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Supplementary Material

Why does the synthesis of *N*-phenylbenzamide from benzenesulfinate and phenylisocyanate via the palladium- mediated Extrusion–Insertion pathway not work? A mechanistic exploration

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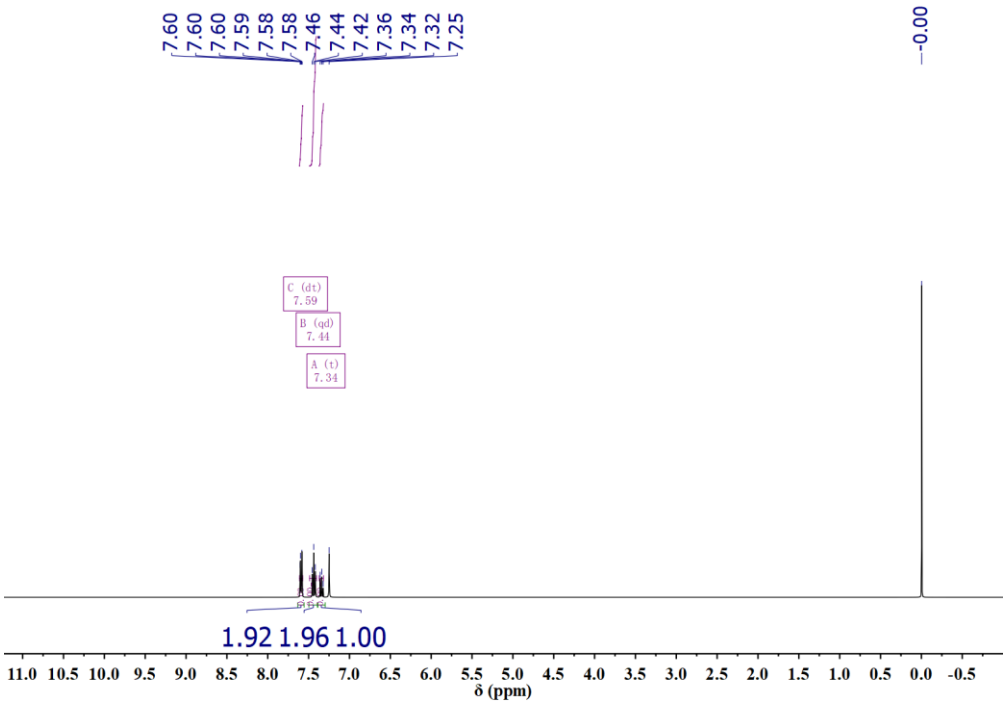

Figure S1. ^{1}H NMR spectra (400 MHz, $CDCl_3$) of biphenyl.

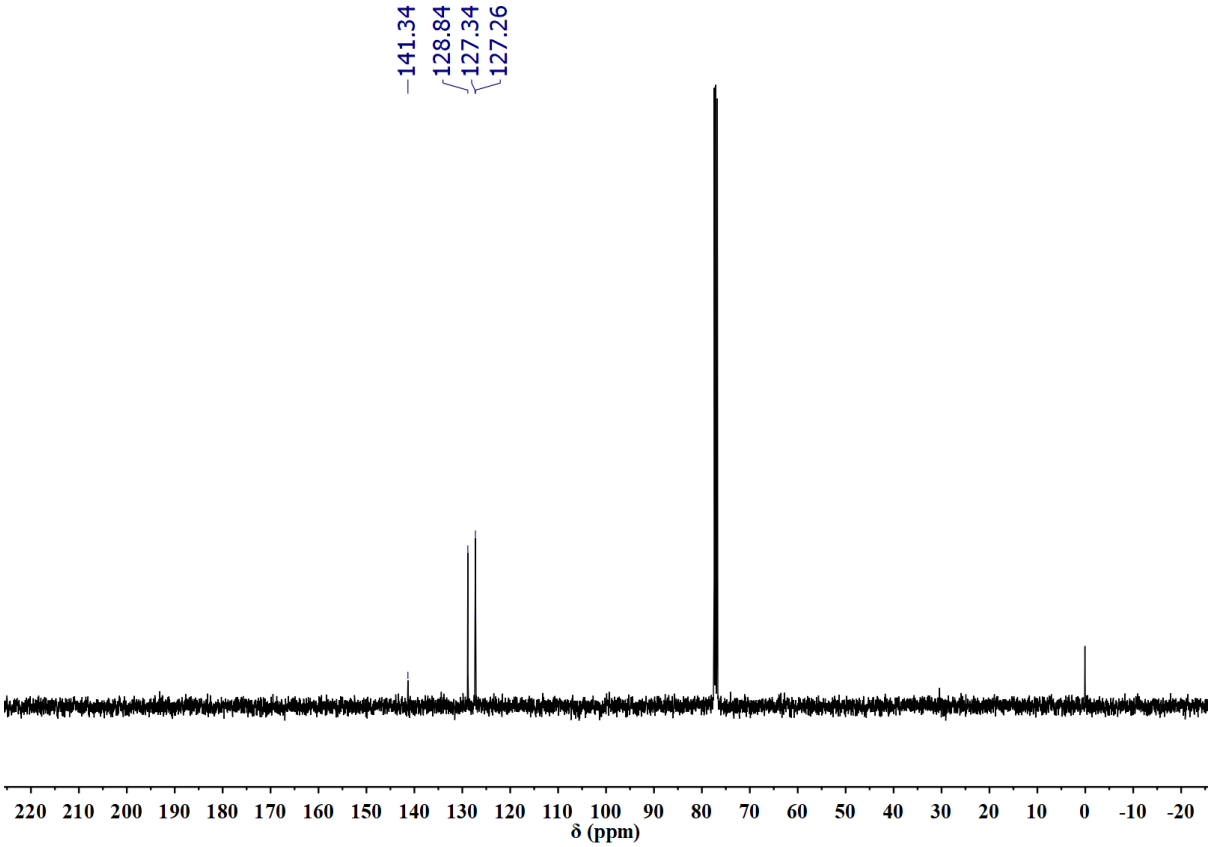

Figure S2. ^{13}C NMR spectra (400 MHz, $CDCl_3$) of biphenyl.

Cartesian coordinates and energies for all DFT calculated structures

4

Zero-point correction= 0.262913 (Hartree/Particle)
Thermal correction to Energy= 0.279320
Thermal correction to Enthalpy= 0.280264
Thermal correction to Gibbs Free Energy= 0.216986
Sum of electronic and zero-point Energies= -928.995980
Sum of electronic and thermal Energies= -928.979573
Sum of electronic and thermal Enthalpies= -928.978629
Sum of electronic and thermal Free Energies= -929.041907
Single Point Energy Calculations with extended basis set: HF = -929.539543

H	5.390653	0.780965	0.011611
C	4.303911	0.839254	-0.008020
C	3.555872	-0.377927	0.036420
C	3.671203	2.039189	-0.076282
C	2.147432	-0.332140	0.012798
C	4.162643	-1.648077	0.101052
C	2.243242	2.118774	-0.102306
H	4.237624	2.967796	-0.113229
N	1.388408	-1.454672	0.045349
C	1.478447	0.935010	-0.051822
C	3.378687	-2.777964	0.135441
H	5.248887	-1.718465	0.122581
C	1.555533	3.344987	-0.178493
C	1.983123	-2.635412	0.104607
N	0.113762	0.965681	-0.065538
H	3.817150	-3.770307	0.185264
C	0.180954	3.352687	-0.201197
H	2.122493	4.273392	-0.220372
H	1.330606	-3.506471	0.129275
C	-0.510110	2.136191	-0.142023
H	-0.382420	4.278919	-0.262920
H	-1.596676	2.110407	-0.150946
Pd	-0.751944	-0.935593	0.017315
C	-2.611638	-0.313398	0.020644
C	-3.418356	-0.758807	-1.023238
C	-3.138261	0.421661	1.079934
C	-4.786883	-0.484247	-0.987535
H	-2.994524	-1.318175	-1.858952
C	-4.508423	0.687611	1.104556
C	-5.329070	0.237367	0.073205
H	-5.425876	-0.830211	-1.798874
H	-4.931860	1.249906	1.935653
H	-6.395588	0.454249	0.093329
H	-2.496050	0.779676	1.885962

5

Zero-point correction= 0.345264 (Hartree/Particle)
Thermal correction to Energy= 0.368260
Thermal correction to Enthalpy= 0.369204
Thermal correction to Gibbs Free Energy= 0.291873
Sum of electronic and zero-point Energies= -1482.018722
Sum of electronic and thermal Energies= -1481.995726
Sum of electronic and thermal Enthalpies= -1481.994781
Sum of electronic and thermal Free Energies= -1482.072112
Single Point Energy Calculations with extended basis set: HF = -1483.105848

H	5.893687	0.015388	0.019613
C	4.848119	0.318305	0.013123
C	3.845529	-0.701111	0.005433
C	4.504009	1.632469	0.011870
C	2.483777	-0.339007	-0.002735
C	4.151775	-2.076793	0.005412
C	3.130782	2.031287	0.003613
H	5.265656	2.410037	0.017212
N	1.489247	-1.264054	-0.011249
C	2.120552	1.048033	-0.002613
C	3.133212	-3.000286	-0.003391
H	5.194366	-2.390581	0.012288
C	2.729809	3.381358	0.001376
C	1.803427	-2.551272	-0.012008
N	0.799349	1.375918	-0.008852
H	3.337597	-4.067049	-0.003831
C	1.390454	3.693360	-0.006366
H	3.488193	4.162494	0.005614
H	0.962696	-3.246022	-0.019895
C	0.448906	2.655888	-0.010849
H	1.047410	4.723684	-0.008716
H	-0.618586	2.869192	-0.016086
Pd	-0.486332	-0.319492	-0.010085
C	-2.120560	0.838179	-0.000201
C	-2.642645	1.306295	-1.206698
C	-2.630705	1.305092	1.211724
C	-3.671985	2.249133	-1.197329
H	-2.244776	0.949116	-2.158079
C	-3.660334	2.247959	1.213202
C	-4.179046	2.721398	0.010747
H	-4.074721	2.616095	-2.140529
H	-4.053684	2.614245	2.160606
H	-4.979819	3.458792	0.014939
H	-2.221872	0.949344	2.159006
S	-1.868997	-2.181064	-0.002865
O	-1.171154	-3.503765	-0.050974
C	-3.066513	-2.135540	-1.337529
H	-3.678961	-1.233066	-1.243811
H	-2.505547	-2.115585	-2.276672
H	-3.676350	-3.043293	-1.272017
C	-2.958119	-2.174939	1.422072

H -3.573489 -1.269727 1.400984
H -3.574231 -3.079918 1.379414
H -2.325950 -2.181249 2.315093

TS5-6

Zero-point correction= 0.448747 (Hartree/Particle)
Thermal correction to Energy= 0.480246
Thermal correction to Enthalpy= 0.481190
Thermal correction to Gibbs Free Energy= 0.383594
Sum of electronic and zero-point Energies= -1881.357486
Sum of electronic and thermal Energies= -1881.325988
Sum of electronic and thermal Enthalpies= -1881.325044
Sum of electronic and thermal Free Energies= -1881.422640
Single Point Energy Calculations with extended basis set: HF = -1882.988175

H 6.018340 -1.876793 0.121320
C 5.170851 -1.195366 0.075576
C 3.884567 -1.731431 -0.243042
C 5.329342 0.132374 0.312485
C 2.765511 -0.874525 -0.302784
C 3.673914 -3.098664 -0.508236
C 4.217322 1.029522 0.246469
H 6.307873 0.543351 0.554190
N 1.522015 -1.338265 -0.591239
C 2.933721 0.530691 -0.059059
C 2.410778 -3.548714 -0.817764
H 4.518455 -3.784672 -0.468206
C 4.347307 2.412999 0.475086
C 1.354814 -2.627512 -0.845467
N 1.848355 1.349911 -0.139318
H 2.217584 -4.595623 -1.032117
C 3.238920 3.222334 0.392493
H 5.326584 2.824515 0.713659
H 0.338605 -2.951892 -1.068822
C 1.998645 2.648849 0.082160
H 3.303342 4.293376 0.560313
H 1.101315 3.260350 0.011871
Pd 0.025277 0.269635 -0.440828
C -1.098609 1.899679 -0.361153
C -1.600670 2.409248 -1.557123
C -1.377723 2.527384 0.851086
C -2.430253 3.532116 -1.529905
H -1.360990 1.942633 -2.513422
C -2.212905 3.646168 0.867014
C -2.746129 4.143153 -0.319043
H -2.828834 3.926348 -2.463719
H -2.439889 4.131142 1.815543
H -3.398003 5.014641 -0.301754
S -0.562538 -0.544526 1.965854
O 0.326557 0.332641 2.816229
C -0.108857 -2.254733 2.333064

H -0.779498 -2.934372 1.793552
H 0.924723 -2.401326 2.001086
H -0.179737 -2.413072 3.415177
C -2.182401 -0.559200 2.768631
H -2.812127 -1.337089 2.319559
H -2.028287 -0.744093 3.838287
C -2.874931 -1.227138 -0.718035
C -3.829765 -0.267217 -0.392549
C -4.929023 -0.646259 0.371136
C -5.062236 -1.960765 0.813199
C -4.092073 -2.906212 0.489043
C -2.988396 -2.543233 -0.278685
H -3.705940 0.757976 -0.739357
H -5.684631 0.094554 0.623806
H -5.923158 -2.248793 1.412570
H -4.191614 -3.934415 0.830196
H -2.227379 -3.273864 -0.548576
N -1.727070 -0.840658 -1.481247
C -1.476128 -0.944236 -2.674314
O -1.136970 -0.990743 -3.789349
H -0.933919 2.163923 1.780552
H -2.638314 0.424433 2.614615
Imaginary Vibrational Frequency = -24.5479 cm^{-1}

6

Zero-point correction= 0.368497 (Hartree/Particle)
Thermal correction to Energy= 0.393435
Thermal correction to Enthalpy= 0.394380
Thermal correction to Gibbs Free Energy= 0.311157
Sum of electronic and zero-point Energies= -1328.375753
Sum of electronic and thermal Energies= -1328.350815
Sum of electronic and thermal Enthalpies= -1328.349871
Sum of electronic and thermal Free Energies= -1328.433094
Single Point Energy Calculations with extended basis set: HF = -1329.462879
C -2.332263 -0.255743 1.919181
H 5.656206 -2.321127 -0.099191
C 4.851555 -1.589213 -0.137335
C 3.527933 -2.015907 0.193564
C 5.097268 -0.300934 -0.491031
C 2.466399 -1.089773 0.152123
C 3.220216 -3.339843 0.565994
C 4.041429 0.662785 -0.540586
H 6.104124 0.026083 -0.743932
N 1.190973 -1.439933 0.453906
C 2.726362 0.271936 -0.217627
C 1.922504 -3.678524 0.872404
H 4.017358 -4.080387 0.607184
C 4.257837 2.006716 -0.901485
C 0.929816 -2.689492 0.803234
N 1.689285 1.158018 -0.245676

H 1.654145 -4.689732 1.163931
C 3.198678 2.883193 -0.927589
H 5.263937 2.335557 -1.156006
H -0.107839 -2.922955 1.039545
C 1.920744 2.419315 -0.591008
H 3.329953 3.925631 -1.201719
H 1.062064 3.086744 -0.596182
N -2.001908 -0.671482 0.806363
Pd -0.142491 0.300582 0.276781
C -1.165563 1.985051 0.053300
C -1.952566 2.154794 -1.084033
C -1.094977 2.980475 1.026368
C -2.664175 3.343438 -1.253329
H -2.016241 1.369850 -1.839122
C -1.815808 4.163517 0.850140
H -0.475768 2.846489 1.915016
C -2.595555 4.346106 -0.288928
H -3.275362 3.482413 -2.144261
H -1.762677 4.943728 1.608415
H -3.153309 5.271138 -0.424428
O -2.572971 0.167459 2.974804
C -2.747760 -1.494074 -0.093267
C -2.156377 -1.854413 -1.300301
C -4.032698 -1.923732 0.235488
C -2.865373 -2.655296 -2.189856
H -1.149950 -1.508012 -1.536304
C -4.727747 -2.723941 -0.662179
H -4.486703 -1.635510 1.182910
C -4.148714 -3.091201 -1.874880
H -2.406703 -2.937319 -3.135060
H -5.730960 -3.060167 -0.409350
H -4.699378 -3.716512 -2.574122

TS6-7

Zero-point correction= 0.368074 (Hartree/Particle)
Thermal correction to Energy= 0.392116
Thermal correction to Enthalpy= 0.393060
Thermal correction to Gibbs Free Energy= 0.312624
Sum of electronic and zero-point Energies= -1328.356427
Sum of electronic and thermal Energies= -1328.332385
Sum of electronic and thermal Enthalpies= -1328.331441
Sum of electronic and thermal Free Energies= -1328.411878
Single Point Energy Calculations with extended basis set: HF = -1329.443553
C 2.625038 1.255342 -0.229344
H -4.994321 -3.428615 -0.143126
C -4.374006 -2.535395 -0.099101
C -2.952954 -2.693817 -0.131920
C -4.936343 -1.301071 -0.015515
C -2.128311 -1.554050 -0.068333
C -2.319961 -3.948441 -0.229275

C	-4.123325	-0.125338	0.034212
H	-6.017775	-1.181448	0.010960
N	-0.771981	-1.635556	-0.079459
C	-2.721174	-0.254126	0.003013
C	-0.946389	-4.014851	-0.263253
H	-2.926743	-4.850905	-0.280821
C	-4.656395	1.175961	0.110574
C	-0.203632	-2.827591	-0.183837
N	-1.893915	0.825946	0.032862
H	-0.426584	-4.964826	-0.345354
C	-3.806088	2.256973	0.149687
H	-5.736291	1.310828	0.137782
H	0.885415	-2.849148	-0.198151
C	-2.422184	2.041580	0.107594
H	-4.183731	3.273241	0.210369
H	-1.726480	2.877925	0.132785
N	2.167749	0.096850	0.039146
Pd	0.138912	0.324548	0.008732
C	0.861141	2.238175	-0.017424
C	1.035031	2.879598	1.223790
C	0.673830	3.007722	-1.183550
C	1.045799	4.267490	1.293469
H	1.187823	2.282000	2.122832
C	0.691652	4.391470	-1.108084
H	0.537410	2.510073	-2.143845
C	0.878063	5.016034	0.129222
H	1.189071	4.767953	2.248850
H	0.560751	4.992017	-2.005961
H	0.895553	6.103055	0.182869
O	3.518877	1.984865	-0.492446
C	2.992858	-1.066243	0.082807
C	2.808113	-1.965695	1.131776
C	3.958234	-1.296815	-0.895644
C	3.600684	-3.106521	1.200081
H	2.046911	-1.758209	1.883548
C	4.750065	-2.437603	-0.811796
H	4.084873	-0.588561	-1.712796
C	4.572431	-3.343929	0.230495
H	3.459432	-3.810039	2.018015
H	5.506347	-2.620334	-1.572527
H	5.191322	-4.236944	0.286759

Imaginary Vibrational Frequency = -419.9637 cm^{-1}

7

Zero-point correction= 0.371209 (Hartree/Particle)
Thermal correction to Energy= 0.394898
Thermal correction to Enthalpy= 0.395842
Thermal correction to Gibbs Free Energy= 0.316986
Sum of electronic and zero-point Energies= -1328.389784
Sum of electronic and thermal Energies= -1328.366095

Sum of electronic and thermal Enthalpies= -1328.365150
Sum of electronic and thermal Free Energies= -1328.444007
Single Point Energy Calculations with extended basis set: HF = -1329.47691

C	2.308612	1.877749	-0.424623
H	-3.664366	-4.526442	-0.465249
C	-3.359573	-3.491625	-0.321967
C	-1.963775	-3.184803	-0.366218
C	-4.282356	-2.514534	-0.120586
C	-1.544149	-1.855458	-0.165589
C	-0.970800	-4.150263	-0.621530
C	-3.882150	-1.152867	0.050832
H	-5.345436	-2.746374	-0.098639
N	-0.231437	-1.496695	-0.195338
C	-2.511779	-0.830605	0.039288
C	0.346774	-3.763167	-0.687219
H	-1.259823	-5.187950	-0.778131
C	-4.798106	-0.095991	0.215107
C	0.679294	-2.418783	-0.468901
N	-2.061955	0.445227	0.183653
H	1.139030	-4.473626	-0.903225
C	-4.329918	1.190686	0.339818
H	-5.865129	-0.310297	0.232073
H	1.714641	-2.090752	-0.523038
C	-2.947314	1.421825	0.319221
H	-5.005578	2.032576	0.456578
H	-2.551399	2.429413	0.415887
N	2.088063	0.709539	0.227942
Pd	0.055499	0.572432	0.199790
C	1.067224	2.709472	-0.289749
C	0.443926	2.808032	0.981020
C	0.580111	3.469712	-1.370967
C	-0.630470	3.701509	1.156965
H	0.924906	2.367754	1.854335
C	-0.494656	4.312162	-1.182991
H	1.075955	3.389871	-2.336289
C	-1.091775	4.441011	0.086640
H	-1.074534	3.818307	2.143285
H	-0.874734	4.900685	-2.015103
H	-1.915370	5.139089	0.222127
O	3.311969	2.265324	-1.011401
C	2.997791	-0.351371	0.286985
C	3.031419	-1.114287	1.463028
C	3.827626	-0.701909	-0.788277
C	3.873473	-2.213372	1.562274
H	2.370385	-0.834465	2.283146
C	4.676691	-1.797134	-0.674811
H	3.800900	-0.108359	-1.698263
C	4.699219	-2.558084	0.492809
H	3.886944	-2.803834	2.476275
H	5.320065	-2.064773	-1.511003

H 5.360095 -3.419204 0.568937

8

Zero-point correction= 0.371389 (Hartree/Particle)
Thermal correction to Energy= 0.394973
Thermal correction to Enthalpy= 0.395917
Thermal correction to Gibbs Free Energy= 0.315841
Sum of electronic and zero-point Energies= -1328.395656
Sum of electronic and thermal Energies= -1328.372072
Sum of electronic and thermal Enthalpies= -1328.371128
Sum of electronic and thermal Free Energies= -1328.451204
Single Point Energy Calculations with extended basis set: HF = -1329.482782

C -2.069754 -0.981377 -0.283398
H 6.203412 1.721615 0.259422
C 5.377912 1.014876 0.202822
C 4.050962 1.533061 0.058468
C 5.606821 -0.325239 0.269701
C 2.979302 0.628764 -0.017293
C 3.739037 2.905578 -0.011005
C 4.526786 -1.261870 0.199020
H 6.618509 -0.710520 0.380315
N 1.687743 1.034208 -0.154820
C 3.219127 -0.770837 0.055295
C 2.425967 3.299538 -0.144200
H 4.539252 3.641575 0.042962
C 4.679459 -2.661658 0.266435
C 1.415027 2.329247 -0.213399
N 2.135478 -1.584244 -0.016184
H 2.154342 4.349441 -0.197698
C 3.569353 -3.474660 0.192146
H 5.675226 -3.087051 0.377229
H 0.365557 2.607434 -0.319020
C 2.298368 -2.896984 0.049878
H 3.658174 -4.555630 0.242375
H 1.396671 -3.503557 -0.011417
Pd 0.355953 -0.537183 -0.228454
C -3.497503 -1.293938 -0.134727
C -3.850885 -2.521124 0.436891
C -4.494814 -0.422012 -0.587444
C -5.189357 -2.863559 0.574079
H -3.066664 -3.194683 0.775498
C -5.831224 -0.775442 -0.458319
H -4.225115 0.523127 -1.054976
C -6.179341 -1.991199 0.127238
H -5.462034 -3.813782 1.028388
H -6.605192 -0.100782 -0.817900
H -7.228418 -2.261541 0.231759
N -1.523057 0.215720 -0.453393
C -2.039688 1.464978 -0.070386
C -2.040072 2.508546 -1.001688

C -2.493070 1.693470 1.233830
C -2.514972 3.764101 -0.636206
H -1.673604 2.314620 -2.009328
C -2.969440 2.949101 1.588387
H -2.467037 0.879498 1.957789
C -2.982124 3.986395 0.656815
H -2.519909 4.571250 -1.366028
H -3.327299 3.121605 2.601656
H -3.351676 4.969410 0.941442
O -1.196806 -1.930991 -0.287557

9

Zero-point correction= 0.444426 (Hartree/Particle)
Thermal correction to Energy= 0.476748
Thermal correction to Enthalpy= 0.477692
Thermal correction to Gibbs Free Energy= 0.378403
Sum of electronic and zero-point Energies= -2262.029153
Sum of electronic and thermal Energies= -2261.996831
Sum of electronic and thermal Enthalpies= -2261.995887
Sum of electronic and thermal Free Energies= -2262.095177
Single Point Energy Calculations with extended basis set: HF = -2263.659842
H 4.789426 -2.659358 -1.226863
C 3.725159 -2.541559 -1.029710
C 3.106285 -1.297927 -1.366792
C 3.005961 -3.546854 -0.465320
C 1.731236 -1.113872 -1.118042
C 3.820753 -0.213491 -1.912945
C 1.608361 -3.392112 -0.205095
H 3.478501 -4.490634 -0.198556
N 1.102768 0.062270 -1.375176
C 0.966830 -2.181817 -0.540922
C 3.169638 0.970924 -2.164025
H 4.885076 -0.324709 -2.115509
C 0.828028 -4.403967 0.387023
C 1.801157 1.073053 -1.870637
N -0.360124 -1.985753 -0.314278
H 3.695483 1.830995 -2.569119
C -0.510464 -4.184458 0.615236
H 1.296498 -5.348524 0.659012
H 1.247266 1.999195 -2.030798
C -1.070369 -2.952797 0.249451
H -1.140225 -4.942617 1.071609
H -2.126265 -2.745088 0.418099
Pd -0.971472 0.043357 -0.665093
C -2.824219 -0.316859 0.009026
C -3.145235 -0.113251 1.352298
C -3.746070 -0.924986 -0.845501
C -4.381139 -0.542696 1.839695
H -2.441019 0.389426 2.020028
C -4.979921 -1.350773 -0.349666

C -5.295649 -1.165384 0.993904
H -4.627044 -0.388036 2.889860
H -5.693411 -1.830274 -1.018939
H -6.256461 -1.501361 1.380413
H -3.502357 -1.082866 -1.897744
S -1.640382 2.211109 -1.138161
O -0.580354 3.102356 -1.712701
C -2.280756 2.993038 0.344371
H -3.240370 2.532102 0.601527
H -1.559864 2.813759 1.156261
H -2.399293 4.059795 0.123102
C -3.075970 2.301253 -2.212829
H -3.886296 1.709804 -1.773786
H -3.360597 3.353972 -2.320701
H -2.782623 1.879652 -3.179002
C 1.952263 1.300777 1.709662
C 2.060693 2.641433 1.346553
C 3.305453 3.172748 1.020339
C 4.437371 2.358907 1.041521
C 4.323511 1.015119 1.392047
C 3.078911 0.484146 1.723636
H 1.168491 3.269065 1.343591
H 3.395630 4.224313 0.750354
H 5.410228 2.773099 0.780812
H 5.207620 0.377711 1.404339
H 2.968807 -0.563953 2.005840
S 0.296785 0.578295 1.981627
O 0.598585 -0.642364 2.828212
O -0.419649 1.676560 2.758432

TS9-10

Zero-point correction= 0.442851 (Hartree/Particle)
Thermal correction to Energy= 0.474202
Thermal correction to Enthalpy= 0.475146
Thermal correction to Gibbs Free Energy= 0.376135
Sum of electronic and zero-point Energies= -2262.012170
Sum of electronic and thermal Energies= -2261.980819
Sum of electronic and thermal Enthalpies= -2261.979875
Sum of electronic and thermal Free Energies= -2262.078886
Single Point Energy Calculations with extended basis set: HF = -2263.642859
H 5.918867 -2.505824 -0.803063
C 5.141849 -1.746298 -0.730580
C 3.864106 -2.130588 -0.214694
C 5.378486 -0.468588 -1.124785
C 2.835597 -1.170441 -0.100252
C 3.573141 -3.450672 0.181869
C 4.355095 0.525997 -1.035892
H 6.349886 -0.175122 -1.520406
N 1.601289 -1.491342 0.369581
C 3.087546 0.182292 -0.516576

C	2.321939	-3.755578	0.665609
H	4.344698	-4.215004	0.094505
C	4.553947	1.854059	-1.459520
C	1.357411	-2.739074	0.742273
N	2.086387	1.095891	-0.414658
H	2.064220	-4.764752	0.974890
C	3.522534	2.758838	-1.363550
H	5.521869	2.146518	-1.864497
H	0.343297	-2.948807	1.074972
C	2.296579	2.335456	-0.833600
H	3.634301	3.789030	-1.689049
H	1.457780	3.025378	-0.748140
Pd	0.187006	0.199947	0.242268
C	-0.694126	1.960841	-0.042868
C	-1.265312	2.262996	-1.276606
C	-0.506732	2.977965	0.900262
C	-1.693297	3.564116	-1.549201
H	-1.338558	1.483964	-2.037257
C	-0.948584	4.274731	0.626285
C	-1.548966	4.568799	-0.595997
H	-2.136237	3.788885	-2.519213
H	-0.811178	5.058232	1.371603
H	-1.891332	5.580608	-0.808875
H	0.000469	2.786382	1.849622
S	-0.662275	0.350001	2.808113
O	0.226520	1.116102	3.759361
C	-1.119662	-1.199042	3.620801
H	-1.995708	-1.620578	3.116421
H	-0.274014	-1.890790	3.551771
H	-1.341856	-0.970351	4.669896
C	-2.304092	1.108589	2.853956
H	-2.999663	0.454083	2.314681
H	-2.611615	1.244480	3.896990
C	-3.220878	-1.267879	-1.056409
C	-3.917546	-0.237408	-1.683268
C	-5.303038	-0.313236	-1.791599
C	-5.984439	-1.419250	-1.283077
C	-5.282281	-2.443865	-0.652583
C	-3.895480	-2.367855	-0.531368
H	-3.374371	0.604152	-2.112083
H	-5.849688	0.483134	-2.294245
H	-7.066615	-1.486279	-1.388450
H	-5.815164	-3.314512	-0.269855
H	-3.325645	-3.175462	-0.074846
S	-1.396607	-1.255225	-1.080703
O	-1.075699	-2.689282	-0.767124
O	-1.108105	-0.850022	-2.503319
H	-2.242151	2.072991	2.344138

Imaginary Vibrational Frequency = -52.2801 cm^{-1}

10

Zero-point correction= 0.363525 (Hartree/Particle)
Thermal correction to Energy= 0.388703
Thermal correction to Enthalpy= 0.389647
Thermal correction to Gibbs Free Energy= 0.306540
Sum of electronic and zero-point Energies= -1709.058020
Sum of electronic and thermal Energies= -1709.032843
Sum of electronic and thermal Enthalpies= -1709.031899
Sum of electronic and thermal Free Energies= -1709.115006
Single Point Energy Calculations with extended basis set: HF = -1710.145146

N	-1.890441	-1.346471	-0.136989
C	-3.011064	-0.614819	0.091177
C	-4.284001	-1.207779	0.216912
C	-4.364195	-2.608979	0.092224
C	-3.220245	-3.336031	-0.138741
C	-1.992629	-2.663436	-0.245061
Pd	-0.089345	-0.082195	-0.312903
H	-5.333341	-3.097585	0.182206
H	-3.248441	-4.417554	-0.237656
H	-1.053801	-3.192997	-0.413127
N	-1.645751	1.360681	0.080494
C	-1.511454	2.675359	0.184848
C	-2.596793	3.529424	0.425557
C	-3.854472	2.988708	0.558191
C	-4.028103	1.595115	0.450527
C	-2.881856	0.810013	0.208309
H	-0.500337	3.066201	0.078577
H	-2.428407	4.599662	0.502607
H	-4.720820	3.621386	0.745119
C	-5.304852	0.962980	0.574720
C	-5.427905	-0.385165	0.461414
H	-6.175270	1.589823	0.760865
H	-6.399958	-0.866582	0.554402
H	1.578248	1.170973	-2.587164
C	1.896547	1.673280	-1.673078
C	2.850635	2.690227	-1.742432
C	1.370870	1.284099	-0.440243
C	3.294353	3.317670	-0.581206
C	1.818008	1.917951	0.723148
C	2.775745	2.929903	0.652644
H	1.420131	1.623107	1.696497
H	3.252137	2.988536	-2.710878
H	3.118640	3.414412	1.566737
H	4.042733	4.106977	-0.636769
C	2.964473	-1.327721	0.303353
C	2.827022	-1.507304	1.676500
C	3.889956	-1.183591	2.512536
C	5.075201	-0.686631	1.971168
C	5.202182	-0.517626	0.594570
C	4.139741	-0.834557	-0.248406

H 1.891372 -1.890602 2.083858
H 3.795746 -1.319031 3.588543
H 5.904600 -0.430060 2.627944
H 6.129942 -0.131758 0.175440
H 4.208956 -0.696199 -1.325697
S 1.543226 -1.660299 -0.751322
O 2.052356 -1.606943 -2.150405
O 1.063455 -3.005430 -0.301237

TS10-11
Zero-point correction= 0.360743 (Hartree/Particle)
Thermal correction to Energy= 0.386140
Thermal correction to Enthalpy= 0.387084
Thermal correction to Gibbs Free Energy= 0.303930
Sum of electronic and zero-point Energies= -1709.012771
Sum of electronic and thermal Energies= -1708.987374
Sum of electronic and thermal Enthalpies= -1708.986430
Sum of electronic and thermal Free Energies= -1709.069584
Single Point Energy Calculations with extended basis set: HF = -1710.099897

N -1.485776 -1.344289 0.170995
C -2.671671 -0.682165 0.173122
C -3.908812 -1.356352 0.266828
C -3.883305 -2.761011 0.365290
C -2.676144 -3.418546 0.363707
C -1.498602 -2.664750 0.259732
Pd 0.252518 0.080330 0.037562
H -4.821997 -3.307626 0.441664
H -2.617081 -4.500519 0.438043
H -0.530697 -3.164984 0.249240
N -1.462507 1.391723 -0.011601
C -1.443284 2.714661 -0.103410
C -2.609975 3.490827 -0.117553
C -3.829281 2.861537 -0.031431
C -3.881569 1.458030 0.068110
C -2.659194 0.752312 0.074137
H -0.460774 3.180647 -0.169284
H -2.532516 4.571418 -0.195463
H -4.757774 3.430240 -0.038553
C -5.115934 0.742727 0.163038
C -5.129080 -0.611317 0.259371
H -6.043656 1.312356 0.157239
H -6.067968 -1.157522 0.332653
H 1.590851 1.641168 -2.201806
C 1.854468 2.163757 -1.280430
C 2.545642 3.375071 -1.336635
C 1.508878 1.616437 -0.044475
C 2.908030 4.032008 -0.162362
C 1.898214 2.256351 1.132902
C 2.590722 3.466848 1.071073

H 1.659542 1.817770 2.103955
H 2.803826 3.804829 -2.304390
H 2.884720 3.968140 1.993113
H 3.445778 4.977823 -0.208343
C 1.981973 -1.173738 0.213131
C 1.809445 -1.793046 1.470005
C 2.852060 -1.862646 2.389395
C 4.103504 -1.351116 2.052131
C 4.315426 -0.771329 0.798645
C 3.266386 -0.685514 -0.101818
H 0.842418 -2.219651 1.743017
H 2.694683 -2.323210 3.363450
H 4.925692 -1.420542 2.762861
H 5.301801 -0.392621 0.534480
H 3.426130 -0.265774 -1.097090
S 1.337002 -2.243639 -1.578805
O 1.684566 -1.235923 -2.621760
O 2.305403 -3.373473 -1.521058
Imaginary Vibrational Frequency = -100.9725 cm^{-1}

11
Zero-point correction= 0.361445 (Hartree/Particle)
Thermal correction to Energy= 0.387578
Thermal correction to Enthalpy= 0.388522
Thermal correction to Gibbs Free Energy= 0.303438
Sum of electronic and zero-point Energies= -1709.040600
Sum of electronic and thermal Energies= -1709.014468
Sum of electronic and thermal Enthalpies= -1709.013524
Sum of electronic and thermal Free Energies= -1709.098608
Single Point Energy Calculations with extended basis set: HF = -1710.127726
N -1.269712 -1.343145 -0.278011
C -2.463116 -0.701320 -0.333788
C -3.688719 -1.400889 -0.345657
C -3.636684 -2.807228 -0.289588
C -2.417638 -3.442114 -0.227080
C -1.250486 -2.665321 -0.222258
Pd 0.481712 0.029957 -0.223695
H -4.565608 -3.375545 -0.296209
H -2.344111 -4.524946 -0.181890
H -0.265106 -3.129479 -0.175000
N -1.281136 1.390720 -0.359404
C -1.273818 2.713054 -0.401738
C -2.447996 3.477313 -0.474379
C -3.661069 2.829530 -0.499952
C -3.700518 1.422073 -0.452674
C -2.469083 0.736716 -0.384312
H -0.293581 3.189948 -0.370668
H -2.383228 4.561153 -0.508357
H -4.594604 3.387600 -0.555229
C -4.924740 0.682273 -0.467877

C -4.919153 -0.674845 -0.414663
H -5.861500 1.234613 -0.521137
H -5.851127 -1.237675 -0.424375
H 2.793513 0.803372 -2.141259
C 2.796268 1.556055 -1.351860
C 3.684143 2.628593 -1.438257
C 1.921720 1.436159 -0.265113
C 3.725995 3.590943 -0.432176
C 1.974590 2.407680 0.740767
C 2.868316 3.477007 0.658161
H 1.298185 2.351469 1.597028
H 4.352816 2.706555 -2.295561
H 2.890216 4.223526 1.452018
H 4.424385 4.424051 -0.497184
C 1.975250 -1.319380 -0.321562
C 3.011834 -1.483902 0.601129
C 3.961685 -2.491401 0.436043
C 3.900244 -3.343950 -0.664277
C 2.882807 -3.180136 -1.599573
C 1.929307 -2.174486 -1.429565
H 3.092406 -0.816957 1.462362
H 4.758470 -2.606570 1.170955
H 4.643697 -4.129324 -0.792661
H 2.825975 -3.836688 -2.467670
H 1.139167 -2.064809 -2.175852
S 0.456677 -0.217448 2.375098
O 0.078339 -1.628138 2.577210
O -0.621391 0.749799 2.666848

12

Zero-point correction= 0.352206 (Hartree/Particle)
Thermal correction to Energy= 0.374114
Thermal correction to Enthalpy= 0.375058
Thermal correction to Gibbs Free Energy= 0.299671
Sum of electronic and zero-point Energies= -1160.525647
Sum of electronic and thermal Energies= -1160.503738
Sum of electronic and thermal Enthalpies= -1160.502794
Sum of electronic and thermal Free Energies= -1160.578181
Single Point Energy Calculations with extended basis set: HF = -1161.340992
N 1.260862 -1.363712 -0.028261
C 2.455363 -0.719165 -0.016282
C 3.684132 -1.412657 -0.033372
C 3.637896 -2.820176 -0.065271
C 2.420015 -3.459751 -0.076378
C 1.248984 -2.687692 -0.057024
Pd -0.481306 -0.000076 0.000091
H 4.569141 -3.384601 -0.079903
H 2.349481 -4.543591 -0.099947
H 0.264695 -3.157152 -0.057683
N 1.260915 1.363654 0.028683

C 1.249071 2.687623 0.057314
C 2.420130 3.459661 0.076313
C 3.637987 2.820050 0.065023
C 3.684178 1.412520 0.033259
C 2.455391 0.719061 0.016475
H 0.264788 3.157104 0.058190
H 2.349619 4.543506 0.099760
H 4.569257 3.384439 0.079417
C 4.912102 0.678882 0.015973
C 4.912078 -0.679051 -0.016301
H 5.847316 1.236369 0.028907
H 5.847274 -1.236564 -0.029400
H -2.851047 0.750982 1.923688
C -2.860970 1.487102 1.117721
C -3.790320 2.526165 1.164655
C -1.950363 1.368973 0.057065
C -3.849029 3.465893 0.137432
C -2.029658 2.322484 -0.970336
C -2.965802 3.357774 -0.933524
H -1.342443 2.265697 -1.818404
H -4.479193 2.597588 2.007108
H -3.003004 4.082794 -1.747239
H -4.579110 4.273773 0.170286
C -1.950537 -1.368935 -0.057212
C -2.861316 -1.486782 -1.117738
C -3.790846 -2.525689 -1.164649
C -3.849560 -3.465526 -0.137528
C -2.966151 -3.357682 0.933307
C -2.029818 -2.322570 0.970089
H -2.851384 -0.750557 -1.923610
H -4.479858 -2.596908 -2.007009
H -4.579787 -4.273275 -0.170364
H -3.003370 -4.082799 1.746937
H -1.342469 -2.265990 1.818059

TS12-13

Zero-point correction= 0.350535 (Hartree/Particle)
Thermal correction to Energy= 0.372322
Thermal correction to Enthalpy= 0.373266
Thermal correction to Gibbs Free Energy= 0.295815
Sum of electronic and zero-point Energies= -1160.509374
Sum of electronic and thermal Energies= -1160.487588
Sum of electronic and thermal Enthalpies= -1160.486643
Sum of electronic and thermal Free Energies= -1160.564094
Single Point Energy Calculations with extended basis set: HF = -1161.324719
N 1.367777 -1.359061 0.000265
C 2.560711 -0.721004 0.000113
C 3.790236 -1.414411 0.000032
C 3.741386 -2.822128 0.000136
C 2.521563 -3.460179 0.000301

C	1.353432	-2.682491	0.000354
Pd	-0.468282	-0.000326	0.000180
H	4.671431	-3.389029	0.000080
H	2.449851	-4.544413	0.000384
H	0.368020	-3.152071	0.000467
N	1.367651	1.358528	0.000118
C	1.353129	2.681953	0.000012
C	2.521168	3.459776	-0.000200
C	3.741065	2.821862	-0.000296
C	3.790087	1.414149	-0.000184
C	2.560644	0.720603	0.000018
H	0.367646	3.151397	0.000093
H	2.449332	4.544001	-0.000285
H	4.671042	3.388871	-0.000461
C	5.018149	0.679237	-0.000272
C	5.018218	-0.679366	-0.000162
H	5.954075	1.236103	-0.000429
H	5.954203	-1.236138	-0.000227
H	-2.386418	1.143513	2.156092
C	-2.663776	1.594485	1.201767
C	-3.427107	2.758466	1.201709
C	-2.252182	0.987934	0.000061
C	-3.814692	3.349278	0.000084
C	-2.663535	1.594665	-1.201636
C	-3.426864	2.758647	-1.201553
H	-2.385988	1.143834	-2.155973
H	-3.722886	3.207591	2.150051
H	-3.722453	3.207914	-2.149887
H	-4.417288	4.256251	0.000093
C	-2.252680	-0.987838	-0.000077
C	-2.664424	-1.594090	-1.201888
C	-3.428778	-2.757396	-1.202037
C	-3.817246	-3.347839	-0.000517
C	-3.429200	-2.757559	1.201222
C	-2.664839	-1.594255	1.201505
H	-2.386434	-1.143355	-2.156142
H	-3.724680	-3.206271	-2.150458
H	-4.420668	-4.254264	-0.000685
H	-3.725435	-3.206565	2.149477
H	-2.387182	-1.143654	2.155918

Imaginary Vibrational Frequency = -277.4155 cm^{-1}

13

Zero-point correction= 0.352711 (Hartree/Particle)
Thermal correction to Energy= 0.374636
Thermal correction to Enthalpy= 0.375580
Thermal correction to Gibbs Free Energy= 0.298695
Sum of electronic and zero-point Energies= -1160.553282
Sum of electronic and thermal Energies= -1160.531357
Sum of electronic and thermal Enthalpies= -1160.530413

Sum of electronic and thermal Free Energies= -1160.607298
Single Point Energy Calculations with extended basis set: HF = -1161.368627

N	0.950266	1.192765	0.487964
C	2.267741	0.986576	0.256721
C	3.243875	1.976099	0.512024
C	2.802349	3.215106	1.014584
C	1.459022	3.418244	1.231880
C	0.567064	2.371672	0.952490
Pd	-0.436385	-0.620857	0.001849
H	3.531477	3.997475	1.221439
H	1.082149	4.363146	1.614141
H	-0.505006	2.502616	1.108748
N	1.733808	-1.220264	-0.531300
C	2.110681	-2.394414	-1.014300
C	3.448373	-2.724977	-1.278453
C	4.421678	-1.785269	-1.026480
C	4.055193	-0.527257	-0.511235
C	2.682426	-0.290607	-0.273928
H	1.313705	-3.114756	-1.203516
H	3.695611	-3.705774	-1.675752
H	5.472677	-1.997179	-1.219055
C	5.015197	0.495607	-0.231226
C	4.624668	1.700420	0.258359
H	6.066247	0.284460	-0.423448
H	5.354305	2.481325	0.468162
H	-2.737741	1.793257	1.352610
C	-3.098273	1.726579	0.325455
C	-3.552424	2.875488	-0.309361
C	-3.072329	0.487022	-0.336236
C	-4.001331	2.821975	-1.627933
C	-3.541979	0.448959	-1.656839
C	-3.995411	1.599708	-2.294005
H	-3.569018	-0.499463	-2.192065
H	-3.552168	3.821761	0.230234
H	-4.356195	1.535781	-3.319878
H	-4.356508	3.721682	-2.127151
C	-2.570374	-0.731444	0.353019
C	-2.130674	-1.897383	-0.375516
C	-2.010799	-3.148910	0.294179
C	-2.258860	-3.262549	1.642243
C	-2.657355	-2.122250	2.376527
C	-2.810574	-0.904104	1.755834
H	-2.183113	-1.914705	-1.466431
H	-1.737180	-4.027256	-0.291113
H	-2.164592	-4.226118	2.140966
H	-2.872785	-2.212204	3.440690
H	-3.183976	-0.057870	2.332888

9b

Zero-point correction= 0.654956 (Hartree/Particle)

Thermal correction to Energy= 0.698657
Thermal correction to Enthalpy= 0.699601
Thermal correction to Gibbs Free Energy= 0.576664
Sum of electronic and zero-point Energies= -2095.411437
Sum of electronic and thermal Energies= -2095.367736
Sum of electronic and thermal Enthalpies= -2095.366792
Sum of electronic and thermal Free Energies= -2095.489730
Single Point Energy Calculations with extended basis set: HF = -2097.042126

Pd	1.703128	0.000182	-0.427327
C	2.739300	-1.631480	0.091044
C	2.803691	-2.751316	-0.738813
C	3.370007	-1.670627	1.335573
C	3.496789	-3.900199	-0.339651
C	4.063802	-2.813634	1.753972
C	4.117695	-3.913578	0.905366
H	3.559670	-4.774385	-0.982679
H	4.559788	-2.851276	2.720653
H	4.656766	-4.805131	1.222134
O	2.191039	-2.631436	-1.953017
O	3.287419	-0.532176	2.087494
C	3.767376	-0.580513	3.412340
H	4.855083	-0.738210	3.448506
H	3.533359	0.388763	3.860502
H	3.271247	-1.374917	3.990027
C	2.223372	-3.742882	-2.820858
H	1.670635	-3.450443	-3.717071
H	3.252958	-4.006738	-3.103196
H	1.739739	-4.621739	-2.370336
C	0.930240	4.171809	-0.174696
C	1.462361	2.909230	-0.423653
C	-0.677084	2.007096	-0.633342
C	-1.273063	3.245510	-0.417797
C	-0.451505	4.336607	-0.170631
H	1.573475	5.025488	0.016988
H	-2.357726	3.309754	-0.458898
H	-0.875589	5.320365	0.017926
C	2.911179	2.634706	-0.527183
C	3.847746	3.657486	-0.455256
C	4.580009	1.069487	-1.039979
C	5.189547	3.368308	-0.658773
H	3.536200	4.678348	-0.259310
C	5.550155	2.073443	-0.979552
H	5.936728	4.155857	-0.599315
H	6.583867	1.816235	-1.197074
N	0.649222	1.853640	-0.635405
N	3.288731	1.345588	-0.767471
C	-0.054576	-0.285520	2.305130
C	-1.284539	-0.095915	3.187151
C	-2.240974	-1.192842	2.720943
C	-0.609153	-0.955021	1.078293

H	0.476298	0.641374	2.057506
H	0.691025	-0.968493	2.742109
H	-1.725744	0.885983	2.975083
H	-1.069546	-0.151232	4.257879
H	-2.139525	-2.120682	3.304308
H	-3.297308	-0.889284	2.737767
O	-0.034254	-1.113935	-0.026522
C	-2.580267	-2.256912	0.416784
H	-3.595226	-2.371807	0.811252
H	-2.629344	-1.748872	-0.556817
H	-2.117709	-3.248278	0.320032
N	-1.825177	-1.428601	1.339791
C	-4.630702	0.217841	-0.553709
C	-4.620426	0.679731	0.763613
C	-5.606270	-0.714974	-0.922204
C	-5.563733	0.236906	1.697783
C	-6.554519	-1.175056	-0.003659
C	-6.520120	-0.690065	1.299759
H	-5.557299	0.604590	2.721152
H	-7.315808	-1.895065	-0.291640
H	-7.257806	-1.040498	2.019860
O	-3.620755	1.556455	1.080299
O	-5.567683	-1.115445	-2.222874
C	-6.545913	-2.029146	-2.662106
H	-7.561212	-1.620114	-2.554146
H	-6.344746	-2.211601	-3.720890
H	-6.485569	-2.981965	-2.116043
C	-3.796809	2.354482	2.229494
H	-2.984995	3.088955	2.224094
H	-4.763410	2.878282	2.208667
H	-3.733802	1.767383	3.158775
C	-3.612427	0.728680	-1.570699
O	-3.781406	1.892906	-1.987118
O	-2.692721	-0.074640	-1.875749
C	4.987483	-0.304831	-1.453690
H	5.187747	-0.944307	-0.584201
H	4.202311	-0.788127	-2.043930
H	5.904693	-0.252000	-2.050721
H	-1.277733	1.116354	-0.836364

TS9-10b

Zero-point correction= 0.653323 (Hartree/Particle)
Thermal correction to Energy= 0.696657
Thermal correction to Enthalpy= 0.697601
Thermal correction to Gibbs Free Energy= 0.577257
Sum of electronic and zero-point Energies= -2095.406188
Sum of electronic and thermal Energies= -2095.362854
Sum of electronic and thermal Enthalpies= -2095.361910
Sum of electronic and thermal Free Energies= -2095.482254
Single Point Energy Calculations with extended basis set: HF = -2097.690200

Pd	-0.935475	0.130754	-0.343390
C	-0.987717	1.962726	0.421221
C	-0.708953	3.094176	-0.354406
C	-1.407203	2.135150	1.747352
C	-0.801988	4.379509	0.199547
C	-1.488983	3.416211	2.310268
C	-1.183025	4.523330	1.527320
H	-0.587318	5.258680	-0.403651
H	-1.797554	3.556589	3.342760
H	-1.253627	5.519928	1.960641
O	-0.404432	2.884897	-1.657398
O	-1.751367	1.009247	2.435868
C	-2.244467	1.165517	3.746961
H	-3.142356	1.799959	3.771056
H	-2.509938	0.164609	4.099720
H	-1.486306	1.592499	4.419613
C	0.228459	3.927264	-2.364733
H	0.592788	3.479917	-3.291748
H	-0.464267	4.752740	-2.588559
H	1.089191	4.314520	-1.799823
C	-3.178491	-3.502506	-1.033729
C	-2.661352	-2.212227	-1.016155
C	-0.469995	-3.013549	-1.022055
C	-0.939929	-4.331994	-1.064714
C	-2.299415	-4.579131	-1.050139
H	-4.249963	-3.676373	-1.014423
H	-0.219167	-5.146673	-1.095446
H	-2.680753	-5.597529	-1.057255
C	-3.548865	-1.030197	-1.023827
C	-4.895135	-1.121685	-1.375511
C	-3.776739	1.261819	-0.684261
C	-5.691341	0.013964	-1.367084
H	-5.318922	-2.075280	-1.675461
C	-5.123800	1.229295	-1.009700
H	-6.740551	-0.052568	-1.643865
H	-5.704346	2.147121	-0.988954
N	-1.326125	-1.978554	-0.981060
N	-3.004811	0.165451	-0.692205
C	-0.708145	-2.072308	2.456094
C	-0.315074	-3.473209	2.915548
C	1.156902	-3.324007	3.304126
C	0.592524	-1.463656	1.979643
H	-1.472947	-2.043212	1.671033
H	-1.074524	-1.448508	3.284310
H	-0.403772	-4.178720	2.077515
H	-0.928931	-3.852695	3.737887
H	1.289803	-3.080110	4.370395
H	1.755631	-4.218568	3.087709
O	0.750878	-0.460875	1.277564
C	2.997218	-1.906292	2.286674

H 3.502628 -2.721566 1.747927
H 3.078374 -0.986950 1.698343
H 3.497828 -1.764221 3.254299
N 1.602803 -2.213384 2.476305
C 3.114084 0.642757 -1.055440
C 3.987135 -0.440180 -1.188727
C 3.322265 1.542881 -0.007869
C 5.055748 -0.625044 -0.305538
C 4.378866 1.369867 0.892991
C 5.238303 0.289094 0.726184
H 5.736942 -1.465090 -0.412134
H 4.541722 2.068798 1.709009
H 6.065887 0.152519 1.420931
O 3.721644 -1.279415 -2.230831
O 2.442488 2.578804 0.060589
C 2.456595 3.370885 1.225938
H 3.387952 3.949718 1.316255
H 1.607997 4.056335 1.140022
H 2.331507 2.752456 2.128397
C 4.439786 -2.488918 -2.293808
H 4.017782 -3.058193 -3.126626
H 5.510440 -2.321158 -2.482176
H 4.327253 -3.069109 -1.364339
C 2.003607 0.853807 -2.076788
O 2.288889 1.561301 -3.058129
O 0.915045 0.244753 -1.867573
H -3.285008 2.189465 -0.399879
C 1.002214 -2.759788 -1.011148
H 1.495908 -3.427661 -1.728966
H 1.232443 -1.716388 -1.254903
H 1.423243 -2.995633 -0.021079
Imaginary Vibrational Frequency = -56.7136 cm^{-1}

10b
Zero-point correction= 0.513142 (Hartree/Particle)
Thermal correction to Energy= 0.549101
Thermal correction to Enthalpy= 0.550046
Thermal correction to Gibbs Free Energy= 0.442190
Sum of electronic and zero-point Energies= -1769.841152
Sum of electronic and thermal Energies= -1769.805193
Sum of electronic and thermal Enthalpies= -1769.804248
Sum of electronic and thermal Free Energies= -1769.912104
Single Point Energy Calculations with extended basis set: HF = -1771.44142
Pd 0.969726 0.054744 0.170271
C 0.309616 -1.823780 0.339901
C 0.093418 -2.636800 -0.775165
C 0.027771 -2.333110 1.610295
C -0.382030 -3.947178 -0.628394
C -0.463365 -3.634989 1.773031
C -0.660715 -4.425786 0.646804

H	-0.540549	-4.588661	-1.492120
H	-0.683731	-4.036061	2.759054
H	-1.037144	-5.440751	0.765859
O	0.397382	-2.093959	-1.989649
O	0.271544	-1.496494	2.661287
C	-0.019898	-1.962795	3.959192
H	0.581101	-2.846695	4.218460
H	0.231055	-1.147933	4.643008
H	-1.085616	-2.210491	4.071380
C	0.033983	-2.817064	-3.143206
H	0.283487	-2.182507	-3.997443
H	0.589138	-3.762852	-3.227405
H	-1.045230	-3.033359	-3.156651
C	4.196154	2.976135	-0.213174
C	3.339224	1.881708	-0.146860
C	1.489208	3.266219	0.158517
C	2.305881	4.399021	0.101043
C	3.667825	4.253446	-0.088520
H	5.264881	2.847504	-0.348408
H	1.855680	5.382957	0.208456
H	4.319608	5.122708	-0.133959
C	3.848479	0.498123	-0.249023
C	5.189550	0.212542	-0.501904
C	3.374182	-1.778307	-0.127235
C	5.618313	-1.104974	-0.561290
H	5.905008	1.013308	-0.657602
C	4.695429	-2.122316	-0.364098
H	2.610055	-2.535231	0.030769
H	6.663752	-1.329391	-0.757910
H	4.982122	-3.169433	-0.394694
N	2.006410	2.031145	0.033912
N	2.955897	-0.505256	-0.074816
C	0.019475	3.410272	0.344500
H	-0.240704	4.443563	0.597596
H	-0.514153	3.126836	-0.571970
H	-0.350312	2.738034	1.125962
C	-3.209773	0.783685	-0.348399
C	-3.905802	1.959196	-0.059668
C	-3.911217	-0.420832	-0.454458
C	-5.290999	1.940395	0.127776
C	-5.296746	-0.455880	-0.271892
C	-5.965008	0.729045	0.017362
H	-5.841088	2.848948	0.356509
H	-5.851951	-1.386120	-0.353878
H	-7.044033	0.707773	0.161327
O	-3.140938	3.078119	0.028600
O	-3.154151	-1.508910	-0.747681
C	-3.798995	-2.760967	-0.835567
H	-4.547491	-2.773700	-1.640993
H	-3.013666	-3.490924	-1.052617

H -4.286396 -3.028154 0.113506
C -3.784642 4.300470 0.313943
H -3.002180 5.063410 0.330673
H -4.522328 4.557359 -0.459585
H -4.284119 4.274178 1.292876
C -1.717512 0.800103 -0.581194
O -1.279940 1.079583 -1.699372
O -1.037594 0.507004 0.468039

11b

Zero-point correction= 0.513878 (Hartree/Particle)
Thermal correction to Energy= 0.549142
Thermal correction to Enthalpy= 0.550086
Thermal correction to Gibbs Free Energy= 0.447062
Sum of electronic and zero-point Energies= -1769.841453
Sum of electronic and thermal Energies= -1769.806188
Sum of electronic and thermal Enthalpies= -1769.805244
Sum of electronic and thermal Free Energies= -1769.908268
Single Point Energy Calculations with extended basis set: HF = -1771.442456
Pd -0.472076 0.421061 -0.645329
C 1.328096 1.243652 -0.379249
C 1.997902 1.831162 -1.456766
C 1.932437 1.262710 0.882639
C 3.267209 2.402444 -1.290405
C 3.193797 1.845115 1.066476
C 3.848880 2.398015 -0.028303
H 3.794060 2.858214 -2.124814
H 3.667558 1.863849 2.045036
H 4.833246 2.843881 0.107626
O 1.336791 1.838880 -2.650162
O 1.215758 0.718826 1.905423
C 1.712392 0.876783 3.213404
H 1.831354 1.940289 3.471803
H 0.974933 0.421457 3.880130
H 2.673996 0.359202 3.347288
C 1.982068 2.417166 -3.761260
H 1.294384 2.314755 -4.604653
H 2.194372 3.484304 -3.599393
H 2.922434 1.899065 -4.000257
C -4.682084 0.030864 0.394653
C -3.375017 0.412771 0.109799
C -3.125119 -1.330096 -1.417460
C -4.446393 -1.734113 -1.194757
C -5.221998 -1.064052 -0.266898
H -5.282491 0.572441 1.118298
H -4.841279 -2.582019 -1.749994
H -6.243284 -1.377715 -0.064041
C -2.775795 1.621449 0.715488
C -3.514857 2.503898 1.502545
C -0.899228 2.983298 0.929810

C -2.916184 3.646585 2.011426
H -4.561978 2.311661 1.711960
C -1.583368 3.896436 1.715813
H -3.491240 4.335929 2.624665
H -1.072093 4.781892 2.082006
N -2.603091 -0.280627 -0.760113
N -1.472720 1.872473 0.445576
C 1.305705 -2.205989 0.127678
C 0.334064 -2.650917 1.024464
C 2.596158 -1.945079 0.598086
C 0.624916 -2.808835 2.381966
C 2.909033 -2.111967 1.949330
C 1.915353 -2.540350 2.823088
H -0.131132 -3.152059 3.083068
H 3.908514 -1.907349 2.324282
H 2.154604 -2.667071 3.878139
O -0.881760 -2.928904 0.476941
O 3.483332 -1.525916 -0.340172
C 4.791368 -1.209151 0.082455
H 5.304458 -2.088073 0.499323
H 5.326894 -0.867712 -0.807476
H 4.783099 -0.399279 0.826833
C -1.981953 -3.056419 1.349998
H -2.870436 -3.148293 0.716776
H -1.902813 -3.951219 1.983343
H -2.082934 -2.165522 1.989140
C 1.007352 -2.094505 -1.347888
O 1.319624 -3.034449 -2.080928
O 0.449849 -1.020292 -1.787493
H 0.147140 3.126829 0.672768
C -2.278208 -2.090183 -2.380863
H -1.565006 -1.439331 -2.893436
H -1.681683 -2.838176 -1.840234
H -2.906392 -2.610984 -3.111789

TS11-12b

Zero-point correction= 0.510880 (Hartree/Particle)
Thermal correction to Energy= 0.546411
Thermal correction to Enthalpy= 0.547355
Thermal correction to Gibbs Free Energy= 0.444094
Sum of electronic and zero-point Energies= -1769.795961
Sum of electronic and thermal Energies= -1769.760430
Sum of electronic and thermal Enthalpies= -1769.759486
Sum of electronic and thermal Free Energies= -1769.862747
Single Point Energy Calculations with extended basis set: HF = -1771.393967
Pd -0.280420 0.183122 -0.493826
C 1.455240 0.984356 0.123361
C 2.355120 1.528202 -0.799241
C 1.785380 1.048368 1.478627
C 3.555650 2.117749 -0.387925

C	2.987372	1.625039	1.913165
C	3.860849	2.151521	0.969768
H	4.252168	2.543344	-1.106242
H	3.239693	1.672173	2.969911
H	4.795733	2.604121	1.297544
O	1.974953	1.480068	-2.113202
O	0.864718	0.534449	2.350143
C	1.264442	0.314556	3.681382
H	1.437442	1.256599	4.223038
H	0.445486	-0.226359	4.165600
H	2.176088	-0.300573	3.728858
C	2.775279	2.154031	-3.055681
H	2.276382	2.043072	-4.022070
H	2.863905	3.225297	-2.815585
H	3.784440	1.720753	-3.123810
C	-4.563433	-0.147422	-0.180772
C	-3.243310	0.276091	-0.339662
C	-2.747141	-1.621347	-1.565755
C	-4.044839	-2.102495	-1.458228
C	-4.963118	-1.356992	-0.732014
H	-5.287138	0.463946	0.349220
H	-4.319127	-3.039611	-1.934559
H	-5.988866	-1.697963	-0.612101
C	-2.781335	1.602683	0.133975
C	-3.593727	2.419158	0.913323
C	-1.167773	3.275553	-0.048258
C	-3.164364	3.703769	1.221464
H	-4.552240	2.067047	1.281499
C	-1.959329	4.145381	0.708410
H	-3.782143	4.356587	1.833816
H	-1.610459	5.160678	0.884361
N	-2.346075	-0.478890	-1.004789
N	-1.558348	2.011997	-0.291229
C	0.678075	-1.644575	-0.026195
C	0.083693	-2.156848	1.175817
C	2.092117	-1.825851	-0.131133
C	0.804031	-2.848232	2.140467
C	2.831060	-2.524427	0.831782
C	2.174824	-3.016228	1.949902
H	0.333585	-3.241419	3.037404
H	3.899762	-2.683166	0.721512
H	2.749025	-3.554486	2.703315
O	-1.245559	-1.968513	1.270841
O	2.663195	-1.338692	-1.241298
C	4.071575	-1.321384	-1.336837
H	4.491449	-2.335540	-1.387013
H	4.305382	-0.791008	-2.264139
H	4.512378	-0.777224	-0.488652
C	-1.948098	-2.537681	2.355591
H	-3.001064	-2.291737	2.193413

H -1.827105 -3.629526 2.381327
H -1.619584 -2.112500 3.314507
C 0.123919 -2.865468 -1.468947
O -0.283279 -3.878736 -0.956947
O 0.306368 -2.332532 -2.535345
H -1.996345 -2.163318 -2.134591
C 0.118612 3.771810 -0.619716
H 0.934113 3.686510 0.111455
H 0.406465 3.194267 -1.503942
H 0.023063 4.830404 -0.889508
Imaginary Vibrational Frequency = -280.5119 cm^{-1}

12b
Zero-point correction= 0.511438 (Hartree/Particle)
Thermal correction to Energy= 0.548032
Thermal correction to Enthalpy= 0.548976
Thermal correction to Gibbs Free Energy= 0.442296
Sum of electronic and zero-point Energies= -1769.836672
Sum of electronic and thermal Energies= -1769.800079
Sum of electronic and thermal Enthalpies= -1769.799135
Sum of electronic and thermal Free Energies= -1769.905815
Single Point Energy Calculations with extended basis set: HF = -1771.435237
Pd -0.135554 0.060496 -0.281513
C 1.276606 -1.378885 -0.322492
C 1.198937 -2.436942 0.598305
C 2.352732 -1.381277 -1.212807
C 2.171344 -3.443215 0.642809
C 3.346929 -2.368291 -1.174008
C 3.245933 -3.390599 -0.240742
H 2.110250 -4.254215 1.364573
H 4.179281 -2.348110 -1.874773
H 4.009588 -4.166457 -0.203296
O 0.125698 -2.426131 1.446683
O 2.378228 -0.385490 -2.150901
C 3.637785 0.054268 -2.595643
H 4.106957 -0.649732 -3.299906
H 3.471967 1.006247 -3.111070
H 4.319936 0.220411 -1.746714
C -0.026691 -3.500400 2.341918
H -0.958154 -3.319224 2.886034
H -0.102286 -4.464124 1.815692
H 0.803314 -3.557359 3.063307
C -4.406210 1.144812 -0.085569
C -3.135079 0.678346 -0.412274
C -2.132780 2.553216 0.530810
C -3.383837 3.076503 0.866678
C -4.530338 2.361362 0.568967
H -5.289446 0.556272 -0.314210
H -3.438681 4.038923 1.369838
H -5.511697 2.742444 0.841867

C -2.968458 -0.617209 -1.107257
C -4.021173 -1.247862 -1.771042
C -1.540174 -2.361421 -1.644302
C -3.806785 -2.480032 -2.372726
H -4.997442 -0.776749 -1.837719
C -2.545279 -3.057046 -2.301328
H -4.618866 -2.979840 -2.895553
H -2.333557 -4.021649 -2.754177
N -2.011551 1.361578 -0.086095
N -1.742388 -1.172638 -1.067436
C 1.455000 1.221211 0.231995
C 2.229122 1.024963 1.377787
C 1.867609 2.240768 -0.639725
C 3.379361 1.781401 1.645308
C 2.999116 3.023565 -0.389008
C 3.755420 2.775589 0.754089
H 3.964286 1.605974 2.546162
H 3.307440 3.809095 -1.074896
H 4.644107 3.373875 0.951536
O 1.796518 0.069342 2.259697
O 1.081501 2.439241 -1.746609
C 1.378319 3.530384 -2.583352
H 2.368956 3.433634 -3.053272
H 0.615524 3.538061 -3.366848
H 1.339704 4.484932 -2.034803
C 2.771468 -0.604947 3.014338
H 2.284186 -1.490559 3.436506
H 3.611625 -0.927597 2.378482
H 3.164331 0.005714 3.842029
C -2.328688 -0.385434 2.581366
O -1.748448 0.541603 2.983153
O -2.926695 -1.308155 2.195142
H -0.526817 -2.754556 -1.569365
C -0.898632 3.321806 0.858080
H -0.235013 2.734877 1.505691
H -0.332235 3.539151 -0.056093
H -1.147968 4.264096 1.356916

13b

Zero-point correction= 0.498086 (Hartree/Particle)
Thermal correction to Energy= 0.530821
Thermal correction to Enthalpy= 0.531765
Thermal correction to Gibbs Free Energy= 0.434012
Sum of electronic and zero-point Energies= -1581.340734
Sum of electronic and thermal Energies= -1581.308000
Sum of electronic and thermal Enthalpies= -1581.307056
Sum of electronic and thermal Free Energies= -1581.404809
Single Point Energy Calculations with extended basis set: HF = -1582.654165
Pd 0.297990 0.139323 -0.127493
C -1.022690 -1.387590 -0.308223

C	-2.086142	-1.398513	-1.210573
C	-0.895449	-2.498453	0.538757
C	-3.011855	-2.450285	-1.264108
C	-1.794486	-3.569660	0.496425
C	-2.856971	-3.528363	-0.404085
H	-3.831935	-2.434211	-1.979819
H	-1.687314	-4.424267	1.160567
H	-3.565817	-4.354904	-0.437187
O	-2.163132	-0.344244	-2.083318
O	0.173807	-2.481128	1.396827
C	0.459627	-3.651819	2.120518
H	0.609042	-4.515612	1.453032
H	1.386366	-3.460540	2.669070
H	-0.334293	-3.898832	2.842460
C	-3.444507	0.063431	-2.492698
H	-3.331188	1.061709	-2.929333
H	-3.879952	-0.605131	-3.251512
H	-4.133014	0.124359	-1.634492
C	4.068637	2.195706	0.600356
C	3.045590	1.301335	0.282820
C	1.456061	2.959426	0.606625
C	2.420761	3.899256	0.940546
C	3.752503	3.505179	0.934068
H	5.108748	1.885271	0.572078
H	2.127597	4.914196	1.194089
H	4.542956	4.210144	1.180718
C	3.315246	-0.102250	-0.109102
C	4.579719	-0.663493	0.041791
C	2.512654	-2.025351	-1.146707
C	4.801512	-1.956342	-0.413534
H	5.384794	-0.109611	0.514649
C	3.767972	-2.631428	-1.036791
H	5.779685	-2.417995	-0.300078
H	3.913206	-3.629196	-1.445121
N	1.757015	1.698271	0.282938
N	2.286618	-0.797374	-0.650638
C	-1.356991	1.170611	0.397480
C	-1.785122	2.233085	-0.413904
C	-2.132794	0.872974	1.520766
C	-2.942154	2.964897	-0.120981
C	-3.306869	1.576244	1.821715
C	-3.700646	2.618654	0.993596
H	-3.268323	3.783440	-0.758094
H	-3.894774	1.324773	2.702561
H	-4.607390	3.177811	1.220931
O	-1.011701	2.508851	-1.510850
O	-1.674958	-0.124259	2.338893
C	-2.633161	-0.901420	3.013486
H	-3.449476	-1.198055	2.335691
H	-2.115362	-1.801751	3.361734

H -3.062794 -0.381479 3.883608
C -1.291193 3.680143 -2.237641
H -0.518061 3.760981 -3.006784
H -2.275568 3.638813 -2.728714
H -1.254970 4.573746 -1.594643
H 0.396397 3.209957 0.598442
C 1.411755 -2.744933 -1.854100
H 0.834910 -3.370870 -1.159419
H 0.708687 -2.038634 -2.307621
H 1.826671 -3.399291 -2.629657

TS13-14b

Zero-point correction= 0.496044 (Hartree/Particle)
Thermal correction to Energy= 0.528673
Thermal correction to Enthalpy= 0.529617
Thermal correction to Gibbs Free Energy= 0.430926
Sum of electronic and zero-point Energies= -1581.309022
Sum of electronic and thermal Energies= -1581.276394
Sum of electronic and thermal Enthalpies= -1581.275450
Sum of electronic and thermal Free Energies= -1581.374141
Single Point Energy Calculations with extended basis set: HF = -1582.620411
Pd 0.403532 0.078970 -0.027554
C -1.498516 -0.852277 -0.104231
C -2.292225 -1.248886 -1.222898
C -1.464367 -1.806413 0.960534
C -3.045023 -2.424952 -1.231375
C -2.232505 -2.971083 0.961982
C -3.027918 -3.274861 -0.133202
H -3.653716 -2.683467 -2.093024
H -2.168479 -3.669522 1.792922
H -3.620990 -4.187709 -0.142667
O -2.314933 -0.401781 -2.286071
O -0.551224 -1.596050 1.956284
C -0.774483 -2.210171 3.202525
H -0.513282 -3.279147 3.188849
H -0.127756 -1.700505 3.923464
H -1.822865 -2.105756 3.518362
C -3.132703 -0.718051 -3.386899
H -3.002182 0.092591 -4.109929
H -2.833541 -1.665459 -3.858628
H -4.194157 -0.779712 -3.104938
C 4.510175 1.815729 0.192851
C 3.389777 0.982950 0.168146
C 1.992397 2.786181 0.543045
C 3.056342 3.677199 0.597144
C 4.339890 3.175895 0.413642
H 5.505012 1.414277 0.019106
H 2.878173 4.734824 0.772109
H 5.202920 3.837641 0.433423
C 3.494972 -0.477853 -0.068305

C 4.703472 -1.153969 0.091266
C 2.410886 -2.425032 -0.724645
C 4.747650 -2.515606 -0.175289
H 5.593564 -0.634164 0.435254
C 3.593866 -3.156875 -0.599450
H 5.676626 -3.068706 -0.054581
H 3.595938 -4.219675 -0.831729
N 2.151046 1.477066 0.335872
N 2.368739 -1.111713 -0.448208
C -1.531872 0.897432 0.193277
C -1.621683 1.855379 -0.867678
C -2.283865 1.245491 1.358251
C -2.471612 2.960475 -0.824596
C -3.125539 2.358773 1.405410
C -3.233028 3.203891 0.309071
H -2.503001 3.660448 -1.656091
H -3.706101 2.571486 2.298327
H -3.893665 4.068154 0.350359
O -0.761430 1.700090 -1.918394
O -2.188803 0.404762 2.422835
C -2.961762 0.671714 3.568030
H -4.039705 0.651249 3.349836
H -2.728608 -0.118898 4.287217
H -2.707025 1.643720 4.015161
C -1.100006 2.294834 -3.148116
H -0.464957 1.827742 -3.907213
H -2.156222 2.119861 -3.400118
H -0.910563 3.378911 -3.148784
H 0.962167 3.123401 0.669226
C 1.146806 -3.079662 -1.179175
H 0.407092 -3.112700 -0.366558
H 0.687507 -2.504270 -1.993346
H 1.333226 -4.102366 -1.525319
Imaginary Vibrational Frequency = -164.2397 cm^{-1}

14b

Zero-point correction= 0.498724 (Hartree/Particle)
Thermal correction to Energy= 0.531844
Thermal correction to Enthalpy= 0.532788
Thermal correction to Gibbs Free Energy= 0.433499
Sum of electronic and zero-point Energies= -1581.364994
Sum of electronic and thermal Energies= -1581.331875
Sum of electronic and thermal Enthalpies= -1581.330931
Sum of electronic and thermal Free Energies= -1581.430220
Single Point Energy Calculations with extended basis set: HF = -1582.679063
Pd -1.460844 0.224031 -1.452109
C 2.612849 0.553671 0.533647
C 4.013798 0.589435 0.518468
C 1.939178 1.047512 1.660868
C 4.731582 1.099790 1.604454

C	2.644354	1.565123	2.751109
C	4.033283	1.580897	2.705526
H	5.817447	1.129366	1.597914
H	2.126142	1.945441	3.626923
H	4.588013	1.980410	3.553073
O	4.598518	0.113477	-0.609330
O	0.582779	0.980791	1.612540
C	-0.151180	1.600461	2.645400
H	0.112336	2.663058	2.745221
H	-1.207245	1.517477	2.364936
H	0.003276	1.099773	3.612805
C	6.007298	0.122176	-0.679543
H	6.268505	-0.298594	-1.653687
H	6.409739	1.142866	-0.608589
H	6.455261	-0.495972	0.111641
C	-1.377228	-1.906327	1.859842
C	-2.379462	-1.563458	0.951337
C	-2.212061	-3.579856	-0.114257
C	-1.197220	-4.010937	0.736689
C	-0.769772	-3.151100	1.741200
H	-1.069597	-1.199161	2.628434
H	-0.764164	-5.001663	0.615945
H	0.026361	-3.444074	2.423514
C	-3.073691	-0.253681	1.060555
C	-3.707117	0.103075	2.245578
C	-3.740977	1.713738	0.020495
C	-4.390983	1.313109	2.301313
H	-3.678266	-0.572213	3.098024
C	-4.417898	2.117364	1.172920
H	-4.905976	1.616007	3.210366
H	-4.951892	3.065264	1.172442
N	-2.796741	-2.386115	-0.022431
N	-3.072428	0.545560	-0.026936
C	1.842069	0.016549	-0.612687
C	1.225105	0.885071	-1.515314
C	1.667749	-1.373474	-0.776183
C	0.400900	0.396114	-2.565817
C	0.853791	-1.887496	-1.780934
C	0.202501	-1.000526	-2.654241
H	0.129662	1.038314	-3.402434
H	0.707465	-2.957798	-1.898313
H	-0.332437	-1.403608	-3.512744
O	1.487665	2.201553	-1.349570
O	2.320857	-2.147012	0.128147
C	2.389546	-3.533240	-0.122451
H	2.840433	-3.738039	-1.104254
H	3.019249	-3.958227	0.663422
H	1.397415	-4.003812	-0.081016
C	0.769154	3.127573	-2.135664
H	1.020573	4.118933	-1.750658

H 1.054845 3.072046 -3.195368
H -0.316023 2.954498 -2.045310
H -2.575285 -4.234331 -0.908238
C -3.707903 2.582367 -1.193948
H -2.818144 3.227713 -1.180693
H -3.649966 1.968107 -2.101674
H -4.589286 3.232624 -1.243587

CO_2
Zero-point correction= 0.010383 (Hartree/Particle)
Thermal correction to Energy= 0.013348
Thermal correction to Enthalpy= 0.014292
Thermal correction to Gibbs Free Energy= -0.007614
Sum of electronic and zero-point Energies= -188.490254
Sum of electronic and thermal Energies= -188.487288
Sum of electronic and thermal Enthalpies= -188.486344
Sum of electronic and thermal Free Energies= -188.508250
Single Point Energy Calculations with extended basis set: HF = -188.7620355
C 0.000000 0.001178 0.000000
O 1.164214 0.035034 0.000000
O -1.164214 -0.035918 -0.000000

$DMPhCO_2$
Zero-point correction= 0.167807 (Hartree/Particle)
Thermal correction to Energy= 0.180023
Thermal correction to Enthalpy= 0.180967
Thermal correction to Gibbs Free Energy= 0.128312
Sum of electronic and zero-point Energies= -648.816912
Sum of electronic and thermal Energies= -648.804695
Sum of electronic and thermal Enthalpies= -648.803751
Sum of electronic and thermal Free Energies= -648.856407
Single Point Energy Calculations with extended basis set: HF = -649.5282815
C -0.000052 0.305025 0.000063
C -1.199031 -0.411263 -0.000732
C 1.198781 -0.411542 0.000600
C -1.212360 -1.809873 -0.000992
C 1.211845 -1.810147 0.000387
C -0.000334 -2.492369 -0.000433
H -2.145815 -2.366715 -0.001677
H 2.145199 -2.367165 0.000818
H -0.000481 -3.581443 -0.000646
O -2.330963 0.351943 -0.001715
O 2.330880 0.351442 0.001749
C 3.571825 -0.312745 0.001694
H 3.697997 -0.940118 -0.893281
H 4.340029 0.465161 0.002408
H 3.697532 -0.941319 0.895881
C -3.572035 -0.312018 0.000026
H -4.340102 0.466021 0.000450
H -3.699123 -0.940509 -0.894019

H -3.697032 -0.939440 0.895129
C 0.000337 1.837069 -0.000254
O 0.008336 2.376148 -1.128607
O -0.007259 2.377056 1.127671

NMP

Zero-point correction= 0.138815 (Hartree/Particle)
Thermal correction to Energy= 0.145748
Thermal correction to Enthalpy= 0.146693
Thermal correction to Gibbs Free Energy= 0.107964
Sum of electronic and zero-point Energies= -325.584342
Sum of electronic and thermal Energies= -325.577408
Sum of electronic and thermal Enthalpies= -325.576464
Sum of electronic and thermal Free Energies= -325.615193
Single Point Energy Calculations with extended basis set: HF = -326.2667199
C -1.330689 0.896410 0.143543
C -1.773604 -0.522910 -0.199276
C -0.543748 -1.372945 0.128223
C 0.178124 0.866751 -0.003980
H -1.769588 1.676874 -0.486801
H -1.556139 1.157174 1.188287
H -1.995070 -0.597333 -1.271486
H -2.662466 -0.849682 0.349082
H -0.560380 -1.754420 1.163202
H -0.425054 -2.235403 -0.541479
O 0.932682 1.830221 -0.050307
C 1.928296 -0.871151 -0.012251
H 2.138391 -1.568588 -0.833924
H 2.566897 0.011301 -0.114330
H 2.159704 -1.375031 0.937509
N 0.555997 -0.440512 -0.046451

DMSO

Zero-point correction= 0.079329 (Hartree/Particle)
Thermal correction to Energy= 0.084955
Thermal correction to Enthalpy= 0.085899
Thermal correction to Gibbs Free Energy= 0.051025
Sum of electronic and zero-point Energies= -552.975987
Sum of electronic and thermal Energies= -552.970361
Sum of electronic and thermal Enthalpies= -552.969417
Sum of electronic and thermal Free Energies= -553.004290
Single Point Energy Calculations with extended basis set: HF = -553.51955
S 0.000032 0.233677 -0.446735
O -0.000069 1.493091 0.388837
C -1.344177 -0.806331 0.183924
H -1.311043 -1.788257 -0.300791
H -1.240785 -0.906485 1.271007
H -2.289169 -0.309305 -0.055405
C 1.344195 -0.806211 0.183959
H 1.241061 -0.906043 1.271093

H 1.310532 -1.788418 -0.300176
H 2.289337 -0.309794 -0.055957

PhNCO

Zero-point correction= 0.103865 (Hartree/Particle)
Thermal correction to Energy= 0.110983
Thermal correction to Enthalpy= 0.111927
Thermal correction to Gibbs Free Energy= 0.071441
Sum of electronic and zero-point Energies= -399.353897
Sum of electronic and thermal Energies= -399.346779
Sum of electronic and thermal Enthalpies= -399.345835
Sum of electronic and thermal Free Energies= -399.386321
Single Point Energy Calculations with extended basis set: HF = -399.89746
C -2.548419 -0.067211 -0.000262
N -1.444712 -0.541665 0.000830
O -3.675839 0.270973 -0.000625
C -0.084007 -0.233729 0.000416
C 0.831886 -1.285620 0.000083
C 0.359760 1.091347 0.000422
C 2.194291 -1.008925 -0.000323
H 0.463375 -2.309262 0.000114
C 1.723972 1.354362 0.000000
H -0.366210 1.902666 0.000736
C 2.644845 0.308627 -0.000388
H 2.907829 -1.830680 -0.000566
H 2.068791 2.386697 -0.000078
H 3.711949 0.521338 -0.000713

PhSOO

Zero-point correction= 0.097682 (Hartree/Particle)
Thermal correction to Energy= 0.105361
Thermal correction to Enthalpy= 0.106305
Thermal correction to Gibbs Free Energy= 0.064270
Sum of electronic and zero-point Energies= -779.982297
Sum of electronic and thermal Energies= -779.974618
Sum of electronic and thermal Enthalpies= -779.973674
Sum of electronic and thermal Free Energies= -780.015709
Single Point Energy Calculations with extended basis set: HF = -780.52586
C -0.075482 -0.007919 -0.107889
C -0.782319 -1.207538 -0.092011
C -2.171315 -1.199563 0.007502
C -2.856315 0.012224 0.087892
C -2.149234 1.213261 0.069212
C -0.759837 1.201291 -0.033635
H -0.230904 -2.146908 -0.141693
H -2.723401 -2.138945 0.027629
H -3.942727 0.020032 0.165789
H -2.684429 2.160125 0.138786
H -0.186704 2.128629 -0.040551
S 1.748015 -0.025723 -0.356931

O 2.161354 1.284766 0.293696
O 2.159514 -1.245002 0.453119

SO_2
Zero-point correction= 0.007013 (Hartree/Particle)
Thermal correction to Energy= 0.010087
Thermal correction to Enthalpy= 0.011031
Thermal correction to Gibbs Free Energy= -0.017204
Sum of electronic and zero-point Energies= -548.492452
Sum of electronic and thermal Energies= -548.489378
Sum of electronic and thermal Enthalpies= -548.488434
Sum of electronic and thermal Free Energies= -548.516670
Single Point Energy Calculations with extended basis set: HF = -548.7642335
S -0.000000 -0.000000 0.379816
O 0.000000 1.242708 -0.379816
O -0.000000 -1.242708 -0.379816