181100	0.371196
H	-1.791534	0.037637	1.140084
H	-0.881294	2.355449	0.100195
H	1.771685	-0.532674	-1.085163
H	2.248187	-0.342672	0.629385
H	-1.273231	-1.838019	-0.202747
H	-2.288534	0.361226	-0.544339
H	1.548643	1.977493	-0.160687

R1a
 SCF Energy: -286.118222470
 ZPE-corrected Energy: -286.011056
 ΔU : -286.004080
 ΔH : -286.003136
 ΔG : -286.042027
 Num. Imaginary Frequencies: 0

C	-3.044746	-0.022808	-0.224104
C	-1.774428	-0.215218	0.032042
H	-3.425154	-0.043004	-1.252488
H	-3.764886	0.161204	0.582272
C	-0.503265	-0.394430	0.293498
C	0.512394	0.717787	0.376753
H	-0.128339	-1.409174	0.481184
N	1.642698	0.452845	-0.505482
H	0.063317	1.670843	0.056544
H	0.849048	0.825572	1.427753
H	2.272157	1.256851	-0.464870
O	2.384224	-0.608195	0.059742
H	2.421450	-1.278625	-0.639098

TS2a3a
 SCF Energy: -881.832814509
 ZPE-corrected Energy: -881.723201
 ΔU : -881.713558
 ΔH : -881.712614
 ΔG : -881.760977
 Num. Imaginary Frequencies: 1
 Imaginary Frequency: -409.0988

C	-1.389855	-0.857461	0.630367
C	-1.148015	0.395467	0.091676
Au	0.881263	0.029839	0.020057
Cl	3.246202	-0.161151	-0.163198
C	-2.007852	1.349065	-0.224202
C	-3.465860	1.019970	0.094226
N	-3.607201	-0.393565	0.382681
O	-3.762112	-1.161834	-0.763789
H	-4.363483	-0.598158	1.037873
H	-1.282926	-1.039819	1.707559
H	-1.755810	2.317698	-0.660033
H	-4.117412	1.316726	-0.749392
H	-3.801365	1.580251	0.983187
H	-4.562662	-0.852877	-1.230512
H	-1.504750	-1.734142	-0.019680

TS4a5a
 SCF Energy: -1107.84879186
 ZPE-corrected Energy: -1107.60848
 ΔU : -1107.58879
 ΔH : -1107.58785
 ΔG : -1107.66093
 Num. Imaginary Frequencies: 1
 Imaginary Frequency: -358.2843

C	-2.581653	1.121776	-0.186705
C	-2.341183	-0.225889	-0.185445
C	-3.135334	-1.277826	-0.261402
C	-4.620074	-0.950697	-0.426214
N	-4.885101	0.440470	-0.126522
O	-5.235624	0.547394	1.225076
Au	-0.190859	-0.048139	-0.037264
H	-5.673726	0.789525	-0.674493
H	-2.496368	1.711817	-1.109642
H	-2.813428	-2.320987	-0.251116
H	-5.222920	-1.600015	0.231218
H	-4.922601	-1.143612	-1.468919
H	-4.809321	1.358594	1.545915
H	-2.644734	1.687307	0.753799
P	2.113725	-0.052252	0.104329
O	2.598380	1.063994	1.146530
C	3.972947	1.218855	1.516606
H	4.273816	0.397274	2.184920
H	4.616037	1.239939	0.622140
H	4.051912	2.174634	2.049542
O	2.961404	0.218195	-1.236297
C	2.705398	1.369992	-2.041051
H	1.645974	1.399474	-2.347145
H	2.961375	2.288596	-1.489785
H	3.342019	1.281334	-2.929962
O	2.727166	-1.449345	0.562174
C	3.990542	-1.988142	0.150466
H	4.024931	-2.074293	-0.944287
H	4.818994	-1.355674	0.503029
H	4.061257	-2.980764	0.611944

TS4a6a
 SCF Energy: -1107.81991458
 ZPE-corrected Energy: -1107.58012
 ΔU : -1107.56042
 ΔH : -1107.55947
 ΔG : -1107.63215
 Num. Imaginary Frequencies: 1
 Imaginary Frequency: -299.9938

C	-2.882580	1.214240	0.837247
C	-2.233955	0.119722	0.301704
C	-3.045736	-0.977901	-0.039825
C	-4.505813	-1.221579	-0.021515
N	-5.401935	-0.109278	0.140758
O	-5.358382	0.626113	-1.059385
Au	-0.151495	0.013645	0.154368
H	-6.353708	-0.472578	0.221324
H	-5.415712	1.559664	-0.797147
H	-2.307049	2.029986	1.291250
H	-2.515636	-1.886203	-0.358333
H	-4.682074	-1.956899	0.790513
H	-4.710494	-1.788396	-0.957945
H	-3.974249	1.301244	0.874614
P	2.158786	-0.099575	-0.021800
O	2.853853	0.597170	1.248657
C	4.269768	0.588659	1.443888
H	4.599382	-0.414837	1.755907
H	4.791806	0.891343	0.521636
H	4.486723	1.310163	2.241869
O	2.863729	0.583718	-1.304066
C	2.563362	1.934448	-1.650506
H	1.472322	2.083449	-1.720782
H	2.985572	2.625805	-0.903835
H	3.022558	2.121823	-2.629292
O	2.753027	-1.579314	-0.133343
C	3.916113	-1.961494	-0.875243
H	3.793344	-1.697018	-1.934761
H	4.817849	-1.475398	-0.472989
H	4.004440	-3.049584	-0.764774

Reaction 2

2b
SCF Energy: -881.849576947
ZPE-corrected Energy: -881.739743
 ΔU : -881.729028
 ΔH : -881.728084
 ΔG : -881.779376
Num. Imaginary Frequencies: 0

C	0.315343	1.925042	-0.181438
Au	-1.002184	0.165486	-0.018371
Cl	-2.844198	-1.294789	0.038420
C	1.090310	0.840537	0.082656
C	2.088565	0.025531	0.328733
C	3.523696	0.498856	0.402713
O	4.355121	-0.229739	-0.464585
N	4.465820	-1.560292	-0.009702
H	0.195581	2.283863	-1.211454
H	0.005065	2.597777	0.627908
H	1.917080	-1.044297	0.492564
H	3.603231	1.550653	0.090832
H	3.882871	0.402010	1.443712
H	4.245954	-2.136151	-0.826678
H	5.464955	-1.695648	0.169882

3b
 SCF Energy: -881.867271381
 ZPE-corrected Energy: -881.753037
 ΔU : -881.744021
 ΔH : -881.743077
 ΔG : -881.790119
 Num. Imaginary Frequencies: 0

C	1.976610	-1.391054	-0.696627
O	2.305582	-1.449682	0.719315
N	2.433012	-0.136797	1.177338
C	2.176142	0.778416	0.020644
C	1.315351	-0.026488	-0.868773
C	2.741727	1.981301	0.007527
Au	-0.653192	0.021964	-0.182260
Cl	-2.928442	0.071246	0.598886
H	1.726453	-0.004910	1.921093
H	1.377848	0.336485	-1.903413
H	2.918387	-1.491039	-1.265465
H	1.329866	-2.257170	-0.879624
H	3.375064	-0.014541	1.580938
H	3.365328	2.340209	0.830640
H	2.558032	2.646630	-0.839194

4b

SCF Energy: -1107.86676890
ZPE-corrected Energy: -1107.62590
 ΔU : -1107.60554
 ΔH : -1107.60460
 ΔG : -1107.67854

Num. Imaginary Frequencies: 0

H	3.077476	-3.503878	0.147203
H	1.603767	-2.907964	0.531608
N	2.582059	-2.640923	0.393084
O	2.569663	-1.870847	-0.791579
C	3.400768	-0.749238	-0.636805
H	3.422776	-0.250812	-1.616108
H	4.425188	-1.060453	-0.363235
H	2.893790	-0.174470	1.467151
C	2.893979	0.201355	0.434109
C	2.635298	1.491682	0.204284
C	2.525207	2.774918	-0.023085
H	1.568770	3.241755	-0.282353
H	3.415985	3.411268	0.049940
Au	0.515016	0.224568	0.153439
P	-1.723655	-0.116385	0.018460
O	-2.041341	-1.120212	-1.182262
C	-3.366149	-1.605390	-1.437784
H	-3.659255	-2.318238	-0.651838
H	-4.081284	-0.769032	-1.485747
H	-3.331396	-2.117703	-2.406996
O	-2.639285	1.178299	-0.220381
C	-2.335618	2.119865	-1.252535
H	-1.301421	2.489220	-1.142258
H	-2.466021	1.657522	-2.243232
H	-3.039271	2.952675	-1.133863
O	-2.375979	-0.714320	1.339040
C	-3.678083	-0.394374	1.852165
H	-3.764529	0.689355	2.009241
H	-4.462939	-0.738323	1.162097
H	-3.764403	-0.925787	2.807601

5b
 SCF Energy: -1107.88669979
 ZPE-corrected Energy: -1107.64171
 ΔU : -1107.62278
 ΔH : -1107.62184
 ΔG : -1107.69454
 Num. Imaginary Frequencies: 0

N	-3.401606	0.051953	1.188241
C	-3.061411	-0.815546	0.006665
C	-2.274460	0.065398	-0.876105
C	-2.946853	1.405365	-0.601597
O	-3.188990	1.381416	0.828500
C	-3.510489	-2.066894	-0.018928
Au	-0.207791	0.019513	-0.332640
P	2.049658	-0.031707	0.227716
O	3.011890	-0.861446	-0.748334
C	2.962257	-0.668280	-2.161032
O	2.796945	1.383942	0.295442
C	2.220132	2.486325	0.992774
O	2.420383	-0.661696	1.654886
C	1.915013	-1.937426	2.043225
H	-2.791243	-0.141556	1.999069
H	-2.374571	-0.247835	-1.924074
H	-3.919322	1.519156	-1.113953
H	-2.329876	2.295806	-0.770780
H	-4.385332	-0.067136	1.481924
H	-4.095560	-2.492299	0.800359
H	-3.273854	-2.699620	-0.877242
H	2.815667	3.371145	0.735307
H	1.173464	2.643609	0.679285
H	2.263484	2.312852	2.079281
H	2.170715	-2.070716	3.101904
H	0.818443	-1.979937	1.921603
H	2.387256	-2.731825	1.444636
H	3.543830	-1.481311	-2.613394
H	1.921674	-0.713082	-2.526249
H	3.410107	0.301787	-2.426482

6b
 SCF Energy: -1107.89619584
 ZPE-corrected Energy: -1107.64901
 ΔU : -1107.63148
 ΔH : -1107.63054
 ΔG : -1107.69725
 Num. Imaginary Frequencies: 1
 Imaginary Frequency: -42.0877

O	-5.076535	0.010579	0.394985
N	-4.481158	-1.124193	-0.137573
C	-3.037740	-1.232815	0.268484
C	-2.301450	0.040001	-0.050591
C	-3.031994	1.139284	-0.297687
C	-4.532339	1.191424	-0.211736
Au	-0.228316	-0.008103	-0.056271
H	-4.574314	-1.117561	-1.169217
H	-5.039337	-1.915194	0.215907
H	-2.649544	-2.103508	-0.280909
H	-3.040379	-1.467706	1.344108
H	-2.558512	2.087834	-0.571717
H	-4.870836	1.995597	0.457316
H	-5.010392	1.344438	-1.198409
P	2.099808	-0.049355	-0.068382
O	2.641133	-1.347817	0.712692
C	4.029890	-1.675861	0.775792
H	4.372774	-2.050186	-0.201767
H	4.624574	-0.797901	1.076370
H	4.138250	-2.466988	1.528860
O	2.902173	1.189052	0.592050
C	2.552563	1.652657	1.894413
H	1.476829	1.892131	1.944241
H	2.799357	0.893378	2.653753
H	3.139559	2.561637	2.077340
O	2.777066	-0.068323	-1.519039
C	4.016245	0.553465	-1.871519
H	3.967026	1.634302	-1.678501
H	4.853761	0.114920	-1.307878
H	4.157391	0.367729	-2.943824

7b

SCF Energy: -881.874719665
ZPE-corrected Energy: -881.758478
 ΔU : -881.749721
 ΔH : -881.748777
 ΔG : -881.795201

Num. Imaginary Frequencies: 0

C	3.402747	1.221954	0.030379
C	1.901150	1.200976	0.107332
C	1.152727	0.090151	0.002557
C	1.876330	-1.223329	-0.134654
N	3.311122	-1.079667	0.291438
O	3.941880	-0.043273	-0.382178
Au	-0.868700	0.023449	-0.002001
Cl	-3.279662	-0.050093	-0.003953
H	1.461461	-2.010611	0.511647
H	1.899096	-1.593140	-1.171217
H	1.439108	2.183746	0.245263
H	3.371999	-0.922581	1.313535
H	3.864639	-1.921019	0.073253
H	3.758723	1.910246	-0.749994
H	3.875923	1.517797	0.986424

P1b

SCF Energy: -286.196666685
ZPE-corrected Energy: -286.087159
 ΔU : -286.081321
 ΔH : -286.080377
 ΔG : -286.116484

Num. Imaginary Frequencies: 0

C	0.206465	1.174089	-0.106928
C	1.556050	0.500201	0.128204
O	1.304416	-0.897461	-0.081131
N	-0.052609	-1.134940	-0.005832
C	-0.694260	-0.033946	0.000715
C	-2.183972	0.020857	0.044794
H	1.905447	0.643792	1.165199
H	2.346430	0.810305	-0.568329
H	-2.522643	0.587304	0.928103
H	-2.571592	0.539412	-0.848368
H	0.106640	1.625171	-1.109517
H	-0.034566	1.946047	0.638798
H	-2.602481	-0.994971	0.083277

P1btau
SCF Energy: -286.166466652
ZPE-corrected Energy: -286.056499
 ΔU : -286.051004
 ΔH : -286.050060
 ΔG : -286.085423

Num. Imaginary Frequencies: 0

O	1.321457	-0.776087	-0.193606
N	-0.033499	-1.158629	-0.108778
C	-0.820715	0.021372	-0.060552
C	0.123658	1.193617	-0.198492
C	1.411427	0.551831	0.304380
H	1.451285	0.550348	1.410858
H	2.333392	0.990377	-0.100139
C	-2.147427	0.041302	0.092548
H	-2.677889	0.994519	0.141686
H	-2.723727	-0.884695	0.176041
H	0.227845	1.480649	-1.258460
H	-0.207197	2.067410	0.379043
H	-0.142534	-1.728233	0.733961

P2b
SCF Energy: -286.165927984
ZPE-corrected Energy: -286.054373
 ΔU : -286.049294
 ΔH : -286.048350
 ΔG : -286.082645

Num. Imaginary Frequencies: 0

O	0.669863	-1.103542	-0.372144
C	1.417586	0.015304	0.061219
C	0.602596	1.279386	0.072408
C	-0.725164	1.232029	-0.042526
C	-1.426623	-0.099118	-0.119301
N	-0.572368	-1.211396	0.278377
H	1.137459	2.228694	0.175345
H	-2.307024	-0.118992	0.544479
H	-1.797123	-0.288294	-1.142735
H	1.854887	-0.178317	1.064005
H	2.256218	0.099565	-0.648549
H	-1.324528	2.147215	-0.079292
H	-0.382581	-1.147372	1.284456

R1b
 SCF Energy: -286.112302501
 ZPE-corrected Energy: -286.005096
 ΔU : -285.998146
 ΔH : -285.997201
 ΔG : -286.036160
 Num. Imaginary Frequencies: 0

C	-2.978240	-0.023187	-0.292358
C	-1.735345	-0.219617	0.067587
C	-0.489405	-0.396426	0.435349
C	0.538965	0.711726	0.413631
O	1.570812	0.505187	-0.530296
N	2.422872	-0.554237	-0.213279
H	-3.295175	-0.172464	-1.331335
H	-3.735198	0.292927	0.435173
H	-0.181185	-1.387255	0.795020
H	0.063234	1.660684	0.126229
H	0.983030	0.831897	1.422652
H	2.756761	-0.406821	0.747091
H	1.866082	-1.415776	-0.204759

TS2b3b
 SCF Energy: -881.819082207
 ZPE-corrected Energy: -881.710226
 ΔU : -881.700619
 ΔH : -881.699674
 ΔG : -881.747630
 Num. Imaginary Frequencies: 1
 Imaginary Frequency: -447.8306

C	1.507118	0.077074	-1.009512
C	2.169933	-1.256709	-0.789422
O	1.940718	-1.604722	0.584895
N	2.117384	-0.479015	1.359584
C	1.839803	1.023426	-0.066883
C	2.181178	2.221038	0.367709
Au	-0.558144	0.055310	-0.180720
Cl	-2.813468	-0.127533	0.502163
H	1.445709	-0.527905	2.131119
H	1.215138	0.401544	-2.015561
H	3.260340	-1.221079	-0.973320
H	1.724226	-2.062939	-1.385706
H	3.078554	-0.446240	1.722450
H	1.928429	2.581225	1.368325
H	2.734318	2.875823	-0.314769

TS2b7b
 SCF Energy: -881.829390986
 ZPE-corrected Energy: -881.719021
 ΔU : -881.709425
 ΔH : -881.708481
 ΔG : -881.756595
 Num. Imaginary Frequencies: 1
 Imaginary Frequency: -454.7833

O	3.937991	-0.024754	-0.545350
C	3.475688	1.141349	0.111878
C	1.976022	1.314350	0.110478
C	1.183399	0.252696	0.065696
C	1.333247	-1.121248	0.107292
N	3.578400	-1.196241	0.143506
Au	-0.874431	0.000382	0.005231
Cl	-3.252253	0.006788	-0.062171
H	1.263186	-1.653696	1.062144
H	1.283932	-1.726813	-0.805138
H	1.579835	2.334013	0.134446
H	4.143481	-1.239770	1.003530
H	3.908755	-1.946944	-0.467466
H	3.949242	1.964338	-0.443530
H	3.877077	1.172103	1.145892

TS4b5b
 SCF Energy: -1107.84108817
 ZPE-corrected Energy: -1107.60086
 ΔU : -1107.58173
 ΔH : -1107.58078
 ΔG : -1107.65169
 Num. Imaginary Frequencies: 1
 Imaginary Frequency: -427.6423

H	-4.283511	1.118794	-0.957993
C	-3.179470	1.056572	-0.939646
H	-2.767638	1.602042	-1.797973
O	-2.697055	1.735489	0.233988
N	-2.912637	0.920178	1.325119
H	-2.162959	1.105316	1.997384
H	-3.824913	1.133764	1.747479
C	-2.672683	-0.356438	-0.834248
H	-2.454188	-0.965036	-1.721067
C	-2.989660	-0.969550	0.348606
C	-3.363767	-1.928592	1.167011
H	-4.018585	-2.714140	0.772762
H	-3.049533	-1.969441	2.213402
Au	-0.431301	-0.241942	-0.319274
P	1.798050	-0.062036	0.046369
O	2.112188	-0.278827	1.602146
C	3.451475	-0.323024	2.107597
H	3.925994	-1.274889	1.823296
H	4.038667	0.527350	1.725462
H	3.379654	-0.259325	3.200500
O	2.495913	1.332246	-0.345064
C	1.962483	2.572632	0.121675
H	0.889891	2.649258	-0.126194
H	2.103248	2.664718	1.210025
H	2.516039	3.367516	-0.393070
O	2.695994	-1.086218	-0.777490
C	4.012215	-0.828773	-1.286146
H	3.997681	0.052894	-1.941449
H	4.724895	-0.673032	-0.462368
H	4.295887	-1.721595	-1.856630

TS4b6b
 SCF Energy: -1107.84327860
 ZPE-corrected Energy: -1107.60243
 ΔU : -1107.58282
 ΔH : -1107.58187
 ΔG : -1107.65469
 Num. Imaginary Frequencies: 1
 Imaginary Frequency: -406.8356

H	5.047535	-1.859801	-0.577895
N	4.730896	-1.152750	0.089879
H	5.391490	-1.182735	0.879393
O	4.955601	0.059927	-0.594055
H	4.883162	1.197606	1.139738
C	4.458160	1.175417	0.115687
H	4.865607	2.043148	-0.423935
C	2.950214	1.269739	0.166233
H	2.498533	2.263821	0.237200
C	2.229609	0.161526	0.101653
C	2.382020	-1.192612	0.107047
H	2.363230	-1.745445	1.053851
H	2.316183	-1.780320	-0.817555
Au	0.044344	-0.011311	0.045119
P	-2.271025	0.019440	-0.040857
O	-2.953722	1.461044	-0.083039
C	-2.544905	2.447468	-1.032206
H	-1.444730	2.533763	-1.055939
H	-2.921750	2.183888	-2.031781
H	-2.981023	3.399350	-0.705706
O	-3.035398	-0.695918	1.163516
C	-2.758613	-0.375367	2.527763
H	-1.672365	-0.392213	2.720436
H	-3.168104	0.616638	2.770514
H	-3.251290	-1.142496	3.137568
O	-2.906227	-0.690993	-1.319562
C	-2.606698	-2.047600	-1.651766
H	-1.517549	-2.202285	-1.729854
H	-3.030219	-2.723458	-0.893030
H	-3.073541	-2.242128	-2.625038

Reaction 3

2c
SCF Energy: -1227.26936064
ZPE-corrected Energy: -1227.03198
 ΔU : -1227.01341
 ΔH : -1227.01246
 ΔG : -1227.08338
Num. Imaginary Frequencies: 0

C	2.026880	-2.052325	-0.286508
C	1.071026	-1.091480	-0.192918
C	-0.065161	-0.435516	-0.145706
C	-1.398550	-1.126080	-0.300595
O	-2.155983	-0.575884	-1.365173
N	-2.529561	0.720299	-1.089475
C	-3.825115	0.949898	-0.649561
O	-4.327758	-0.127609	-0.065896
C	-5.646438	-0.108050	0.556503
C	-5.799399	-1.529844	1.081600
O	-4.341370	2.035377	-0.755531
C	-5.661962	0.895929	1.705291
C	-6.712160	0.196310	-0.492181
H	2.380322	-2.388981	-1.269211
H	2.280243	-2.671557	0.583102
H	-0.078143	0.647754	0.019680
H	-1.267011	-2.186324	-0.557264
H	-1.975948	-1.048954	0.637128
H	-2.209905	1.366949	-1.807916
H	-6.617069	0.810433	2.248688
H	-4.841765	0.677405	2.409359
H	-5.555002	1.925164	1.334476
H	-6.775936	-1.643624	1.578124
H	-5.736173	-2.252205	0.251770
H	-5.003154	-1.756982	1.809196
H	-7.709996	0.075911	-0.039733
H	-6.615055	1.223698	-0.870732
H	-6.625326	-0.510132	-1.334420
Au	3.019911	-0.116195	0.067127
Cl	4.597059	1.589447	0.421664

3c
 SCF Energy: -1227.26815652
 ZPE-corrected Energy: -1227.02761
 ΔU : -1227.01054
 ΔH : -1227.00959
 ΔG : -1227.07411
 Num. Imaginary Frequencies: 0

C	1.065576	1.896659	0.207508
C	0.558848	2.293414	1.589080
O	-0.857276	1.973304	1.555248
N	-1.291937	2.090882	0.249277
C	-0.077643	2.306240	-0.632759
C	-2.121272	0.890706	-0.218168
O	-1.803009	-0.142951	0.461488
C	-2.390754	-1.486025	0.165714
C	-1.963647	-1.893329	-1.236217
C	-0.263937	2.788626	-1.858277
O	-2.880878	1.098011	-1.107144
C	-1.754826	-2.372333	1.222355
C	-3.900677	-1.393688	0.333681
H	0.655264	3.374847	1.794021
H	0.962884	1.713872	2.426920
H	0.606081	2.955198	-2.497600
H	-1.260725	2.994132	-2.256945
H	1.963642	2.461833	-0.076817
H	-2.385939	-2.888838	-1.449900
H	-2.340710	-1.190282	-1.995079
H	-0.864178	-1.964966	-1.292374
H	-2.160015	-3.391902	1.121511
H	-0.661685	-2.412807	1.081344
H	-1.989256	-1.997370	2.231553
H	-4.323311	-2.406960	0.243311
H	-4.152840	-1.001976	1.332735
H	-4.358803	-0.755997	-0.436755
H	-1.920441	2.907188	0.173507
Au	1.403193	-0.148302	-0.020708
Cl	1.755330	-2.524988	-0.307217

4c

SCF Energy: -1453.28310020
ZPE-corrected Energy: -1452.91472
 ΔU : -1452.88640
 ΔH : -1452.88546
 ΔG : -1452.97918

Num. Imaginary Frequencies: 0

C	7.105250	-0.905371	-1.296081
C	6.752934	0.407650	-0.608993
C	6.595613	1.528157	-1.632130
O	5.463274	0.118504	0.010523
C	4.820526	1.027794	0.724927
O	5.160028	2.162691	0.950290
C	7.779978	0.745954	0.467186
N	3.590326	0.543361	1.157298
O	3.449259	-0.821109	1.292612
C	2.777967	-1.373857	0.177724
C	1.332415	-0.931051	0.125648
C	0.347816	-1.788200	0.059822
C	-0.553350	-2.772273	-0.020218
Au	-1.930766	-0.851288	-0.063698
H	7.170700	-1.718682	-0.555399
H	8.075988	-0.812130	-1.807897
H	6.335843	-1.166374	-2.041003
H	7.813214	-0.056416	1.222825
H	8.776455	0.826886	0.003394
H	7.540188	1.698256	0.961110
H	5.807008	1.269664	-2.358389
H	7.543531	1.653241	-2.180407
H	6.340107	2.479082	-1.143438
H	3.213685	1.036969	1.964359
H	3.293277	-1.075594	-0.751405
H	2.854003	-2.462855	0.299389
H	1.139516	0.149116	0.133077
H	-0.921001	-3.266838	0.888596
H	-0.806331	-3.219330	-0.990745
P	-3.629469	0.660201	-0.171844
O	-3.020578	2.134372	-0.267692
C	-3.845481	3.289216	-0.474208
H	-4.200369	3.309695	-1.515991
H	-4.698242	3.286250	0.223177
H	-3.214137	4.165231	-0.281533
O	-4.684696	0.695390	1.035176
C	-4.256296	0.843778	2.391414
H	-3.550641	0.040794	2.662014
H	-3.782119	1.826712	2.537672
H	-5.156209	0.768232	3.013651
O	-4.593738	0.434321	-1.414273
C	-6.002174	0.711527	-1.449281
H	-6.509083	0.189789	-0.626302
H	-6.185378	1.794030	-1.380135
H	-6.359341	0.336216	-2.415868

5c
 SCF Energy: -1453.28599787
 ZPE-corrected Energy: -1452.91425
 ΔU : -1452.88779
 ΔH : -1452.88684
 ΔG : -1452.97309
 Num. Imaginary Frequencies: 0

H	0.302941	3.653904	-1.046252
C	-0.258421	2.716970	-1.190002
H	0.431921	1.867424	-1.064258
H	-0.656618	2.697487	-2.216834
C	-0.875400	2.627982	1.253295
H	-0.376736	3.587718	1.465761
H	-0.138137	1.817870	1.385245
H	-1.699868	2.504242	1.973014
C	-2.417171	3.746560	-0.428933
H	-1.903433	4.719861	-0.382195
H	-2.856094	3.636856	-1.433977
H	-3.217716	3.737784	0.324271
C	-1.388938	2.652571	-0.177958
O	-2.009002	1.323091	-0.454677
C	-3.064119	0.941474	0.163267
O	-3.790905	1.451502	0.950564
N	-3.365069	-0.507380	-0.201724
H	-4.388221	-0.617701	-0.106800
C	-2.655624	-1.459128	0.746294
H	-2.545615	-2.166820	2.710046
C	-3.042631	-1.481961	2.019084
H	-3.831431	-0.827453	2.399391
O	-2.987565	-0.823302	-1.491830
C	-2.331201	-2.115598	-1.456171
C	-1.655584	-2.147890	-0.091232
H	-3.103717	-2.895157	-1.579878
H	-1.502746	-3.174014	0.270120
H	-1.659048	-2.115743	-2.322074
Au	0.216035	-1.129681	-0.015340
P	2.270394	-0.067926	0.063104
O	2.743427	0.469779	-1.380514
O	2.288839	1.236787	1.012282
O	3.477000	-0.990427	0.589622
C	3.029000	2.432264	0.764677
C	4.599767	-0.526840	1.342093
C	4.095903	0.525080	-1.836166
H	4.056935	0.719763	-2.915496
H	4.643456	1.341801	-1.338380
H	4.599459	-0.436334	-1.652473
H	5.113529	-1.419147	1.721627
H	5.290747	0.045807	0.702252
H	4.262696	0.092718	2.187113
H	2.626577	3.197030	1.442151
H	4.099264	2.281706	0.981284
H	2.896820	2.757423	-0.279320

6c

SCF Energy: -1453.29181636

ZPE-corrected Energy: -1452.91798

ΔU : -1452.89162

ΔH : -1452.89067

ΔG : -1452.97785

Num. Imaginary Frequencies: 0

C	2.056213	-1.342428	1.324746
N	3.500093	-1.126265	0.941436
O	3.991439	-2.215678	0.246892
C	3.305558	-2.445616	-1.004717
C	1.887805	-1.950682	-1.009206
C	1.246703	-1.445170	0.058730
C	3.717979	0.177069	0.142787
O	2.976504	1.081459	0.679030
C	2.761798	2.406658	0.026366
C	2.189601	2.158205	-1.361754
Au	-0.696292	-0.729202	0.035114
O	4.470148	0.170940	-0.768653
C	1.744009	3.062729	0.942918
C	4.082925	3.158696	0.007019
H	1.393938	-2.033911	-1.983372
H	1.783169	-0.492457	1.960342
H	2.050222	-2.263174	1.928671
H	3.895299	-1.988777	-1.815136
H	3.346377	-3.540326	-1.114903
H	4.092628	-1.084119	1.785301
H	1.902387	3.126523	-1.801697
H	2.925594	1.681338	-2.026783
H	1.291351	1.520083	-1.295628
H	3.903970	4.173945	-0.381631
H	4.490736	3.244568	1.027015
H	4.819621	2.662301	-0.642155
H	1.491104	4.060152	0.550912
H	0.824922	2.455084	0.991820
H	2.154400	3.175737	1.958804
P	-2.877038	0.087399	0.018146
O	-3.652434	-0.389853	-1.307298
C	-5.036187	-0.111119	-1.527112
H	-5.655721	-0.759489	-0.887720
H	-5.257716	0.948927	-1.321813
H	-5.243830	-0.331440	-2.582093
O	-3.106985	1.688027	0.070058
C	-2.447786	2.532562	-0.869898
H	-1.363387	2.326559	-0.885369
H	-2.865937	2.386968	-1.878890
H	-2.618737	3.566815	-0.545076
O	-3.767064	-0.355987	1.271649
C	-4.805878	0.417801	1.879419
H	-4.406883	1.380279	2.229103
H	-5.632527	0.593099	1.174277
H	-5.168329	-0.172386	2.730566

7c
 SCF Energy: -1227.27158615
 ZPE-corrected Energy: -1227.02897
 ΔU : -1227.01219
 ΔH : -1227.01125
 ΔG : -1227.07577
 Num. Imaginary Frequencies: 0

C	-1.857361	-2.727420	0.914361
C	-0.572075	-1.952092	0.973344
C	-0.014856	-1.301631	-0.064068
C	-0.799155	-1.338405	-1.351886
N	-2.265506	-1.410202	-0.999037
O	-2.556040	-2.592964	-0.345764
Au	1.686021	-0.213579	-0.003978
Cl	3.707173	1.097526	0.084264
C	-2.733355	-0.196243	-0.167488
O	-3.497039	-0.369119	0.718410
O	-2.155768	0.844047	-0.654523
C	-2.157677	2.153565	0.062224
C	-1.592897	1.929579	1.457364
C	-1.221205	2.991605	-0.790210
C	-3.577448	2.696778	0.067898
H	-0.100192	-1.951450	1.961554
H	-0.679977	-0.439901	-1.967291
H	-0.602670	-2.230885	-1.966675
H	-2.544245	-2.431282	1.723134
H	-1.678867	-3.811809	0.984836
H	-2.841692	-1.453196	-1.853608
H	-1.458921	2.910492	1.940704
H	-2.271144	1.326330	2.079848
H	-0.610972	1.429475	1.393712
H	-3.567818	3.702573	0.517587
H	-3.962388	2.779725	-0.961263
H	-4.249027	2.056919	0.660220
H	-1.130890	3.997349	-0.351419
H	-0.221819	2.526138	-0.824429
H	-1.611522	3.085584	-1.816096

P1c
 SCF Energy: -631.586197541
 ZPE-corrected Energy: -631.348717
 ΔU : -631.335017
 ΔH : -631.334073
 ΔG : -631.389557
 Num. Imaginary Frequencies: 0

C	2.590699	-1.675736	0.325665
O	1.337972	-1.404405	-0.295412
N	1.175866	-0.029190	-0.164831
C	2.413312	0.631285	-0.060257
C	3.445697	-0.476567	-0.067286
C	2.631030	1.947113	0.036219
H	2.460623	-1.737899	1.421023
H	2.938023	-2.637713	-0.070796
H	3.662826	2.291645	0.137049
H	1.819056	2.672090	0.016590
H	3.850381	-0.607595	-1.084399
H	4.274271	-0.274944	0.624465
C	-0.088615	0.491091	-0.033597
O	-0.279590	1.679777	0.090898
O	-1.006883	-0.465139	-0.079294
C	-2.425873	-0.150933	0.013271
C	-3.085501	-1.520751	-0.089626
C	-2.733244	0.491682	1.363061
C	-2.843143	0.734444	-1.157764
H	-3.938935	0.853739	-1.149852
H	-2.376581	1.727419	-1.091608
H	-2.552592	0.260752	-2.110294
H	-4.180522	-1.416101	-0.033010
H	-2.822620	-1.999887	-1.046566
H	-2.746879	-2.170116	0.733873
H	-3.824935	0.594457	1.475799
H	-2.359305	-0.149080	2.179000
H	-2.272044	1.485930	1.444882

P2c
 SCF Energy: -631.589119569
 ZPE-corrected Energy: -631.350387
 ΔU : -631.337202
 ΔH : -631.336257
 ΔG : -631.390185
 Num. Imaginary Frequencies: 0

C	-1.862191	1.599396	-0.007356
C	-2.936013	0.912785	0.791228
C	-3.195307	-0.384951	0.624009
C	-2.366107	-1.221771	-0.316528
N	-1.187213	-0.483809	-0.723572
O	-1.463519	0.805757	-1.119140
C	0.052986	-0.757483	-0.185447
O	0.313624	-1.822541	0.328052
O	0.883137	0.268106	-0.343664
C	2.267712	0.194780	0.098595
C	3.001473	-0.909019	-0.657768
C	2.820832	1.563084	-0.281525
C	2.324610	-0.004054	1.610843
H	-3.503471	1.518766	1.503758
H	-2.018375	-2.143686	0.169688
H	-2.947776	-1.512429	-1.209275
H	-0.979790	1.844556	0.615267
H	-2.237230	2.535589	-0.448516
H	4.075414	-0.864776	-0.413210
H	2.614979	-1.901206	-0.385532
H	2.886710	-0.761377	-1.744582
H	3.370152	0.081606	1.949425
H	1.731832	0.777026	2.116275
H	1.937246	-0.991912	1.896753
H	3.882515	1.632578	0.003647
H	2.732893	1.721632	-1.368501
H	2.261267	2.358897	0.236806
H	-4.009781	-0.875786	1.164713

R1c

SCF Energy: -631.536944557

ZPE-corrected Energy: -631.302270

ΔU : -631.287345

ΔH : -631.286401

ΔG : -631.345353

Num. Imaginary Frequencies: 0

C	-5.600275	0.605300	0.098090
C	-4.356126	0.249780	0.296362
C	-3.105104	-0.087542	0.494659
C	-1.947879	0.571577	-0.210183
O	-1.202227	-0.347459	-1.001042
N	-0.548767	-1.261713	-0.210099
H	-6.209424	0.123310	-0.675837
H	-6.067543	1.392233	0.702038
H	-2.863459	-0.883195	1.211594
H	-2.303178	1.330711	-0.920950
H	-1.266573	1.048291	0.516111
C	0.810940	-1.106597	-0.005889
H	-0.841565	-2.218070	-0.398968
O	1.504851	-2.030585	0.346154
O	1.180825	0.154721	-0.177543
C	2.554273	0.580105	0.055848
C	2.927377	0.354168	1.518154
C	3.495551	-0.147439	-0.899934
C	2.511779	2.069207	-0.263779
H	3.917246	0.798252	1.713039
H	2.191252	0.845996	2.175800
H	2.965082	-0.718130	1.756862
H	3.510956	2.511799	-0.126090
H	2.193509	2.226502	-1.307054
H	1.800712	2.583331	0.403292
H	4.507636	0.279182	-0.806813
H	3.540158	-1.221907	-0.672722
H	3.155750	-0.011094	-1.940133

TS2c3c
 SCF Energy: -1227.23433875
 ZPE-corrected Energy: -1226.99815
 ΔU : -1226.98071
 ΔH : -1226.97977
 ΔG : -1227.04467
 Num. Imaginary Frequencies: 1
 Imaginary Frequency: -512.7653

C	-1.086304	2.110280	0.804865
N	0.581527	2.254178	-0.415584
O	0.055811	1.900166	-1.618924
C	-1.376919	2.082719	-1.571279
H	-1.778659	1.514311	-2.418663
H	1.488304	-1.586762	1.355807
Cl	-0.770152	-2.876137	0.241387
Au	-1.228902	-0.543836	0.024651
C	-1.815172	1.548006	-0.230584
H	-2.881864	1.359514	-0.038520
H	-1.638399	3.149815	2.507739
C	-0.826335	2.637371	1.978504
H	0.164541	2.569400	2.440521
O	1.768909	0.331852	-0.509156
H	1.559573	-2.205765	-1.005080
O	2.309987	1.939028	1.000808
C	1.672097	1.483395	0.089652
H	2.716854	-1.417012	-2.139002
H	3.308203	-2.586319	-0.918021
H	4.346827	0.746648	0.482183
C	4.172575	-0.048034	-0.257072
H	4.924691	-0.839435	-0.108411
H	4.300867	0.363437	-1.272100
C	2.784358	-0.661403	-0.109795
C	2.574147	-1.787497	-1.110798
H	0.780315	3.258821	-0.345834
H	3.233774	-1.893843	1.590585
C	2.490996	-1.128842	1.310287
H	-1.595021	3.158141	-1.705203
H	2.560835	-0.297141	2.027613

TS2c7c
 SCF Energy: -1227.24118166
 ZPE-corrected Energy: -1227.00284
 ΔU : -1226.98535
 ΔH : -1226.98440
 ΔG : -1227.05154
 Num. Imaginary Frequencies: 1
 Imaginary Frequency: -447.5549

C	0.961984	2.883542	0.421640
C	-0.383487	2.224842	0.555154
C	-0.638580	1.038825	0.013237
C	0.143687	0.134119	-0.701570
N	1.970568	1.194600	-0.906848
O	1.704467	2.540567	-0.756707
Au	-2.330935	-0.148221	0.004264
Cl	-4.379205	-1.358456	0.112824
C	3.044931	0.702679	-0.106730
O	3.466386	1.285054	0.849979
O	3.375017	-0.481845	-0.575616
C	4.384835	-1.319182	0.086639
C	3.911509	-1.655306	1.496131
C	4.426198	-2.563216	-0.788607
C	5.727306	-0.597149	0.076777
H	-1.136451	2.762102	1.139789
H	0.609909	-0.716862	-0.187479
H	0.008933	0.023110	-1.784698
H	1.587156	2.696820	1.311413
H	0.844408	3.971381	0.316610
H	2.127398	1.025234	-1.902674
H	4.609280	-2.380001	1.945710
H	3.878146	-0.758983	2.132379
H	2.909575	-2.114921	1.461723
H	6.503482	-1.279703	0.458661
H	5.995669	-0.308271	-0.952757
H	5.704827	0.300355	0.711632
H	5.159726	-3.277351	-0.382888
H	3.436974	-3.047942	-0.814467
H	4.720072	-2.299107	-1.817169

TS4c5canti
 SCF Energy: -1453.26550891
 ZPE-corrected Energy: -1452.89663
 ΔU : -1452.86987
 ΔH : -1452.86893
 ΔG : -1452.95752
 Num. Imaginary Frequencies: 1
 Imaginary Frequency: -341.4188

C	-1.601740	-0.900794	2.077632
C	-1.524437	-0.731343	0.782649
C	-1.076919	-0.342813	-0.470912
C	-1.394339	-1.425433	-1.468213
O	-2.827245	-1.660727	-1.365034
N	-3.200752	-1.719681	-0.065490
H	-2.514267	-1.281116	2.550492
H	-0.741662	-0.644734	2.706656
H	-1.231019	-1.126136	-2.510085
H	-0.866821	-2.369000	-1.254088
H	-3.266035	-2.676726	0.295730
C	-4.289600	-0.905981	0.347065
O	-4.398934	0.147690	-0.416983
C	-5.333735	1.234641	-0.091566
O	-4.900319	-1.203420	1.338278
C	-4.958071	1.826411	1.262096
H	-5.143222	1.112724	2.078081
H	-3.893990	2.117041	1.266734
H	-5.564821	2.728860	1.439535
C	-5.092142	2.234719	-1.212500
H	-4.042296	2.570006	-1.207303
H	-5.745006	3.110700	-1.075302
H	-5.313521	1.775684	-2.189263
C	-6.762530	0.706045	-0.125144
H	-7.458752	1.551245	-0.001193
H	-6.967644	0.227252	-1.096649
H	-6.940851	-0.018565	0.682366
Au	1.085656	-0.080775	-0.153645
P	3.338781	0.210717	0.049287
O	3.846179	0.214257	1.571484
C	5.096891	-0.312784	2.023553
H	5.924250	0.362404	1.752358
H	5.265345	-1.313241	1.597062
H	5.029789	-0.383770	3.116377
O	3.848098	1.594612	-0.582506
C	4.942205	2.368682	-0.082360
H	4.829828	2.530643	1.000373
H	5.902333	1.871784	-0.295997
H	4.907878	3.332446	-0.605525
O	4.181735	-0.939517	-0.686194
C	5.429613	-0.744318	-1.357623
H	6.246271	-0.609145	-0.630288
H	5.613730	-1.652045	-1.945813
H	5.369178	0.125813	-2.028730
H	-1.449287	0.650779	-0.768878

TS4c5c
 SCF Energy: -1453.25175746
 ZPE-corrected Energy: -1452.88423
 ΔU : -1452.85747
 ΔH : -1452.85653
 ΔG : -1452.94260
 Num. Imaginary Frequencies: 1
 Imaginary Frequency: -510.3371

H	0.508987	3.787545	-0.864196
C	-0.056584	2.869748	-1.090372
H	-0.424160	2.923437	-2.127691
H	0.621781	2.006226	-1.004537
C	-1.220551	2.734533	-0.120292
C	-2.232207	3.854755	-0.335007
H	-2.634141	3.812836	-1.360623
H	-3.061294	3.795864	0.383939
H	-1.719276	4.821190	-0.204728
H	-0.027973	1.812178	1.439854
H	-0.218918	3.579999	1.583929
C	-0.741243	2.645101	1.322872
H	-1.586713	2.513156	2.014344
O	-1.820490	1.444281	-0.504001
C	-2.903437	1.005170	0.075463
O	-3.566425	1.498516	0.946566
N	-3.254933	-0.295944	-0.388160
H	-4.267132	-0.454167	-0.316987
O	-2.733146	-0.712979	-1.572554
C	-2.526613	-1.752944	0.895253
H	-3.353884	-0.632211	2.480590
H	-3.253692	-2.513483	2.678244
H	-1.194806	-3.201767	0.101148
H	-3.388356	-2.684378	-1.566604
C	-2.439876	-2.125627	-1.469408
H	-1.784227	-2.358691	-2.317089
C	-1.774109	-2.294878	-0.128373
Au	0.111821	-1.060838	-0.016675
C	-3.074065	-1.612672	2.079438
P	2.185548	-0.114090	0.053605
O	2.313680	1.172809	1.005627
O	3.298169	-1.145650	0.572275
O	2.679324	0.381823	-1.391917
C	4.651556	-1.202605	0.111250
C	3.539732	1.499997	-1.628683
C	3.463004	1.512281	1.786847
H	5.070250	-2.143846	0.488645
H	4.679029	-1.200334	-0.988931
H	5.234838	-0.357686	0.511287
H	3.516664	1.687630	-2.709476
H	3.169172	2.386341	-1.090492
H	4.572341	1.270632	-1.319849
H	3.145347	2.299122	2.482528
H	3.811246	0.635043	2.352587
H	4.269797	1.896945	1.142617

TS4c6c
 SCF Energy: -1453.22774549
 ZPE-corrected Energy: -1452.86053
 ΔU : -1452.83298
 ΔH : -1452.83204
 ΔG : -1452.92381
 Num. Imaginary Frequencies: 1
 Imaginary Frequency: -610.2723

C	-5.817477	2.458083	-0.017620
C	-5.987190	0.949647	0.118117
C	-7.277236	0.481148	-0.538479
C	-5.901737	0.474427	1.564266
O	-4.950050	0.265907	-0.668328
C	-3.683411	0.369972	-0.358042
N	-2.932093	-0.545346	-1.143184
C	-1.537478	-0.331659	-1.320763
C	-0.714947	-0.987230	-0.196873
Au	1.312338	-0.309686	-0.036319
O	-3.144336	1.080205	0.443135
C	-1.065201	-1.816878	0.738139
C	-2.623028	-2.337297	1.011356
O	-3.462230	-2.049977	0.070935
H	-1.338216	0.748242	-1.294192
H	-1.221205	-0.739199	-2.289772
H	-3.458271	-1.068634	-1.839370
H	-2.864005	-1.939680	2.015911
H	-2.353489	-3.416101	0.994153
H	-0.433975	-2.311450	1.478875
H	-4.885862	2.800851	0.455079
H	-5.813494	2.745491	-1.081862
H	-6.667563	2.958788	0.473111
H	-7.363814	-0.615349	-0.474864
H	-7.297672	0.779098	-1.599089
H	-4.977964	0.824296	2.048428
H	-5.936793	-0.626933	1.601002
H	-8.139624	0.935832	-0.026621
H	-6.763208	0.871623	2.124797
P	3.482347	0.419947	0.107414
O	3.780239	1.470952	-1.066853
C	5.028206	2.163231	-1.170685
H	5.091122	2.939322	-0.392121
H	5.871551	1.459759	-1.078868
H	5.048623	2.634297	-2.161476
O	4.663688	-0.670529	0.004783
C	4.713848	-1.585586	-1.089690
H	3.773754	-2.158660	-1.158105
H	4.892449	-1.046623	-2.033738
H	5.547406	-2.270541	-0.890744
O	3.856551	1.120689	1.490230
C	5.134519	1.079796	2.137166
H	5.443493	0.037951	2.299169
H	5.893152	1.606500	1.538769
H	5.004238	1.590640	3.099203