

**Supporting Information:**

**The Key Role of Protodeauration in the  
Gold-Catalyzed Reaction of 1,3-Diynes with  
Pyrrole and Indole to Form Complex  
Heterocycles**

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# Solvation Effects

Structure	Gas phase SCF energy	Solv. Effect	Solution phase SCF energy
Pyrrole series	A.U.	kcal/mol	A.U.
1a	-209.84360087	-3.38	-209.848983061
2a	-1211.03477496	<b>-34.57</b>	-1211.089859610
10a	-1420.89950864	<b>-35.28</b>	-1420.955724140
3a1	-1420.90950949	<b>-32.43</b>	-1420.961193420
3a	-1420.90574240	<b>-36.27</b>	-1420.963540690
4a'	-1420.95486577	<b>-34.92</b>	-1421.010509440
4a	-1420.95476697	<b>-34.41</b>	-1421.009594860
5a	-1420.97372745	<b>-32.69</b>	<b>-34.57</b> -1421.025814960
6a	-1420.96009921	<b>-33.10</b>	-1421.012841870
7a1	-1420.91284172	<b>-35.04</b>	-1420.968685420
7a	-1420.90003616	<b>-37.18</b>	-1420.959278870
8a'	-1420.95080312	<b>-33.28</b>	-1421.003837740
8a	-1420.94447008	<b>-36.22</b>	-1421.002184800
9a	-1420.95052642	<b>-34.09</b>	-1421.004860200
TS_2a_3a	-1420.87531684	<b>-32.91</b>	-1420.927759040
TS_2a_7a	-1420.88231236	<b>-32.32</b>	-1420.933824540
TS_3a1_4a'	-1420.89437105	<b>-32.38</b>	-1420.945967200
TS_3a_3a1	-1420.86520474	<b>-32.24</b>	-1420.916582910
TS_4a_5a	-1420.93327642	<b>-31.10</b>	-1420.982840900
TS_4a_6a	-1420.93246316	<b>-32.43</b>	<b>-32.64</b> -1420.984140970
TS_7a1_8a'	-1420.87879273	<b>-34.27</b>	-1420.933401430
TS_7a_7a1	-1420.85162928	<b>-32.73</b>	-1420.903792470
TS_8a_10a	-1420.89845568	<b>-34.10</b>	-1420.952801570
TS_8a_9a	-1420.91662082	<b>-31.90</b>	-1420.967448920
P1	-824.66425008	-4.80	-824.671903421
P2	-824.60986717	-5.53	-824.618672133
P3	-824.60981150	-5.29	-824.618234218
P4	-824.55295966	-6.15	-824.562758701

average values in boldface

Structure	Gas phase SCF energy	Solv. Effect	Solution phase SCF energy
Substituted diynes series	A.U.	kcal/mol	A.U.
4c	-1428.17122465	-33.34	-1428.22435949
5c	-1428.18501587	-32.03	-1428.23606384
6c	-1428.17176255	-32.19	-1428.22306481
TS_4c_5c	-1428.14137830	-31.11	-1428.19094761
TS_4c_6c	-1428.14448818	-31.81	-1428.19517273
4e	-1876.13402412	-38.83	-1876.19590840
5e	-1876.15315286	-37.38	-1876.21272032
6e	-1876.13983381	-38.40	-1876.20103320
TS_4e_5e	-1876.11161867	-35.48	-1876.16816125
TS_4e_6e	-1876.11132546	-37.48	-1876.17104680
4d	-1649.70767629	-34.51	-1649.76266656
5d	-1649.72620714	-32.46	-1649.77792896
6d	-1649.71199006	-32.98	-1649.76455482
TS_4d_5d	-1649.68808426	-30.86	-1649.73726564
TS_4d_6d	-1649.68475176	-32.50	-1649.73655130

average values in boldface

Structure	Gas phase SCF energy	Solv. Effect	Solution phase SCF energy
Indole series	A.U.	kcal/mol	A.U.
11a	-363.260459274	-3.96	-363.266770063
2a	-1211.034774960	<b>-34.57</b>	-1211.089859610
12a1	-1574.325994990	<b>-32.85</b>	-1574.378341700
12a	-1574.319431370	<b>-32.52</b>	-1574.371247640
13a'	-1574.364529040	<b>-35.67</b>	-1574.421380440
13a	-1574.368188610	<b>-35.60</b>	-1574.424913650
14a	-1574.399607430	<b>-31.42</b>	-1574.449683700
15a1	-1574.333044490	<b>-31.40</b>	<b>-34.02</b> -1574.383090660
15a	-1574.324975630	<b>-36.48</b>	-1574.383103650
16a'	-1574.366056440	<b>-35.89</b>	-1574.423243570
16a	-1574.369499470	<b>-35.64</b>	-1574.426302540
17a	-1574.389280840	<b>-30.93</b>	-1574.438567400
18a	-1574.371694730	<b>-35.22</b>	-1574.427826270
TS_12a1_13a'	-1574.308056390	<b>-32.69</b>	-1574.360157840
TS_12a_12a1	-1574.281740880	<b>-31.03</b>	-1574.331184660
TS_13a_14a	-1574.355734640	<b>-30.86</b>	-1574.404909650
TS_15a1_16a'	-1574.312048130	<b>-32.37</b>	-1574.363636200
TS_15a_15a1	-1574.283456960	<b>-32.50</b>	<b>-32.13</b> -1574.335254890
TS_16a_18a	-1574.356158710	<b>-32.81</b>	-1574.408442320
TS_18a_17a	-1574.355806210	<b>-31.63</b>	-1574.406212830
TS_2a_12a	-1574.287285080	<b>-31.84</b>	-1574.338033040
TS_2a_15a	-1574.294627310	<b>-33.43</b>	-1574.347897520
P	-978.082978848	-4.69	-978.090456570

average values in boldface

# Cartesian coordinates of the pyrrole mechanism

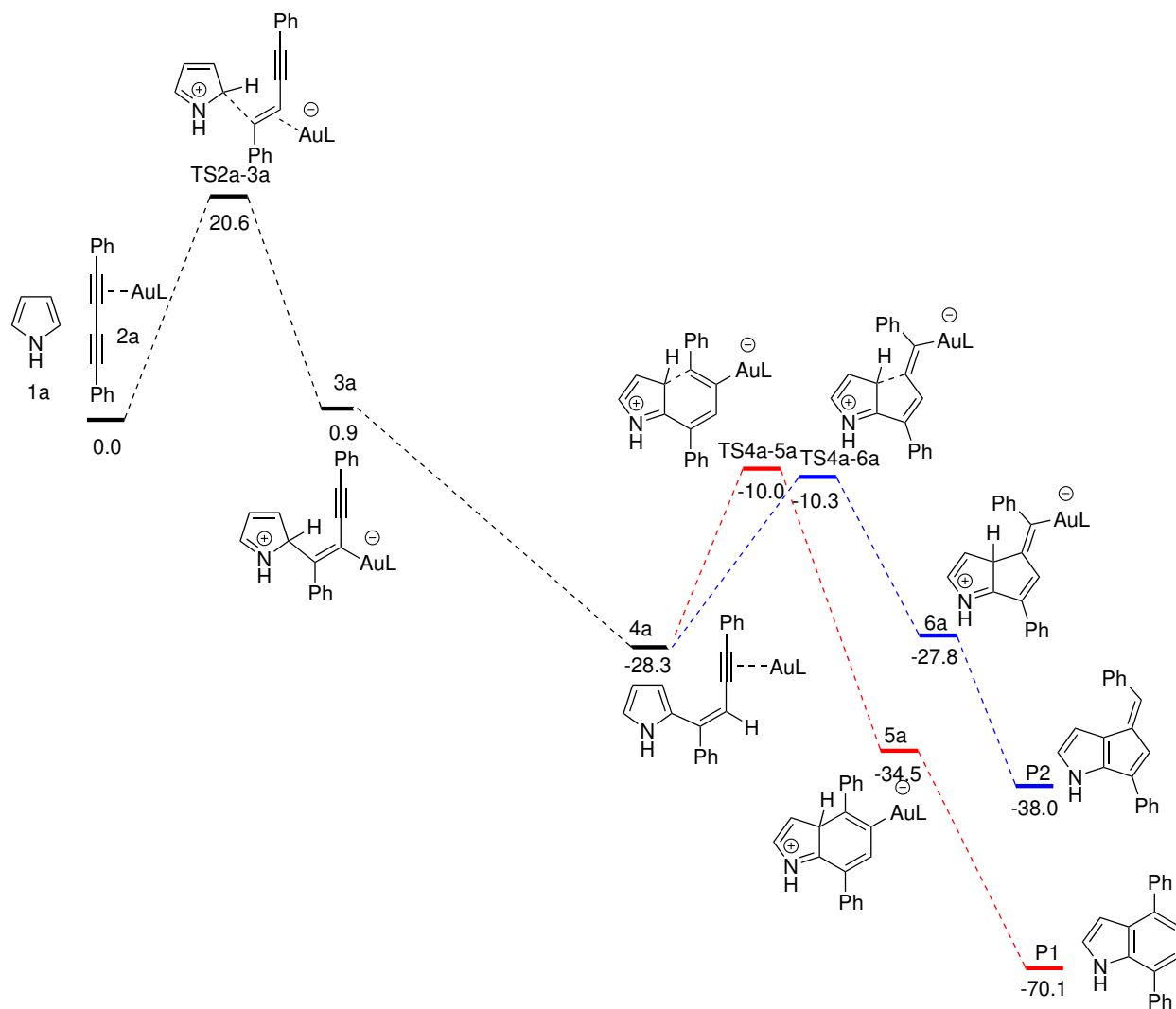


Figure S1: Pyrrole reaction mechanism, part 1.

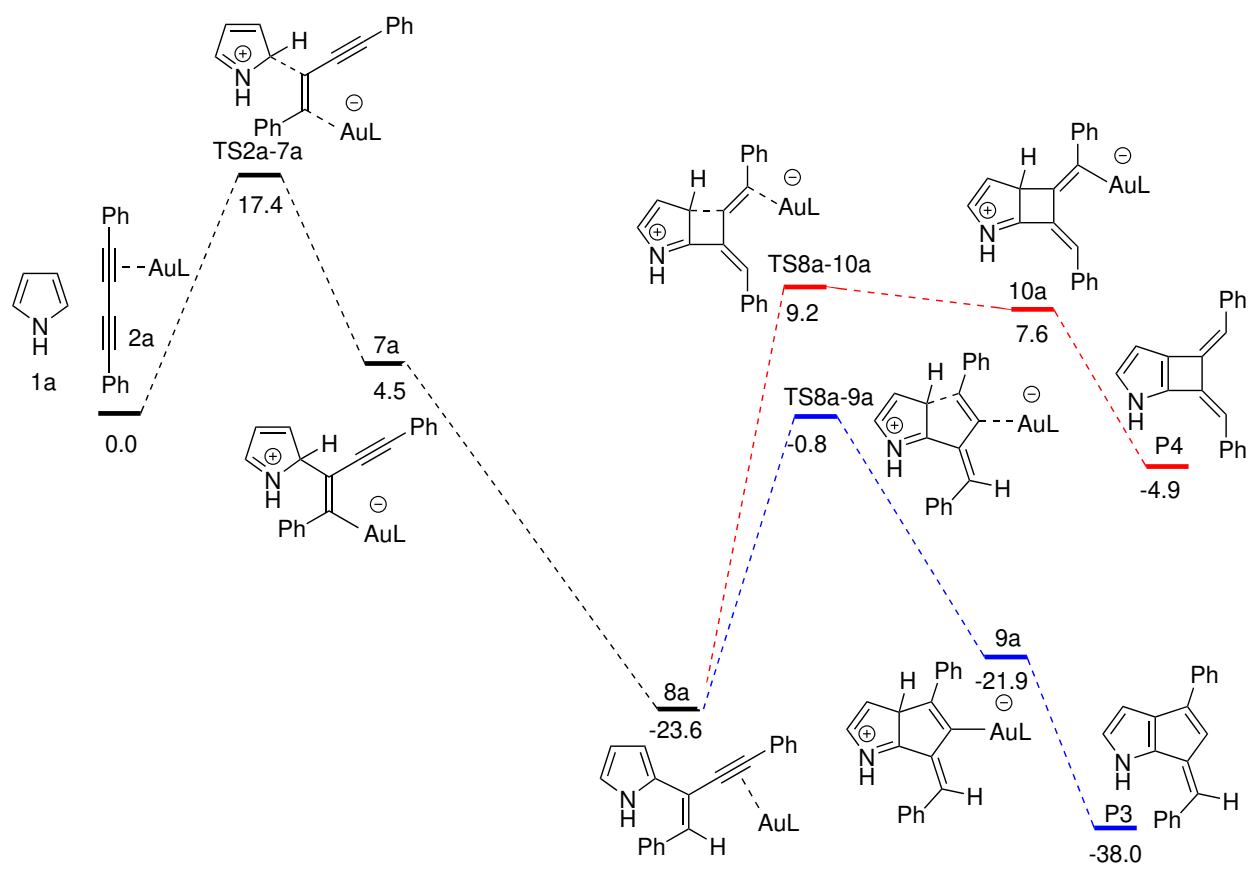


Figure S2: Pyrrole reaction mechanism, part 2.

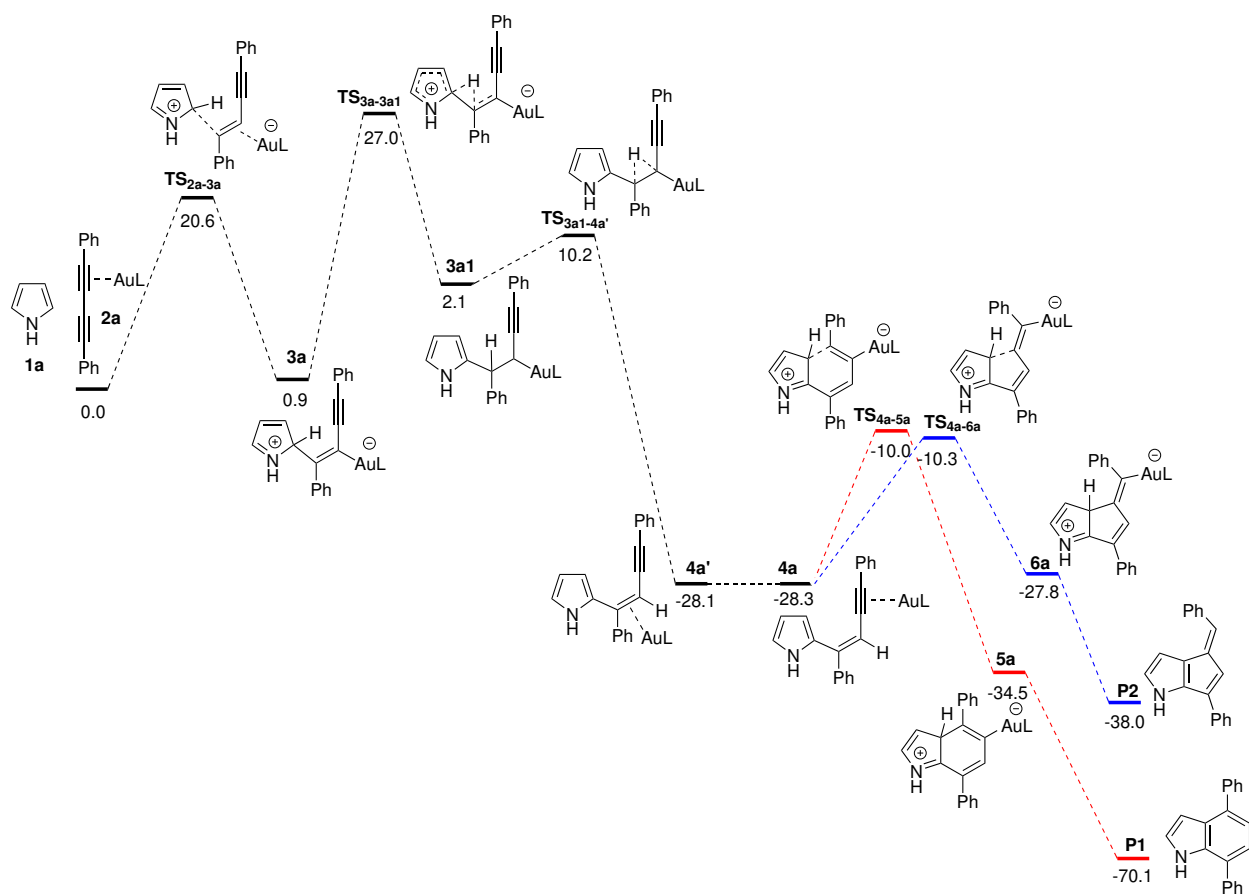


Figure S3: Pyrrole reaction mechanism, part 3.



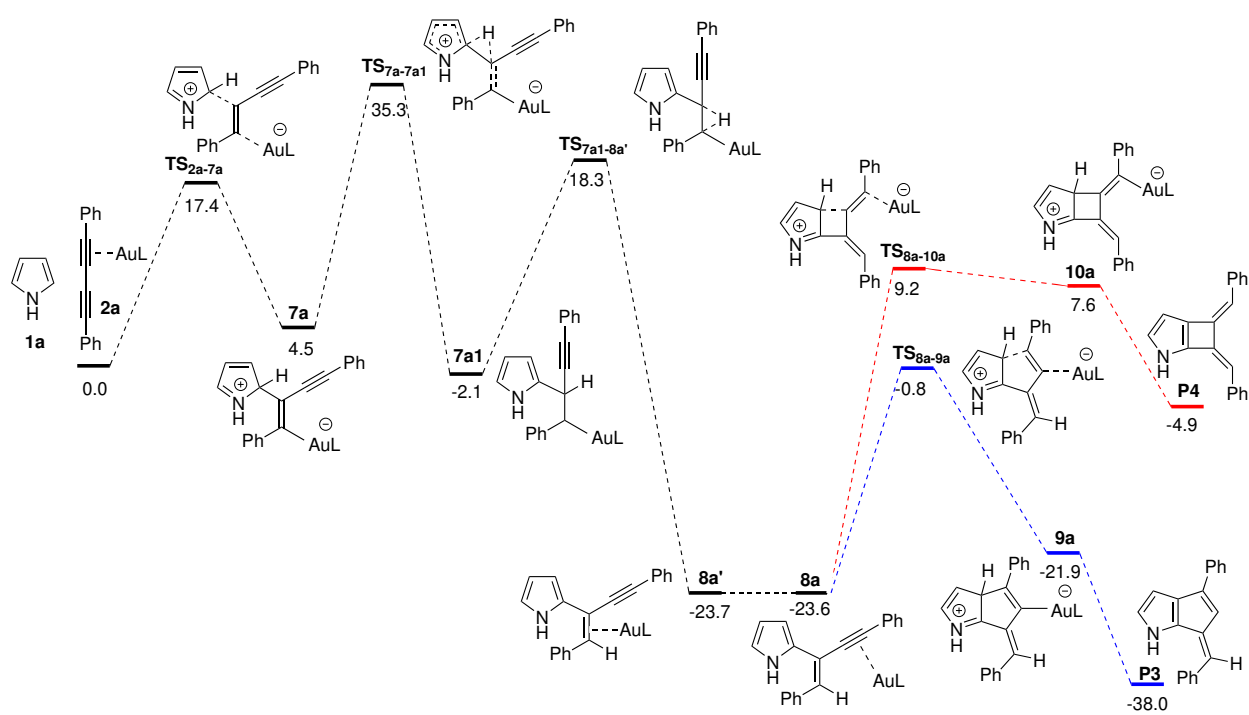


Figure S4: Pyrrole reaction mechanism, part 4.

10a  
SCF Energy: -1420.95572414  
ZPE-corrected Energy: -1420.55501  
 $\Delta U$ : -1420.52829  
 $\Delta H$ : -1420.52734  
 $\Delta G$ : -1420.61550

Num. Imaginary Frequencies: 0

C	2.512032	1.506871	-0.198976
C	3.440820	1.051094	0.754072
C	4.707772	1.618223	0.852824
C	5.092456	2.633250	-0.024054
C	4.196590	3.075999	-0.997837
C	2.920247	2.525254	-1.080037
H	3.146730	0.241272	1.434563
H	5.407451	1.256424	1.615138
H	6.095331	3.070154	0.042588
H	4.497248	3.856692	-1.706371
H	2.237151	2.865771	-1.867450
C	1.170008	0.910553	-0.262721
C	0.386545	4.266861	0.422275
C	-0.082230	3.273753	-0.570747
C	-0.587922	4.415789	1.345797
N	-1.654122	3.526752	1.066359
C	-1.388490	2.862645	-0.039968
C	-1.373640	1.461850	-0.440663
C	-2.241468	0.432121	-0.528271
C	-3.680317	0.459404	-0.339588
C	-4.428410	1.650765	-0.286454
C	-5.799251	1.616782	-0.063378
C	-6.455322	0.394156	0.101522
C	-5.731560	-0.796334	0.031489
C	-4.359607	-0.763774	-0.193099
C	0.079186	1.679235	-0.493602
H	1.293278	4.870223	0.351627
H	-0.040181	3.591361	-1.628267
H	-0.660480	5.079160	2.208794
H	-3.938216	2.618280	-0.453861
H	-6.367473	2.552909	-0.030089
H	-7.537110	0.371134	0.273548
H	-6.242332	-1.758252	0.150440
H	-3.787921	-1.699035	-0.246865
H	-2.370616	3.263932	1.746925
H	-1.795970	-0.550753	-0.749783
Au	0.920488	-1.159174	-0.059534
P	0.544337	-3.503876	0.154965
C	2.030563	-4.560764	0.111130
C	-0.310485	-3.991265	1.692664
C	-0.524235	-4.171918	-1.166021
H	1.749231	-5.626967	0.197781
H	2.572198	-4.402310	-0.838200
H	2.702523	-4.292184	0.945285
H	-1.278963	-3.463772	1.760144
H	-0.488518	-5.083202	1.707020
H	0.301734	-3.710033	2.567672
H	-1.494485	-3.642564	-1.159490
H	-0.046963	-4.011837	-2.149025
H	-0.698088	-5.254058	-1.016107

1a  
 SCF Energy: -209.848983061  
 ZPE-corrected Energy: -209.767134  
 $\Delta U$ : -209.763200  
 $\Delta H$ : -209.762255  
 $\Delta G$ : -209.793504  
 Num. Imaginary Frequencies: 0

N	-1.119940	-0.002327	0.000194
C	-0.331237	-1.120754	-0.000020
C	0.985951	-0.709769	-0.000189
C	0.982947	0.713731	0.000102
C	-0.335870	1.119486	-0.000153
H	1.860301	-1.364504	0.000859
H	1.854458	1.372266	-0.000423
H	-0.779644	2.116300	0.000469
H	-2.135472	-0.004523	-0.000510
H	-0.770807	-2.119418	-0.000196

2a  
 SCF Energy: -1211.08985961  
 ZPE-corrected Energy: -1210.77538  
 $\Delta U$ : -1210.75188  
 $\Delta H$ : -1210.75094  
 $\Delta G$ : -1210.83407  
 Num. Imaginary Frequencies: 0

C	2.263116	-3.407703	0.834993
C	2.025446	-2.386296	-0.102300
C	3.026257	-2.041097	-1.027855
C	4.242010	-2.714396	-1.015256
C	4.473098	-3.727508	-0.083225
C	3.484024	-4.072051	0.839061
C	0.750358	-1.733395	-0.104313
C	-0.453279	-1.423727	-0.062375
Au	0.806350	0.595694	0.012371
C	-1.805337	-1.215738	-0.059869
C	-3.015050	-1.036132	-0.057256
C	-4.421492	-0.838012	-0.057516
C	-5.077162	-0.419084	-1.230331
C	-6.453738	-0.229329	-1.225418
C	-7.188380	-0.456506	-0.060311
C	-6.544830	-0.873500	1.106172
C	-5.168305	-1.063475	1.113958
H	-4.654377	-1.390389	2.024476
H	-8.273874	-0.307748	-0.061645
H	-6.960771	0.097051	-2.139916
H	-4.492688	-0.246915	-2.140738
H	-7.123335	-1.052138	2.019020
H	1.480207	-3.671739	1.554066
H	3.665708	-4.867951	1.569280
H	5.433759	-4.254066	-0.076101
H	5.017927	-2.447090	-1.740537
H	2.836783	-1.247655	-1.760445
P	1.486194	2.824201	0.138581
C	3.148366	3.086795	-0.548997
C	1.554679	3.455504	1.841447
C	0.393460	3.963870	-0.761987
H	0.552554	3.396415	2.300675
H	2.254699	2.845238	2.438132
H	0.358238	3.684439	-1.829400
H	-0.627643	3.908132	-0.346204
H	1.895556	4.507735	1.838165
H	0.772142	4.998503	-0.665228
H	3.426499	4.153490	-0.460217
H	3.880588	2.470781	0.001496
H	3.163991	2.791702	-1.612662

3a1  
 SCF Energy: -1420.96119342  
 ZPE-corrected Energy: -1420.56153  
 $\Delta U$ : -1420.53401  
 $\Delta H$ : -1420.53306  
 $\Delta G$ : -1420.62426

Num. Imaginary Frequencies: 0

N	1.731712	3.872032	0.861732
C	1.509674	2.681253	0.214983
C	2.401495	2.611885	-0.839815
C	3.185736	3.798219	-0.814477
C	2.744816	4.556293	0.249671
C	0.380441	1.791154	0.641611
C	-0.982277	2.297732	0.198340
C	-1.996536	2.539587	1.126329
C	-3.268211	2.924807	0.698002
C	-3.532462	3.069028	-0.662845
C	-2.518228	2.837700	-1.594728
C	-1.248280	2.460184	-1.165274
C	0.539892	0.327257	0.369248
Au	-1.168171	-0.854749	0.169647
C	1.766424	-0.235812	0.275836
C	2.861626	-0.812410	0.169495
C	4.137412	-1.374628	0.045782
C	5.277298	-0.535002	0.069532
C	6.541664	-1.085982	-0.061056
C	6.683400	-2.469269	-0.212811
C	5.566224	-3.310969	-0.237659
C	4.296654	-2.772066	-0.110808
H	7.685491	-2.900654	-0.313946
H	7.427060	-0.442452	-0.044859
H	5.137001	0.545254	0.188457
H	3.406975	-3.410346	-0.128739
H	5.696306	-4.391228	-0.357739
H	-1.794695	2.413392	2.198479
H	-4.057016	3.114139	1.435129
H	-4.530919	3.369409	-1.000603
H	-2.718970	2.955207	-2.665805
H	-0.447725	2.278854	-1.895909
H	2.477374	1.793971	-1.560739
H	3.988545	4.066416	-1.504012
H	3.075560	5.525383	0.625449
H	1.208203	4.201890	1.668590
H	0.366934	1.776613	1.761807
P	-3.198046	-2.055875	-0.123230
C	-3.199122	-3.226776	-1.519439
C	-3.732121	-3.046324	1.309953
C	-4.592292	-0.929143	-0.454348
H	-2.427227	-3.999762	-1.358225
H	-2.968994	-2.689598	-2.456254
H	-3.834167	-2.395361	2.195919
H	-2.978372	-3.822948	1.528760
H	-4.188631	-3.712417	-1.609504
H	-4.704252	-3.529447	1.097146
H	-5.526819	-1.500906	-0.607497
H	-4.719450	-0.240391	0.400327
H	-4.377377	-0.326259	-1.355175

3a  
 SCF Energy: -1420.96354069  
 ZPE-corrected Energy: -1420.56314  
 $\Delta U$ : -1420.53564  
 $\Delta H$ : -1420.53470  
 $\Delta G$ : -1420.62617

Num. Imaginary Frequencies: 0

N	-1.604615	3.612512	0.727600
C	-1.292418	2.880041	-0.499723
C	-2.640745	2.449060	-0.942030
C	-3.586505	2.948101	-0.099093
C	-2.894732	3.639225	0.938244
C	-0.156643	1.882694	-0.297595
C	1.180493	2.514326	-0.173723
C	1.641044	3.456550	-1.106757
C	2.909281	4.021567	-0.990406
C	3.738957	3.670283	0.073963
C	3.288194	2.753386	1.023415
C	2.021735	2.185896	0.902830
C	-0.369584	0.548014	-0.158304
Au	1.191964	-0.861646	-0.021824
C	-1.664603	-0.008629	-0.142761
C	-2.763301	-0.549987	-0.097810
C	-4.072846	-1.106902	-0.033303
C	-5.014169	-0.594705	0.880045
C	-6.295989	-1.130748	0.944494
C	-6.661722	-2.179542	0.099566
C	-5.736726	-2.694131	-0.810497
C	-4.451401	-2.167156	-0.877717
H	-7.672484	-2.599649	0.151747
H	-7.018594	-0.726561	1.662516
H	-4.720938	0.226369	1.545057
H	-3.721330	-2.570273	-1.588777
H	-6.020547	-3.518788	-1.474124
H	1.015280	3.732484	-1.965758
H	3.253795	4.739514	-1.743355
H	4.734583	4.118429	0.167942
H	3.924229	2.485736	1.875131
H	1.661191	1.484694	1.665535
H	-2.809960	1.898900	-1.870361
H	-4.669959	2.847582	-0.171071
H	-3.319983	4.147200	1.808757
H	-0.890987	4.028066	1.328694
H	-0.962641	3.644889	-1.240415
P	2.968305	-2.435215	0.087460
C	2.655083	-4.030666	-0.740286
C	4.513056	-1.831593	-0.674106
C	3.461171	-2.900894	1.782094
H	2.436140	-3.858620	-1.808901
H	1.781024	-4.523960	-0.279544
H	4.831963	-0.898497	-0.175788
H	4.338598	-1.612998	-1.742635
H	3.537248	-4.691892	-0.650521
H	5.314437	-2.588783	-0.581710
H	4.307164	-3.613330	1.757331
H	3.761925	-1.997798	2.342353
H	2.606624	-3.367169	2.303698

4a.  
 SCF Energy: -1421.01050944  
 ZPE-corrected Energy: -1420.60963  
 $\Delta U$ : -1420.58211  
 $\Delta H$ : -1420.58116  
 $\Delta G$ : -1420.67233

Num. Imaginary Frequencies: 0

N	0.797088	3.056052	1.783662
C	0.112860	2.066572	1.095216
C	-0.943039	1.664320	1.926317
C	-0.877507	2.423285	3.104394
C	0.205551	3.285748	2.975462
C	0.515791	1.641231	-0.215998
C	1.853416	2.059709	-0.707498
C	1.983938	2.677790	-1.958518
C	3.238151	3.063128	-2.426981
C	4.376030	2.826075	-1.657864
C	4.257769	2.207783	-0.412039
C	3.005607	1.832969	0.064633
C	-0.308304	0.909216	-1.093925
Au	0.711806	-0.950340	-0.222256
C	-1.702951	0.691679	-0.923161
C	-2.902606	0.497150	-0.816609
C	-4.302096	0.284999	-0.653910
C	-4.984629	0.867764	0.429996
C	-6.348791	0.654356	0.595005
C	-7.051043	-0.137190	-0.315275
C	-6.382909	-0.716562	-1.395181
C	-5.018560	-0.509821	-1.567064
H	-8.126265	-0.302141	-0.183132
H	-6.871595	1.112666	1.441994
H	-4.429732	1.494690	1.137954
H	-4.488855	-0.963432	-2.412427
H	-6.932561	-1.337251	-2.111695
H	1.089947	2.880483	-2.559978
H	3.324980	3.556167	-3.401368
H	5.362127	3.125154	-2.030114
H	5.150381	2.011391	0.191949
H	2.916597	1.331880	1.037702
H	-1.658755	0.872959	1.698037
H	-1.543061	2.357413	3.966125
H	0.586052	4.050264	3.654058
H	1.588549	3.577806	1.413563
H	0.072863	0.790586	-2.122052
P	1.683496	-2.936182	0.532341
C	3.356602	-2.652500	1.189396
C	0.759736	-3.756755	1.866512
C	1.879595	-4.200196	-0.759832
H	3.305959	-1.956698	2.045601
H	3.988424	-2.200765	0.404055
H	-0.251977	-4.018642	1.510081
H	0.665888	-3.076571	2.730711
H	3.807008	-3.607742	1.518003
H	1.287001	-4.677390	2.179098
H	2.356562	-5.101516	-0.331010
H	0.891374	-4.470229	-1.171199
H	2.508702	-3.806314	-1.576952

4a  
SCF Energy: -1421.00959486  
ZPE-corrected Energy: -1420.60912  
 $\Delta U$ : -1420.58149  
 $\Delta H$ : -1420.58055  
 $\Delta G$ : -1420.67266

Num. Imaginary Frequencies: 0

C	2.649040	3.522316	1.692552
C	3.593617	2.730789	2.327288
N	3.705468	1.566201	1.640740
C	2.830444	1.559125	0.570772
C	2.166569	2.787367	0.590465
C	2.731140	0.437375	-0.335065
C	3.920335	-0.420517	-0.528750
C	3.791766	-1.815501	-0.617688
C	4.908705	-2.619690	-0.825158
C	6.172534	-2.043017	-0.953058
C	6.314316	-0.658066	-0.867435
C	5.199569	0.146939	-0.651249
H	2.355609	4.530682	1.989010
H	4.194440	2.917959	3.218275
H	4.304894	0.786979	1.901830
H	1.448710	3.128469	-0.158378
H	2.803037	-2.274659	-0.495732
H	4.792651	-3.707885	-0.880494
H	7.051534	-2.676399	-1.117242
H	7.303193	-0.198698	-0.975429
H	5.315724	1.236280	-0.602213
C	1.585354	0.141357	-1.031690
C	0.343513	0.781142	-0.856829
C	-0.745593	1.365409	-0.722074
C	-1.799071	2.344120	-0.681734
C	-2.855432	2.297384	-1.607721
C	-3.852324	3.265632	-1.573051
C	-3.811900	4.281352	-0.616006
C	-2.770423	4.326056	0.311416
C	-1.767706	3.361773	0.286562
H	-2.878740	1.496975	-2.356884
H	-4.670242	3.228844	-2.300948
H	-4.600095	5.041950	-0.591161
H	-2.739826	5.119987	1.065740
H	-0.951893	3.385026	1.018482
Au	-1.379389	-0.736971	-0.081325
H	1.623071	-0.652418	-1.790229
P	-2.478986	-2.662524	0.643842
C	-3.878182	-3.137237	-0.416040
C	-1.401041	-4.126137	0.711531
C	-3.180119	-2.496801	2.313091
H	-3.524025	-3.321584	-1.445170
H	-4.621495	-2.321116	-0.437696
H	-0.554606	-3.936134	1.394586
H	-1.002551	-4.342350	-0.295101
H	-1.975188	-4.999311	1.073789
H	-4.353518	-4.054861	-0.021764
H	-3.694014	-3.433555	2.598667
H	-2.375800	-2.283257	3.038342
H	-3.903334	-1.662814	2.330812

5a  
 SCF Energy: -1421.02581496  
 ZPE-corrected Energy: -1420.62347  
 $\Delta U$ : -1420.59741  
 $\Delta H$ : -1420.59647  
 $\Delta G$ : -1420.68255

Num. Imaginary Frequencies: 0

C	2.405666	3.480256	0.114848
C	3.720543	3.344153	0.373725
N	4.096058	2.000680	0.254310
C	3.047631	1.239918	-0.072046
C	1.895649	2.136297	-0.291362
C	2.926963	-0.158147	-0.156507
C	4.098602	-1.052061	-0.062980
C	4.067171	-2.183415	0.764899
C	5.167245	-3.033027	0.846062
C	6.317929	-2.763907	0.105009
C	6.361361	-1.642232	-0.722115
C	5.260187	-0.792992	-0.806767
H	1.844745	4.414524	0.079848
H	4.471101	4.092767	0.629303
H	5.035000	1.644483	0.433166
H	1.912090	2.216295	-1.420198
H	3.174602	-2.386792	1.369158
H	5.128669	-3.909699	1.502341
H	7.184439	-3.431124	0.172574
H	7.257517	-1.430089	-1.315902
H	5.291517	0.068118	-1.487174
C	1.619169	-0.627153	-0.220714
C	0.418010	0.157958	-0.177526
C	0.533537	1.531411	-0.146815
C	-0.621051	2.447205	-0.103864
C	-1.687370	2.327088	-1.009593
C	-2.795840	3.164514	-0.913268
C	-2.861173	4.127673	0.094672
C	-1.806845	4.259200	0.998150
C	-0.689775	3.434453	0.891027
H	-1.630927	1.577998	-1.808839
H	-3.615111	3.067353	-1.634919
H	-3.736400	4.782503	0.172943
H	-1.854951	5.009644	1.795156
H	0.128204	3.531632	1.616075
Au	-1.444979	-0.799128	-0.048704
H	1.506627	-1.719973	-0.267599
P	-3.591680	-1.816641	0.097903
C	-4.613527	-1.552219	-1.392179
C	-3.625138	-3.624102	0.347238
C	-4.623990	-1.159032	1.452526
H	-4.117945	-2.003665	-2.270009
H	-4.724624	-0.467656	-1.573316
H	-3.107283	-3.880152	1.288463
H	-3.102165	-4.124916	-0.486638
H	-4.668661	-3.988061	0.394707
H	-5.614533	-2.005553	-1.264483
H	-5.623045	-1.634312	1.445902
H	-4.134223	-1.351498	2.423573
H	-4.738204	-0.066871	1.330261



6a  
SCF Energy: -1421.01284187  
ZPE-corrected Energy: -1420.61113  
 $\Delta U$ : -1420.58464  
 $\Delta H$ : -1420.58370  
 $\Delta G$ : -1420.67195

Num. Imaginary Frequencies: 0

C	2.232469	3.200516	0.671406
C	2.031805	1.986351	-0.178473
C	3.496982	3.155947	1.133850
N	4.114934	1.938138	0.756715
C	3.249201	1.196633	0.079640
C	0.953613	0.902980	-0.224352
C	1.680773	-0.330007	-0.315028
C	3.057769	-0.187231	-0.176521
C	-0.400544	1.068989	-0.197313
C	-0.936732	2.438083	-0.219568
C	-1.739309	2.905908	0.834854
C	-2.185102	4.224604	0.857507
C	-1.877692	5.089473	-0.194231
C	-1.118701	4.625289	-1.268802
C	-0.643979	3.315997	-1.277678
Au	-1.747071	-0.520990	-0.047065
P	-3.323544	-2.305692	0.103487
C	-2.849294	-3.812054	-0.811179
C	-4.981211	-1.897237	-0.539991
C	-3.636337	-2.897910	1.801239
H	5.010599	1.614108	1.121808
H	1.543669	4.043540	0.758988
H	2.126255	2.346947	-1.234810
H	4.070254	3.888622	1.703631
H	1.175760	-1.289049	-0.487971
C	4.087946	-1.225512	-0.150780
H	-1.993200	2.222381	1.655446
H	-2.788987	4.579078	1.700839
H	-2.241943	6.122963	-0.182290
H	-0.890898	5.291302	-2.109160
H	-0.053331	2.956101	-2.129879
H	-3.626437	-4.591439	-0.699688
H	-2.723727	-3.573652	-1.882196
H	-1.889386	-4.196901	-0.423411
H	-5.658765	-2.766007	-0.441720
H	-5.399097	-1.043707	0.022495
H	-4.906833	-1.611369	-1.604143
H	-4.376147	-3.720386	1.792914
H	-2.693920	-3.260456	2.248496
H	-4.020568	-2.068090	2.420476
C	3.769788	-2.554180	0.170719
C	5.421181	-0.905814	-0.451459
C	6.410486	-1.885409	-0.424598
C	6.082073	-3.201396	-0.102645
C	4.758310	-3.532256	0.192289
H	2.737188	-2.820897	0.425533
H	5.685913	0.119342	-0.741824
H	7.445417	-1.619082	-0.666300
H	6.859524	-3.973144	-0.081723
H	4.494872	-4.564157	0.449976

7a1  
 SCF Energy: -1420.96868542  
 ZPE-corrected Energy: -1420.56870  
 $\Delta U$ : -1420.54132  
 $\Delta H$ : -1420.54038  
 $\Delta G$ : -1420.63088

Num. Imaginary Frequencies: 0

C	2.779573	3.200221	2.177213
C	2.912983	2.638661	0.932425
C	1.494891	2.833781	2.651351
N	0.884161	2.083022	1.754543
C	1.717380	1.897040	0.624686
C	1.124633	1.902868	-0.825275
C	1.646220	0.634446	-0.272173
C	2.947032	0.113621	-0.770691
C	3.856066	-0.490498	0.111884
C	5.055034	-1.018360	-0.353482
C	5.364219	-0.967470	-1.715812
C	4.464151	-0.381156	-2.602129
C	3.265494	0.159348	-2.133256
Au	0.184075	-0.841751	0.243660
P	-1.586638	-2.347288	0.699357
C	-3.034672	-1.496650	1.415505
C	-2.252970	-3.184299	-0.777451
C	-1.226728	-3.700468	1.866945
C	-0.297040	2.070706	-0.943251
C	-1.513230	2.046131	-0.969587
C	-2.928354	1.854098	-0.992694
C	-3.462989	0.804117	-1.761741
C	-4.830158	0.548362	-1.745136
C	-5.678714	1.331865	-0.960882
C	-5.156634	2.378008	-0.198970
C	-3.790483	2.643277	-0.214123
H	3.499103	3.817148	2.715727
H	3.768990	2.707249	0.256500
H	1.014449	3.092022	3.597897
H	3.609012	-0.537197	1.181768
H	5.756901	-1.478806	0.351603
H	6.307072	-1.388172	-2.083235
H	4.694792	-0.339265	-3.673010
H	2.559207	0.611834	-2.840880
H	-3.855296	-2.216669	1.594525
H	-2.753733	-1.021149	2.372082
H	-3.385492	-0.710862	0.719630
H	-1.461852	-3.788445	-1.255455
H	-3.096570	-3.842544	-0.496683
H	-2.605730	-2.429106	-1.502780
H	-0.414795	-4.331821	1.465134
H	-0.898730	-3.280826	2.834309
H	-2.128298	-4.321855	2.024621
H	-2.786258	0.192198	-2.370882
H	-5.238354	-0.270950	-2.347763
H	-6.755129	1.127463	-0.945718
H	-5.822688	2.995109	0.414344
H	-3.375886	3.461983	0.384722
H	-0.052780	1.686070	1.838100
H	1.756393	2.487165	-1.516026

7a

SCF Energy: -1420.95927887

ZPE-corrected Energy: -1420.55847

$\Delta U$ : -1420.53110

$\Delta H$ : -1420.53016

$\Delta G$ : -1420.62046

Num. Imaginary Frequencies: 0

C	3.556939	3.627139	0.886702
C	2.217218	3.420583	0.962347
C	3.978582	3.135506	-0.388458
N	2.963154	2.638897	-1.042845
C	1.727636	2.803669	-0.295527
C	0.811724	1.573828	-0.175168
C	1.245826	0.290714	-0.079676
C	2.685314	-0.009952	-0.014422
C	3.407728	0.227736	1.164682
C	4.784487	0.016922	1.208191
C	5.461804	-0.444265	0.078408
C	4.745539	-0.726015	-1.087193
C	3.368234	-0.527396	-1.128931
Au	-0.080173	-1.327000	-0.011955
P	-1.555090	-3.198670	0.069467
C	-3.322887	-2.771037	0.224850
C	-1.491180	-4.277973	-1.401219
C	-1.253296	-4.334789	1.465853
C	-0.571060	1.920010	-0.144382
C	-1.746615	2.244624	-0.110035
C	-3.136310	2.559356	-0.065606
C	-4.079232	1.535944	0.142325
C	-5.437737	1.829478	0.184736
C	-5.877179	3.144499	0.022917
C	-4.949567	4.166814	-0.182588
C	-3.588938	3.880875	-0.228178
H	4.214861	4.073243	1.633050
H	1.547029	3.677066	1.787197
H	4.984876	3.141764	-0.817264
H	2.877718	0.594359	2.053534
H	5.336072	0.216729	2.134515
H	6.545250	-0.605344	0.112259
H	5.266896	-1.108399	-1.972505
H	2.803046	-0.750075	-2.044034
H	-3.940108	-3.688411	0.262415
H	-3.484602	-2.185674	1.147567
H	-3.634949	-2.157854	-0.639285
H	-0.467548	-4.672418	-1.528860
H	-2.196794	-5.123002	-1.291562
H	-1.756251	-3.695843	-2.301615
H	-0.224782	-4.732688	1.406745
H	-1.362432	-3.788753	2.419634
H	-1.972376	-5.175126	1.441872
H	-3.726195	0.505398	0.269569
H	-6.162997	1.023969	0.346557
H	-6.948231	3.373659	0.057103
H	-5.291455	5.200214	-0.309889
H	-2.858069	4.681177	-0.391349
H	3.005637	2.234311	-1.979501
H	1.141129	3.584870	-0.831562

8a.

SCF Energy: -1421.00383774  
ZPE-corrected Energy: -1420.60262  
 $\Delta U$ : -1420.57519  
 $\Delta H$ : -1420.57425  
 $\Delta G$ : -1420.66535

Num. Imaginary Frequencies: 0

C	0.178296	3.390198	3.150574
C	-0.557454	2.628375	2.232778
C	1.468748	3.494825	2.643286
N	1.533920	2.821677	1.473515
C	0.299406	2.272866	1.181528
C	-0.034891	1.530256	-0.001707
C	0.831268	1.042885	-1.008922
C	2.268279	1.381053	-1.188180
C	3.273966	1.018306	-0.276129
C	4.604088	1.365735	-0.503656
C	4.959472	2.067075	-1.655757
C	3.975618	2.412717	-2.581119
C	2.645348	2.069387	-2.351204
Au	0.620897	-1.033339	-0.104574
P	0.538380	-3.266786	0.607029
C	0.305358	-3.452447	2.402415
C	-0.820495	-4.204524	-0.157543
C	2.045292	-4.208763	0.217175
C	-1.433385	1.314899	-0.191313
C	-2.630141	1.158364	-0.357832
C	-4.031669	0.983747	-0.534407
C	-4.532176	0.300731	-1.657586
C	-5.903098	0.135733	-1.818392
C	-6.787144	0.646816	-0.866524
C	-6.298597	1.325871	0.251053
C	-4.929533	1.495880	0.420212
H	-0.179351	3.825462	4.084368
H	-1.610204	2.346820	2.299548
H	2.344240	4.009990	3.041325
H	3.012557	0.446065	0.625034
H	5.371690	1.072681	0.221334
H	6.006260	2.335400	-1.836426
H	4.245152	2.956657	-3.493445
H	1.876071	2.344075	-3.083542
H	0.276627	-4.524548	2.672919
H	1.137177	-2.962379	2.937976
H	-0.641657	-2.973182	2.706324
H	-0.700893	-4.200743	-1.255118
H	-0.814051	-5.248489	0.207792
H	-1.787091	-3.733731	0.094033
H	2.215525	-4.203173	-0.873651
H	2.915701	-3.744762	0.713114
H	1.939022	-5.253287	0.565399
H	-3.831196	-0.096072	-2.400436
H	-6.287877	-0.396277	-2.695387
H	-7.867061	0.515188	-0.997291
H	-6.993227	1.727087	0.997121
H	-4.536157	2.028309	1.293948
H	2.359340	2.761565	0.879632
H	0.306061	0.831238	-1.955790

8a  
SCF Energy: -1421.00218480  
ZPE-corrected Energy: -1420.60190  
 $\Delta U$ : -1420.57420  
 $\Delta H$ : -1420.57325  
 $\Delta G$ : -1420.66518

Num. Imaginary Frequencies: 0

Au	1.230431	-0.817336	-0.002279
P	1.889308	-3.065829	-0.065108
C	2.778279	-3.545313	-1.576409
C	2.966242	-3.566196	1.310539
C	0.438609	-4.161000	0.017891
H	3.023280	-4.623280	-1.537924
H	2.149546	-3.343266	-2.460943
H	3.711236	-2.961608	-1.663727
H	2.457900	-3.378238	2.272083
H	3.205235	-4.642589	1.224760
H	3.902242	-2.981579	1.284060
H	-0.116296	-3.975064	0.954802
H	-0.231195	-3.954010	-0.835568
H	0.759461	-5.218913	-0.015539
C	2.217423	2.304317	0.063211
C	3.438842	1.886771	-0.490895
C	4.543041	2.730885	-0.452280
C	4.439901	3.995309	0.128819
C	3.227320	4.418849	0.675398
C	2.119296	3.580569	0.648990
H	3.514471	0.898421	-0.959933
H	5.493407	2.400712	-0.885169
H	5.312208	4.657657	0.154656
H	3.145383	5.411907	1.130335
H	1.163337	3.901268	1.078867
C	-2.816963	4.332341	-0.538621
C	-1.820071	3.344181	-0.723047
C	-3.803093	3.770654	0.250310
N	-3.440408	2.488736	0.538810
C	-2.234439	2.198409	-0.054313
C	-1.555016	0.910954	0.093102
C	-2.130675	-0.315108	0.260940
C	-3.527648	-0.714415	0.119806
C	-4.424616	-0.088998	-0.767057
C	-5.731274	-0.547846	-0.892414
C	-6.173939	-1.636483	-0.137894
C	-5.291706	-2.279484	0.730105
C	-3.980304	-1.830176	0.847218
C	-0.126609	1.057231	0.110069
C	1.035342	1.494682	0.037478
H	-2.815833	5.348611	-0.936176
H	-0.894519	3.438376	-1.296651
H	-4.732815	4.190186	0.636743
H	-4.084571	0.750315	-1.384794
H	-6.412371	-0.054838	-1.595304
H	-7.205858	-1.991424	-0.237497
H	-5.626348	-3.143088	1.315771
H	-3.283471	-2.345429	1.520634
H	-3.973048	1.846297	1.119037
H	-1.449802	-1.135389	0.536757

9a  
SCF Energy: -1421.00486020  
ZPE-corrected Energy: -1420.60260  
 $\Delta U$ : -1420.57629  
 $\Delta H$ : -1420.57534  
 $\Delta G$ : -1420.66243

Num. Imaginary Frequencies: 0

C	-1.181845	2.709577	0.056212
C	-2.317103	2.216459	-0.613760
C	-3.520890	2.912426	-0.591824
C	-3.621003	4.127802	0.088304
C	-2.500590	4.643276	0.738126
C	-1.295033	3.946390	0.715590
H	-2.240927	1.277638	-1.177448
H	-4.389824	2.507851	-1.124121
H	-4.569017	4.677319	0.101427
H	-2.564063	5.599006	1.270774
H	-0.431224	4.366139	1.246282
Au	-1.147466	-0.874265	0.016210
P	-2.896629	-2.494966	0.021722
C	-4.541577	-1.708197	-0.082142
C	-2.884199	-3.680281	-1.366538
C	-3.000951	-3.552345	1.505582
H	-5.344017	-2.469806	-0.080033
H	-4.681085	-1.028002	0.777397
H	-4.606888	-1.112222	-1.010562
H	-1.954870	-4.276340	-1.340504
H	-3.754610	-4.360038	-1.302112
H	-2.920422	-3.131377	-2.324274
H	-2.075043	-4.145690	1.606444
H	-3.110935	-2.920924	2.404942
H	-3.866846	-4.236876	1.431996
C	1.967995	3.909932	-0.430837
C	1.400532	2.721850	0.280983
C	3.176964	3.558016	-0.902431
N	3.399457	2.177156	-0.651501
C	2.368333	1.654235	-0.027998
C	1.755169	0.348178	0.054109
C	2.352494	-0.877188	0.019107
C	3.764021	-1.201419	0.110003
C	4.695463	-0.389907	0.786216
C	6.041551	-0.734445	0.821263
C	6.483790	-1.901601	0.194443
C	5.568215	-2.733793	-0.451326
C	4.220625	-2.394540	-0.481805
C	0.300785	0.624879	0.026334
C	0.085102	1.978939	0.066078
H	1.545863	4.916337	-0.440536
H	1.501510	2.946220	1.374866
H	3.951593	4.137903	-1.405757
H	4.353191	0.498562	1.331201
H	6.751797	-0.097783	1.360211
H	7.544710	-2.173103	0.227232
H	5.908585	-3.658919	-0.929240
H	3.498918	-3.049628	-0.984637
H	4.182602	1.645952	-1.039365
H	1.666976	-1.730374	-0.102236

AuPMe3  
SCF Energy: -596.392670308  
ZPE-corrected Energy: -596.279720  
 $\Delta U$ : -596.271299  
 $\Delta H$ : -596.270354  
 $\Delta G$ : -596.314078

Num. Imaginary Frequencies: 0

P	-1.330080	0.000581	0.000447
C	-2.016572	-1.078279	1.285961
C	-2.015855	-0.576164	-1.576022
C	-2.015410	1.654267	0.289303
Au	0.957729	-0.000084	0.000021
H	-1.678594	0.081489	-2.395801
H	-1.674770	-1.605853	-1.779808
H	-3.120636	-0.558508	-1.520007
H	-1.675747	2.344250	-0.502384
H	-3.120354	1.599223	0.280273
H	-1.675340	2.036014	1.267261
H	-1.679001	-0.740251	2.280749
H	-3.121345	-1.041207	1.239614
H	-1.676568	-2.116166	1.126329

P1  
SCF Energy: -824.671903421  
ZPE-corrected Energy: -824.381411  
 $\Delta U$ : -824.365799  
 $\Delta H$ : -824.364855  
 $\Delta G$ : -824.425177

Num. Imaginary Frequencies: 0

C	-1.100756	2.239206	-0.015892
C	0.061268	2.966260	0.001981
N	1.138864	2.116151	0.010366
C	0.693795	0.814844	-0.001121
C	-0.727676	0.853151	-0.005133
C	1.430315	-0.385173	0.001156
C	2.907675	-0.413027	0.006668
C	3.599531	-1.287976	0.858339
C	4.991344	-1.335023	0.858881
C	5.722765	-0.506665	0.007500
C	5.049649	0.364945	-0.847861
C	3.656727	0.410533	-0.849157
H	-2.109918	2.652769	-0.044170
H	0.211836	4.047175	0.005545
H	2.111144	2.402226	0.069093
H	3.031161	-1.928938	1.543601
H	5.511068	-2.021756	1.537164
H	6.818211	-0.541746	0.009416
H	5.613965	1.010583	-1.530828
H	3.138955	1.074397	-1.553298
C	0.676464	-1.558643	0.003416
C	-0.726255	-1.545793	-0.010370
C	-1.459065	-0.359028	-0.010895
C	-2.936697	-0.386409	-0.013070
C	-3.632883	-1.285044	-0.836560
C	-5.024850	-1.334441	-0.829063
C	-5.752695	-0.486485	0.005547
C	-5.075144	0.409063	0.832991
C	-3.682874	0.459462	0.822582
H	-3.069005	-1.942794	-1.509636
H	-5.546772	-2.039097	-1.487164
H	-6.848169	-0.524090	0.012087
H	-5.636924	1.072251	1.501332
H	-3.159323	1.148100	1.496726
H	-1.263042	-2.502430	0.000750
H	1.200933	-2.522239	-0.002815

P2

SCF Energy: -824.618672133  
ZPE-corrected Energy: -824.329360  
 $\Delta U$ : -824.313381  
 $\Delta H$ : -824.312437  
 $\Delta G$ : -824.374062

Num. Imaginary Frequencies: 0

C	1.012075	2.181173	-0.396754
C	0.439277	0.904937	-0.127235
C	-0.043652	3.061636	-0.551043
N	-1.229564	2.376303	-0.394159
C	-0.941703	1.069947	-0.140638
C	0.683917	-0.535469	0.019920
C	-0.649456	-1.154057	0.069513
C	-1.636597	-0.207762	-0.007410
C	1.815048	-1.286837	0.072357
C	3.208216	-0.863590	0.109968
C	4.200547	-1.745120	-0.356012
C	5.543748	-1.383303	-0.344429
C	5.927616	-0.138558	0.156438
C	4.958419	0.734196	0.654758
C	3.614141	0.376474	0.633613
H	1.662963	-2.377437	0.067768
H	-2.152926	2.785320	-0.500659
H	2.065348	2.455458	-0.481619
H	-0.044764	4.134458	-0.749024
H	-0.798874	-2.228583	0.219722
C	-3.082355	-0.414368	0.045197
H	3.900749	-2.727525	-0.742688
H	6.299800	-2.080401	-0.723738
H	6.985789	0.146549	0.172313
H	5.256105	1.701854	1.075152
H	2.863087	1.048110	1.063340
C	-3.654250	-1.638789	-0.340612
C	-3.938449	0.604393	0.494605
C	-5.316010	0.407676	0.558500
C	-5.867834	-0.813050	0.172719
C	-5.029326	-1.836109	-0.275419
H	-3.005688	-2.439375	-0.716458
H	-3.514542	1.557341	0.835021
H	-5.963571	1.215206	0.919228
H	-6.951777	-0.968336	0.218871
H	-5.454987	-2.797290	-0.586340



P3

SCF Energy: -824.618234218  
ZPE-corrected Energy: -824.329087  
 $\Delta U$ : -824.313065  
 $\Delta H$ : -824.312121  
 $\Delta G$ : -824.374064

Num. Imaginary Frequencies: 0

C	-3.112585	-0.378243	0.038218
C	-3.695794	-1.627678	-0.238261
C	-5.073716	-1.802718	-0.180257
C	-5.906440	-0.731799	0.153178
C	-5.344535	0.514066	0.427692
C	-3.963632	0.689207	0.368102
H	-3.054042	-2.470333	-0.522299
H	-5.506236	-2.784667	-0.405276
H	-6.993023	-0.869643	0.194995
H	-5.987936	1.360862	0.693803
H	-3.531566	1.668073	0.605649
H	-0.880949	-2.237352	0.235479
C	-1.130134	2.476324	-0.421648
C	-0.959566	1.095337	-0.144604
C	0.146450	3.007372	-0.538686
N	1.070332	2.011674	-0.347671
C	0.406197	0.841620	-0.104625
C	0.645635	-0.589479	0.038997
C	1.774616	-1.343271	0.081157
C	3.162958	-0.899829	0.115784
C	3.559392	0.297581	0.737944
C	4.895577	0.687304	0.749570
C	5.866357	-0.113590	0.145890
C	5.493144	-1.319268	-0.449821
C	4.158848	-1.713020	-0.453722
C	-0.707333	-1.166848	0.083711
C	-1.663559	-0.192567	-0.005051
H	-2.055525	3.044144	-0.538930
H	0.467784	4.031843	-0.733200
H	2.811163	0.905018	1.262069
H	5.185387	1.619228	1.248645
H	6.917934	0.194696	0.154683
H	6.251860	-1.961611	-0.911425
H	3.868442	-2.664420	-0.917036
H	2.076652	2.133255	-0.416950
H	1.626464	-2.433818	0.062081

P4

SCF Energy: -824.562758701  
ZPE-corrected Energy: -824.274558  
 $\Delta U$ : -824.258091  
 $\Delta H$ : -824.257146  
 $\Delta G$ : -824.321257

Num. Imaginary Frequencies: 0

C	3.139428	-0.874520	-0.051332
C	3.915449	-2.047129	-0.026681
C	5.306430	-1.993424	-0.006780
C	5.960325	-0.761430	-0.013366
C	5.205586	0.413251	-0.042399
C	3.815861	0.359008	-0.061637
H	3.406189	-3.019617	-0.021628
H	5.886130	-2.923862	0.013674
H	7.055318	-0.715215	0.001906
H	5.708597	1.387463	-0.051857
H	3.244006	1.292422	-0.091587
C	1.684989	-0.985294	-0.067107
C	1.071699	2.845252	0.152304
C	0.691522	1.483766	0.049278
C	-0.125788	3.547553	0.206912
N	-1.201702	2.680047	0.140268
C	-0.692779	1.427745	0.044541
C	-0.737296	-0.038144	-0.033394
C	-1.625520	-1.048730	-0.055554
C	-3.080417	-0.941283	-0.058829
C	-3.752386	0.235440	-0.435675
C	-5.141537	0.308174	-0.407131
C	-5.897442	-0.796222	-0.009522
C	-5.247808	-1.978744	0.345963
C	-3.858059	-2.050839	0.316184
C	0.774554	0.004656	-0.028892
H	2.062784	3.302453	0.188463
H	-0.297713	4.622130	0.290065
H	-3.176025	1.095279	-0.798106
H	-5.642278	1.234928	-0.711208
H	-6.991675	-0.738028	0.011365
H	-5.831263	-2.856163	0.648768
H	-3.351892	-2.983329	0.597295
H	-2.176586	2.964156	0.191896
H	-1.210592	-2.067464	-0.041714
H	1.286038	-2.009995	-0.110500

TS\_2a\_3a  
SCF Energy: -1420.92775904  
ZPE-corrected Energy: -1420.53041  
 $\Delta U$ : -1420.50227  
 $\Delta H$ : -1420.50133  
 $\Delta G$ : -1420.59481

Num. Imaginary Frequencies: 1

Imaginary Frequency: -455.6020

N	2.158900	3.188453	-0.794399
C	0.840959	3.565044	-0.651626
C	0.704378	4.049387	0.663384
C	1.934526	3.876887	1.315025
C	2.811312	3.337782	0.381070
C	-0.359376	1.749338	-0.239176
C	-1.695173	2.300347	-0.211417
C	-2.366385	2.448139	1.014786
C	-3.664747	2.944146	1.042525
C	-4.301998	3.303385	-0.147027
C	-3.640392	3.163120	-1.367399
C	-2.341201	2.666390	-1.402788
C	0.382800	0.702985	-0.147625
Au	-1.018150	-0.968153	-0.002701
C	1.711249	0.281674	-0.140354
C	2.841296	-0.184712	-0.131625
C	4.185621	-0.653820	-0.101872
C	5.048835	-0.254190	0.935590
C	6.363521	-0.706679	0.965810
C	6.837565	-1.554983	-0.035755
C	5.988883	-1.954962	-1.069301
C	4.670678	-1.513508	-1.104322
H	7.874613	-1.907885	-0.010290
H	7.026891	-0.392954	1.779579
H	4.670615	0.411008	1.720590
H	3.999684	-1.827647	-1.911775
H	6.358682	-2.622004	-1.856100
H	-1.853484	2.164780	1.942053
H	-4.185759	3.052862	1.999998
H	-5.324177	3.697007	-0.121635
H	-4.142315	3.441191	-2.300453
H	-1.818246	2.546320	-2.359309
H	-0.213820	4.463328	1.086157
H	2.168753	4.104242	2.355721
H	3.850700	3.022128	0.490379
H	2.562890	2.786868	-1.636928
H	0.237717	3.789099	-1.534244
P	-2.372361	-2.875305	0.170287
C	-1.735816	-4.296061	-0.773207
C	-2.552717	-3.485832	1.876084
C	-4.074991	-2.634870	-0.428575
H	-0.728142	-4.562608	-0.408799
H	-1.665161	-4.032061	-1.842959
H	-3.015430	-2.704546	2.504284
H	-1.558614	-3.728362	2.290785
H	-2.410560	-5.164260	-0.653897
H	-3.186821	-4.392104	1.891714
H	-4.651661	-3.572851	-0.321658
H	-4.564941	-1.835560	0.154645
H	-4.057388	-2.335582	-1.491173

TS\_2a\_7a  
SCF Energy: -1420.93382454  
ZPE-corrected Energy: -1420.53654  
 $\Delta U$ : -1420.50851  
 $\Delta H$ : -1420.50756  
 $\Delta G$ : -1420.60137

Num. Imaginary Frequencies: 1

Imaginary Frequency: -402.0224

N	2.618829	2.843782	-1.227518
C	1.519953	3.102598	-0.436976
C	1.999854	3.269582	0.878632
C	3.368019	2.987654	0.870236
C	3.715969	2.709604	-0.452504
C	-0.650834	1.199493	-0.035497
C	-1.568703	2.336480	-0.038484
C	-1.615600	3.225265	1.046944
C	-2.486548	4.312288	1.026550
C	-3.315711	4.529518	-0.073730
C	-3.280131	3.645024	-1.152659
C	-2.424178	2.547736	-1.131649
C	0.643332	1.101662	-0.065985
Au	-1.539409	-0.749848	0.029550
C	1.773954	0.331393	-0.042802
C	2.868622	-0.221563	-0.040982
C	4.107222	-0.920041	-0.029733
C	4.433409	-1.805132	-1.073886
C	5.643673	-2.488778	-1.054126
C	6.542000	-2.292607	-0.004156
C	6.228499	-1.411589	1.032825
C	5.017820	-0.729317	1.026426
H	7.496388	-2.830732	0.006048
H	5.891369	-3.179694	-1.867358
H	3.723749	-1.949599	-1.896038
H	4.760265	-0.037600	1.836740
H	6.935060	-1.258305	1.855828
H	-0.973545	3.046701	1.918100
H	-2.516638	4.997529	1.881313
H	-3.997384	5.387263	-0.087707
H	-3.932192	3.807421	-2.018364
H	-2.403514	1.843265	-1.972487
H	1.387779	3.547131	1.738954
H	4.047352	2.972316	1.723853
H	4.681740	2.435903	-0.882061
H	2.586031	2.669651	-2.229104
H	0.595310	3.480777	-0.880620
P	-2.624828	-2.842247	0.115658
C	-3.455016	-3.173287	1.702865
C	-3.930704	-3.044399	-1.138822
C	-1.517741	-4.267163	-0.135584
H	-4.208703	-2.390732	1.899604
H	-2.713980	-3.161097	2.521264
H	-3.496662	-2.942592	-2.148987
H	-4.699351	-2.262898	-1.005651
H	-3.951789	-4.161129	1.673388
H	-4.401167	-4.040813	-1.040782
H	-2.093904	-5.210091	-0.085292
H	-1.029359	-4.189679	-1.122882
H	-0.735927	-4.274304	0.644158

TS\_3a1.4a\_  
 SCF Energy: -1420.94596720  
 ZPE-corrected Energy: -1420.54914  
 $\Delta U$ : -1420.52192  
 $\Delta H$ : -1420.52097  
 $\Delta G$ : -1420.61126

Num. Imaginary Frequencies: 1

Imaginary Frequency: -937.8825

N	-0.982161	4.233929	-0.330749
C	-1.264780	2.920168	-0.004144
C	-2.566306	2.898094	0.498666
C	-3.056260	4.217188	0.470087
C	-2.050350	5.016665	-0.054853
C	-0.268225	1.879920	-0.190023
C	1.170213	2.303991	-0.154580
C	2.028432	2.116464	-1.242748
C	3.378522	2.446254	-1.135956
C	3.878455	2.965062	0.057579
C	3.022180	3.167877	1.140256
C	1.670880	2.847222	1.033861
C	-0.533941	0.470230	-0.148010
Au	1.072836	-0.909333	-0.047098
C	-1.836017	-0.046082	-0.134858
C	-2.928232	-0.600992	-0.107289
C	-4.215903	-1.198478	-0.066316
C	-5.370826	-0.394330	-0.123938
C	-6.630295	-0.979111	-0.081431
C	-6.753119	-2.366055	0.023856
C	-5.614620	-3.172467	0.082757
C	-4.351252	-2.596485	0.034707
H	-7.747932	-2.824063	0.059444
H	-7.525933	-0.350367	-0.129386
H	-5.262283	0.693006	-0.208876
H	-3.450572	-3.218870	0.077568
H	-5.715863	-4.260086	0.164633
H	1.640577	1.707669	-2.185218
H	4.042411	2.300086	-1.995207
H	4.940278	3.221573	0.142361
H	3.409501	3.579531	2.078810
H	0.996565	3.001545	1.885585
H	-3.087625	2.015071	0.869789
H	-4.036982	4.559551	0.803491
H	-2.025233	6.090389	-0.245241
H	-0.101754	4.557250	-0.725673
H	-0.372861	1.240469	-1.291000
P	2.928022	-2.360781	0.135470
C	4.498574	-1.436301	0.170190
C	2.956825	-3.383995	1.642670
C	3.119580	-3.547610	-1.233752
H	4.508489	-0.758381	1.042576
H	4.588642	-0.825891	-0.746279
H	2.070236	-4.041775	1.663899
H	2.932238	-2.732295	2.533696
H	5.357494	-2.130281	0.234833
H	3.872690	-4.003696	1.667370
H	4.026597	-4.161980	-1.080585
H	2.235810	-4.207680	-1.282678
H	3.205014	-3.002594	-2.190320

TS\_3a\_3a1  
 SCF Energy: -1420.91658291  
 ZPE-corrected Energy: -1420.52108  
 $\Delta U$ : -1420.49354  
 $\Delta H$ : -1420.49259  
 $\Delta G$ : -1420.58453

Num. Imaginary Frequencies: 1

Imaginary Frequency: -1176.7902

N	0.854396	4.255561	0.081281
C	1.246850	2.924624	-0.033722
C	2.613671	2.937863	-0.399037
C	3.003557	4.273761	-0.513106
C	1.892555	5.060601	-0.214014
C	0.230731	1.802531	0.110362
C	-1.194399	2.242966	0.182341
C	-1.948024	2.058135	1.346885
C	-3.304802	2.377140	1.363819
C	-3.917920	2.878626	0.215658
C	-3.169851	3.074801	-0.945745
C	-1.810991	2.766838	-0.960559
C	0.548360	0.446648	0.061850
Au	-1.039585	-0.934534	-0.015741
C	1.848371	-0.048349	0.062010
C	2.961506	-0.569294	0.075253
C	4.253220	-1.158671	0.084007
C	5.396419	-0.375216	0.338466
C	6.657794	-0.957745	0.342507
C	6.798403	-2.323663	0.089178
C	5.673168	-3.110559	-0.164926
C	4.407795	-2.536970	-0.164875
H	7.794773	-2.779677	0.091014
H	7.541720	-0.342799	0.544005
H	5.278459	0.695706	0.540255
H	3.518281	-3.146048	-0.360770
H	5.786018	-4.182194	-0.362543
H	-1.464149	1.647088	2.242244
H	-3.887737	2.230918	2.280078
H	-4.986053	3.123238	0.226845
H	-3.649168	3.468704	-1.848879
H	-1.220168	2.914346	-1.874155
H	3.227657	2.051574	-0.557698
H	3.992692	4.644511	-0.783768
H	1.783384	6.145643	-0.193839
H	-0.089614	4.563319	0.309475
H	0.988984	2.274574	1.073129
P	-2.944979	-2.339474	-0.119447
C	-2.924985	-3.626982	-1.409908
C	-3.328876	-3.240059	1.418968
C	-4.446622	-1.361123	-0.460524
H	-2.082025	-4.317889	-1.232850
H	-2.791642	-3.158015	-2.400619
H	-3.446787	-2.521814	2.249456
H	-2.501137	-3.927966	1.665790
H	-3.872610	-4.197382	-1.400098
H	-4.263721	-3.819847	1.302080
H	-5.342394	-2.009670	-0.486374
H	-4.570330	-0.594532	0.326272
H	-4.338856	-0.845863	-1.432088

TS.4a\_5a  
 SCF Energy: -1420.98284090  
 ZPE-corrected Energy: -1420.58255  
 $\Delta U$ : -1420.55599  
 $\Delta H$ : -1420.55504  
 $\Delta G$ : -1420.64348  
 Num. Imaginary Frequencies: 1  
 Imaginary Frequency: -486.3716

C	2.720672	3.383319	-0.246912
C	3.670293	2.988351	-1.149483
N	3.841837	1.624624	-1.036889
C	3.014869	1.124652	-0.085889
C	2.263905	2.203198	0.428698
C	2.836737	-0.286103	0.185613
C	4.008967	-1.182012	0.177512
C	5.244207	-0.727742	0.669881
C	6.351615	-1.570387	0.702162
C	6.248011	-2.880866	0.236963
C	5.030111	-3.341779	-0.264239
C	3.921829	-2.501100	-0.296455
H	2.389016	4.406888	-0.065260
H	4.250816	3.560362	-1.873872
H	4.434712	1.057543	-1.640765
H	1.831558	2.199297	1.436106
H	5.331415	0.296093	1.054335
H	7.303483	-1.200820	1.099785
H	7.120370	-3.543611	0.258822
H	4.945044	-4.365537	-0.645668
H	2.979102	-2.865096	-0.721355
C	1.560190	-0.751916	0.341641
C	0.390977	0.082679	0.199389
C	0.299509	1.373573	0.063680
Au	-1.553233	-0.789735	0.014406
H	1.414303	-1.824166	0.518182
C	-0.544052	2.537220	0.159232
C	-1.376069	2.709503	1.281456
C	-2.216359	3.813849	1.364470
C	-2.231935	4.756485	0.334839
C	-1.405950	4.597162	-0.780281
C	-0.561543	3.497018	-0.867389
H	-1.354477	1.959729	2.081393
H	-2.863919	3.943112	2.238481
H	-2.894246	5.626833	0.402424
H	-1.422840	5.338414	-1.586506
H	0.096221	3.363020	-1.734095
P	-3.665920	-1.824868	-0.181744
C	-4.398078	-2.329726	1.408794
C	-4.929784	-0.762693	-0.954082
C	-3.662873	-3.344606	-1.187360
H	-5.386004	-2.799055	1.243098
H	-3.731490	-3.050883	1.913713
H	-4.518625	-1.446875	2.060836
H	-4.683558	-3.767476	-1.241960
H	-3.306835	-3.117672	-2.207596
H	-2.983669	-4.089126	-0.735975
H	-5.894040	-1.300923	-1.018736
H	-5.062644	0.154706	-0.353737
H	-4.603835	-0.473509	-1.968786

TS\_4a\_6a  
SCF Energy: -1420.98414097  
ZPE-corrected Energy: -1420.58444  
 $\Delta U$ : -1420.55786  
 $\Delta H$ : -1420.55691  
 $\Delta G$ : -1420.64530

Num. Imaginary Frequencies: 1

Imaginary Frequency: -472.6982

C	2.248216	3.191148	0.896685
C	2.223667	2.175845	-0.113020
C	3.145287	2.781833	1.849724
N	3.678760	1.563545	1.482678
C	3.118728	1.161564	0.315216
C	0.819196	0.671381	-0.509347
C	1.774286	-0.329854	-0.785087
C	3.039083	-0.147071	-0.262929
C	-0.417051	1.073731	-0.405403
C	-0.924874	2.447588	-0.420057
C	-0.589676	3.322004	-1.467065
C	-1.024081	4.645067	-1.449679
C	-1.790501	5.118185	-0.384411
C	-2.138184	4.254238	0.654887
C	-1.723063	2.925446	0.630718
Au	-1.756639	-0.549577	-0.080699
P	-3.309439	-2.297060	0.268042
C	-5.047597	-1.756449	0.183609
C	-3.160976	-3.111501	1.892136
C	-3.192213	-3.656140	-0.941009
H	4.247265	0.974028	2.088640
H	1.720896	4.146848	0.874387
H	2.025042	2.391390	-1.171427
H	3.473510	3.268219	2.769488
H	1.507142	-1.174682	-1.434693
C	4.126662	-1.122990	-0.260941
H	0.003402	2.950487	-2.312218
H	-0.760581	5.313519	-2.277344
H	-2.126641	6.161073	-0.368887
H	-2.745883	4.617733	1.491392
H	-2.001176	2.243359	1.443917
H	-5.235259	-0.986799	0.952885
H	-5.252987	-1.318508	-0.809027
H	-5.724714	-2.614702	0.351904
H	-3.914392	-3.915924	1.986554
H	-2.150551	-3.542714	2.003822
H	-3.316530	-2.369573	2.695093
H	-3.948302	-4.431996	-0.717052
H	-3.362244	-3.263565	-1.959022
H	-2.184710	-4.106535	-0.901867
C	3.861682	-2.498387	-0.369890
C	5.461344	-0.697581	-0.154181
C	6.501691	-1.621780	-0.156377
C	6.224982	-2.983944	-0.268374
C	4.902575	-3.419441	-0.375694
H	2.824668	-2.849293	-0.429092
H	5.688427	0.374115	-0.093277
H	7.537819	-1.274723	-0.078613
H	7.043794	-3.712006	-0.270592
H	4.681663	-4.489434	-0.456190



TS\_7a1\_8a\_  
SCF Energy: -1420.93340143  
ZPE-corrected Energy: -1420.53660  
 $\Delta U$ : -1420.50934  
 $\Delta H$ : -1420.50839  
 $\Delta G$ : -1420.59845

Num. Imaginary Frequencies: 1

Imaginary Frequency: -696.4171

C	3.117403	4.614665	-0.037825
C	1.919089	3.896782	0.180227
C	4.005110	3.746107	-0.644596
N	3.395434	2.536378	-0.786337
C	2.117687	2.603436	-0.281398
C	1.155638	1.483293	-0.272226
C	1.437884	0.079874	-0.081427
C	2.807546	-0.387599	0.134414
C	3.613598	0.216006	1.119102
C	4.866160	-0.308786	1.416493
C	5.350197	-1.410277	0.708820
C	4.563920	-2.012555	-0.275122
C	3.289549	-1.524402	-0.538941
Au	-0.146661	-1.308241	-0.110647
P	-1.936007	-2.867162	-0.075135
C	-2.776228	-2.983369	1.538652
C	-3.266504	-2.478313	-1.259139
C	-1.458225	-4.582231	-0.463825
C	-0.221802	1.894043	-0.156608
C	-1.385755	2.227021	-0.048770
C	-2.764485	2.561393	0.091113
C	-3.660677	1.605771	0.602153
C	-5.009318	1.915074	0.736170
C	-5.476229	3.177556	0.365907
C	-4.592382	4.132206	-0.139454
C	-3.242140	3.829906	-0.279051
H	3.312013	5.658093	0.214244
H	0.997680	4.265632	0.634831
H	5.026482	3.900050	-0.994637
H	3.241424	1.087046	1.671728
H	5.475613	0.151615	2.201596
H	6.345722	-1.809132	0.933165
H	4.940411	-2.881821	-0.824889
H	2.650801	-2.014056	-1.284585
H	-3.597018	-3.723155	1.489433
H	-2.053117	-3.292368	2.313798
H	-3.189972	-1.998172	1.818103
H	-2.860642	-2.469933	-2.286032
H	-4.073754	-3.231563	-1.192060
H	-3.680883	-1.478553	-1.038786
H	-1.016119	-4.627884	-1.474542
H	-0.706724	-4.933663	0.264988
H	-2.343839	-5.243507	-0.422665
H	-3.278140	0.619741	0.893752
H	-5.703880	1.167364	1.134582
H	-6.539460	3.419833	0.472977
H	-4.960852	5.122582	-0.428484
H	-2.541710	4.572530	-0.677009
H	3.827988	1.719949	-1.210221
H	1.246028	0.849643	-1.324802

TS\_7a\_7a1  
 SCF Energy: -1420.90379247  
 ZPE-corrected Energy: -1420.50817  
 $\Delta U$ : -1420.48070  
 $\Delta H$ : -1420.47975  
 $\Delta G$ : -1420.57134  
 Num. Imaginary Frequencies: 1  
 Imaginary Frequency: -1138.9310

C	2.614246	4.812366	0.596266
C	1.531144	4.084702	0.083122
C	3.578631	3.891795	0.985224
N	3.124517	2.641601	0.729130
C	1.859075	2.723355	0.187458
C	0.950948	1.521304	-0.111817
C	1.378086	0.190532	-0.135158
C	2.787927	-0.148786	-0.322356
C	3.427704	-1.000661	0.598201
C	4.781947	-1.293407	0.467298
C	5.509081	-0.791072	-0.612743
C	4.874590	0.012303	-1.560876
C	3.530892	0.340206	-1.414520
Au	-0.024561	-1.347526	0.044729
P	-1.602922	-3.118669	0.241249
C	-3.269373	-2.700022	-0.368834
C	-1.150037	-4.629018	-0.674565
C	-1.877674	-3.689124	1.951475
C	-0.443680	1.857044	-0.135209
C	-1.628161	2.131932	-0.162794
C	-3.027335	2.407306	-0.205717
C	-3.893127	1.523428	-0.873925
C	-5.259465	1.779154	-0.913364
C	-5.776979	2.917318	-0.292873
C	-4.923857	3.801176	0.369495
C	-3.556460	3.550878	0.416560
H	2.696861	5.896718	0.674022
H	0.596594	4.471544	-0.327208
H	4.561813	4.045424	1.431607
H	2.850489	-1.412023	1.435452
H	5.271331	-1.934418	1.208862
H	6.570059	-1.039618	-0.724691
H	5.432160	0.388340	-2.425731
H	3.041808	0.959409	-2.178799
H	-3.948699	-3.565481	-0.255221
H	-3.670524	-1.844049	0.202438
H	-3.215770	-2.416359	-1.434944
H	-0.182295	-5.012587	-0.305867
H	-1.926070	-5.405861	-0.540987
H	-1.047961	-4.396487	-1.749252
H	-0.927369	-4.051860	2.381097
H	-2.244137	-2.850153	2.569013
H	-2.621745	-4.507588	1.967954
H	-3.475851	0.635275	-1.363439
H	-5.928276	1.085759	-1.435359
H	-6.853834	3.117332	-0.326271
H	-5.329736	4.694888	0.856358
H	-2.881402	4.238634	0.938246
H	3.619544	1.777508	0.943951
H	1.616798	2.112792	-1.019586

TS.8a\_10a  
 SCF Energy: -1420.95280157  
 ZPE-corrected Energy: -1420.55307  
 $\Delta U$ : -1420.52648  
 $\Delta H$ : -1420.52554  
 $\Delta G$ : -1420.61299  
 Num. Imaginary Frequencies: 1  
 Imaginary Frequency: -326.7739

C	2.012529	2.099186	-0.040466
C	1.914938	3.233492	0.784815
C	2.964906	4.144804	0.867150
C	4.126579	3.946934	0.121091
C	4.240445	2.819838	-0.694772
C	3.202299	1.896109	-0.761758
H	1.011457	3.380416	1.387981
H	2.875785	5.017171	1.524909
H	4.950812	4.666437	0.183972
H	5.153274	2.654141	-1.278288
H	3.298015	1.003523	-1.393140
C	0.914410	1.138876	-0.133310
C	-1.005068	4.373365	-0.163031
C	-1.003215	3.110323	-0.863207
C	-2.021362	4.330105	0.746836
N	-2.649656	3.093761	0.672011
C	-2.087094	2.361718	-0.300012
C	-1.724438	0.945036	-0.336434
C	-2.350475	-0.244456	-0.217790
C	-3.781740	-0.490594	-0.150993
C	-4.744454	0.483944	-0.475227
C	-6.101184	0.199629	-0.377355
C	-6.528261	-1.063672	0.039340
C	-5.586864	-2.045288	0.348052
C	-4.228346	-1.762836	0.248535
C	-0.368023	1.404415	-0.320512
H	-0.377863	5.237552	-0.385889
H	-0.649893	2.996472	-1.894275
H	-2.381326	5.083602	1.448418
H	-4.430456	1.470608	-0.837974
H	-6.836728	0.968373	-0.639286
H	-7.598901	-1.284565	0.113225
H	-5.914671	-3.041106	0.666612
H	-3.487837	-2.535718	0.490054
H	-3.302118	2.728903	1.366675
H	-1.696915	-1.127145	-0.139786
Au	1.273714	-0.947602	-0.023188
P	1.613863	-3.287528	0.124621
C	2.963020	-3.945731	-0.909634
C	1.991052	-3.885671	1.805073
C	0.143682	-4.242485	-0.380463
H	3.033362	-5.043676	-0.794077
H	2.773168	-3.701806	-1.969688
H	3.920838	-3.485563	-0.609545
H	1.172936	-3.604099	2.491317
H	2.106627	-4.985785	1.805833
H	2.925679	-3.420206	2.164658
H	-0.109697	-4.006160	-1.429347
H	0.336168	-5.327829	-0.287544
H	-0.715513	-3.968637	0.258099

TS\_8a\_9a  
SCF Energy: -1420.96744892  
ZPE-corrected Energy: -1420.56767  
 $\Delta U$ : -1420.54092  
 $\Delta H$ : -1420.53997  
 $\Delta G$ : -1420.62891

Num. Imaginary Frequencies: 1

Imaginary Frequency: -451.1525

C	0.920247	2.856549	0.020622
C	1.068247	3.934514	-0.874195
C	2.011397	4.921398	-0.626258
C	2.823200	4.848641	0.509440
C	2.683994	3.788521	1.405712
C	1.730150	2.804761	1.175372
H	0.433841	3.993182	-1.765463
H	2.120040	5.757265	-1.325513
H	3.566550	5.630776	0.699081
H	3.316109	3.735432	2.298651
H	1.601939	1.973186	1.877839
Au	1.335115	-0.842430	-0.103143
P	3.129059	-2.390822	-0.061049
C	4.718697	-1.679468	0.478485
C	2.864135	-3.810506	1.051717
C	3.491694	-3.139777	-1.683088
H	5.507302	-2.455201	0.468814
H	5.008010	-0.856425	-0.198554
H	4.618173	-1.274071	1.500741
H	1.962308	-4.366302	0.739836
H	3.738198	-4.487853	1.023522
H	2.715121	-3.451051	2.085194
H	2.601740	-3.679426	-2.052091
H	3.746363	-2.347482	-2.408866
H	4.339399	-3.845544	-1.600103
C	-2.611871	3.749192	-0.422957
C	-1.893130	2.599747	-0.894473
C	-3.505868	3.308958	0.513463
N	-3.374835	1.934433	0.633309
C	-2.412325	1.488559	-0.195374
C	-1.716038	0.192680	-0.145379
C	-2.237343	-1.047400	0.022871
C	-3.638494	-1.454235	0.043287
C	-4.652542	-0.747776	-0.629032
C	-5.972805	-1.182172	-0.579147
C	-6.309526	-2.332368	0.137311
C	-5.312052	-3.056823	0.790276
C	-3.990104	-2.627142	0.734886
C	-0.289530	0.504504	-0.158177
C	0.009558	1.780900	-0.198164
H	-2.505802	4.775290	-0.778753
H	-1.403051	2.530574	-1.871166
H	-4.232251	3.847410	1.122834
H	-4.399302	0.137048	-1.225570
H	-6.747937	-0.623745	-1.116083
H	-7.350717	-2.672004	0.174010
H	-5.566266	-3.968231	1.343060
H	-3.205211	-3.201794	1.242510
H	-3.823496	1.367958	1.351772
H	-1.505307	-1.853278	0.181965

# Cartesian coordinates of the indole mechanism

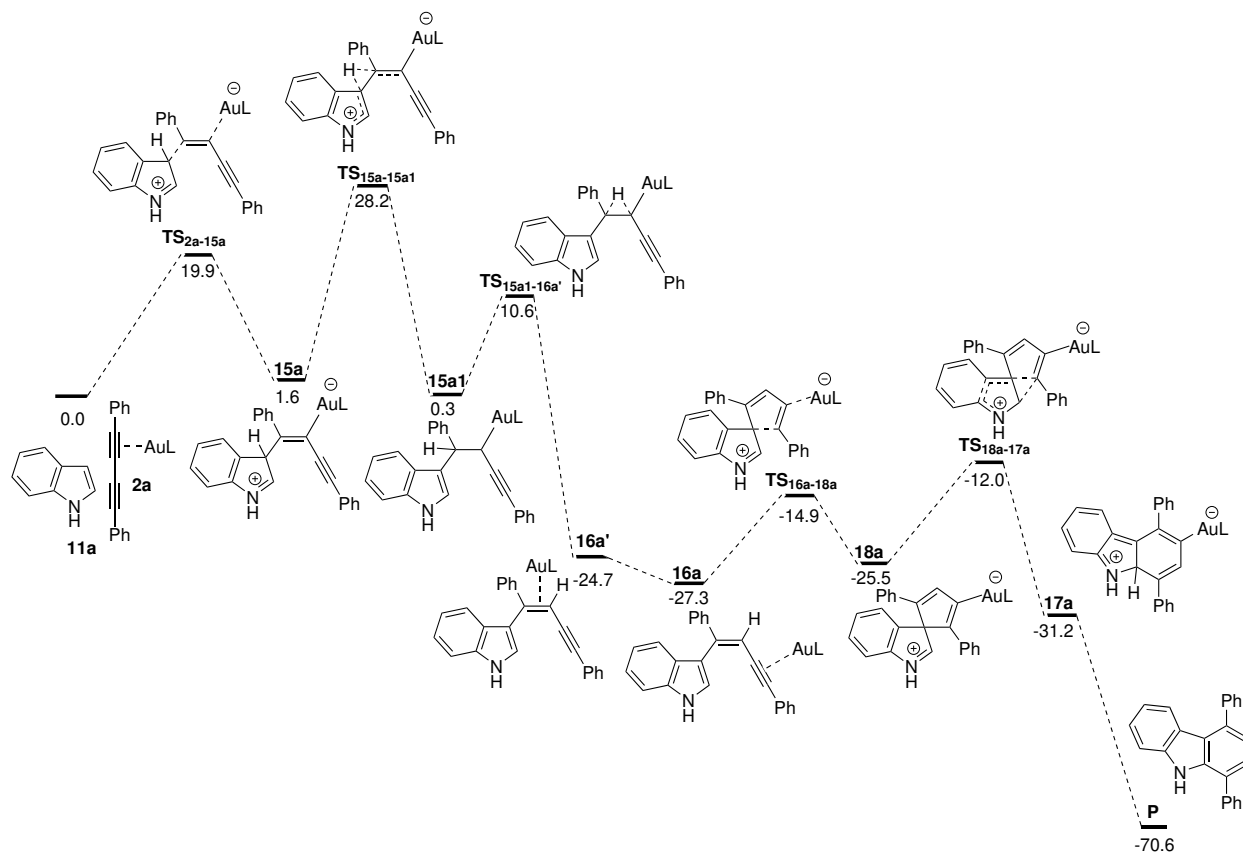


Figure S5: Indole reaction mechanism, part 1.

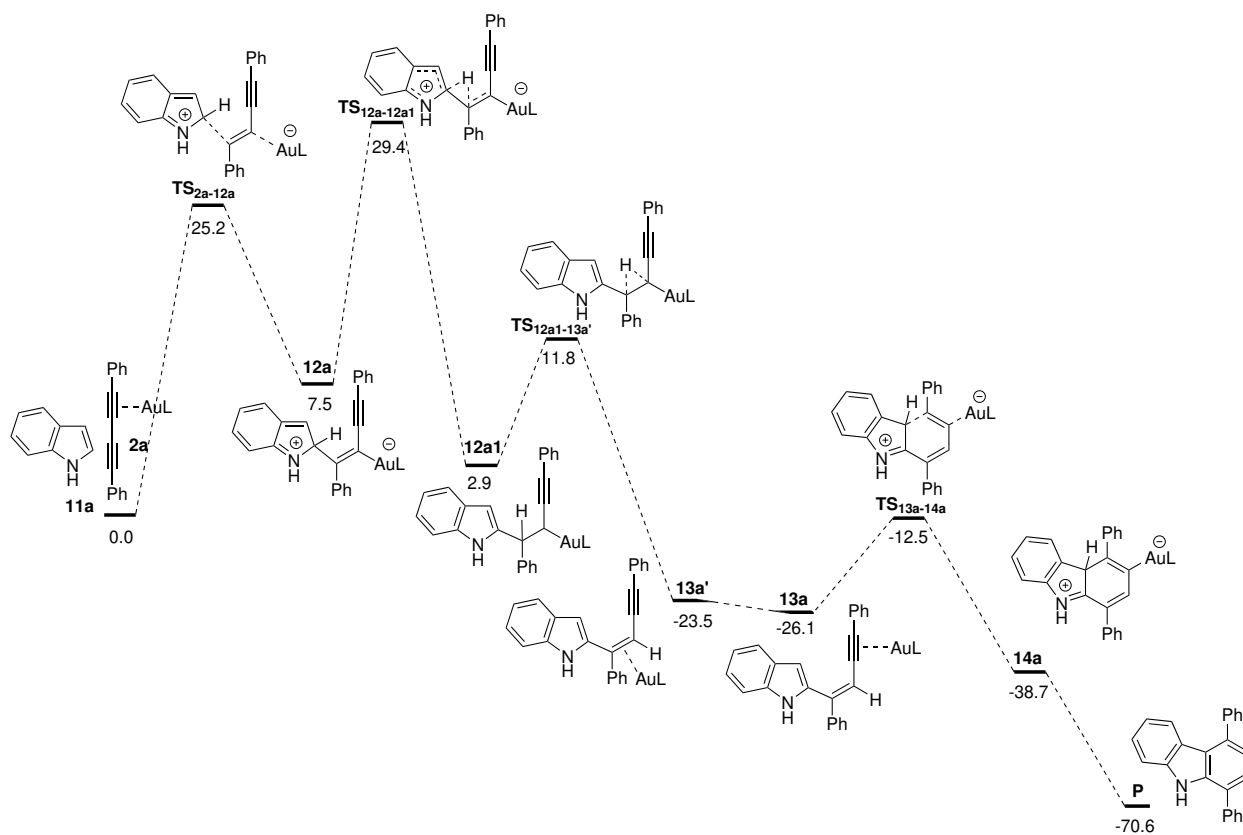


Figure S6: Indole reaction mechanism, part 2.

11a  
SCF Energy: -363.266770063  
ZPE-corrected Energy: -363.137589  
 $\Delta U$ : -363.131363  
 $\Delta H$ : -363.130419  
 $\Delta G$ : -363.167843  
Num. Imaginary Frequencies: 0

N	1.565369	-1.076954	-0.000089
C	0.252735	-0.668905	-0.000011
C	0.249066	0.752535	0.000013
C	1.622033	1.169353	-0.000018
C	2.383102	0.028386	-0.000017
C	-0.984714	1.427031	0.000032
H	1.998505	2.193859	-0.000038
H	3.468155	-0.091144	-0.000033
H	1.882103	-2.041034	0.000171
C	-0.929497	-1.417146	-0.000001
C	-2.131276	-0.722028	0.000030
C	-2.158918	0.687628	0.000041
H	-1.015027	2.523638	0.000036
H	-3.126362	1.203965	0.000053
H	-3.076115	-1.278588	0.000039
H	-0.904031	-2.513140	-0.000019

12a1  
SCF Energy: -1574.37834170  
ZPE-corrected Energy: -1573.93164  
 $\Delta U$ : -1573.90148  
 $\Delta H$ : -1573.90054  
 $\Delta G$ : -1573.99734

Num. Imaginary Frequencies: 0

N	2.156584	-1.552121	0.740747
C	1.645456	-1.670643	-0.538970
C	2.656524	-2.027838	-1.396336
C	3.861601	-2.109215	-0.624915
C	3.510624	-1.791977	0.713811
C	0.236173	-1.281263	-0.871518
C	-0.870082	-2.233354	-0.450864
C	-1.986882	-2.383428	-1.281342
C	-3.074080	-3.156550	-0.880281
C	-3.055710	-3.795342	0.360566
C	-1.939175	-3.666992	1.184598
C	-0.850219	-2.893248	0.779584
C	-0.071946	0.155175	-0.501780
Au	-2.033736	0.733194	-0.121093
C	0.979125	1.003296	-0.421724
C	1.981707	1.728284	-0.303883
C	3.201534	2.402227	-0.184297
C	4.404802	1.667825	-0.337651
C	5.624651	2.310045	-0.205548
C	5.659760	3.680689	0.071670
C	4.479903	4.418546	0.221100
C	3.253107	3.788077	0.097465
H	6.626780	4.185796	0.173333
H	6.556688	1.746902	-0.319444
H	4.349665	0.593409	-0.556433
H	2.317076	4.344500	0.212990
H	4.528347	5.490640	0.436644
H	-2.007206	-1.877311	-2.256234
H	-3.938962	-3.266648	-1.544724
H	-3.908813	-4.404699	0.679605
H	-1.910059	-4.175603	2.154856
H	0.023380	-2.812424	1.436552
H	2.546408	-2.186426	-2.471298
C	5.208879	-2.370800	-0.930791
C	4.459014	-1.729702	1.739502
H	1.649302	-1.201512	1.548348
H	0.202223	-1.226006	-1.985730
P	-4.327042	1.170057	0.330712
C	-4.793704	2.893908	0.687129
C	-5.401132	0.669377	-1.054242
C	-4.940700	0.210819	1.754282
H	-4.530513	3.536647	-0.171033
H	-4.246969	3.252871	1.576647
H	-5.239145	-0.401328	-1.275027
H	-5.148241	1.256220	-1.954903
H	-5.881652	2.961950	0.874227
H	-6.464134	0.834482	-0.797062
H	-6.023994	0.382757	1.897836
H	-4.760407	-0.865000	1.577169
H	-4.399186	0.511456	2.668494
C	6.154524	-2.298453	0.081860
C	5.782732	-1.980310	1.404161
H	4.166787	-1.480825	2.765870
H	6.553212	-1.931306	2.182360
H	7.208987	-2.493636	-0.145413
H	5.506175	-2.618176	-1.956699



12a

SCF Energy: -1574.37124764

ZPE-corrected Energy: -1573.92432

$\Delta U$ : -1573.89424

$\Delta H$ : -1573.89330

$\Delta G$ : -1573.99000

Num. Imaginary Frequencies: 0

N	-2.082152	2.591646	0.519785
C	-1.456622	2.092099	-0.695322
C	-2.524173	1.256029	-1.291463
C	-3.676263	1.382189	-0.549197
C	-3.355979	2.198383	0.598086
C	-0.062746	1.511504	-0.450461
C	1.021923	2.514311	-0.338731
C	1.207598	3.511292	-1.309412
C	2.253061	4.426311	-1.205872
C	3.124738	4.375988	-0.118302
C	2.940144	3.406380	0.867142
C	1.898193	2.488364	0.759119
C	0.115124	0.180205	-0.245920
Au	1.993716	-0.733373	0.010592
C	-1.002575	-0.674888	-0.237028
C	-1.987811	-1.404995	-0.206757
C	-3.229180	-2.096012	-0.155773
C	-4.063508	-1.948461	0.968763
C	-5.309250	-2.565820	1.003711
C	-5.744811	-3.327681	-0.081073
C	-4.925173	-3.478543	-1.202039
C	-3.674570	-2.872459	-1.242056
H	-6.728516	-3.809699	-0.053104
H	-5.950943	-2.446123	1.884082
H	-3.720304	-1.335384	1.811392
H	-3.026850	-2.987752	-2.118534
H	-5.265715	-4.078128	-2.053690
H	0.547013	3.555359	-2.185547
H	2.390451	5.182911	-1.986781
H	3.943812	5.099305	-0.034927
H	3.607186	3.371353	1.736308
H	1.741187	1.742535	1.548065
H	-2.411695	0.739409	-2.248370
C	-4.988492	0.845769	-0.705724
C	-4.332847	2.473442	1.577356
H	-1.600505	3.188713	1.188963
H	-1.351664	2.954341	-1.397207
P	4.132062	-1.741213	0.239715
C	4.282308	-3.420370	-0.457368
C	5.460752	-0.791985	-0.575387
C	4.707139	-1.918185	1.962706
H	4.042692	-3.398049	-1.535226
H	3.567976	-4.096122	0.045381
H	5.493666	0.230173	-0.157059
H	5.253538	-0.718113	-1.657662
H	5.309462	-3.807046	-0.319302
H	6.441090	-1.281841	-0.423448
H	5.715685	-2.371989	1.989248
H	4.741987	-0.925465	2.445593
H	4.004849	-2.557046	2.526739
C	-5.925710	1.137787	0.247487
C	-5.587963	1.942890	1.377680
H	-4.099089	3.089437	2.450290
H	-6.368051	2.147493	2.119877
H	-6.944100	0.746079	0.161376
H	-5.222441	0.217526	-1.572380

13a\_

SCF Energy: -1574.42138044

ZPE-corrected Energy: -1573.97356

$\Delta U$ : -1573.94340

$\Delta H$ : -1573.94245

$\Delta G$ : -1574.03940

Num. Imaginary Frequencies: 0

N	-1.274309	-2.347807	0.508101
C	-0.416256	-1.796069	-0.433824
C	0.809936	-2.432043	-0.340605
C	0.704491	-3.408249	0.690071
C	-0.615282	-3.318750	1.210876
C	-0.860660	-0.732948	-1.322041
C	-2.255020	-0.778110	-1.830193
C	-2.842865	-2.025381	-2.101022
C	-4.115907	-2.106309	-2.659448
C	-4.829435	-0.945854	-2.951701
C	-4.258494	0.299682	-2.687629
C	-2.985068	0.382830	-2.135990
C	0.015821	0.244206	-1.814279
Au	-0.669118	1.331314	0.143901
C	1.417172	0.304104	-1.595076
C	2.625217	0.395200	-1.447242
C	4.033585	0.451549	-1.250627
C	4.645366	-0.380636	-0.294268
C	6.021602	-0.331185	-0.103783
C	6.803606	0.543890	-0.859785
C	6.204924	1.372829	-1.810050
C	4.829389	1.331000	-2.007298
H	7.888019	0.580292	-0.706824
H	6.490737	-0.981617	0.642755
H	4.024783	-1.063588	0.298142
H	4.353032	1.978336	-2.752087
H	6.818352	2.059529	-2.403852
H	-2.284442	-2.946281	-1.898496
H	-4.550479	-3.089149	-2.872142
H	-5.833866	-1.010401	-3.384306
H	-4.813625	1.218125	-2.907213
H	-2.562317	1.373188	-1.921304
H	1.676697	-2.240551	-0.973903
C	1.597391	-4.352131	1.234616
C	-1.055035	-4.135232	2.260977
H	-2.230103	-2.044029	0.673863
H	-0.361094	0.874587	-2.633954
P	-1.055280	2.718247	1.981632
C	0.347462	3.817090	2.342711
C	-2.490963	3.810582	1.757123
C	-1.370743	1.802380	3.520062
H	0.557033	4.455815	1.467006
H	1.245485	3.214218	2.563877
H	-3.402467	3.204655	1.611931
H	-2.342082	4.445826	0.866575
H	0.110065	4.455327	3.214235
H	-2.615709	4.453313	2.648527
H	-1.549900	2.512145	4.349221
H	-2.256671	1.155948	3.394634
H	-0.499947	1.168308	3.761908
C	1.162741	-5.160235	2.269817
C	-0.152006	-5.050476	2.777258
H	-2.074636	-4.053116	2.652379
H	-0.464522	-5.707183	3.597326
H	1.843776	-5.898948	2.707232
H	2.617719	-4.438021	0.843212

13a

SCF Energy: -1574.42491365

ZPE-corrected Energy: -1573.97758

$\Delta U$ : -1573.94736

$\Delta H$ : -1573.94641

$\Delta G$ : -1574.04355

Num. Imaginary Frequencies: 0

C	3.906577	1.677575	0.057139
C	4.503288	0.737557	0.940881
N	3.860057	-0.459591	0.769341
C	2.853410	-0.315126	-0.170975
C	2.867330	0.989345	-0.634479
C	1.990211	-1.423570	-0.547224
C	2.557103	-2.787450	-0.568952
C	1.792116	-3.894279	-0.167457
C	2.322180	-5.180018	-0.218168
C	3.625204	-5.382975	-0.673109
C	4.397273	-4.292043	-1.072607
C	3.870983	-3.004867	-1.016628
C	4.393075	2.998661	0.027104
C	5.558400	1.087701	1.792606
H	4.043817	-1.309749	1.294754
H	2.237807	1.387480	-1.433078
H	0.776088	-3.739789	0.215415
H	1.715034	-6.031433	0.109106
H	4.042445	-6.395457	-0.711936
H	5.419379	-4.445207	-1.436429
H	4.478828	-2.154168	-1.347386
C	0.678938	-1.229517	-0.889501
C	0.004225	0.007367	-0.788843
C	-0.502771	1.140240	-0.713357
C	-0.719901	2.558587	-0.730508
C	-1.841305	3.127627	-1.358283
C	-1.993361	4.509001	-1.387446
C	-1.037309	5.334111	-0.792204
C	0.074775	4.774281	-0.161994
C	0.235792	3.393420	-0.122990
H	-2.585587	2.476020	-1.831460
H	-2.866336	4.948209	-1.882377
H	-1.162156	6.422272	-0.817439
H	0.824116	5.419820	0.309427
H	1.101029	2.944301	0.379356
Au	-2.243510	-0.186675	-0.013280
H	0.101404	-2.079911	-1.275250
P	-4.256248	-1.091864	0.755645
C	-5.717772	-0.480076	-0.136494
C	-4.317454	-2.902701	0.599726
C	-4.574361	-0.744617	2.511911
H	-5.626070	-0.717667	-1.210658
H	-5.795044	0.615098	-0.020952
H	-3.496832	-3.356341	1.182552
H	-4.202176	-3.190750	-0.459772
H	-5.286652	-3.277342	0.978414
H	-6.630935	-0.956421	0.267181
H	-5.528641	-1.209766	2.822202
H	-3.752341	-1.151178	3.126595
H	-4.629691	0.346210	2.672352
C	5.437629	3.344632	0.867348
C	6.013492	2.396381	1.741516
H	6.006167	0.353411	2.471195
H	6.839389	2.702455	2.394033
H	5.826896	4.369137	0.858954
H	3.944021	3.737665	-0.647782

14a

SCF Energy: -1574.44968370

ZPE-corrected Energy: -1573.99996

$\Delta U$ : -1573.97114

$\Delta H$ : -1573.97020

$\Delta G$ : -1574.06358

Num. Imaginary Frequencies: 0

C	2.868279	2.275842	-0.138818
C	4.141286	1.763971	0.156945
N	4.091229	0.362807	0.102205
C	2.865357	-0.069608	-0.189657
C	1.996300	1.097850	-0.477831
C	2.364312	-1.384848	-0.205259
C	3.252410	-2.558854	-0.079994
C	2.952840	-3.588782	0.823016
C	3.784458	-4.700552	0.929977
C	4.929538	-4.799012	0.139630
C	5.237409	-3.781466	-0.762788
C	4.404790	-2.670275	-0.873140
C	2.684421	3.653263	-0.190461
H	4.883966	-0.250368	0.295447
H	1.995093	1.082968	-1.605883
H	2.066047	-3.505339	1.463277
H	3.540084	-5.494405	1.644665
H	5.584865	-5.672754	0.227406
H	6.129025	-3.857145	-1.395162
H	4.637342	-1.890394	-1.610098
C	0.978848	-1.482883	-0.234323
C	0.039967	-0.395071	-0.198462
C	0.529331	0.889510	-0.236710
C	-0.353226	2.072075	-0.168639
C	-1.344195	2.300486	-1.134574
C	-2.216140	3.380180	-1.009873
C	-2.116661	4.236662	0.087374
C	-1.135607	4.016294	1.054447
C	-0.253019	2.946590	0.922429
H	-1.420529	1.624129	-1.995030
H	-2.980004	3.554287	-1.776458
H	-2.806878	5.081870	0.188422
H	-1.058891	4.681280	1.922034
H	0.510747	2.769437	1.690394
Au	-2.021731	-0.739830	-0.021747
H	0.571622	-2.504341	-0.232855
P	-4.384884	-0.967572	0.129458
C	-5.228056	-0.393161	-1.384944
C	-5.058494	-2.639128	0.414246
C	-5.128360	0.049570	1.450754
H	-4.916720	-1.014528	-2.243496
H	-4.937029	0.653826	-1.588098
H	-4.669195	-3.040194	1.366717
H	-4.742675	-3.310985	-0.403284
H	-6.163556	-2.609208	0.455317
H	-6.326777	-0.452672	-1.270261
H	-6.231425	-0.033663	1.433371
H	-4.752550	-0.282265	2.434805
H	-4.839707	1.106414	1.305918
C	3.769253	4.483192	0.100671
C	5.025189	3.950970	0.410713
C	5.235666	2.573649	0.433701
H	1.712147	4.084984	-0.449726
H	3.633754	5.569791	0.082459
H	5.859506	4.625180	0.632137
H	6.217791	2.145829	0.658096

15a1

SCF Energy: -1574.38309066

ZPE-corrected Energy: -1573.93579

$\Delta U$ : -1573.90580

$\Delta H$ : -1573.90485

$\Delta G$ : -1574.00143

Num. Imaginary Frequencies: 0

N	3.364966	2.995006	-0.932379
C	2.011267	2.780365	-0.974806
C	1.628279	1.978908	0.074951
C	2.825589	1.690590	0.821826
C	3.895304	2.341894	0.154876
C	0.252839	1.458490	0.377990
C	-0.865624	2.240585	-0.278841
C	-1.652490	3.129360	0.457315
C	-2.708561	3.808154	-0.150183
C	-2.985626	3.606527	-1.502161
C	-2.198044	2.728157	-2.247359
C	-1.144270	2.049287	-1.638263
C	0.040942	-0.019747	0.153088
Au	-1.903424	-0.758720	0.263811
C	1.102607	-0.797985	-0.153307
C	2.089828	-1.511634	-0.398103
C	3.302543	-2.165902	-0.643007
C	3.365515	-3.570114	-0.801203
C	4.588997	-4.182658	-1.017655
C	5.753756	-3.409086	-1.077243
C	5.706224	-2.019581	-0.924927
C	4.488809	-1.394695	-0.710864
H	6.718378	-3.900783	-1.245884
H	4.646653	-5.269017	-1.139500
H	2.441702	-4.155594	-0.746356
H	4.420261	-0.306730	-0.585499
H	6.626629	-1.428543	-0.973607
H	-1.440247	3.285893	1.522663
H	-3.321041	4.500095	0.439074
H	-3.816702	4.138836	-1.978594
H	-2.407666	2.567696	-3.311066
H	-0.530060	1.350630	-2.223894
H	0.087398	1.536367	1.481222
C	3.098374	0.951116	1.985777
C	5.215784	2.262004	0.611345
H	3.885443	3.568866	-1.588149
H	1.404239	3.229828	-1.763358
P	-4.203397	-1.359278	0.285926
C	-4.731687	-2.425026	-1.094357
C	-4.804455	-2.210161	1.780574
C	-5.244135	0.131657	0.145820
H	-4.200731	-3.391871	-1.045044
H	-4.487537	-1.938133	-2.054849
H	-4.598055	-1.591810	2.671709
H	-4.283879	-3.177165	1.894873
H	-5.821954	-2.603624	-1.041502
H	-5.893365	-2.388136	1.702678
H	-6.315388	-0.141193	0.104358
H	-5.067204	0.787029	1.017548
H	-4.968935	0.689735	-0.768006
C	5.455505	1.519378	1.759810
C	4.406035	0.872373	2.443284
H	6.028763	2.771182	0.081751
H	6.478844	1.438357	2.144341
H	4.629817	0.298784	3.350134
H	2.291525	0.438759	2.525415

15a

SCF Energy: -1574.38310365

ZPE-corrected Energy: -1573.93491

$\Delta U$ : -1573.90520

$\Delta H$ : -1573.90425

$\Delta G$ : -1573.99943

Num. Imaginary Frequencies: 0

N	3.525224	1.551342	-1.480400
C	2.289140	1.792812	-1.801070
C	1.495853	2.175397	-0.606308
C	2.494016	1.949329	0.497857
C	3.719768	1.606819	-0.080247
C	0.093900	1.568559	-0.495320
C	-1.033067	2.524960	-0.439637
C	-0.929237	3.712210	0.303697
C	-1.999294	4.599220	0.399279
C	-3.196217	4.327342	-0.262190
C	-3.309391	3.164004	-1.024008
C	-2.240073	2.276185	-1.114634
C	-0.048409	0.215989	-0.407012
Au	-1.853139	-0.796646	-0.048322
C	1.115478	-0.580217	-0.456091
C	2.153197	-1.230621	-0.455189
C	3.443477	-1.834764	-0.423497
C	4.001648	-2.249171	0.800032
C	5.296688	-2.753073	0.846085
C	6.054869	-2.855918	-0.322085
C	5.507352	-2.456881	-1.541824
C	4.211783	-1.950429	-1.596618
H	7.075583	-3.252496	-0.281496
H	5.722370	-3.068045	1.805661
H	3.407712	-2.152666	1.716563
H	3.778385	-1.636871	-2.554234
H	6.096125	-2.542363	-2.462291
H	-0.002692	3.939651	0.848749
H	-1.896375	5.509648	1.000703
H	-4.036988	5.026762	-0.192586
H	-4.237111	2.951319	-1.568275
H	-2.327106	1.381078	-1.743033
H	1.378639	3.277651	-0.748023
C	2.384869	2.000230	1.879465
C	4.861531	1.313750	0.649118
H	4.258831	1.302393	-2.150084
H	1.946192	1.777168	-2.839433
P	-3.913921	-1.895914	0.389591
C	-4.220478	-3.410289	-0.581421
C	-4.156713	-2.417716	2.121240
C	-5.357688	-0.835508	0.036022
H	-3.435935	-4.156664	-0.364528
H	-4.188353	-3.173582	-1.659690
H	-4.073073	-1.540975	2.787446
H	-3.375758	-3.145912	2.403036
H	-5.209697	-3.837090	-0.330595
H	-5.152507	-2.881680	2.250843
H	-6.300838	-1.369900	0.257530
H	-5.302629	0.079850	0.652523
H	-5.348017	-0.539096	-1.028440
C	4.739557	1.375648	2.036756
C	3.520896	1.708865	2.640121
H	5.799504	1.027161	0.161952
H	5.607885	1.146209	2.663284
H	3.455227	1.734066	3.733114
H	1.430099	2.238324	2.362531

16a\_

SCF Energy: -1574.42324357

ZPE-corrected Energy: -1573.97543

$\Delta U$ : -1573.94529

$\Delta H$ : -1573.94434

$\Delta G$ : -1574.04120

Num. Imaginary Frequencies: 0

N	-0.565278	2.389591	2.636745
C	0.404192	1.981276	1.778436
C	-0.110960	1.875183	0.496536
C	-1.493058	2.290490	0.580960
C	-1.739220	2.598062	1.941766
C	0.644399	1.418714	-0.670201
C	1.939241	2.073577	-0.975642
C	2.170660	3.385705	-0.530577
C	3.348950	4.054630	-0.854591
C	4.324056	3.425218	-1.623824
C	4.111208	2.119818	-2.072481
C	2.934460	1.453622	-1.754498
C	0.110423	0.469095	-1.555077
Au	1.263677	-0.980979	-0.125540
C	-1.173975	-0.124482	-1.416266
C	-2.280026	-0.624874	-1.295909
C	-3.586975	-1.156096	-1.104558
C	-4.146308	-2.053614	-2.031571
C	-5.426109	-2.559157	-1.830442
C	-6.162595	-2.179236	-0.707367
C	-5.615321	-1.287967	0.217766
C	-4.337049	-0.776382	0.024985
H	-7.170849	-2.579512	-0.552167
H	-5.855180	-3.257434	-2.557771
H	-3.563106	-2.347814	-2.911509
H	-3.901580	-0.068875	0.741874
H	-6.193599	-0.987185	1.098652
H	1.401859	3.899656	0.056056
H	3.501404	5.081129	-0.503422
H	5.253772	3.948402	-1.873499
H	4.875805	1.611674	-2.670255
H	2.803526	0.419809	-2.099128
H	0.601802	0.340898	-2.531142
C	-2.519387	2.503189	-0.355921
C	-2.979918	3.052627	2.397462
H	-0.442415	2.523914	3.636283
H	1.414361	1.757780	2.131228
P	2.231344	-2.739096	1.062953
C	1.061446	-3.595615	2.159426
C	2.925570	-4.028253	-0.014905
C	3.604110	-2.211734	2.132396
H	0.227862	-4.009598	1.565863
H	0.651882	-2.882458	2.895878
H	3.709099	-3.592886	-0.659329
H	2.130970	-4.447619	-0.656426
H	1.577205	-4.416878	2.691360
H	3.364381	-4.835527	0.600946
H	4.029314	-3.087491	2.657254
H	4.389955	-1.734104	1.521663
H	3.239296	-1.481252	2.875403
C	-3.984381	3.220564	1.454555
C	-3.750835	2.960262	0.089774
H	-3.144014	3.277463	3.457085
H	-4.970126	3.576735	1.774797
H	-4.558876	3.123311	-0.632618
H	-2.352022	2.316805	-1.422290

16a

SCF Energy: -1574.42630254

ZPE-corrected Energy: -1573.97880

$\Delta U$ : -1573.94862

$\Delta H$ : -1573.94768

$\Delta G$ : -1574.04541

Num. Imaginary Frequencies: 0

C	-4.289614	0.019263	1.559727
C	-5.108968	0.507600	2.567782
C	-5.263311	1.891665	2.777851
C	-4.593779	2.815510	1.987532
C	-3.769889	2.318019	0.974699
C	-3.610127	0.931635	0.734861
C	-2.676797	0.804521	-0.365469
C	-2.336423	2.097365	-0.731058
N	-2.984859	2.992739	0.061424
C	-2.184171	-0.414430	-0.982892
C	-3.124328	-1.537424	-1.168187
C	-4.458678	-1.292390	-1.529534
C	-5.347973	-2.346047	-1.713494
C	-4.923419	-3.662117	-1.525137
C	-3.602121	-3.918969	-1.159080
C	-2.708500	-2.865495	-0.986170
C	-0.888529	-0.550467	-1.413306
C	0.127259	0.394572	-1.172192
C	1.017387	1.236699	-0.952996
H	-2.939837	4.002766	-0.039996
H	-4.178157	-1.061486	1.410372
H	-5.647105	-0.195404	3.213893
H	-5.919806	2.245073	3.581170
H	-4.702379	3.893678	2.148910
H	-1.704516	2.435888	-1.555740
H	-4.793688	-0.258797	-1.678512
H	-6.383620	-2.139284	-2.005720
H	-5.627201	-4.491209	-1.660231
H	-3.266287	-4.949625	-0.998523
H	-1.677705	-3.071451	-0.672372
H	-0.605858	-1.444304	-1.986173
Au	2.034764	-0.571902	-0.015516
P	3.401428	-2.141149	1.044625
C	3.735313	-1.745599	2.787856
C	2.679361	-3.810612	1.059440
C	5.034803	-2.328479	0.267673
H	4.377122	-2.528099	3.234054
H	4.244753	-0.768767	2.859504
H	2.784425	-1.690517	3.346077
H	2.518971	-4.157819	0.023823
H	3.361147	-4.509598	1.578862
H	1.707021	-3.791020	1.581982
H	5.625654	-3.087949	0.813078
H	4.913415	-2.644873	-0.783045
H	5.571457	-1.364007	0.287305
C	1.730226	2.485078	-0.886181
C	1.113403	3.588655	-0.272057
C	1.771672	4.812898	-0.218926
C	3.047149	4.948688	-0.768043
C	3.667241	3.853396	-1.371824
C	3.018696	2.624774	-1.429002
H	0.114807	3.471721	0.165724
H	1.284938	5.669866	0.259632
H	3.563519	5.913888	-0.722528
H	4.668979	3.958055	-1.802749
H	3.500885	1.761726	-1.903618



17a

SCF Energy: -1574.43856740

ZPE-corrected Energy: -1573.98944

$\Delta U$ : -1573.96054

$\Delta H$ : -1573.95959

$\Delta G$ : -1574.05166

Num. Imaginary Frequencies: 0

C	5.240023	0.376314	0.474603
C	6.248772	1.241257	0.835304
C	6.018955	2.638903	0.890425
C	4.787512	3.194858	0.604454
C	3.744935	2.318139	0.261290
C	3.964409	0.907333	0.166494
C	2.723150	0.321599	-0.179996
C	1.766058	1.425225	-0.434298
N	2.452152	2.610219	-0.010645
C	2.247247	-1.003569	-0.213671
C	3.156411	-2.168095	-0.241635
C	4.151061	-2.250437	-1.226981
C	5.000480	-3.351267	-1.286407
C	4.868538	-4.386198	-0.359534
C	3.880774	-4.315949	0.622110
C	3.027098	-3.215703	0.679407
C	0.866533	-1.162792	-0.113215
C	-0.118888	-0.121841	-0.056355
C	0.313206	1.182537	-0.165387
C	-0.573217	2.356013	-0.216155
C	-1.619709	2.508814	0.709930
C	-0.390643	3.356745	-1.185792
C	-2.460720	3.617166	0.654879
C	-2.277551	4.593244	-0.324955
C	-1.238492	4.459224	-1.244951
Au	-2.148723	-0.646615	0.042708
P	-4.465035	-1.184529	0.126664
C	-5.426197	0.034350	1.088357
C	-4.887007	-2.789654	0.885284
C	-5.298365	-1.227175	-1.496494
H	2.078773	3.550463	-0.112427
H	1.754845	1.426586	-1.565748
H	5.418885	-0.702530	0.425053
H	7.242739	0.852278	1.077812
H	6.846516	3.299622	1.172480
H	4.618684	4.274792	0.655047
H	4.251184	-1.440323	-1.961080
H	5.769116	-3.404870	-2.065598
H	5.539043	-5.251844	-0.403364
H	3.776103	-5.123384	1.355537
H	2.260855	-3.156491	1.462443
H	0.510048	-2.201443	-0.053871
H	-1.749540	1.761438	1.501999
H	0.401070	3.256623	-1.939503
H	-3.263011	3.724197	1.393885
H	-2.943021	5.462554	-0.368269
H	-1.089752	5.215554	-2.023582
H	-6.502468	-0.222020	1.085508
H	-5.059733	0.055888	2.130434
H	-5.288428	1.039403	0.650036
H	-5.983724	-2.933093	0.901256
H	-4.421437	-3.607897	0.307878
H	-4.499532	-2.826946	1.918758
H	-6.375674	-1.446427	-1.373441
H	-5.179836	-0.251587	-2.000640
H	-4.838398	-2.005839	-2.130291

18a

SCF Energy: -1574.42782627

ZPE-corrected Energy: -1573.97853

$\Delta U$ : -1573.94938

$\Delta H$ : -1573.94843

$\Delta G$ : -1574.04256

Num. Imaginary Frequencies: 0

C	-0.197021	-0.593344	-0.133087
C	0.572289	0.540113	-0.185099
C	0.121924	1.941468	-0.268377
C	-0.873405	2.292595	-1.198234
C	-1.348823	3.598015	-1.284723
C	-0.831272	4.587947	-0.448615
C	0.158647	4.258366	0.475730
C	0.631039	2.950120	0.566716
H	-1.266853	1.519899	-1.870890
H	-2.123495	3.847080	-2.019218
H	-1.201184	5.617326	-0.517106
H	0.562964	5.026259	1.145166
H	1.385655	2.706700	1.323296
C	0.688497	-1.744834	-0.138125
C	2.006224	-1.398982	-0.188973
C	3.179148	-2.269620	-0.192781
H	0.325907	-2.778245	-0.102694
Au	-2.268111	-0.650058	0.044698
P	-4.643440	-0.668872	0.258206
C	-5.304121	-1.753964	1.568926
H	-5.002069	-2.798357	1.374841
H	-4.893283	-1.447772	2.547286
H	-6.408368	-1.693559	1.601297
C	-5.349941	0.970433	0.641278
H	-4.943310	1.333380	1.601986
H	-6.452673	0.913726	0.709215
C	-5.538902	-1.196364	-1.242926
H	-5.068528	1.689492	-0.148852
H	-6.631669	-1.155940	-1.075794
H	-5.248491	-2.229032	-1.506144
H	-5.274835	-0.533590	-2.086006
C	3.052938	-3.629856	0.147164
C	4.156646	-4.473855	0.146476
C	5.420016	-3.983648	-0.190600
C	5.564669	-2.638836	-0.524999
C	4.458748	-1.792467	-0.524452
H	2.073729	-4.030236	0.433038
H	4.030922	-5.528045	0.418346
H	6.289920	-4.649870	-0.189439
H	6.549719	-2.239786	-0.791805
H	4.604321	-0.740382	-0.796950
C	2.282657	0.566814	-1.676639
N	3.102933	1.584964	-1.704837
C	3.620858	1.856990	-0.412700
C	4.520046	2.834107	-0.016633
C	4.868098	2.844825	1.335434
C	4.337143	1.908619	2.230284
C	3.424386	0.938467	1.807467
C	3.060159	0.928052	0.469802
H	3.345005	2.112786	-2.546215
H	1.791045	0.170751	-2.570035
H	4.936839	3.556684	-0.724785
H	5.577695	3.595502	1.698808
H	4.643480	1.938901	3.281247
H	3.001609	0.211602	2.510281
C	2.070653	0.105109	-0.290526

2a  
SCF Energy: -1211.08985961  
ZPE-corrected Energy: -1210.77538  
 $\Delta U$ : -1210.75188  
 $\Delta H$ : -1210.75094  
 $\Delta G$ : -1210.83407

Num. Imaginary Frequencies: 0

C	2.263116	-3.407703	0.834993
C	2.025446	-2.386296	-0.102300
C	3.026257	-2.041097	-1.027855
C	4.242010	-2.714396	-1.015256
C	4.473098	-3.727508	-0.083225
C	3.484024	-4.072051	0.839061
C	0.750358	-1.733395	-0.104313
C	-0.453279	-1.423727	-0.062375
Au	0.806350	0.595694	0.012371
C	-1.805337	-1.215738	-0.059869
C	-3.015050	-1.036132	-0.057256
C	-4.421492	-0.838012	-0.057516
C	-5.077162	-0.419084	-1.230331
C	-6.453738	-0.229329	-1.225418
C	-7.188380	-0.456506	-0.060311
C	-6.544830	-0.873500	1.106172
C	-5.168305	-1.063475	1.113958
H	-4.654377	-1.390389	2.024476
H	-8.273874	-0.307748	-0.061645
H	-6.960771	0.097051	-2.139916
H	-4.492688	-0.246915	-2.140738
H	-7.123335	-1.052138	2.019020
H	1.480207	-3.671739	1.554066
H	3.665708	-4.867951	1.569280
H	5.433759	-4.254066	-0.076101
H	5.017927	-2.447090	-1.740537
H	2.836783	-1.247655	-1.760445
P	1.486194	2.824201	0.138581
C	3.148366	3.086795	-0.548997
C	1.554679	3.455504	1.841447
C	0.393460	3.963870	-0.761987
H	0.552554	3.396415	2.300675
H	2.254699	2.845238	2.438132
H	0.358238	3.684439	-1.829400
H	-0.627643	3.908132	-0.346204
H	1.895556	4.507735	1.838165
H	0.772142	4.998503	-0.665228
H	3.426499	4.153490	-0.460217
H	3.880588	2.470781	0.001496
H	3.163991	2.791702	-1.612662

AuPMe3  
SCF Energy: -596.392670308  
ZPE-corrected Energy: -596.279720  
 $\Delta U$ : -596.271299  
 $\Delta H$ : -596.270354  
 $\Delta G$ : -596.314078  
Num. Imaginary Frequencies: 0

P	-1.330080	0.000581	0.000447
C	-2.016572	-1.078279	1.285961
C	-2.015855	-0.576164	-1.576022
C	-2.015410	1.654267	0.289303
Au	0.957729	-0.000084	0.000021
H	-1.678594	0.081489	-2.395801
H	-1.674770	-1.605853	-1.779808
H	-3.120636	-0.558508	-1.520007
H	-1.675747	2.344250	-0.502384
H	-3.120354	1.599223	0.280273
H	-1.675340	2.036014	1.267261
H	-1.679001	-0.740251	2.280749
H	-3.121345	-1.041207	1.239614
H	-1.676568	-2.116166	1.126329

P

SCF Energy: -978.090456570  
ZPE-corrected Energy: -977.753166  
 $\Delta U$ : -977.734831  
 $\Delta H$ : -977.733887  
 $\Delta G$ : -977.800394

Num. Imaginary Frequencies: 0

C	-2.300008	2.099306	-0.089639
C	-2.412657	3.484974	-0.074501
C	-1.272743	4.301183	0.016537
C	0.000903	3.748887	0.079067
C	0.108220	2.356594	0.053891
C	-1.028337	1.510637	-0.013997
C	-0.524544	0.147572	-0.019289
C	0.892523	0.245997	0.006057
C	1.737071	-0.877618	-0.025700
C	1.101175	-2.119788	-0.078208
C	-0.292211	-2.241369	-0.101510
C	-1.130585	-1.124470	-0.059675
N	1.243784	1.577538	0.066261
C	-2.598646	-1.318515	-0.028735
C	-3.237875	-2.082596	-1.014166
C	-4.614221	-2.299468	-0.967382
C	-5.372527	-1.762514	0.072169
C	-4.745457	-1.009996	1.066276
C	-3.371061	-0.790666	1.015735
C	3.210920	-0.762334	-0.002520
C	3.883860	0.143518	-0.838162
C	5.274220	0.235763	-0.820295
C	6.020452	-0.578057	0.031194
C	5.365476	-1.488214	0.861037
C	3.975650	-1.578907	0.844075
H	-3.198917	1.477644	-0.165305
H	-3.404551	3.947256	-0.134504
H	-1.387749	5.391349	0.032338
H	0.894998	4.379346	0.138846
H	1.719460	-3.025352	-0.116144
H	-0.744406	-3.240302	-0.131402
H	2.192782	1.928079	0.148593
H	-2.643097	-2.501117	-1.835949
H	-5.098476	-2.892022	-1.752358
H	-6.454576	-1.933373	0.110625
H	-5.332531	-0.594976	1.893909
H	-2.879470	-0.207793	1.805183
H	3.310546	0.764570	-1.538398
H	5.779433	0.944406	-1.486826
H	7.113866	-0.504597	0.046861
H	5.943166	-2.131045	1.535391
H	3.465465	-2.284347	1.511763

TS\_12a1\_13a\_  
 SCF Energy: -1574.36015784  
 ZPE-corrected Energy: -1573.91699  
 $\Delta U$ : -1573.88703  
 $\Delta H$ : -1573.88608  
 $\Delta G$ : -1573.98314

Num. Imaginary Frequencies: 1  
 Imaginary Frequency: -960.4413

N	3.075626	-0.809260	-0.312492
C	2.001480	-1.658847	-0.115489
C	2.481494	-2.937572	0.125283
C	3.900834	-2.871381	0.082304
C	4.239449	-1.520342	-0.201974
C	0.602843	-1.245594	-0.151311
C	-0.404696	-2.337937	0.022052
C	-0.615856	-3.288809	-0.980589
C	-1.591280	-4.270847	-0.816979
C	-2.343347	-4.319644	0.356480
C	-2.118858	-3.386980	1.370081
C	-1.155647	-2.395082	1.202313
C	0.114626	0.103475	-0.122840
Au	-1.979819	0.473610	-0.092089
C	0.955550	1.224329	-0.104929
C	1.600447	2.264972	-0.033814
C	2.372937	3.453191	0.054199
C	3.749013	3.383891	0.346914
C	4.502697	4.547458	0.432891
C	3.896241	5.788282	0.226944
C	2.532812	5.868297	-0.063765
C	1.770818	4.709904	-0.149063
H	4.493581	6.704332	0.294727
H	5.572004	4.489574	0.662524
H	4.215687	2.405332	0.511004
H	0.700062	4.759679	-0.375286
H	2.061962	6.844208	-0.223721
H	-0.021339	-3.249205	-1.902438
H	-1.764801	-5.003093	-1.613063
H	-3.107084	-5.094792	0.485064
H	-2.698222	-3.431916	2.299046
H	-0.974996	-1.658360	1.995138
H	1.868879	-3.817770	0.326120
C	4.930314	-3.818857	0.253843
C	5.569989	-1.097914	-0.321977
H	3.007931	0.185253	-0.511625
H	0.287403	-0.667865	-1.255448
P	-4.323920	0.739416	-0.013615
C	-5.179286	-0.506898	-1.032046
C	-5.000130	0.499478	1.661761
C	-4.989943	2.341429	-0.566662
H	-4.869048	-1.517815	-0.710715
H	-4.902127	-0.376067	-2.092977
H	-4.594080	1.267678	2.343138
H	-4.702765	-0.496128	2.037739
H	-6.275772	-0.407773	-0.925631
H	-6.103918	0.570295	1.646405
H	-6.093504	2.341781	-0.493598
H	-4.582134	3.151976	0.062432
H	-4.693603	2.525966	-1.613999
C	6.243229	-3.402341	0.135985
C	6.557626	-2.053521	-0.149534
H	5.815168	-0.053316	-0.542596
H	7.609492	-1.757692	-0.235582
H	7.057596	-4.124047	0.264777
H	4.688632	-4.864677	0.474804

TS\_12a\_12a1  
SCF Energy: -1574.33118466  
ZPE-corrected Energy: -1573.88867  
 $\Delta U$ : -1573.85863  
 $\Delta H$ : -1573.85769  
 $\Delta G$ : -1573.95499

Num. Imaginary Frequencies: 1  
Imaginary Frequency: -1136.0767

N	-2.969394	-0.799495	0.382048
C	-1.989620	-1.604946	-0.182636
C	-2.570668	-2.853789	-0.491503
C	-3.919076	-2.797425	-0.092053
C	-4.138616	-1.497814	0.455100
C	-0.527230	-1.215863	-0.286091
C	0.422764	-2.358408	-0.399866
C	0.465111	-3.335946	0.601320
C	1.422207	-4.346195	0.557613
C	2.334816	-4.399798	-0.497089
C	2.286595	-3.440978	-1.508716
C	1.336358	-2.422537	-1.458884
C	-0.073692	0.097020	-0.175038
Au	1.984615	0.469330	0.061953
C	-0.910234	1.210206	-0.196381
C	-1.591424	2.233277	-0.228798
C	-2.403205	3.397152	-0.263170
C	-3.783275	3.293578	-0.529847
C	-4.577626	4.432900	-0.559037
C	-4.010532	5.686625	-0.321225
C	-2.644347	5.801827	-0.055926
C	-1.842159	4.667924	-0.027686
H	-4.639812	6.583361	-0.343683
H	-5.649245	4.345594	-0.768801
H	-4.219618	2.305625	-0.718858
H	-0.769031	4.747290	0.178497
H	-2.202590	6.787004	0.129363
H	-0.252390	-3.292766	1.430883
H	1.458087	-5.097339	1.354566
H	3.084383	-5.198421	-0.533141
H	2.993415	-3.486264	-2.344954
H	1.296797	-1.663588	-2.250697
H	-2.049847	-3.683365	-0.973208
C	-4.987166	-3.722518	-0.140879
C	-5.388157	-1.109019	0.955050
H	-2.803899	0.136202	0.746798
H	-1.449003	-1.207300	-1.278851
P	4.313824	0.800984	0.346692
C	4.836338	1.104280	2.066872
C	5.279153	-0.656013	-0.174902
C	5.029135	2.185220	-0.599965
H	4.515769	0.262421	2.705542
H	4.363723	2.029070	2.442178
H	5.092752	-0.858101	-1.244959
H	4.959933	-1.539347	0.407090
H	5.936263	1.207025	2.122697
H	6.360649	-0.484031	-0.018323
H	6.121119	2.241314	-0.432506
H	4.832081	2.039796	-1.676775
H	4.562370	3.134352	-0.282760
C	-6.214833	-3.335635	0.352081
C	-6.409385	-2.040893	0.895045
H	-5.544867	-0.110201	1.374884
H	-7.399976	-1.770596	1.277744
H	-7.058092	-4.034054	0.327917
H	-4.832517	-4.722451	-0.559955

TS\_13a\_14a  
 SCF Energy: -1574.40490965  
 ZPE-corrected Energy: -1573.95783  
 $\Delta U$ : -1573.92855  
 $\Delta H$ : -1573.92760  
 $\Delta G$ : -1574.02176

Num. Imaginary Frequencies: 1  
 Imaginary Frequency: -444.7518

C	-3.231030	1.848761	-0.336660
C	-3.942765	1.279949	0.744098
N	-3.617256	-0.068129	0.797170
C	-2.720836	-0.366381	-0.176701
C	-2.419632	0.798865	-0.897760
C	-2.061764	-1.659893	-0.304853
C	-2.868185	-2.891951	-0.250997
C	-4.188153	-2.889457	-0.732812
C	-4.955648	-4.050736	-0.715090
C	-4.421216	-5.235209	-0.209996
C	-3.114791	-5.249493	0.280731
C	-2.346402	-4.090143	0.263974
C	-3.377841	3.212118	-0.616869
C	-4.786139	2.031297	1.560883
H	-3.919464	-0.719833	1.518991
H	-1.984953	0.797023	-1.902711
H	-4.613851	-1.967116	-1.147271
H	-5.979987	-4.030067	-1.103538
H	-5.026024	-6.148710	-0.191674
H	-2.693067	-6.172814	0.693519
H	-1.333711	-4.108675	0.682984
C	-0.700468	-1.656703	-0.390193
C	0.091763	-0.445728	-0.289426
C	-0.305987	0.789242	-0.288713
Au	2.205782	-0.516142	0.007385
H	-0.175371	-2.615190	-0.476920
C	-0.029199	2.194330	-0.359121
C	0.569107	2.741821	-1.509801
C	0.827388	4.105748	-1.576945
C	0.492527	4.933724	-0.502398
C	-0.104443	4.400318	0.641020
C	-0.374997	3.038722	0.711480
H	0.830031	2.078150	-2.343126
H	1.296798	4.529385	-2.471473
H	0.698842	6.008429	-0.558551
H	-0.366890	5.053440	1.480269
H	-0.860149	2.608132	1.596084
P	4.541864	-0.669813	0.319646
C	5.441061	-1.287689	-1.140069
C	5.343162	0.918575	0.716068
C	5.037211	-1.784666	1.673582
H	6.526566	-1.331043	-0.932307
H	5.078818	-2.297765	-1.400678
H	5.260665	-0.617433	-1.998877
H	6.139016	-1.804546	1.770044
H	4.594438	-1.436470	2.623319
H	4.670528	-2.805840	1.468454
H	6.432385	0.775150	0.845650
H	5.164477	1.640417	-0.100194
H	4.915253	1.328929	1.647611
C	-4.217778	3.969089	0.191691
C	-4.910854	3.385384	1.267140
H	-5.326171	1.575113	2.397223
H	-5.564773	4.009410	1.886544
H	-4.343039	5.039178	-0.007840
H	-2.828847	3.672686	-1.447407



TS\_15a1\_16a\_  
 SCF Energy: -1574.36363620  
 ZPE-corrected Energy: -1573.92012  
 $\Delta U$ : -1573.89032  
 $\Delta H$ : -1573.88938  
 $\Delta G$ : -1573.98507

Num. Imaginary Frequencies: 1  
 Imaginary Frequency: -973.9968

N	3.307758	3.447628	-0.940327
C	1.979510	3.186845	-1.020365
C	1.653568	2.135314	-0.178837
C	2.875866	1.759161	0.496827
C	3.890649	2.604755	-0.015342
C	0.308525	1.559927	-0.102480
C	-0.830443	2.503135	-0.276706
C	-0.907683	3.654895	0.518192
C	-1.969372	4.541946	0.369441
C	-2.949847	4.300426	-0.593996
C	-2.866276	3.171403	-1.408481
C	-1.814033	2.271947	-1.248159
C	0.052419	0.147728	-0.065806
Au	-1.883396	-0.700026	0.108525
C	1.121319	-0.755702	-0.168473
C	2.017905	-1.578096	-0.301132
C	3.126972	-2.453206	-0.454657
C	2.965308	-3.848905	-0.376396
C	4.064523	-4.687041	-0.521359
C	5.332049	-4.145183	-0.742806
C	5.503456	-2.761325	-0.821004
C	4.409955	-1.916150	-0.679511
H	6.196698	-4.808967	-0.855310
H	3.934824	-5.773093	-0.460452
H	1.966146	-4.262776	-0.200499
H	4.529330	-0.827040	-0.733148
H	6.499882	-2.340148	-0.993680
H	-0.133248	3.842334	1.272181
H	-2.032514	5.429152	1.008890
H	-3.781365	5.003498	-0.716814
H	-3.622435	2.991879	-2.180877
H	-1.734820	1.396844	-1.904685
H	0.131588	0.950243	1.035112
C	3.206284	0.858618	1.524368
C	5.215784	2.540623	0.422122
H	3.795539	4.160818	-1.475041
H	1.333925	3.746474	-1.700251
P	-4.048943	-1.632945	0.276107
C	-4.679823	-1.766248	1.980577
C	-5.301800	-0.640049	-0.600742
C	-4.217217	-3.311673	-0.412453
H	-4.692447	-0.767315	2.451129
H	-4.019503	-2.424649	2.571804
H	-5.042472	-0.576494	-1.672659
H	-5.319840	0.382847	-0.183638
H	-5.704661	-2.182372	1.979171
H	-6.303931	-1.096062	-0.493849
H	-5.261153	-3.663848	-0.315278
H	-3.931051	-3.307582	-1.478994
H	-3.547168	-4.003330	0.127966
C	5.517946	1.619973	1.416105
C	4.518984	0.797595	1.970393
H	5.981345	3.201319	0.001051
H	6.547003	1.542513	1.784726
H	4.784168	0.094056	2.767759
H	2.447127	0.210290	1.976665

TS\_15a\_15a1  
SCF Energy: -1574.33525489  
ZPE-corrected Energy: -1573.89189  
 $\Delta U$ : -1573.86206  
 $\Delta H$ : -1573.86111  
 $\Delta G$ : -1573.95703

Num. Imaginary Frequencies: 1  
Imaginary Frequency: -1145.8692

N	-4.519489	-0.559619	0.829487
C	-3.295405	-0.030652	0.701713
C	-2.424233	-0.993687	0.155128
C	-3.236174	-2.191650	-0.070765
C	-4.536459	-1.870021	0.374720
C	-0.908384	-0.855540	-0.030062
C	-0.163763	-2.144752	-0.077252
C	-0.176012	-2.984907	1.040704
C	0.556823	-4.169485	1.037493
C	1.295370	-4.530892	-0.090109
C	1.306195	-3.700388	-1.211291
C	0.583381	-2.508554	-1.202936
C	-0.221957	0.357250	-0.021479
Au	1.882401	0.345331	0.030651
C	-0.848489	1.601349	-0.055108
C	-1.326917	2.732200	-0.097843
C	-1.915612	4.024129	-0.137035
C	-1.124882	5.176580	0.038879
C	-1.709368	6.436802	0.010866
C	-3.083730	6.567100	-0.199175
C	-3.877161	5.432593	-0.380299
C	-3.301327	4.168437	-0.348134
H	-3.540559	7.562790	-0.223789
H	-1.088916	7.328670	0.151484
H	-0.047026	5.064221	0.200631
H	-3.916341	3.272516	-0.493649
H	-4.954730	5.537002	-0.548057
H	-0.769260	-2.702796	1.920202
H	0.549333	-4.818150	1.920654
H	1.864338	-5.467524	-0.095872
H	1.881231	-3.983453	-2.100282
H	0.588227	-1.850952	-2.081777
H	-1.800493	-0.651934	-0.948766
C	-3.005975	-3.465678	-0.610606
C	-5.603106	-2.766091	0.319643
H	-5.327054	-0.061977	1.199386
H	-3.079374	0.989561	1.020086
P	4.248846	0.223738	0.085894
C	4.852706	-1.414448	-0.443197
C	5.120996	1.405171	-0.995013
C	4.998629	0.472650	1.729517
H	4.514516	-1.618225	-1.475095
H	4.433816	-2.193025	0.219799
H	4.880109	2.438408	-0.688552
H	4.794616	1.264556	-2.040507
H	5.957564	-1.455236	-0.405031
H	6.214261	1.250316	-0.929543
H	6.097786	0.361846	1.670740
H	4.753248	1.482221	2.103351
H	4.594082	-0.271371	2.438276
C	-5.347154	-4.023310	-0.209781
C	-4.064496	-4.363840	-0.672640
H	-6.597618	-2.483250	0.680130
H	-6.156627	-4.758857	-0.270393
H	-3.893934	-5.361628	-1.091525
H	-2.018078	-3.755843	-0.983812

TS\_16a\_18a  
SCF Energy: -1574.40844232  
ZPE-corrected Energy: -1573.96124  
 $\Delta U$ : -1573.93187  
 $\Delta H$ : -1573.93092  
 $\Delta G$ : -1574.02567

Num. Imaginary Frequencies: 1

Imaginary Frequency: -379.4592

C	-0.175547	-0.560575	-0.290325
C	0.334505	0.615148	-0.529314
C	0.266391	2.043953	-0.533925
C	0.370238	2.787184	-1.723980
C	0.333163	4.176631	-1.686939
C	0.190823	4.837826	-0.465758
C	0.074636	4.111959	0.722017
C	0.118488	2.724217	0.692191
H	0.474308	2.258360	-2.678601
H	0.410981	4.750746	-2.616512
H	0.164359	5.933036	-0.439822
H	-0.044801	4.635115	1.677005
H	0.038358	2.139517	1.616469
C	0.680023	-1.728552	-0.183607
C	2.016886	-1.502982	-0.280460
C	3.069957	-2.525331	-0.191498
H	0.251273	-2.723317	-0.026072
Au	-2.276295	-0.564947	-0.035346
P	-4.622639	-0.642736	0.256211
C	-5.254249	0.406691	1.606545
H	-4.798054	0.097756	2.563428
H	-4.987566	1.460874	1.414494
H	-6.354394	0.315437	1.679564
C	-5.572046	-0.116970	-1.208814
H	-5.315456	0.926561	-1.463324
H	-6.657380	-0.187569	-1.007265
C	-5.255564	-2.309180	0.637394
H	-5.317978	-0.760973	-2.069071
H	-6.355227	-2.285340	0.754353
H	-4.796973	-2.676438	1.572488
H	-4.990559	-3.003206	-0.179601
C	2.762620	-3.886234	-0.007044
C	3.767433	-4.841327	0.079573
C	5.109476	-4.465194	-0.015168
C	5.432715	-3.122827	-0.197198
C	4.425397	-2.164490	-0.283545
H	1.718776	-4.209792	0.069266
H	3.501124	-5.894745	0.222326
H	5.900470	-5.220407	0.053592
H	6.481321	-2.813468	-0.271886
H	4.701304	-1.112096	-0.423001
C	2.693529	0.490937	-1.732029
N	3.271952	1.690993	-1.552177
C	3.427815	1.946231	-0.193923
C	3.962507	3.057033	0.457686
C	3.992979	3.018679	1.846817
C	3.503896	1.908884	2.560703
C	2.964492	0.809903	1.902401
C	2.923244	0.830436	0.504942
H	3.520511	2.334846	-2.300483
H	2.502461	0.090515	-2.730269
H	4.342458	3.918909	-0.100713
H	4.410025	3.869140	2.397509
H	3.552745	1.914007	3.655294
H	2.577987	-0.053342	2.458314
C	2.391720	-0.086922	-0.488924

TS\_18a\_17a  
SCF Energy: -1574.40621283  
ZPE-corrected Energy: -1573.95811  
 $\Delta U$ : -1573.92949  
 $\Delta H$ : -1573.92855  
 $\Delta G$ : -1574.02106

Num. Imaginary Frequencies: 1  
Imaginary Frequency: -140.4639

C	0.002523	-0.546675	-0.579833
C	0.482949	0.685986	-0.901195
C	-0.206449	1.966739	-0.643727
C	-0.573435	2.821114	-1.694060
C	-1.255831	4.006213	-1.436523
C	-1.565481	4.364104	-0.122423
C	-1.193842	3.530024	0.930726
C	-0.518237	2.337902	0.671852
H	-0.337827	2.538362	-2.729038
H	-1.552731	4.656088	-2.267503
H	-2.098460	5.300175	0.079577
H	-1.429321	3.809605	1.963915
H	-0.221282	1.675837	1.495803
C	0.969670	-1.635420	-0.489749
C	2.268446	-1.275007	-0.337883
C	3.432946	-2.150171	-0.209912
H	0.649368	-2.682855	-0.511900
Au	-2.015933	-0.808480	-0.110030
P	-4.319143	-1.032351	0.453418
C	-4.866351	0.207311	1.676236
H	-4.285433	0.091498	2.608476
H	-4.688300	1.222458	1.278216
H	-5.942829	0.084482	1.898980
C	-5.474732	-0.815577	-0.942410
H	-5.320093	0.176824	-1.401637
H	-6.521150	-0.896982	-0.592391
C	-4.805148	-2.630046	1.188466
H	-5.285089	-1.588494	-1.708005
H	-5.883474	-2.627028	1.435582
H	-4.220997	-2.811004	2.107994
H	-4.597453	-3.447423	0.475524
C	3.276545	-3.529061	0.027725
C	4.382654	-4.360247	0.138166
C	5.673483	-3.838924	0.012063
C	5.845475	-2.476752	-0.221647
C	4.737695	-1.639065	-0.327343
H	2.273207	-3.953746	0.143525
H	4.239054	-5.429430	0.330130
H	6.544358	-4.497784	0.101239
H	6.852568	-2.057130	-0.322058
H	4.892815	-0.569964	-0.516230
C	1.965012	0.883932	-1.612708
N	2.450187	2.201561	-1.503424
C	2.962960	2.402481	-0.264710
C	3.411927	3.582788	0.347787
C	3.892975	3.477825	1.639086
C	3.932910	2.245371	2.343358
C	3.477362	1.085206	1.759821
C	2.984556	1.156325	0.436856
H	2.266969	2.938410	-2.179551
H	1.978206	0.427869	-2.613537
H	3.381267	4.541298	-0.178888
H	4.256955	4.380666	2.142162
H	4.327769	2.228906	3.364146
H	3.492559	0.128090	2.292609
C	2.446738	0.194545	-0.435031

TS\_2a\_12a  
 SCF Energy: -1574.3380304  
 ZPE-corrected Energy: -1573.89389  
 $\Delta U$ : -1573.86328  
 $\Delta H$ : -1573.86234  
 $\Delta G$ : -1573.96174

Num. Imaginary Frequencies: 1  
 Imaginary Frequency: -523.6491

N	-1.729186	3.239471	0.086458
C	-1.563538	2.567448	-1.125801
C	-2.644188	1.684731	-1.274073
C	-3.412546	1.745430	-0.092125
C	-2.801244	2.724544	0.747551
C	0.193049	1.378428	-0.685133
C	1.188066	2.426044	-0.646304
C	1.744414	2.936205	-1.831009
C	2.716157	3.928970	-1.773039
C	3.135461	4.426900	-0.537859
C	2.583395	3.929726	0.643707
C	1.610804	2.936314	0.593998
C	-0.037773	0.122507	-0.479323
Au	1.838624	-0.847358	0.005172
C	-1.145131	-0.717297	-0.505679
C	-2.135755	-1.432606	-0.523824
C	-3.376231	-2.128396	-0.543461
C	-3.945903	-2.601388	0.652542
C	-5.198397	-3.204967	0.637518
C	-5.895111	-3.348383	-0.563637
C	-5.333028	-2.888703	-1.755903
C	-4.081550	-2.282182	-1.751118
H	-6.882972	-3.822435	-0.570880
H	-5.638503	-3.565985	1.573804
H	-3.398454	-2.475347	1.593491
H	-3.637849	-1.910719	-2.682269
H	-5.878175	-3.001919	-2.699621
H	1.409944	2.539126	-2.797063
H	3.153049	4.317845	-2.699111
H	3.899812	5.210764	-0.496105
H	2.915229	4.319135	1.612333
H	1.173060	2.532422	1.515302
H	-2.838901	1.068112	-2.154317
C	-4.560043	1.055560	0.362545
C	-3.305550	3.015575	2.024951
H	-1.090787	3.939634	0.454666
H	-1.027872	3.056225	-1.944326
P	3.812836	-2.012118	0.525865
C	3.853557	-3.705992	-0.140852
C	5.325095	-1.222576	-0.112075
C	4.104549	-2.206303	2.312852
H	3.767106	-3.675632	-1.241292
H	3.005789	-4.286689	0.262982
H	5.422551	-0.207626	0.311759
H	5.267602	-1.141421	-1.211746
H	4.802853	-4.199977	0.139112
H	6.212050	-1.822892	0.164662
H	5.041602	-2.768404	2.485500
H	4.180972	-1.212710	2.788274
H	3.261220	-2.752282	2.770854
C	-5.055008	1.350628	1.615275
C	-4.429488	2.323121	2.436389
H	-2.828498	3.766389	2.663378
H	-4.852134	2.531791	3.425950
H	-5.943520	0.829524	1.988825
H	-5.039070	0.299780	-0.272638

TS\_2a\_15a  
 SCF Energy: -1574.34789752  
 ZPE-corrected Energy: -1573.90369  
 $\Delta U$ : -1573.87307  
 $\Delta H$ : -1573.87213  
 $\Delta G$ : -1573.97026

Num. Imaginary Frequencies: 1  
 Imaginary Frequency: -435.5541

N	2.369553	2.896986	-1.550146
C	1.222884	3.404345	-1.054217
C	1.172633	3.196174	0.329480
C	2.430496	2.580746	0.685183
C	3.144213	2.384575	-0.517519
C	-0.372757	1.619651	0.009710
C	-1.574494	2.425691	-0.014819
C	-2.120456	2.937633	1.173510
C	-3.303693	3.667740	1.139567
C	-3.947877	3.900697	-0.076766
C	-3.408799	3.400033	-1.262787
C	-2.226505	2.667500	-1.235817
C	0.117468	0.430338	-0.064257
Au	-1.619681	-0.888447	0.001785
C	1.325362	-0.261178	-0.130539
C	2.332283	-0.951916	-0.184921
C	3.547717	-1.692972	-0.226040
C	4.042467	-2.306128	0.938616
C	5.258746	-2.980361	0.911504
C	5.992440	-3.061075	-0.273047
C	5.500573	-2.467021	-1.436749
C	4.287679	-1.787074	-1.417914
H	6.950858	-3.592011	-0.290367
H	5.639630	-3.448695	1.826181
H	3.467074	-2.231881	1.868688
H	3.904021	-1.307170	-2.325896
H	6.071836	-2.531824	-2.369771
H	-1.610552	2.747016	2.125685
H	-3.729248	4.057820	2.070525
H	-4.878688	4.478150	-0.100330
H	-3.915805	3.580599	-2.216933
H	-1.797397	2.263549	-2.161093
H	0.503716	3.719971	1.014907
C	2.992768	2.150769	1.893572
C	4.384926	1.753614	-0.558346
H	2.612545	2.862735	-2.537230
H	0.488482	3.881629	-1.706830
P	-3.422514	-2.388774	0.074343
C	-3.718137	-3.261793	-1.495952
C	-3.234212	-3.705732	1.317458
C	-5.007458	-1.586391	0.476650
H	-2.823690	-3.849164	-1.768281
H	-3.916266	-2.529233	-2.297994
H	-3.130121	-3.257428	2.321031
H	-2.327574	-4.297132	1.100171
H	-4.585870	-3.940715	-1.397641
H	-4.117515	-4.371279	1.303454
H	-5.821101	-2.335519	0.499092
H	-4.934253	-1.096246	1.463542
H	-5.238402	-0.817251	-0.281280
C	4.917363	1.325415	0.652535
C	4.234997	1.528591	1.865227
H	4.914247	1.592627	-1.503794
H	5.886222	0.810930	0.659156
H	4.690325	1.182536	2.800138
H	2.459413	2.296812	2.839803

## Cartesian coordinates of substituted dyines

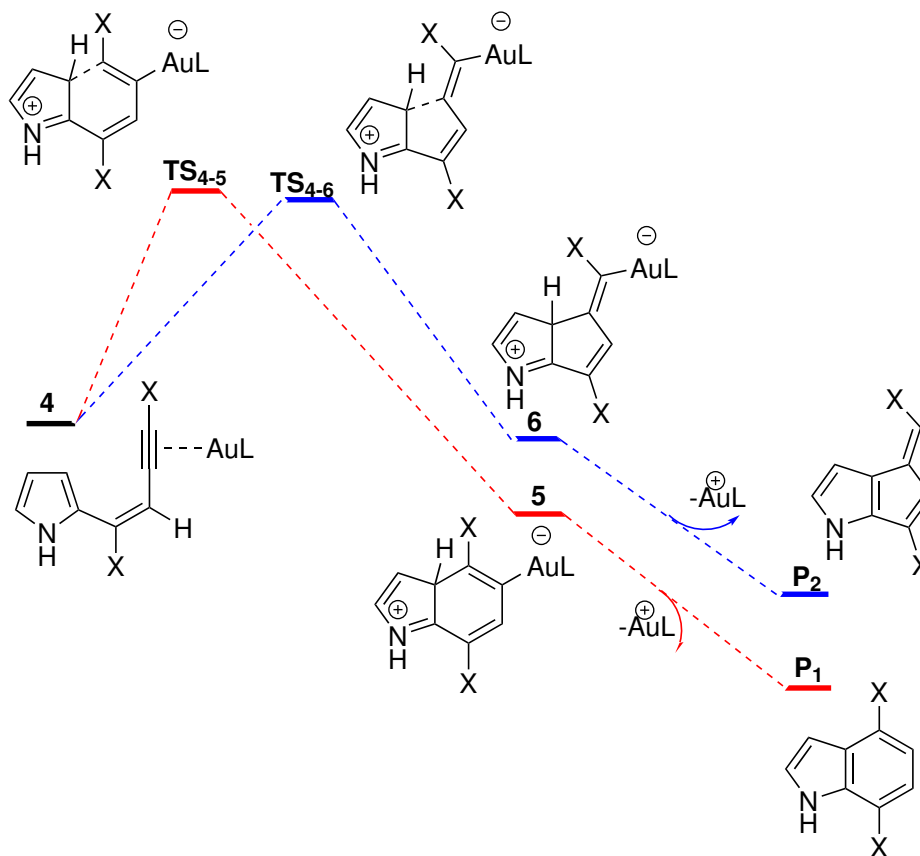


Figure S7: Reaction mechanism.

**Ester**



4e  
 SCF Energy: -1876.19590840  
 ZPE-corrected Energy: -1875.70960  
 $\Delta U$ : -1875.67305  
 $\Delta H$ : -1875.67211  
 $\Delta G$ : -1875.78514

Num. Imaginary Frequencies: 0

C	-0.504670	-4.035131	1.836031
C	-1.675187	-3.777125	2.533957
N	-2.348526	-2.791520	1.891129
C	-1.630822	-2.368724	0.787437
C	-0.473666	-3.150540	0.740588
C	-2.099714	-1.321331	-0.086473
C	-3.556038	-1.087349	-0.199423
C	-4.062964	0.221145	-0.246126
C	-5.426693	0.446098	-0.372525
C	-6.314359	-0.631025	-0.460428
C	-5.819697	-1.938779	-0.416347
C	-4.454838	-2.163621	-0.280990
H	0.235456	-4.796517	2.087077
H	-2.074602	-4.230714	3.441966
H	-3.222817	-2.379115	2.208038
H	0.279594	-3.114971	-0.049156
H	-3.376492	1.071100	-0.155092
H	-5.827610	1.464768	-0.398314
C	-7.765323	-0.330553	-0.595419
H	-6.510511	-2.783624	-0.494156
H	-4.074085	-3.191417	-0.264119
C	-1.254657	-0.532409	-0.830038
C	0.146214	-0.524677	-0.722507
C	1.386466	-0.511671	-0.634979
C	2.774159	-0.885959	-0.647820
C	3.655532	-0.340936	-1.598048
C	4.986096	-0.730133	-1.608795
C	5.461487	-1.657357	-0.673818
C	4.587436	-2.193949	0.278239
C	3.253009	-1.809781	0.296780
H	3.280295	0.383823	-2.329461
H	5.683304	-0.319568	-2.346503
C	6.899822	-2.031385	-0.734304
H	4.960278	-2.915517	1.011152
H	2.568150	-2.219097	1.047901
Au	0.993852	1.650875	-0.011210
H	-1.690972	0.154337	-1.568092
P	1.067966	3.883361	0.663416
C	2.064800	4.926161	-0.443268
C	-0.573082	4.665356	0.724616
C	1.776972	4.115116	2.321359
H	1.643234	4.896083	-1.463128
H	3.102098	4.549731	-0.477707
H	-1.221677	4.116343	1.429483
H	-1.036222	4.640803	-0.277333
H	-0.476490	5.715393	1.058384
H	2.065612	5.969672	-0.077203
H	1.793164	5.191950	2.573880
H	1.168760	3.573019	3.066301
H	2.806500	3.717500	2.347578
O	7.234159	-2.921019	0.200219
O	7.682380	-1.582574	-1.537552
C	8.589427	-3.340240	0.220730
H	8.677629	-4.065716	1.042072
H	8.864502	-3.814609	-0.737128
H	9.259797	-2.481459	0.398167
O	-8.508596	-1.433972	-0.673853
O	-8.224540	0.786087	-0.630738
C	-9.908681	-1.247525	-0.807763
H	-10.352075	-2.252144	-0.860729
H	-10.312875	-0.698502	0.060298
H	-10.139428	-0.680709	-1.726306

5e  
 SCF Energy: -1876.21272032  
 ZPE-corrected Energy: -1875.72489  
 $\Delta U$ : -1875.68966  
 $\Delta H$ : -1875.68871  
 $\Delta G$ : -1875.79727

Num. Imaginary Frequencies: 0

C	-0.350474	-3.899324	0.016751
C	-1.579170	-4.371277	0.302695
N	-2.519104	-3.335774	0.227234
C	-1.932509	-2.182254	-0.097656
C	-0.508143	-2.462959	-0.362002
C	-2.452447	-0.875079	-0.147330
C	-3.898114	-0.601893	-0.033902
C	-4.367489	0.418659	0.806720
C	-5.726787	0.684605	0.901020
C	-6.647802	-0.064403	0.161399
C	-6.189349	-1.083027	-0.680218
C	-4.827807	-1.346919	-0.776572
H	0.567246	-4.483521	-0.055977
H	-1.908109	-5.381034	0.550089
H	-3.512701	-3.441597	0.433737
H	-0.522560	-2.528848	-1.492114
H	-3.656551	0.995437	1.409770
H	-6.098270	1.475807	1.560705
C	-8.091359	0.261934	0.306130
H	-6.904703	-1.663787	-1.270083
H	-4.479883	-2.125286	-1.467525
C	-1.497219	0.132533	-0.207651
C	-0.070130	-0.032634	-0.203854
C	0.438738	-1.312409	-0.221374
C	1.884069	-1.605935	-0.234701
C	2.742329	-0.992295	-1.161989
C	4.109482	-1.231345	-1.121651
C	4.649879	-2.082077	-0.150752
C	3.802121	-2.703661	0.772123
C	2.431422	-2.476245	0.720124
H	2.321285	-0.335202	-1.931872
H	4.782550	-0.762682	-1.847615
C	6.122367	-2.291099	-0.147552
H	4.221797	-3.364799	1.536159
H	1.776446	-2.952713	1.459864
Au	1.171408	1.654921	-0.062604
H	-1.886093	1.160682	-0.225099
P	2.646247	3.514949	0.100158
C	3.570468	3.841207	-1.439996
C	1.885190	5.119467	0.519255
C	3.954983	3.298103	1.354206
H	2.865249	4.072672	-2.257867
H	4.146327	2.940339	-1.719716
H	1.371879	5.043747	1.494252
H	1.138915	5.390119	-0.248429
H	2.656012	5.911016	0.573599
H	4.265664	4.691226	-1.305468
H	4.636569	4.169562	1.359175
H	3.499750	3.184973	2.353974
H	4.533336	2.384014	1.128711
O	6.516371	-3.129609	0.811326
O	6.883412	-1.762768	-0.922884
C	7.908666	-3.388491	0.894591
H	8.044458	-4.092007	1.728530
H	8.278475	-3.835741	-0.044327
H	8.467204	-2.456436	1.088857
O	-8.868317	-0.522897	-0.441162
O	-8.519857	1.137868	1.018972
C	-10.265128	-0.285198	-0.369886
H	-10.739258	-1.016796	-1.039796
H	-10.631088	-0.421669	0.662488
H	-10.502736	0.741296	-0.698872

6e  
SCF Energy: -1876.20103320  
ZPE-corrected Energy: -1875.71334  
 $\Delta U$ : -1875.67787  
 $\Delta H$ : -1875.67692  
 $\Delta G$ : -1875.78672

Num. Imaginary Frequencies: 0

C	0.639642	-3.459143	0.596070
C	-0.024647	-2.397793	-0.220833
C	-0.331912	-4.270773	1.055259
N	-1.606221	-3.754296	0.710363
C	-1.457165	-2.614837	0.052656
C	0.069338	-0.872746	-0.238917
C	-1.291763	-0.423039	-0.306116
C	-2.228969	-1.441399	-0.175619
C	1.193117	-0.101528	-0.216951
C	2.498570	-0.774693	-0.247171
C	2.874912	-1.580775	-1.336393
C	4.092811	-2.247718	-1.334308
C	4.958177	-2.140356	-0.239977
C	4.596754	-1.330148	0.843981
C	3.391419	-0.640381	0.830077
Au	1.166480	1.983122	-0.067593
P	1.186715	4.362176	0.076967
C	2.302797	5.026277	1.358560
C	-0.431002	5.114289	0.460012
C	1.718647	5.198230	-1.454982
H	-2.485283	-4.118017	1.079395
H	1.714604	-3.639262	0.664312
H	0.125637	-2.710306	-1.286563
H	-0.271698	-5.211759	1.603821
H	-1.545437	0.633789	-0.458319
C	-3.686643	-1.335540	-0.142982
H	2.205369	-1.668155	-2.201104
H	4.391664	-2.871092	-2.184009
C	6.238897	-2.889607	-0.284231
H	5.273628	-1.236312	1.698706
H	3.116704	0.004064	1.674379
H	1.997655	4.648738	2.350537
H	3.336758	4.692915	1.160143
H	2.270345	6.132096	1.362809
H	-0.341308	6.215671	0.510466
H	-1.162932	4.844579	-0.321847
H	-0.797912	4.734231	1.429928
H	1.703481	6.295963	-1.319237
H	2.742323	4.877054	-1.717216
H	1.042903	4.924036	-2.284235
C	-4.316579	-0.130125	0.205147
C	-4.483894	-2.445258	-0.466148
C	-5.868911	-2.354682	-0.432928
C	-6.488618	-1.151846	-0.081525
C	-5.701195	-0.037829	0.234527
H	-3.712495	0.742875	0.476919
H	-4.013182	-3.386137	-0.777687
H	-6.493243	-3.217252	-0.688091
C	-7.974423	-1.111591	-0.058420
H	-6.182528	0.904186	0.513691
O	6.977243	-2.704288	0.812506
O	6.584974	-3.593401	-1.204032
C	8.222004	-3.381407	0.860433
H	8.684500	-3.114408	1.821639
H	8.075009	-4.473840	0.800416
H	8.871360	-3.064308	0.025952
O	-8.445978	0.086411	0.288993
O	-8.682317	-2.054281	-0.322436
C	-9.857115	0.221870	0.341450
H	-10.058440	1.260516	0.640676
H	-10.305093	0.017300	-0.646369
H	-10.288340	-0.476600	1.079410

TS\_4e\_5e  
SCF Energy: -1876.16816125  
ZPE-corrected Energy: -1875.68250  
 $\Delta U$ : -1875.64681  
 $\Delta H$ : -1875.64587  
 $\Delta G$ : -1875.75623

Num. Imaginary Frequencies: 1  
Imaginary Frequency: -481.8092

C	0.097193	-3.937174	0.210411
C	1.088134	-4.150512	1.129692
N	1.997830	-3.118257	1.040798
C	1.612793	-2.234251	0.088145
C	0.394925	-2.700555	-0.451852
C	2.268701	-0.967455	-0.166636
C	3.741449	-0.893837	-0.150767
C	4.506368	-1.969307	-0.634751
C	5.892769	-1.901183	-0.652056
C	6.550243	-0.761005	-0.180181
C	5.798493	0.311623	0.312918
C	4.411617	0.243325	0.329613
H	-0.748943	-4.596009	0.008906
H	1.234205	-4.955427	1.850573
H	2.795888	-2.988739	1.660878
H	0.048373	-2.441464	-1.459185
H	4.004335	-2.863498	-1.022928
H	6.489418	-2.733993	-1.038846
C	8.036448	-0.743866	-0.218044
H	6.308670	1.200102	0.696894
H	3.838280	1.077229	0.749647
C	1.486875	0.143295	-0.321336
C	0.049538	0.114343	-0.189364
C	-0.753356	-0.897954	-0.059035
Au	-1.061830	1.936953	-0.005888
H	1.975130	1.109502	-0.493172
C	-2.107378	-1.387717	-0.136782
C	-2.915219	-1.044376	-1.236552
C	-4.228315	-1.488055	-1.298401
C	-4.752213	-2.281021	-0.271658
C	-3.951754	-2.629842	0.823159
C	-2.637193	-2.189804	0.887834
H	-2.496650	-0.421840	-2.035693
H	-4.870556	-1.228146	-2.146157
C	-6.169232	-2.726952	-0.393704
H	-4.367620	-3.247258	1.624528
H	-2.000936	-2.461209	1.737705
P	-2.189172	4.001758	0.179331
C	-3.994518	3.879654	-0.035852
C	-1.968193	4.822091	1.791092
C	-1.656251	5.239870	-1.046555
H	-4.459958	4.877833	0.067712
H	-4.223716	3.471650	-1.036054
H	-4.415216	3.199734	0.725839
H	-2.221946	6.180684	-0.910782
H	-0.577381	5.442591	-0.926472
H	-1.829823	4.853669	-2.066311
H	-2.516412	5.782703	1.808537
H	-2.348532	4.169984	2.596789
H	-0.894968	5.010893	1.969145
O	-6.553764	-3.481247	0.633621
O	-6.889039	-2.437337	-1.318474
C	-7.891830	-3.954930	0.607686
H	-8.025716	-4.555969	1.518327
H	-8.602218	-3.110283	0.600578
H	-8.066365	-4.575460	-0.288087
O	8.544812	0.394063	0.256664
O	8.714706	-1.654002	-0.631237
C	9.959072	0.503627	0.259498
H	10.193248	1.491611	0.681348
H	10.410087	-0.290991	0.878821
H	10.357918	0.424199	-0.766663

TS\_4e\_6e  
SCF Energy: -1876.17104680  
ZPE-corrected Energy: -1875.68589  
 $\Delta U$ : -1875.65005  
 $\Delta H$ : -1875.64911  
 $\Delta G$ : -1875.76030

Num. Imaginary Frequencies: 1  
Imaginary Frequency: -470.2797

C	0.570646	-3.486285	0.743219
C	-0.094414	-2.657965	-0.215642
C	-0.342650	-3.765843	1.727355
N	-1.540676	-3.150963	1.427555
C	-1.411459	-2.453803	0.272986
C	0.008994	-0.574319	-0.533034
C	-1.373503	-0.416015	-0.773033
C	-2.207250	-1.380655	-0.249627
C	1.210518	-0.088810	-0.417454
C	2.489065	-0.799485	-0.422788
C	2.854590	-1.611639	-1.509313
C	4.046174	-2.324483	-1.481554
C	4.892581	-2.248159	-0.370220
C	4.537195	-1.433337	0.711467
C	3.354432	-0.705690	0.678586
Au	1.187322	2.018526	-0.086456
P	1.250661	4.354245	0.257093
C	-0.360613	5.097429	0.672530
C	1.831200	5.288869	-1.195381
C	2.356734	4.866198	1.611641
H	-2.328854	-3.077702	2.069401
H	1.581752	-3.891001	0.668076
H	0.154219	-2.656484	-1.285026
H	-0.250665	-4.376333	2.626743
H	-1.726941	0.419260	-1.393135
C	-3.667084	-1.321453	-0.199348
H	2.200463	-1.668552	-2.387658
H	4.339932	-2.956741	-2.326313
C	6.150965	-3.037136	-0.394154
H	5.198914	-1.367189	1.580336
H	3.079914	-0.062105	1.523083
H	-1.081750	4.904513	-0.141051
H	-0.749771	4.647054	1.602621
H	-0.251949	6.189336	0.812830
H	1.845233	6.372295	-0.973270
H	2.849143	4.958181	-1.467539
H	1.159796	5.100611	-2.051591
H	2.344059	5.966831	1.721302
H	2.026619	4.401661	2.557420
H	3.387218	4.532669	1.396998
C	-4.334663	-0.086388	-0.246276
C	-4.426359	-2.499476	-0.102622
C	-5.812632	-2.441301	-0.052476
C	-6.468790	-1.207860	-0.101535
C	-5.720227	-0.028599	-0.200859
H	-3.756842	0.843464	-0.294978
H	-3.925095	-3.474798	-0.090185
H	-6.410020	-3.356085	0.018091
C	-7.955880	-1.205124	-0.040932
H	-6.232020	0.937658	-0.232104
O	6.874853	-2.876425	0.715395
O	6.490899	-3.748028	-1.310365
C	8.098381	-3.590066	0.783014
H	8.550462	-3.340755	1.753829
H	7.920416	-4.677342	0.714871
H	8.771814	-3.288169	-0.037905
O	-8.464489	0.025024	-0.100531
O	-8.630557	-2.202364	0.052373
C	-9.878786	0.129937	-0.049289
H	-10.113012	1.202146	-0.113737
H	-10.339596	-0.411941	-0.893181
H	-10.265657	-0.287914	0.896244

# Cyclohexane

4c  
SCF Energy: -1428.22435949  
ZPE-corrected Energy: -1427.68577  
 $\Delta U$ : -1427.65604  
 $\Delta H$ : -1427.65510  
 $\Delta G$ : -1427.74873

Num. Imaginary Frequencies: 0

C	0.515693	-0.847216	3.229731
C	1.821626	-1.292773	3.121230
N	2.441445	-0.564193	2.155541
C	1.560062	0.345978	1.598160
C	0.347876	0.179740	2.276068
C	1.949690	1.243597	0.530063
H	-0.228911	-1.210222	3.940186
H	2.357596	-2.068627	3.669775
H	3.403759	-0.706974	1.862207
H	-0.545287	0.790758	2.137215
C	1.054529	1.818070	-0.330777
C	-0.336410	1.577328	-0.384111
C	-1.558970	1.396051	-0.506382
Au	-0.840330	-0.787026	-0.552844
H	1.436383	2.486126	-1.114649
P	-0.358531	-3.071482	-0.507327
C	-0.793781	-4.032176	-1.988115
C	1.430985	-3.311942	-0.269262
C	-1.142844	-3.936729	0.886986
H	-0.282337	-3.610018	-2.870721
H	-1.884038	-3.985672	-2.155019
H	1.747664	-2.792765	0.654850
H	1.980541	-2.877840	-1.123347
H	1.668676	-4.389416	-0.188651
H	-0.488304	-5.087159	-1.856955
H	-0.811380	-4.991642	0.913653
H	-0.860008	-3.437104	1.831192
H	-2.241174	-3.901592	0.780956
C	-3.013780	1.618939	-0.470206
C	3.428681	1.458308	0.299737
C	-3.330760	3.095012	-0.746044
H	-3.490795	1.008999	-1.267486
C	-4.831865	3.343885	-0.696524
H	-2.819573	3.709540	0.025063
H	-2.909749	3.393745	-1.724472
C	-5.423326	2.902878	0.636001
H	-5.040759	4.414074	-0.882970
H	-5.320861	2.780950	-1.519578
C	-5.107244	1.439506	0.917644
H	-4.998500	3.529737	1.448607
H	-6.516685	3.071298	0.648967
C	-3.607649	1.180057	0.875511
H	-5.514290	1.132587	1.899330
H	-5.607086	0.802778	0.157228
H	-3.103625	1.753909	1.682224
H	-3.383543	0.109756	1.057066
C	3.822804	2.883155	-0.094761
H	3.957110	1.252455	1.254600
C	5.335881	3.003204	-0.226768
H	3.364491	3.147622	-1.070148
H	3.429750	3.603421	0.648405
C	5.877988	2.012857	-1.249779
H	5.610182	4.038286	-0.504704
H	5.806303	2.809167	0.760376
C	5.470449	0.585969	-0.905846
H	5.477013	2.272490	-2.252698
H	6.979098	2.093134	-1.322691
C	3.960565	0.465804	-0.749700
H	5.828914	-0.120225	-1.678603
H	5.958077	0.283613	0.045344
H	3.460291	0.688110	-1.716572
H	3.673788	-0.573642	-0.489354

5c  
SCF Energy: -1428.23606384  
ZPE-corrected Energy: -1427.69631  
 $\Delta U$ : -1427.66766  
 $\Delta H$ : -1427.66671  
 $\Delta G$ : -1427.75825

Num. Imaginary Frequencies: 0

C	1.895403	3.725167	0.144068
C	3.225178	3.722626	0.356461
N	3.739939	2.437258	0.159200
C	2.765093	1.578651	-0.164136
C	1.515349	2.353072	-0.322537
C	2.810525	0.183890	-0.292647
H	1.248459	4.601719	0.181300
H	3.895982	4.537619	0.630206
H	4.720608	2.189617	0.281083
H	1.498139	2.481115	-1.447742
C	1.564999	-0.426578	-0.292405
C	0.282933	0.219456	-0.211309
C	0.231256	1.594674	-0.183190
Au	-1.423437	-0.995483	-0.067553
H	1.564227	-1.525910	-0.316739
P	-3.328945	-2.418618	0.123523
C	-4.694439	-2.033027	-1.025859
C	-2.989738	-4.187249	-0.177067
C	-4.123482	-2.397357	1.767363
H	-4.339045	-2.116162	-2.068293
H	-5.041580	-0.998205	-0.857064
H	-2.236888	-4.549784	0.545235
H	-2.587716	-4.321079	-1.197037
H	-3.915551	-4.783101	-0.069139
H	-5.539194	-2.730718	-0.871338
H	-4.994112	-3.079540	1.785880
H	-3.396651	-2.713474	2.536497
H	-4.458784	-1.372098	2.004778
C	-1.053284	2.368764	-0.144315
C	4.116367	-0.567217	-0.238645
C	4.166687	-1.784067	-1.164119
H	4.918333	0.122388	-0.585354
C	5.531504	-2.457547	-1.102477
H	3.394766	-2.518787	-0.852220
H	3.918019	-1.482558	-2.200329
C	5.878268	-2.866395	0.323696
H	5.552279	-3.335445	-1.775437
H	6.303218	-1.754228	-1.481498
C	5.816182	-1.672718	1.268084
H	5.155456	-3.637731	0.665405
H	6.878928	-3.337227	0.360193
C	4.460512	-0.983681	1.198532
H	6.031708	-1.984477	2.307652
H	6.607396	-0.944175	0.989618
H	3.666148	-1.673578	1.557262
H	4.431803	-0.101952	1.869507
C	-1.195561	3.407930	-1.263332
H	-1.867173	1.627409	-0.295034
C	-2.546687	4.106036	-1.187471
H	-0.398847	4.176197	-1.188487
H	-1.063302	2.912208	-2.245807
C	-2.753953	4.748581	0.177958
H	-2.628879	4.860656	-1.992491
H	-3.352478	3.363734	-1.369109
C	-2.631481	3.715804	1.290240
H	-1.987792	5.539740	0.328142
H	-3.737763	5.252945	0.224068
C	-1.288653	2.997991	1.237683
H	-2.769612	4.188086	2.281376
H	-3.445618	2.967759	1.182946
H	-0.475852	3.716142	1.475195
H	-1.240343	2.203641	2.008788



6c  
SCF Energy: -1428.22306481  
ZPE-corrected Energy: -1427.68371  
 $\Delta U$ : -1427.65488  
 $\Delta H$ : -1427.65394  
 $\Delta G$ : -1427.74635

Num. Imaginary Frequencies: 0

C	-1.662978	3.715783	-0.496208
C	-1.663506	2.383580	0.190005
C	-2.918248	3.941400	-0.930927
N	-3.728006	2.802198	-0.708368
C	-2.991056	1.843138	-0.158844
C	-0.784518	1.132584	0.129008
C	-1.719189	0.042577	0.056751
C	-3.043740	0.432624	-0.084771
C	0.572871	1.045249	0.232083
C	1.363632	2.309439	0.392438
Au	1.571826	-0.780926	0.026690
P	2.721527	-2.866360	-0.190949
C	2.649505	-3.914497	1.302336
C	4.506738	-2.721131	-0.543108
C	2.100685	-3.952815	-1.520612
H	-4.666110	2.681734	-1.089224
H	-0.852718	4.448028	-0.489158
H	-1.713409	2.622131	1.284100
H	-3.360288	4.829750	-1.384569
H	-1.387514	-1.002270	0.110350
C	-4.275756	-0.401070	-0.239159
H	1.596705	-4.143414	1.545777
H	3.200228	-4.859990	1.139597
H	3.095481	-3.375459	2.156938
H	4.968157	-3.723522	-0.622706
H	4.655450	-2.175792	-1.491959
H	5.001966	-2.155598	0.265954
H	2.678798	-4.895689	-1.549336
H	1.035024	-4.184787	-1.346692
H	2.192254	-3.439858	-2.494410
C	1.855064	2.792213	-0.983026
H	0.709436	3.114321	0.801469
C	2.618344	4.104949	-0.865724
H	2.513354	2.007701	-1.415270
H	0.997162	2.896565	-1.677542
C	3.781482	3.985637	0.110703
H	2.976642	4.425406	-1.862758
H	1.923508	4.898037	-0.513487
C	3.307971	3.494742	1.473061
H	4.522110	3.264398	-0.296281
H	4.307859	4.954443	0.206502
C	2.551547	2.179160	1.348371
H	4.164538	3.378719	2.164140
H	2.642127	4.259339	1.927465
H	3.235511	1.392795	0.959556
H	2.201941	1.827004	2.339055
C	-5.251619	-0.158595	0.921462
H	-4.789240	-0.070174	-1.172839
C	-6.526667	-0.973847	0.758732
H	-4.742133	-0.441192	1.867800
H	-5.486814	0.921854	1.004341
C	-6.216288	-2.457601	0.610625
H	-7.201748	-0.798354	1.617573
H	-7.069588	-0.622254	-0.144341
C	-5.254089	-2.700996	-0.544858
H	-5.756540	-2.828965	1.551314
H	-7.148578	-3.036140	0.467798
C	-3.975849	-1.890684	-0.378273
H	-5.012573	-3.777072	-0.632100
H	-5.745703	-2.412128	-1.498034
H	-3.442928	-2.233314	0.535309
H	-3.289504	-2.064086	-1.230409

TS\_4c\_5c  
SCF Energy: -1428.19094761  
ZPE-corrected Energy: -1427.65331  
 $\Delta U$ : -1427.62439  
 $\Delta H$ : -1427.62344  
 $\Delta G$ : -1427.71545

Num. Imaginary Frequencies: 1  
Imaginary Frequency: -460.4007

C	-2.508627	3.447703	0.119888
C	-3.364989	3.180979	1.152752
N	-3.530618	1.813678	1.237303
C	-2.792448	1.190152	0.288451
C	-2.099016	2.185179	-0.429773
C	-2.687637	-0.250015	0.132126
H	-2.217616	4.440908	-0.228600
H	-3.879238	3.845306	1.847617
H	-4.059843	1.341733	1.967630
H	-1.752272	2.040757	-1.460582
C	-1.452562	-0.771849	-0.084795
C	-0.249511	0.043162	-0.116432
C	-0.109019	1.330639	-0.103818
Au	1.654886	-0.941978	-0.041988
H	-1.337543	-1.857388	-0.168654
P	3.708059	-2.093079	0.102744
C	4.803159	-1.477878	1.423556
C	3.537615	-3.874704	0.444173
C	4.721754	-2.008134	-1.409562
H	5.744744	-2.058412	1.437187
H	5.034558	-0.411995	1.251574
H	4.299948	-1.575225	2.401635
H	5.666540	-2.565875	-1.268202
H	4.164087	-2.443376	-2.257393
H	4.951964	-0.954088	-1.645087
H	4.535537	-4.347695	0.509212
H	3.001802	-4.021448	1.398490
H	2.957480	-4.356335	-0.362410
C	0.796209	2.490692	-0.172850
C	-3.946150	-1.068598	0.264384
C	0.781350	3.357671	1.091354
H	1.796867	2.000871	-0.212597
C	1.851423	4.439262	1.023978
H	-0.218338	3.824301	1.200351
H	0.927979	2.711946	1.978514
C	1.713262	5.278882	-0.239092
H	1.798110	5.076382	1.926748
H	2.855485	3.963929	1.036106
C	1.771812	4.401874	-1.482875
H	0.739628	5.814663	-0.217548
H	2.499048	6.056714	-0.275874
C	0.687116	3.333423	-1.449997
H	1.666586	5.012129	-2.399403
H	2.768121	3.914886	-1.542428
H	-0.302085	3.830982	-1.484751
H	0.746799	2.673102	-2.336702
C	-3.725938	-2.576372	0.318431
H	-4.432494	-0.775469	1.225025
C	-5.043487	-3.322265	0.487964
H	-3.246616	-2.905729	-0.628312
H	-3.026169	-2.833418	1.137249
C	-6.019700	-2.977950	-0.628699
H	-4.857942	-4.412379	0.522667
H	-5.493912	-3.050549	1.466307
C	-6.249049	-1.474812	-0.703740
H	-5.604649	-3.332190	-1.596390
H	-6.978982	-3.510535	-0.485290
C	-4.936298	-0.719260	-0.858265
H	-6.930074	-1.223032	-1.538704
H	-6.754292	-1.135278	0.225521
H	-4.461465	-0.981141	-1.828385
H	-5.119911	0.372966	-0.882719

TS\_4c\_6c  
 SCF Energy: -1428.19517273  
 ZPE-corrected Energy: -1427.65827  
 $\Delta U$ : -1427.62918  
 $\Delta H$ : -1427.62824  
 $\Delta G$ : -1427.72139

Num. Imaginary Frequencies: 1  
 Imaginary Frequency: -469.0055

C	-1.864411	3.640018	-0.688584
C	-1.944794	2.479353	0.154859
C	-2.794240	3.479384	-1.680647
N	-3.450622	2.276393	-1.499326
C	-2.938701	1.643930	-0.417512
C	-0.741984	0.781409	0.378040
C	-1.826384	-0.128120	0.487061
C	-3.035563	0.270415	-0.020263
C	0.537877	1.011531	0.405707
C	1.255291	2.318262	0.533996
Au	1.637274	-0.778609	0.043570
P	2.920994	-2.727685	-0.347619
C	2.971598	-3.883254	1.061658
C	4.672146	-2.385969	-0.721646
C	2.348117	-3.742416	-1.750062
H	-4.083172	1.857808	-2.178689
H	-1.248157	4.526635	-0.526767
H	-1.759202	2.518028	1.237420
H	-3.068392	4.134376	-2.508778
H	-1.666649	-1.089077	0.993832
C	-4.280310	-0.546215	-0.161529
H	1.947796	-4.217085	1.306417
H	3.593718	-4.763750	0.813836
H	3.394971	-3.373894	1.945314
H	5.218512	-3.331979	-0.895005
H	4.743622	-1.753043	-1.623803
H	5.135789	-1.846720	0.123056
H	3.001489	-4.626605	-1.874338
H	1.311355	-4.077105	-1.570344
H	2.367316	-3.141655	-2.676407
C	1.816226	2.765486	-0.821371
H	0.518942	3.089803	0.856518
C	2.509011	4.116705	-0.707342
H	2.539806	1.998570	-1.174646
H	1.000433	2.800070	-1.570440
C	3.605974	4.087908	0.349527
H	2.920452	4.416103	-1.690081
H	1.757717	4.888927	-0.434812
C	3.058295	3.633862	1.696861
H	4.401940	3.383636	0.025815
H	4.084512	5.081651	0.439428
C	2.369093	2.280865	1.582801
H	3.866619	3.586135	2.451064
H	2.329112	4.385234	2.068071
H	3.110853	1.507522	1.285264
H	1.957239	1.961757	2.560175
C	-5.443143	0.072179	0.629732
H	-4.566129	-0.511740	-1.239951
C	-6.727272	-0.724653	0.446724
H	-5.160117	0.089568	1.704165
H	-5.593542	1.127288	0.326939
C	-6.529727	-2.187952	0.819011
H	-7.540084	-0.273656	1.046701
H	-7.046958	-0.657753	-0.615025
C	-5.383537	-2.801433	0.025619
H	-6.301559	-2.260471	1.903833
H	-7.463642	-2.758534	0.656390
C	-4.095516	-2.012194	0.218247
H	-5.227524	-3.857250	0.316600
H	-5.647380	-2.809596	-1.053298
H	-3.791612	-2.068653	1.285861
H	-3.271537	-2.458545	-0.372108

Methoxy

4d

SCF Energy: -1649.7626656  
ZPE-corrected Energy: -1649.29714

$\Delta U$ : -1649.26461

$\Delta H$ : -1649.26367

$\Delta G$ : -1649.36576

Num. Imaginary Frequencies: 0

C	-1.052352	-4.329632	1.121008
C	-2.135822	-4.047718	1.936173
N	-2.689185	-2.878676	1.520483
C	-1.974377	-2.366075	0.455950
C	-0.947673	-3.272162	0.191203
C	-2.331124	-1.120424	-0.193706
C	-3.749211	-0.719322	-0.230837
C	-4.125660	0.633460	-0.122249
C	-5.452945	1.016980	-0.189197
C	-6.462045	0.057649	-0.373729
C	-6.109219	-1.293520	-0.482660
C	-4.769652	-1.665635	-0.406278
H	-0.416444	-5.214475	1.184047
H	-2.552657	-4.597430	2.781137
H	-3.480142	-2.415377	1.960989
H	-0.234667	-3.193493	-0.632654
H	-3.356492	1.396793	0.046651
H	-5.748496	2.067151	-0.090079
O	-7.720206	0.521554	-0.426891
H	-6.868386	-2.066359	-0.635265
H	-4.511376	-2.725999	-0.513804
C	-1.389628	-0.312943	-0.783061
C	0.004685	-0.503243	-0.689225
C	1.223627	-0.742272	-0.613255
C	2.517972	-1.356428	-0.589054
C	3.581640	-0.881748	-1.383408
C	4.812014	-1.509596	-1.354550
C	5.024288	-2.627906	-0.529187
C	3.975650	-3.104623	0.269245
C	2.739047	-2.468345	0.238616
H	3.425306	-0.011099	-2.031648
H	5.645892	-1.154989	-1.969712
O	6.251726	-3.165316	-0.567901
H	4.111550	-3.970001	0.924390
H	1.922540	-2.837418	0.870821
Au	1.166201	1.492182	-0.072553
H	-1.728998	0.547017	-1.375671
P	1.634842	3.697963	0.533360
C	2.837226	4.511851	-0.561749
C	0.162786	4.766821	0.513225
C	2.325994	3.852689	2.208154
H	2.449747	4.527071	-1.595360
H	3.790030	3.954557	-0.548324
H	-0.592591	4.375939	1.217125
H	-0.272037	4.781431	-0.501504
H	0.440127	5.796404	0.807351
H	3.015389	5.549124	-0.221349
H	2.518933	4.916928	2.439107
H	1.614532	3.441163	2.945161
H	3.271599	3.286552	2.274467
C	6.539742	-4.284702	0.233595
H	7.590320	-4.549460	0.040167
H	6.418484	-4.053666	1.309866
H	5.896511	-5.146916	-0.029119
C	-8.779100	-0.385568	-0.606490
H	-9.705984	0.207942	-0.617369
H	-8.688246	-0.929582	-1.566852
H	-8.829979	-1.118305	0.222440

5d

SCF Energy: -1649.77792896

ZPE-corrected Energy: -1649.31065

$\Delta U$ : -1649.27950

$\Delta H$ : -1649.27856

$\Delta G$ : -1649.37633

Num. Imaginary Frequencies: 0

C	-0.946020	3.910204	-0.123589
C	-2.222544	4.213054	-0.429783
N	-3.023441	3.070064	-0.334484
C	-2.295062	2.006704	0.023616
C	-0.918995	2.473644	0.286244
C	-2.649789	0.650663	0.109084
C	-4.048954	0.197672	-0.002115
C	-4.393471	-0.904497	-0.804550
C	-5.703688	-1.343275	-0.892283
C	-6.722653	-0.692434	-0.179091
C	-6.398397	0.405781	0.626051
C	-5.074474	0.835265	0.706816
H	-0.113573	4.610878	-0.057141
H	-2.674327	5.166774	-0.704808
H	-4.017406	3.038394	-0.560494
H	-0.937291	2.550524	1.414355
H	-3.616950	-1.415238	-1.387089
H	-5.976526	-2.196170	-1.523359
O	-7.963352	-1.186511	-0.329697
H	-7.163918	0.929082	1.206610
H	-4.837486	1.676202	1.372065
C	-1.570480	-0.225361	0.198141
C	-0.179187	0.116185	0.190840
C	0.174743	1.451719	0.179529
C	1.564293	1.927137	0.220199
C	2.498230	1.393944	1.131310
C	3.820047	1.803024	1.123956
C	4.263600	2.757970	0.193684
C	3.350090	3.303147	-0.717556
C	2.018334	2.895334	-0.685234
H	2.163603	0.662440	1.876769
H	4.544309	1.404448	1.843073
O	5.562832	3.088848	0.256833
H	3.663513	4.043133	-1.459855
H	1.323650	3.317076	-1.422169
Au	1.256160	-1.409164	0.058909
H	-1.827099	-1.293881	0.237273
P	2.952631	-3.069408	-0.125133
C	3.969947	-3.241283	1.381573
C	2.406746	-4.772417	-0.488604
C	4.174735	-2.702500	-1.431070
H	3.334467	-3.557670	2.227694
H	4.424167	-2.265346	1.631992
H	1.859734	-4.791975	-1.447724
H	1.727423	-5.123617	0.308124
H	3.277423	-5.452024	-0.551153
H	4.771272	-3.988401	1.227151
H	4.966903	-3.474442	-1.452289
H	3.672091	-2.667263	-2.413930
H	4.632126	-1.715226	-1.238279
C	6.071350	4.049199	-0.634874
H	7.139974	4.166239	-0.398452
H	5.969482	3.719820	-1.687364
H	5.565430	5.026450	-0.509590
C	-9.029393	-0.579656	0.355038
H	-9.938911	-1.137481	0.084206
H	-8.889487	-0.631573	1.452660
H	-9.154480	0.479437	0.055209

6d

SCF Energy: -1649.76455482

ZPE-corrected Energy: -1649.29793

$\Delta U$ : -1649.26641

$\Delta H$ : -1649.26547

$\Delta G$ : -1649.36508

Num. Imaginary Frequencies: 0

C	0.034534	-3.810398	0.627419
C	-0.449569	-2.664478	-0.203922
C	-1.054633	-4.463496	1.076083
N	-2.232606	-3.771489	0.707396
C	-1.903248	-2.660949	0.054345
C	-0.122047	-1.170584	-0.238726
C	-1.398317	-0.531042	-0.320597
C	-2.487217	-1.394283	-0.186622
C	1.099079	-0.544829	-0.203270
C	2.342164	-1.315430	-0.242654
C	2.528816	-2.417850	-1.105456
C	3.711317	-3.135695	-1.118169
C	4.760390	-2.795115	-0.248239
C	4.607463	-1.696379	0.607622
C	3.425010	-0.963546	0.582082
Au	1.231067	1.542428	-0.048676
P	1.410991	3.918973	0.080988
C	2.515835	4.524878	1.401438
C	-0.166727	4.783251	0.389535
C	2.058074	4.704745	-1.433845
H	-3.160692	-3.995782	1.064591
H	1.067632	-4.152571	0.711671
H	-0.351409	-3.006450	-1.265947
H	-1.139529	-5.400070	1.629396
H	-1.492118	0.551594	-0.477338
C	-3.911049	-1.068250	-0.152575
H	1.740728	-2.693101	-1.816003
H	3.860088	-3.976072	-1.805224
O	5.862362	-3.558694	-0.317381
H	5.408597	-1.393788	1.288536
H	3.323254	-0.094487	1.245061
H	2.153969	4.169360	2.382461
H	3.535632	4.132157	1.241329
H	2.547011	5.630681	1.402856
H	-0.006688	5.877031	0.431345
H	-0.882367	4.550855	-0.418976
H	-0.597619	4.441818	1.347399
H	2.114520	5.802248	-1.306952
H	3.065933	4.310950	-1.654667
H	1.396952	4.470078	-2.286836
C	-4.362008	0.218185	0.169422
C	-4.878051	-2.045724	-0.450859
C	-6.230702	-1.751272	-0.419324
C	-6.667444	-0.458619	-0.092664
C	-5.718182	0.529778	0.200444
H	-3.637752	1.002055	0.421499
H	-4.562741	-3.055120	-0.745165
H	-6.984037	-2.509902	-0.657530
O	-7.996589	-0.262407	-0.086661
H	-6.024432	1.546483	0.463943
C	-8.499773	1.013416	0.218883
H	-9.596707	0.944145	0.158815
H	-8.215108	1.328420	1.241971
H	-8.147085	1.773202	-0.505879
C	6.951287	-3.269535	0.522966
H	7.727587	-4.018695	0.304598
H	7.359932	-2.259391	0.324766
H	6.669315	-3.343556	1.591525

TS\_4d\_5d  
SCF Energy: -1649.73726564  
ZPE-corrected Energy: -1649.27253  
 $\Delta U$ : -1649.24074  
 $\Delta H$ : -1649.23979  
 $\Delta G$ : -1649.34065

Num. Imaginary Frequencies: 1

Imaginary Frequency: -488.9385

C	-0.753885	4.066240	0.287212
C	-1.805269	4.138876	1.159926
N	-2.572638	3.001977	1.019606
C	-2.033458	2.185514	0.078990
C	-0.860183	2.809795	-0.398588
C	-2.497949	0.850108	-0.214009
C	-3.941538	0.560004	-0.188795
C	-4.871179	1.510305	-0.655628
C	-6.228523	1.239893	-0.672225
C	-6.712647	0.004313	-0.215277
C	-5.805170	-0.949801	0.262956
C	-4.442506	-0.664809	0.272832
H	0.009051	4.830670	0.130722
H	-2.084868	4.908833	1.879821
H	-3.372836	2.759970	1.601590
H	-0.467115	2.627592	-1.405679
H	-4.516322	2.476308	-1.035886
H	-6.950333	1.974154	-1.046197
O	-8.043266	-0.170311	-0.266020
H	-6.149389	-1.915351	0.645298
H	-3.753790	-1.415020	0.679117
C	-1.555160	-0.129898	-0.388485
C	-0.138750	0.080830	-0.225874
C	0.526557	1.195563	-0.072412
Au	1.173903	-1.590299	-0.013307
H	-1.905222	-1.151602	-0.579304
C	1.804334	1.833240	-0.181027
C	2.656600	1.547972	-1.272396
C	3.904678	2.129615	-1.363615
C	4.344398	3.026106	-0.371496
C	3.506244	3.327126	0.715215
C	2.253391	2.736025	0.797357
H	2.315423	0.850168	-2.046382
H	4.577033	1.915017	-2.201050
O	5.564486	3.540245	-0.545800
H	3.824658	4.019048	1.500177
H	1.596152	2.973639	1.642173
P	2.567366	-3.485438	0.202114
C	2.931821	-3.950032	1.926687
C	1.886358	-5.000668	-0.547577
C	4.204316	-3.284825	-0.575011
H	3.585737	-4.841794	1.952804
H	3.436749	-3.112225	2.439039
H	1.990830	-4.171723	2.460290
H	4.812295	-4.198464	-0.435814
H	4.081174	-3.089808	-1.654958
H	4.728116	-2.424746	-0.121643
H	2.587159	-5.845247	-0.408694
H	0.919348	-5.248560	-0.075648
H	1.718674	-4.838981	-1.627065
C	6.080799	4.448661	0.399024
H	7.085225	4.729087	0.048193
H	5.454066	5.358424	0.466475
H	6.163568	3.984063	1.400122
C	-8.591278	-1.390209	0.165475
H	-9.680355	-1.316150	0.023847
H	-8.207438	-2.240872	-0.431149
H	-8.379723	-1.574220	1.237097



TS\_4d.6d  
SCF Energy: -1649.73655130  
ZPE-corrected Energy: -1649.27181  
 $\Delta U$ : -1649.24016  
 $\Delta H$ : -1649.23921  
 $\Delta G$ : -1649.33906

Num. Imaginary Frequencies: 1

Imaginary Frequency: -472.4948

C	-0.067576	-3.661421	0.997936
C	-0.585695	-2.799398	-0.022849
C	-1.046851	-3.782966	1.949859
N	-2.147831	-3.042265	1.572275
C	-1.885020	-2.413830	0.398371
C	-0.182345	-0.800867	-0.455931
C	-1.519908	-0.452409	-0.724876
C	-2.505100	-1.264750	-0.188878
C	1.085226	-0.485316	-0.383599
C	2.245449	-1.371622	-0.456362
C	2.349095	-2.345070	-1.469762
C	3.417790	-3.224596	-1.510807
C	4.421098	-3.170107	-0.530646
C	4.342977	-2.198572	0.475266
C	3.274064	-1.304769	0.492357
Au	1.339787	1.601079	-0.053263
P	1.688035	3.918270	0.266348
C	0.163273	4.915720	0.199203
C	2.784928	4.674237	-0.977779
C	2.447144	4.352793	1.865803
H	-2.941772	-2.838033	2.176674
H	0.888074	-4.189172	0.984047
H	-0.308777	-2.901531	-1.080709
H	-1.066476	-4.359224	2.876104
H	-1.740217	0.401176	-1.380633
C	-3.936501	-0.997689	-0.180655
H	1.585439	-2.391012	-2.256257
H	3.507565	-3.975000	-2.304084
O	5.412922	-4.071437	-0.642867
H	5.113171	-2.121950	1.248709
H	3.224256	-0.543218	1.280880
H	-0.322839	4.786461	-0.783955
H	-0.536632	4.579913	0.984609
H	0.398243	5.985620	0.352519
H	2.905802	5.755305	-0.777370
H	3.774281	4.184788	-0.946879
H	2.356156	4.535306	-1.985804
H	2.578149	5.448725	1.941912
H	1.802554	4.004659	2.691957
H	3.431566	3.860692	1.956561
C	-4.434662	0.305754	-0.327602
C	-4.867362	-2.045800	-0.035356
C	-6.227869	-1.798624	-0.036836
C	-6.710878	-0.488506	-0.188889
C	-5.799117	0.567876	-0.334901
H	-3.736929	1.146532	-0.419441
H	-4.513972	-3.080610	0.054408
H	-6.955040	-2.610949	0.067095
O	-8.042422	-0.343184	-0.181367
H	-6.143904	1.600085	-0.445460
C	-8.598385	0.938975	-0.343337
H	-9.691465	0.814618	-0.315500
H	-8.291808	1.619058	0.474923
H	-8.310384	1.384426	-1.315249
C	6.450945	-4.066288	0.303126
H	7.138542	-4.879669	0.024685
H	7.005848	-3.107511	0.293199
H	6.069357	-4.252514	1.326441