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Supplementary Material

The role of silver carbonate as a catalyst in the synthesis of *N*-phenylbenzamide from benzoic acid and phenyl isocyanate: a mechanistic exploration

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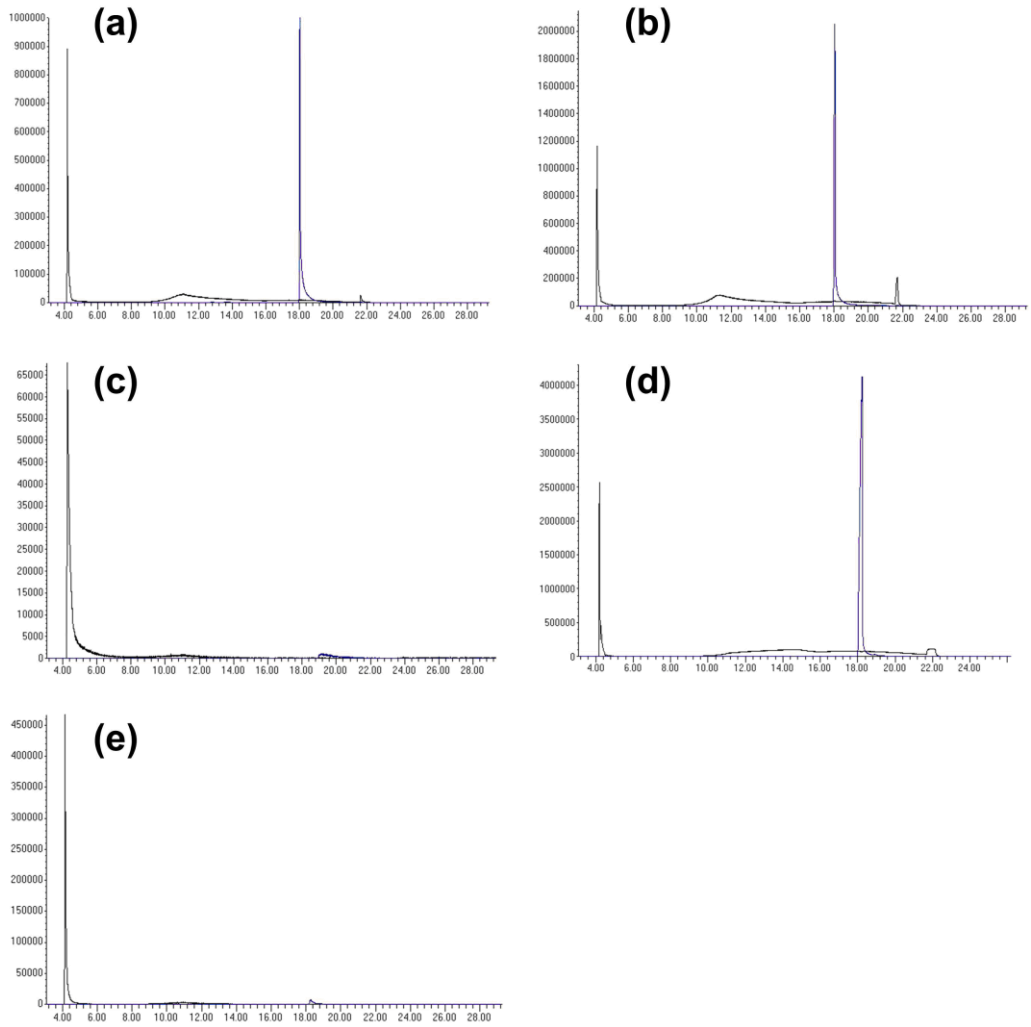

Figure S1: Extracted ion chromatograms for m/z 119 (phenyl isocyanate, black) and 197 (N-phenyl benzamide, blue) with ±0.5 Da window. (a)-(e) represent the entry 1-5 respectively in Table 1.

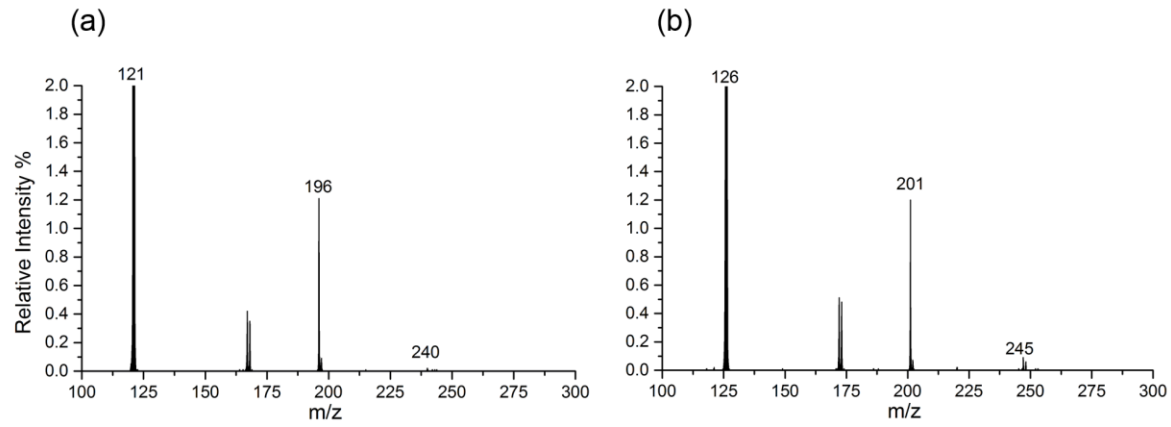

Figure S2. MS^2 experiment involving an ion-molecule reaction of (a) $[C_6H_5COO]^-$ (*m/z* 121) and (b) $[C_6D_5COO]^-$ (*m/z* 126) with phenyl isocyanate (reaction time: 500 ms).

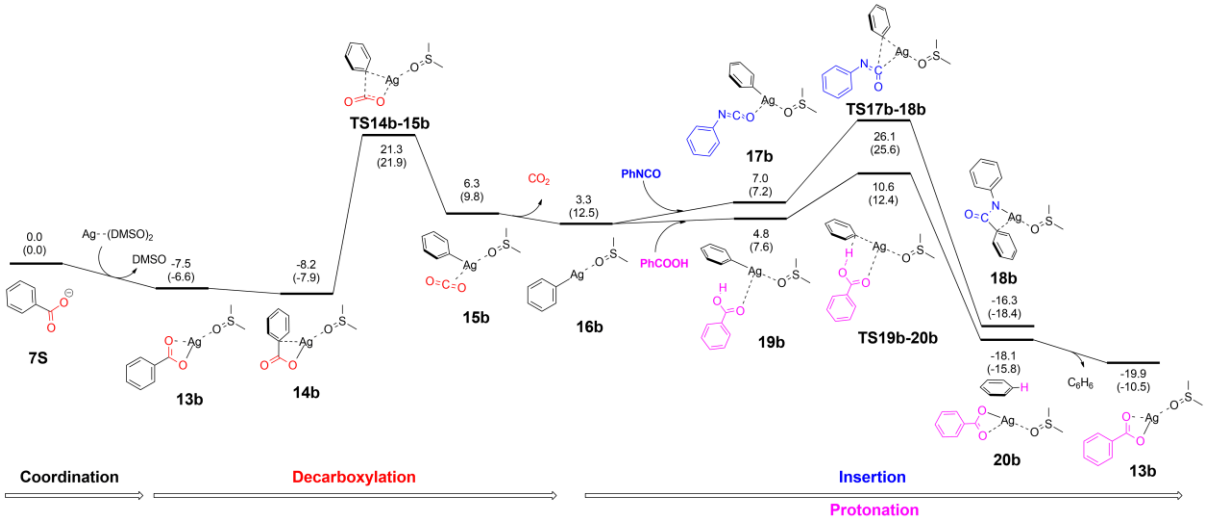

Figure S3. DFT calculated energy surface of the ligand-free reactions mediated by silver ion, including decarboxylation of **13b**, insertion between phenyl isocyanate and **16b,** and protonation between benzoic acid and **16b**. The relative Gibbs and enthalpy energies (in parentheses) are given in kcal/mol and were calculated at the B3LYP-D3BJ/BS2//M06/BS1 level of theory in DMSO using the CPCM approach.

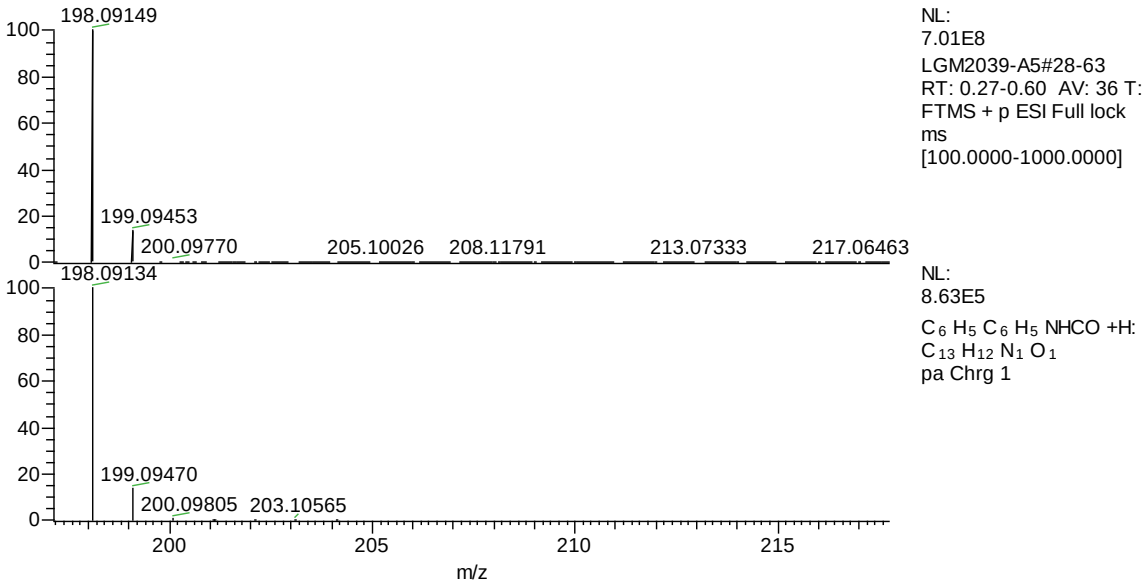

Figure S4. Observed (top) and calculated (bottom) isotopic distribution patterns of **III**.

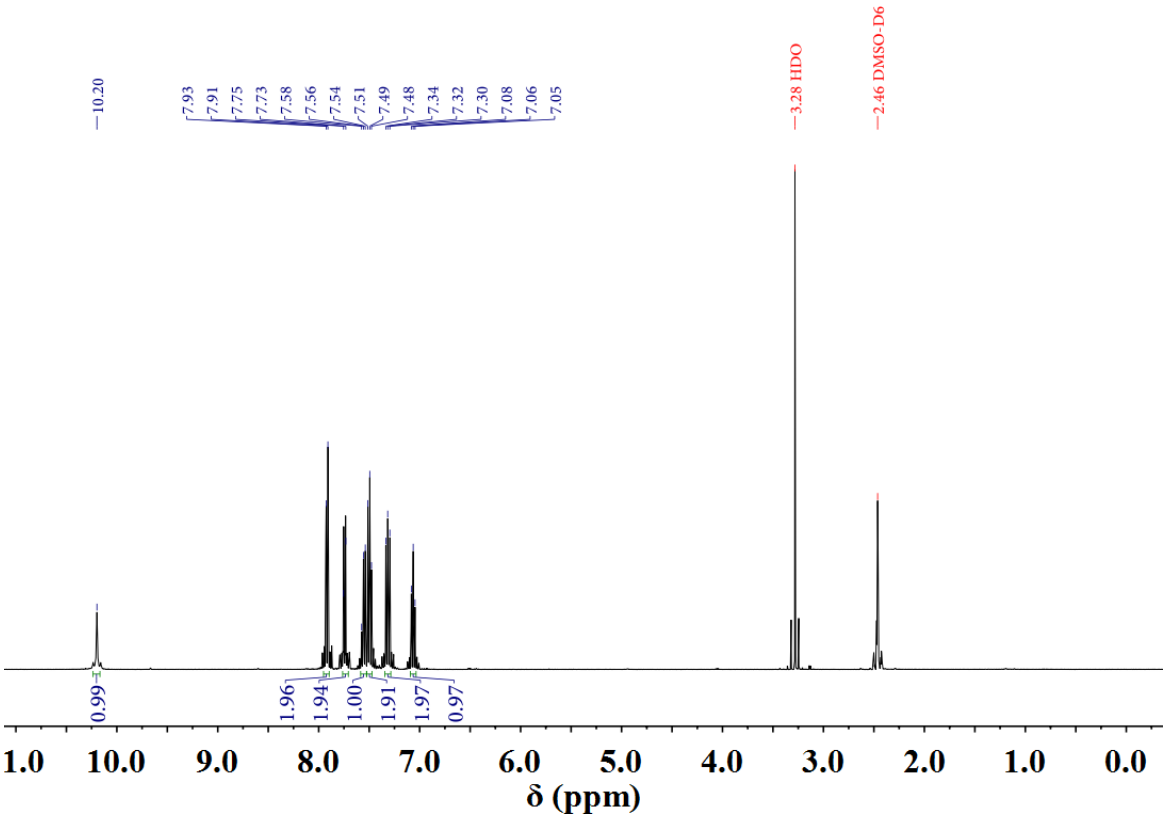

Figure S5. ^{1}H NMR spectra (400 MHz, DMSO-d_6) of **III**.

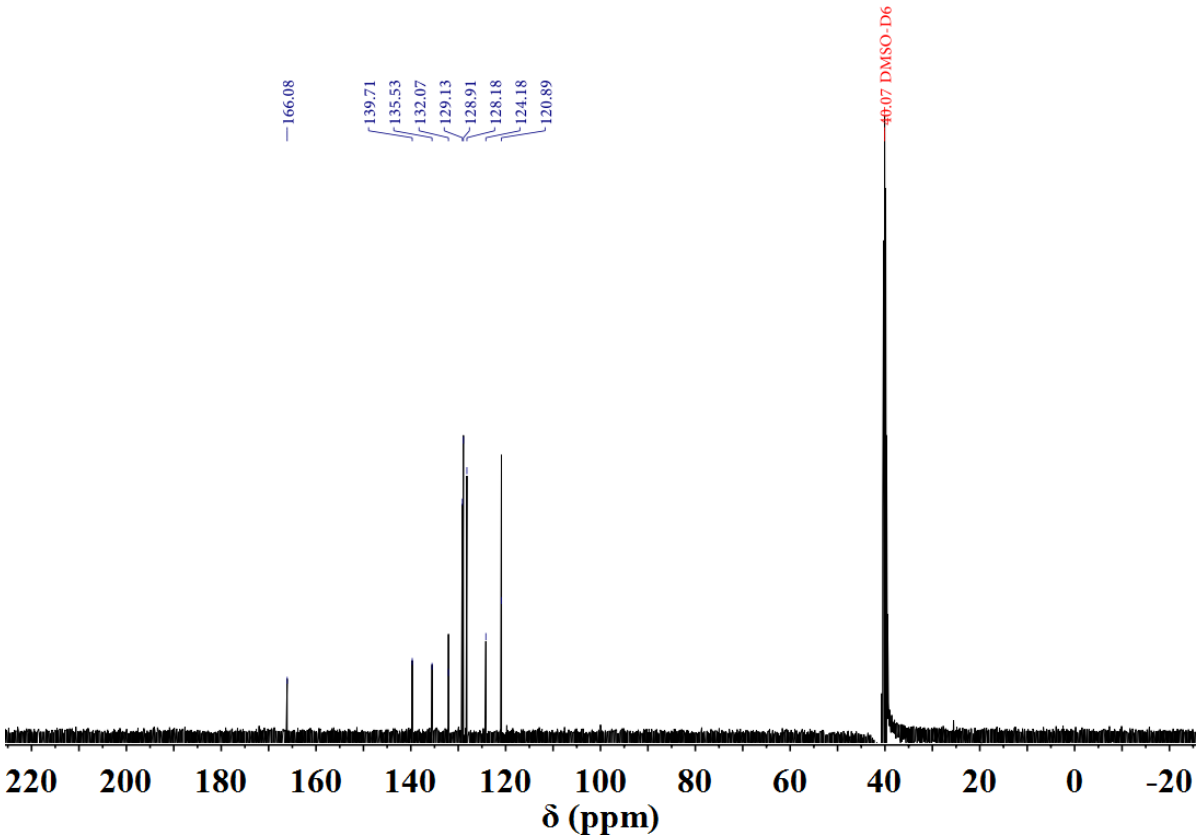

Figure S6. ^{13}C NMR spectra (400 MHz, DMSO-d_6) of **III**.

Cartesian coordinates and energies for all DFT calculated structures

1

Zero-point correction= 0.443631 (Hartree/Particle)
Thermal correction to Energy= 0.481238
Thermal correction to Enthalpy= 0.482182
Thermal correction to Gibbs Free Energy= 0.362630
Sum of electronic and zero-point Energies= -2845.784644
Sum of electronic and thermal Energies= -2845.747037
Sum of electronic and thermal Enthalpies= -2845.746093
Sum of electronic and thermal Free Energies= -2845.865645
Single Point Energy Calculations with extended basis set: HF = -2848.67110025

N	0.795417	-2.295453	0.063709
C	0.222014	-3.488792	0.080017
C	-1.158273	-3.675035	0.107158
C	-2.014167	-2.581383	0.120446
C	-1.414418	-1.286910	0.143196
C	-0.001392	-1.200457	0.098907
N	1.984840	0.131414	0.075837
C	2.604719	1.298433	0.101127
C	1.913292	2.512125	0.129698
C	0.525041	2.534381	0.136120

C	-0.149569	1.275910	0.151037
C	0.637795	0.102090	0.104187
H	0.895094	-4.346956	0.052052
H	-1.569524	-4.681894	0.075025
H	3.695816	1.248935	0.080601
H	2.464722	3.450104	0.105632
C	-2.169463	-0.078240	0.271765
C	-1.567860	1.141534	0.275577
H	-3.247213	-0.153140	0.398060
H	-2.165423	2.041603	0.403898
Ag	3.098828	-1.951197	-0.002524
C	5.874124	-1.586624	-0.045211
C	7.364371	-1.822706	-0.104888
C	8.235533	-0.734243	-0.058691
C	7.887934	-3.111787	-0.207847
C	9.610806	-0.929245	-0.114176
H	7.801194	0.260561	0.020771
C	9.263303	-3.309656	-0.264241
H	7.192651	-3.947964	-0.242842
C	10.127746	-2.218579	-0.217419
H	10.284259	-0.072903	-0.077459
H	9.664810	-4.319931	-0.345454
H	11.206080	-2.373223	-0.261763
C	-3.467224	-2.820926	0.106492
C	-4.008549	-3.810676	0.943733
C	-4.320957	-2.162241	-0.787843
C	-5.354855	-4.127975	0.887110
H	-3.357202	-4.313586	1.660343
C	-5.669816	-2.495981	-0.853395
H	-3.912156	-1.415370	-1.469629
C	-6.191184	-3.480445	-0.021719
H	-5.782282	-4.882695	1.546023
H	-6.344543	-2.008911	-1.555419
C	-0.169293	3.834227	0.122763
C	-1.205232	4.110646	-0.779098
C	0.269861	4.861815	0.972879
C	-1.773487	5.378796	-0.837634
H	-1.536396	3.334415	-1.470416
C	-0.308958	6.119179	0.922196
H	1.060876	4.651109	1.694337
C	-1.327093	6.387751	0.008339
H	-2.569508	5.615074	-1.541802
H	0.013031	6.914066	1.593664
S	-7.926103	-3.982670	-0.123128
S	-1.993489	8.066304	-0.094222
O	-7.832910	-5.373468	-0.606596
O	-8.396455	-3.856364	1.268472
O	-8.523122	-3.031124	-1.077159
O	-2.288941	8.402596	1.310903
O	-3.172577	7.934716	-0.969136

O -0.870518 8.826410 -0.675430
O 5.153290 -2.643873 -0.085905
O 5.459233 -0.420492 0.036134

1b

Zero-point correction= 0.443360 (Hartree/Particle)
Thermal correction to Energy= 0.480770
Thermal correction to Enthalpy= 0.481714
Thermal correction to Gibbs Free Energy= 0.364314
Sum of electronic and zero-point Energies= -2845.784852
Sum of electronic and thermal Energies= -2845.747443
Sum of electronic and thermal Enthalpies= -2845.746498
Sum of electronic and thermal Free Energies= -2845.863899
Single Point Energy Calculations with extended basis set: HF = -2848.66321745
N -1.836888 -4.322233 1.575870
C -0.563200 -4.303059 1.908113
C 0.241737 -3.159179 1.877200
C -0.297613 -1.951171 1.468268
C -1.664144 -1.946891 1.067187
C -2.390353 -3.164980 1.158168
N -4.441876 -4.372682 0.870772
C -5.711008 -4.396312 0.518997
C -6.432607 -3.278445 0.088579
C -5.808065 -2.044216 0.003043
C -4.423238 -1.996300 0.337241
C -3.797075 -3.191173 0.782114
H -0.134187 -5.253048 2.240506
H 1.278870 -3.207493 2.205889
H -6.215470 -5.364609 0.593886
H -7.493316 -3.363787 -0.143134
C -2.316715 -0.790938 0.533368
C -3.630747 -0.814486 0.187888
H -1.732620 0.114424 0.379940
H -4.096970 0.072041 -0.237919
Ag 5.495349 2.078243 -0.232890
C 6.838671 -0.166619 -1.139806
C 7.853727 -1.111775 -1.736047
C 7.589696 -2.481308 -1.751898
C 9.052513 -0.641528 -2.272707
C 8.509155 -3.370192 -2.296868
H 6.647141 -2.820416 -1.326187
C 9.974153 -1.528709 -2.818470
H 9.240144 0.430019 -2.250521
C 9.704343 -2.895096 -2.831876
H 8.294250 -4.438898 -2.305644
H 10.908743 -1.153640 -3.236401
H 10.426573 -3.590884 -3.259974
C 0.564859 -0.749489 1.491431
C 1.865756 -0.823596 0.973407
C 0.159539 0.437824 2.111015

C 2.743694 0.244934 1.078543
H 2.191174 -1.736126 0.474158
C 1.032630 1.515357 2.216991
H -0.837287 0.503805 2.547081
C 2.320497 1.416966 1.704684
H 3.755512 0.151920 0.676476
H 0.735668 2.438571 2.710578
C -6.604312 -0.871731 -0.412005
C -6.609711 0.320833 0.322906
C -7.460731 -0.975613 -1.518372
C -7.458862 1.365646 -0.026500
H -5.969020 0.410911 1.201285
C -8.297745 0.071589 -1.871660
H -7.446734 -1.890539 -2.113053
C -8.311227 1.243889 -1.118844
H -7.479713 2.294669 0.541018
H -8.949038 0.004823 -2.742118
S 3.459934 2.791401 1.890383
S -9.502172 2.543735 -1.522534
O 4.657911 2.225368 2.534720
O 3.766851 3.200703 0.460822
O 2.735509 3.832319 2.620059
O -9.478297 2.593919 -2.996842
O -8.971967 3.742539 -0.847047
O -10.761265 2.022815 -0.954988
O 7.159887 1.071774 -1.170459
O 5.788910 -0.634729 -0.674598

TS1-2

Zero-point correction= 0.440712 (Hartree/Particle)
Thermal correction to Energy= 0.478529
Thermal correction to Enthalpy= 0.479474
Thermal correction to Gibbs Free Energy= 0.361715
Sum of electronic and zero-point Energies= -2845.736001
Sum of electronic and thermal Energies= -2845.698184
Sum of electronic and thermal Enthalpies= -2845.697240
Sum of electronic and thermal Free Energies= -2845.814999
Single Point Energy Calculations with extended basis set: HF = -2848.62312153
N 2.026397 1.196512 -0.162529
C 2.149441 2.507785 -0.290049
C 1.062734 3.379833 -0.289460
C -0.230018 2.891382 -0.152797
C -0.384278 1.475705 -0.057944
C 0.782754 0.673692 -0.055462
N 1.811032 -1.481769 0.125378
C 1.733732 -2.796821 0.245060
C 0.518188 -3.482774 0.271632
C -0.682604 -2.793650 0.171939
C -0.612701 -1.369653 0.092324
C 0.666896 -0.767542 0.057250

H	3.167932	2.888913	-0.380240
H	1.229004	4.453136	-0.354500
H	2.686204	-3.328527	0.301878
H	0.512071	-4.569704	0.323589
C	-1.658230	0.828658	0.002205
C	-1.766722	-0.525124	0.074444
H	-2.554357	1.444288	-0.023759
H	-2.749443	-0.987762	0.129813
Ag	3.843718	-0.271174	-0.065061
C	5.379648	-2.307155	-0.725511
C	6.020224	-0.434449	0.031500
C	6.535932	-0.505812	1.335688
C	6.738606	0.335533	-0.898251
C	7.687924	0.184355	1.707553
H	6.032321	-1.144779	2.064430
C	7.890554	1.030592	-0.539905
H	6.394932	0.360239	-1.934606
C	8.363930	0.959688	0.768920
H	8.067495	0.110451	2.727634
H	8.428841	1.622022	-1.282048
H	9.270320	1.495687	1.052519
O	5.204622	-3.005647	0.234630
O	5.449898	-2.199558	-1.915222
C	-1.344469	3.854456	-0.117742
C	-1.372122	4.898196	-1.056838
C	-2.326097	3.828086	0.881776
C	-2.345433	5.881349	-0.996183
H	-0.627298	4.913690	-1.854092
C	-3.291895	4.826665	0.949096
H	-2.301126	3.043977	1.639743
C	-3.302773	5.858609	0.016922
H	-2.385649	6.681245	-1.734339
H	-4.053056	4.831231	1.727594
C	-1.942317	-3.557772	0.144414
C	-2.140486	-4.598858	1.065638
C	-2.914606	-3.342707	-0.840769
C	-3.274381	-5.391731	1.004556
H	-1.397466	-4.763544	1.847594
C	-4.044368	-4.151237	-0.908358
H	-2.758384	-2.564264	-1.588862
C	-4.228476	-5.178311	0.010150
H	-3.440205	-6.190380	1.726472
H	-4.801539	-4.011269	-1.677953
S	-5.661115	-6.279220	-0.079594
S	-4.487032	7.220680	0.140042
O	-6.485087	-5.712702	-1.162761
O	-6.246536	-6.182452	1.270211
O	-5.049140	-7.587077	-0.381766
O	-4.969271	7.381793	-1.243903
O	-3.647125	8.333203	0.623353

O -5.492173 6.738449 1.104097
Imaginary Vibrational Frequency = -298.5911 cm^{-1}

2

Zero-point correction= 0.440819 (Hartree/Particle)
Thermal correction to Energy= 0.479982
Thermal correction to Enthalpy= 0.480927
Thermal correction to Gibbs Free Energy= 0.356944
Sum of electronic and zero-point Energies= -2845.753319
Sum of electronic and thermal Energies= -2845.714155
Sum of electronic and thermal Enthalpies= -2845.713211
Sum of electronic and thermal Free Energies= -2845.837194
Single Point Energy Calculations with extended basis set: HF = -2848.6426016

N	1.448334	-1.906397	-0.163741
C	1.128904	-3.187196	-0.136835
C	-0.186172	-3.646612	-0.048462
C	-1.240286	-2.745608	0.019560
C	-0.909898	-1.357369	0.029373
C	0.455179	-0.997905	-0.079017
N	2.154778	0.690094	-0.179244
C	2.518403	1.963991	-0.177052
C	1.608854	3.017982	-0.109137
C	0.245189	2.767985	-0.033274
C	-0.162435	1.401163	0.002759
C	0.835726	0.401148	-0.090361
H	1.961927	-3.890445	-0.206557
H	-0.392270	-4.714965	-0.073228
H	3.589855	2.157722	-0.246739
H	1.967312	4.044379	-0.154002
C	-1.876862	-0.318586	0.206458
C	-1.520751	0.993635	0.192975
H	-2.913138	-0.598650	0.383040
H	-2.272378	1.762163	0.359050
Ag	3.755092	-1.004426	-0.299962
C	5.895374	0.751017	1.539244
C	5.695381	-1.825057	-0.394049
C	6.721293	-1.279935	-1.188210
C	6.038603	-2.980837	0.332428
C	7.995073	-1.844783	-1.260285
H	6.524930	-0.376671	-1.771312
C	7.306882	-3.556821	0.271513
H	5.290745	-3.450581	0.976621
C	8.294781	-2.989980	-0.528857
H	8.758898	-1.385349	-1.891105
H	7.525820	-4.453754	0.854419
H	9.289218	-3.435498	-0.580024
C	-2.618053	-3.265548	0.074163
C	-2.915501	-4.338295	0.930443
C	-3.627385	-2.786001	-0.770652
C	-4.176943	-4.909452	0.939442

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C -4.888904 -3.372328 -0.769575
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C -5.167866 -4.436902 0.079934
H -4.418179 -5.729276 1.614845
H -5.680474 -3.023748 -1.430859
C -0.683760 3.910490 0.005737
C -1.805648 3.989056 -0.830056
C -0.391411 5.003073 0.838550
C -2.599126 5.131370 -0.842588
H -2.029499 3.164378 -1.508045
C -1.192857 6.132079 0.834687
H 0.465705 4.942471 1.511050
C -2.295207 6.207167 -0.015809
H -3.465641 5.216618 -1.496256
H -0.982935 6.973618 1.493642
S -6.773596 -5.269352 0.054090
S -3.262221 7.735119 -0.064433
O -6.444200 -6.590923 -0.513149
O -7.163200 -5.301519 1.475889
O -7.610748 -4.414827 -0.807099
O -3.537183 8.008916 1.358105
O -4.442394 7.390544 -0.877399
O -2.329564 8.688342 -0.695451
O 5.918539 1.533508 0.672858
O 5.897202 0.031207 2.454883

3

Zero-point correction= 0.428158 (Hartree/Particle)
Thermal correction to Energy= 0.463038
Thermal correction to Enthalpy= 0.463982
Thermal correction to Gibbs Free Energy= 0.351514
Sum of electronic and zero-point Energies= -2657.258784
Sum of electronic and thermal Energies= -2657.223903
Sum of electronic and thermal Enthalpies= -2657.222959
Sum of electronic and thermal Free Energies= -2657.335427
Single Point Energy Calculations with extended basis set: HF = -2659.9612609
N 2.026684 1.658009 -0.045627
C 1.855725 2.969325 -0.064621
C 0.600810 3.577059 -0.095655
C -0.553420 2.805403 -0.110030
C -0.387323 1.388518 -0.126265
C 0.929265 0.870421 -0.079733
N 2.417949 -0.998268 -0.052448
C 2.635048 -2.301448 -0.075668
C 1.609891 -3.247940 -0.106048
C 0.281657 -2.843673 -0.115239
C 0.029695 -1.439416 -0.129343
C 1.140724 -0.563513 -0.082474
H 2.765654 3.571455 -0.037666

H	0.522945	4.662166	-0.068802
H	3.681125	-2.613208	-0.051540
H	1.849233	-4.309352	-0.081465
C	-1.477369	0.470295	-0.251674
C	-1.279182	-0.875139	-0.252687
H	-2.480587	0.872013	-0.377051
H	-2.124165	-1.548706	-0.378645
Ag	4.196847	0.675544	0.023427
C	6.289174	0.901283	0.103007
C	7.109979	0.742210	-1.029185
C	6.961312	1.217429	1.298543
C	8.496308	0.886238	-0.978348
H	6.654872	0.495318	-1.991629
C	8.346545	1.364060	1.365732
H	6.385840	1.356479	2.217099
C	9.124521	1.198865	0.223576
H	9.090323	0.752519	-1.885035
H	8.821622	1.609889	2.317892
H	10.208567	1.312429	0.269652
C	-1.861133	3.484159	-0.108626
C	-2.066369	4.579070	-0.963732
C	-2.881927	3.133211	0.784307
C	-3.250291	5.296357	-0.925418
H	-1.287367	4.845652	-1.679782
C	-4.063165	3.866491	0.831187
H	-2.727609	2.305687	1.478147
C	-4.250942	4.951210	-0.018055
H	-3.423232	6.133528	-1.600436
H	-4.860952	3.618405	1.529293
C	-0.775224	-3.870391	-0.106275
C	-1.846054	-3.824062	0.795382
C	-0.665222	-4.980756	-0.958971
C	-2.768329	-4.863933	0.852607
H	-1.928717	-2.985580	1.488299
C	-1.594409	-6.006381	-0.910210
H	0.152691	-5.015800	-1.680449
C	-2.645304	-5.959149	0.005058
H	-3.596821	-4.853456	1.558827
H	-1.523711	-6.861060	-1.581747
S	-5.743110	5.969984	0.070294
S	-3.786261	-7.359581	0.100216
O	-5.238720	7.234903	0.638148
O	-6.172609	6.067041	-1.336986
O	-6.647929	5.210842	0.952109
O	-4.222264	-7.538697	-1.296988
O	-4.835508	-6.909226	1.032400
O	-2.925964	-8.444664	0.609501

4N

Zero-point correction= 0.533326 (Hartree/Particle)

Thermal correction to Energy= 0.576859
Thermal correction to Enthalpy= 0.577803
Thermal correction to Gibbs Free Energy= 0.448258
Sum of electronic and zero-point Energies= -3056.628365
Sum of electronic and thermal Energies= -3056.584832
Sum of electronic and thermal Enthalpies= -3056.583888
Sum of electronic and thermal Free Energies= -3056.713433
Single Point Energy Calculations with extended basis set: HF = -3059.8974670

N	2.053853	1.221926	-1.174487
C	3.286319	0.751667	-1.147224
C	3.586117	-0.600969	-0.972112
C	2.563926	-1.531134	-0.837585
C	1.225806	-1.044545	-0.915284
C	1.034051	0.351729	-1.049756
N	-0.442882	2.245295	-1.115457
C	-1.666711	2.754884	-1.093248
C	-2.818324	1.981584	-0.958420
C	-2.724468	0.599747	-0.849833
C	-1.419926	0.028770	-0.925148
C	-0.309157	0.900076	-1.037411
H	4.084079	1.492239	-1.247222
H	4.622622	-0.925960	-0.900793
H	-1.737056	3.842471	-1.153659
H	-3.787446	2.470534	-0.879018
C	0.076004	-1.894913	-0.904809
C	-1.183760	-1.382897	-0.916676
H	0.225961	-2.972654	-0.910390
H	-2.042109	-2.050922	-0.934919
Ag	1.371103	3.629386	-0.817630
C	-2.016477	3.985096	1.799924
C	2.652062	5.222995	-0.315742
C	2.478166	6.563737	-0.703608
C	3.789983	4.961955	0.470811
C	3.368047	7.571920	-0.334398
H	1.614954	6.836905	-1.314944
C	4.689984	5.958409	0.849157
H	3.988162	3.937568	0.804874
C	4.481446	7.273970	0.446673
H	3.189501	8.599804	-0.657336
H	5.558643	5.705587	1.460538
H	5.179250	8.059794	0.739051
O	-3.013299	4.530948	1.491096
N	-0.956818	3.549470	2.160060
C	-0.167267	2.403052	2.240862
C	-0.745971	1.132818	2.295358
C	1.220608	2.551502	2.260409
C	0.071751	0.010929	2.360044
H	-1.831717	1.034949	2.272783
C	2.025858	1.418879	2.319128
H	1.649019	3.551549	2.204825

C 1.458364 0.148375 2.366904
H -0.379979 -0.980216 2.389193
H 3.109328 1.533432 2.306952
H 2.095270 -0.734803 2.401582
C -3.954000 -0.183741 -0.643111
C -5.093904 0.103007 -1.411857
C -4.055175 -1.150126 0.366448
C -6.287015 -0.561144 -1.183684
H -5.021970 0.842285 -2.211119
C -5.260170 -1.803168 0.603958
H -3.188724 -1.363273 0.995358
C -6.378898 -1.512716 -0.168338
H -7.169613 -0.353277 -1.787153
H -5.362686 -2.544020 1.395144
C 2.911467 -2.942220 -0.593860
C 3.931983 -3.545240 -1.346180
C 2.320944 -3.679043 0.441328
C 4.346646 -4.837511 -1.070274
H 4.382944 -2.988433 -2.169176
C 2.750738 -4.971022 0.726067
H 1.544280 -3.216448 1.053548
C 3.766714 -5.553065 -0.023646
H 5.123944 -5.318107 -1.662894
H 2.313475 -5.552730 1.535882
S 4.403961 -7.199675 0.369625
S -7.969624 -2.321726 0.127932
O 4.408388 -7.883201 -0.936968
O 3.445471 -7.732345 1.354491
O 5.747600 -6.907690 0.904571
O -7.693573 -3.271799 1.220369
O -8.279621 -2.936586 -1.175838
O -8.848093 -1.193289 0.489352

TS4-5N

Zero-point correction= 0.532070 (Hartree/Particle)
Thermal correction to Energy= 0.574957
Thermal correction to Enthalpy= 0.575901
Thermal correction to Gibbs Free Energy= 0.446607
Sum of electronic and zero-point Energies= -3056.597096
Sum of electronic and thermal Energies= -3056.554208
Sum of electronic and thermal Enthalpies= -3056.553264
Sum of electronic and thermal Free Energies= -3056.682558
Single Point Energy Calculations with extended basis set: HF = -3059.86873889
N -0.040865 -2.321008 -0.026400
C -0.808192 -3.397007 -0.070337
C -2.199623 -3.340066 -0.138134
C -2.851942 -2.114299 -0.162360
C -2.036935 -0.942824 -0.151056
C -0.633213 -1.106879 -0.069860
N 1.562115 -0.152770 0.014831

C	2.370196	0.895140	0.024359
C	1.905972	2.210322	0.006113
C	0.543412	2.476355	-0.027964
C	-0.337888	1.354448	-0.084629
C	0.228653	0.058716	-0.042057
H	-0.290848	-4.357595	-0.031612
H	-2.781307	-4.259638	-0.129934
H	3.439584	0.675661	0.069529
H	2.615478	3.033412	0.060988
C	-2.562545	0.381106	-0.280243
C	-1.754197	1.474189	-0.246287
H	-3.632425	0.500895	-0.435976
H	-2.178401	2.467725	-0.373864
Ag	2.339040	-2.360627	0.111331
C	4.776124	-2.128359	-0.819722
C	3.875030	-3.837631	0.445818
C	3.858340	-5.029129	-0.295226
C	4.433380	-3.894065	1.731402
C	4.340860	-6.225988	0.229285
H	3.482467	-5.010411	-1.321075
C	4.919000	-5.085008	2.268307
H	4.514983	-2.973541	2.313912
C	4.868663	-6.256945	1.518179
H	4.313907	-7.137047	-0.370678
H	5.348731	-5.097909	3.271180
H	5.254282	-7.189799	1.930870
O	4.715991	-2.570559	-1.924040
N	5.175093	-1.311419	0.052246
C	6.134563	-0.339005	-0.285802
C	6.806053	-0.280288	-1.514987
C	6.425185	0.625141	0.687682
C	7.740018	0.721075	-1.752236
H	6.586506	-1.021647	-2.281311
C	7.356106	1.624615	0.439559
H	5.897294	0.565361	1.638852
C	8.022317	1.679163	-0.782351
H	8.251621	0.753666	-2.714234
H	7.561615	2.369188	1.208123
H	8.750871	2.464425	-0.978771
C	0.089031	3.876825	0.003146
C	0.733821	4.830105	-0.802183
C	-0.909018	4.311993	0.884934
C	0.389296	6.169128	-0.727877
H	1.497620	4.499313	-1.507635
C	-1.240575	5.660203	0.968209
H	-1.395448	3.591184	1.543576
C	-0.592712	6.593324	0.166788
H	0.874557	6.909725	-1.362257
H	-2.000084	6.019754	1.660401
C	-4.324360	-2.095961	-0.195181

C -5.002469 -2.965343 -1.065216
C -5.078830 -1.305115 0.681461
C -6.385166 -3.040577 -1.056668
H -4.425657 -3.566863 -1.769578
C -6.466541 -1.395741 0.698364
H -4.568548 -0.648318 1.387219
C -7.124577 -2.265148 -0.164722
H -6.918086 -3.695944 -1.744309
H -7.068154 -0.800042 1.382874
S -8.921011 -2.469270 -0.103886
S -0.958138 8.360490 0.293479
O -9.319207 -2.417418 -1.522681
O -9.384805 -1.339304 0.720850
O -9.072824 -3.797496 0.520148
O -2.103766 8.427323 1.218543
O -1.252184 8.746359 -1.098831
O 0.302180 8.915585 0.822492
Imaginary Vibrational Frequency = -244.9984 cm^{-1}

5N
Zero-point correction= 0.536046 (Hartree/Particle)
Thermal correction to Energy= 0.578299
Thermal correction to Enthalpy= 0.579243
Thermal correction to Gibbs Free Energy= 0.452029
Sum of electronic and zero-point Energies= -3056.666444
Sum of electronic and thermal Energies= -3056.624192
Sum of electronic and thermal Enthalpies= -3056.623248
Sum of electronic and thermal Free Energies= -3056.750462
Single Point Energy Calculations with extended basis set: HF = -3059.94055965
N 1.449239 1.114110 0.013031
C 1.581947 2.431712 0.042845
C 0.495184 3.303846 0.032839
C -0.802709 2.812811 -0.014323
C -0.960287 1.395244 -0.072017
C 0.203155 0.589074 -0.040494
N 1.218495 -1.583512 -0.052680
C 1.124006 -2.902404 -0.079257
C -0.094437 -3.580056 -0.111947
C -1.290140 -2.874311 -0.123321
C -1.204699 -1.449544 -0.128233
C 0.079633 -0.856150 -0.072998
H 2.603589 2.814865 0.084825
H 0.664191 4.376703 0.097105
H 2.067218 -3.454045 -0.052542
H -0.110720 -4.667841 -0.088510
C -2.230560 0.756073 -0.224197
C -2.347281 -0.598243 -0.249282
H -3.112624 1.380463 -0.347245
H -3.322926 -1.057539 -0.391449
Ag 3.257166 -0.312254 -0.038239

C	6.196614	0.302597	0.358633
C	5.698218	1.669329	-0.055365
C	5.945566	2.751197	0.790916
C	5.079738	1.906507	-1.287504
C	5.542568	4.035212	0.439501
H	6.468468	2.560532	1.726773
C	4.700130	3.194808	-1.654058
H	4.914816	1.070412	-1.967014
C	4.920273	4.262197	-0.786333
H	5.722969	4.866492	1.120608
H	4.226825	3.365208	-2.620688
H	4.612607	5.268925	-1.067249
C	-1.921336	3.770543	-0.008442
C	-1.850995	4.904205	-0.834191
C	-3.017227	3.639501	0.855352
C	-2.841851	5.870923	-0.797694
H	-1.015132	5.002996	-1.528587
C	-4.001388	4.620725	0.901061
H	-3.072543	2.782406	1.527820
C	-3.916979	5.740320	0.079949
H	-2.807494	6.739648	-1.453669
H	-4.853451	4.540788	1.574087
C	-2.558302	-3.622944	-0.124274
C	-3.595912	-3.326330	0.769395
C	-2.705969	-4.726360	-0.980475
C	-4.738477	-4.117770	0.813739
H	-3.484029	-2.494175	1.465746
C	-3.852492	-5.502114	-0.944625
H	-1.913962	-4.952105	-1.696331
C	-4.870902	-5.208340	-0.038675
H	-5.548660	-3.911425	1.511113
H	-3.982827	-6.345388	-1.621551
S	-5.134940	7.073989	0.186576
S	-6.313214	-6.297297	0.043076
O	-4.407412	8.114274	0.938126
O	-5.394635	7.414103	-1.224503
O	-6.269309	6.468047	0.906100
O	-6.723824	-6.422076	-1.367541
O	-7.260409	-5.576214	0.911938
O	-5.753576	-7.532775	0.623223
O	7.278318	0.252729	0.953955
N	5.379557	-0.718595	-0.000580
C	5.750311	-2.060033	0.144769
C	6.878841	-2.542183	0.836514
C	4.916611	-3.018147	-0.466360
C	7.126511	-3.909135	0.914862
H	7.543850	-1.826393	1.305648
C	5.170980	-4.378545	-0.380577
H	4.055375	-2.656434	-1.035227
C	6.283978	-4.841525	0.317929

H 8.004609 -4.249855 1.465511
H 4.495717 -5.081542 -0.870335
H 6.489614 -5.908676 0.393240

4O

Zero-point correction= 0.533430 (Hartree/Particle)
Thermal correction to Energy= 0.577244
Thermal correction to Enthalpy= 0.578188
Thermal correction to Gibbs Free Energy= 0.445913
Sum of electronic and zero-point Energies= -3056.620947
Sum of electronic and thermal Energies= -3056.577133
Sum of electronic and thermal Enthalpies= -3056.576189
Sum of electronic and thermal Free Energies= -3056.708464
Single Point Energy Calculations with extended basis set: HF = -3059.89265601
N 0.533388 -1.878173 -0.589888
C 0.239119 -3.163475 -0.540070
C -1.048088 -3.646536 -0.297337
C -2.098867 -2.763378 -0.089636
C -1.791081 -1.370139 -0.103748
C -0.454803 -0.986941 -0.374168
N 1.193060 0.735803 -0.664073
C 1.533584 2.016969 -0.686989
C 0.620519 3.051660 -0.490876
C -0.718752 2.774342 -0.254088
C -1.095134 1.399660 -0.187280
C -0.100041 0.418679 -0.415711
H 1.068066 -3.852349 -0.720562
H -1.240195 -4.717788 -0.309742
H 2.584460 2.230117 -0.887306
H 0.953067 4.085097 -0.564114
C -2.745823 -0.350445 0.202407
C -2.413785 0.967434 0.161937
H -3.748609 -0.650040 0.499574
H -3.151041 1.722103 0.427022
Ag 2.809976 -0.864221 -0.979723
C 5.806819 1.694878 -0.238956
C 4.685436 -1.783223 -1.254924
C 5.731512 -1.202478 -1.998401
C 4.981437 -3.026675 -0.662596
C 6.982932 -1.805259 -2.132181
H 5.569020 -0.237115 -2.484600
C 6.227347 -3.643207 -0.788399
H 4.213985 -3.534815 -0.072235
C 7.239460 -3.030034 -1.522060
H 7.764892 -1.312882 -2.713578
H 6.409221 -4.607713 -0.309245
H 8.217743 -3.502258 -1.617960
C -3.451747 -3.306962 0.126613
C -3.626603 -4.388928 1.003973
C -4.563409 -2.838987 -0.586305

C -4.868584 -4.982412 1.159669
H -2.772816 -4.744702 1.582999
C -5.805505 -3.447023 -0.438754
H -4.440239 -2.019143 -1.295312
C -5.962710 -4.522632 0.428632
H -5.016275 -5.807099 1.855678
H -6.676905 -3.104085 -0.994167
C -1.659654 3.896009 -0.091380
C -2.869477 3.957808 -0.794739
C -1.299264 4.985670 0.718396
C -3.685332 5.080729 -0.701768
H -3.149168 3.136159 -1.455480
C -2.122037 6.094509 0.821227
H -0.369243 4.938964 1.287161
C -3.315320 6.152994 0.101985
H -4.619733 5.154689 -1.255517
H -1.854450 6.934736 1.460664
S -7.542484 -5.392986 0.567200
S -4.323432 7.651639 0.201850
O -7.294569 -6.634968 -0.189839
O -7.700053 -5.590515 2.020163
O -8.516121 -4.474905 -0.050725
O -4.537409 7.819861 1.650983
O -5.531820 7.328040 -0.577750
O -3.447605 8.673298 -0.402987
O 5.039987 2.030061 -1.065794
N 6.635444 1.518432 0.613942
C 7.259186 0.579624 1.431166
C 6.932554 -0.776025 1.366370
C 8.230292 1.031254 2.326407
C 7.586916 -1.671299 2.202405
H 6.176755 -1.120024 0.659727
C 8.874374 0.124203 3.158355
H 8.463578 2.093933 2.356845
C 8.556012 -1.229976 3.099630
H 7.329432 -2.727599 2.137718
H 9.630145 0.479898 3.857562
H 9.062687 -1.939864 3.751924

TS4-5O

Zero-point correction= 0.532631 (Hartree/Particle)
Thermal correction to Energy= 0.575140
Thermal correction to Enthalpy= 0.576084
Thermal correction to Gibbs Free Energy= 0.448794
Sum of electronic and zero-point Energies= -3056.605845
Sum of electronic and thermal Energies= -3056.563336
Sum of electronic and thermal Enthalpies= -3056.562392
Sum of electronic and thermal Free Energies= -3056.689682
Single Point Energy Calculations with extended basis set: HF = -3059.87740314
N -1.525137 1.084851 -0.391274

C	-1.711579	2.395083	-0.379869
C	-0.669427	3.312649	-0.260291
C	0.643171	2.872523	-0.146459
C	0.856370	1.461826	-0.105255
C	-0.266582	0.610857	-0.244211
N	-1.196633	-1.595683	-0.315521
C	-1.068645	-2.911109	-0.246772
C	0.168449	-3.542698	-0.107925
C	1.336697	-2.796398	-0.028374
C	1.204664	-1.374637	-0.045202
C	-0.089901	-0.828634	-0.208969
H	-2.743925	2.733682	-0.489033
H	-0.878360	4.379604	-0.304159
H	-1.994975	-3.485840	-0.321766
H	0.222713	-4.629507	-0.104782
C	2.135889	0.869291	0.134683
C	2.301526	-0.480267	0.162249
H	2.981800	1.524987	0.328852
H	3.280378	-0.902788	0.378380
Ag	-3.265361	-0.465025	-0.652611
C	-4.855747	-2.393237	0.339696
C	-5.372783	-0.815013	-1.055489
C	-5.658135	-1.496191	-2.250307
C	-6.192646	0.287527	-0.742124
C	-6.692190	-1.103238	-3.095743
H	-5.071192	-2.384241	-2.491419
C	-7.239112	0.679706	-1.575384
H	-6.010159	0.858099	0.169821
C	-7.489607	-0.013445	-2.756256
H	-6.886176	-1.655599	-4.016130
H	-7.857542	1.536388	-1.304030
H	-8.308147	0.292330	-3.408692
O	-4.549342	-3.328786	-0.347283
N	-5.167895	-2.059457	1.515520
C	-5.193410	-0.810372	2.098069
C	-6.393561	-0.306226	2.620909
C	-4.027080	-0.039301	2.236568
C	-6.437433	0.954050	3.200461
H	-7.289180	-0.919061	2.529176
C	-4.081691	1.230413	2.804377
H	-3.070620	-0.463707	1.926493
C	-5.286424	1.738579	3.281067
H	-7.383378	1.335414	3.585241
H	-3.166749	1.817551	2.884861
H	-5.325814	2.729961	3.730172
C	2.628971	-3.496673	0.063147
C	3.711609	-3.158524	-0.759543
C	2.763248	-4.593389	0.930147
C	4.886172	-3.902216	-0.724802
H	3.612638	-2.332161	-1.464768

C 3.940269 -5.321759 0.973031
H 1.934369 -4.851980 1.590921
C 5.005175 -4.986303 0.137486
H 5.731784 -3.664477 -1.367972
H 4.056687 -6.161192 1.657254
C 1.723392 3.870934 -0.082868
C 2.858987 3.782666 -0.898368
C 1.574493 5.000060 0.739529
C 3.806419 4.801038 -0.903954
H 2.973698 2.929961 -1.568856
C 2.528757 6.002952 0.744158
H 0.705035 5.068228 1.395373
C 3.644295 5.915078 -0.088230
H 4.684297 4.760482 -1.546526
H 2.426020 6.872982 1.391348
S 6.495919 -6.010778 0.162297
S 4.822765 7.287288 -0.114527
O 7.447190 -5.284934 -0.698524
O 6.016814 -7.294539 -0.384301
O 6.852050 -6.056636 1.592348
O 5.897000 6.824950 -1.011304
O 5.204793 7.431900 1.302028
O 4.009231 8.400713 -0.638905
Imaginary Vibrational Frequency = -291.5005 cm^{-1}

5O
Zero-point correction= 0.534618 (Hartree/Particle)
Thermal correction to Energy= 0.577074
Thermal correction to Enthalpy= 0.578018
Thermal correction to Gibbs Free Energy= 0.449594
Sum of electronic and zero-point Energies= -3056.643077
Sum of electronic and thermal Energies= -3056.600621
Sum of electronic and thermal Enthalpies= -3056.599677
Sum of electronic and thermal Free Energies= -3056.728101
Single Point Energy Calculations with extended basis set: HF = -3059.91466598
N -1.832765 1.091201 0.594186
C -2.084709 2.385821 0.500278
C -1.082153 3.345974 0.363486
C 0.252590 2.965538 0.310049
C 0.539485 1.572319 0.433340
C -0.547624 0.675751 0.571345
N -1.360597 -1.565599 0.885635
C -1.144943 -2.866447 0.991090
C 0.120215 -3.442942 0.891064
C 1.238926 -2.646313 0.687427
C 1.029711 -1.235143 0.623555
C -0.297963 -0.749094 0.695784
H -3.139413 2.670764 0.518512
H -1.347179 4.395737 0.254885
H -2.028137 -3.490326 1.137403

H	0.227566	-4.524978	0.933042
C	1.868670	1.047325	0.481228
C	2.101484	-0.289919	0.559788
H	2.703082	1.744926	0.473395
H	3.122356	-0.661944	0.610878
Ag	-3.477854	-0.613195	0.692812
C	-5.992879	-1.776099	-1.697300
C	-4.494685	-1.927339	-1.910091
C	-3.940158	-3.208987	-1.940679
C	-3.657986	-0.824049	-2.125666
C	-2.578368	-3.387310	-2.159442
H	-4.612530	-4.054740	-1.804201
C	-2.295416	-1.004010	-2.363714
H	-4.097255	0.174455	-2.139340
C	-1.751523	-2.284756	-2.370637
H	-2.153914	-4.391385	-2.170885
H	-1.657606	-0.136194	-2.531993
H	-0.683353	-2.425161	-2.536778
O	-6.713599	-2.734076	-1.963952
N	-6.409952	-0.536621	-1.339378
C	-6.124580	0.040405	-0.187320
C	-6.233755	1.466152	-0.041366
C	-5.729584	-0.678019	1.010273
C	-6.064810	2.090746	1.171826
H	-6.513900	2.030500	-0.930889
C	-5.602270	0.002631	2.250727
H	-5.875790	-1.761183	1.016815
C	-5.748553	1.374573	2.345505
H	-6.186264	3.174250	1.227386
H	-5.404504	-0.590296	3.145895
H	-5.627994	1.886811	3.297704
C	2.555283	-3.288301	0.541531
C	3.427096	-2.953922	-0.503349
C	2.918161	-4.331988	1.409060
C	4.617577	-3.650177	-0.681828
H	3.145468	-2.170379	-1.208168
C	4.111882	-5.011815	1.237560
H	2.257646	-4.585983	2.239655
C	4.963693	-4.681435	0.183879
H	5.299160	-3.416323	-1.497933
H	4.406826	-5.809467	1.918105
C	1.279971	4.006928	0.137526
C	2.295702	3.905895	-0.822281
C	1.193691	5.183540	0.900243
C	3.188674	4.954029	-1.019429
H	2.356532	3.015537	-1.449654
C	2.093995	6.218074	0.711550
H	0.420283	5.263643	1.665784
C	3.091215	6.112699	-0.257338
H	3.974368	4.900732	-1.771305

H 2.042837 7.124376 1.313566
S 6.476256 -5.645774 -0.050502
S 4.201362 7.515655 -0.526005
O 7.179518 -4.953920 -1.145148
O 5.956431 -6.983773 -0.390252
O 7.132252 -5.567579 1.267473
O 5.190946 7.012607 -1.495297
O 4.727512 7.792197 0.823242
O 3.291411 8.553771 -1.045952

6

Zero-point correction= 0.535341 (Hartree/Particle)
Thermal correction to Energy= 0.577859
Thermal correction to Enthalpy= 0.578803
Thermal correction to Gibbs Free Energy= 0.449663
Sum of electronic and zero-point Energies= -3056.654861
Sum of electronic and thermal Energies= -3056.612343
Sum of electronic and thermal Enthalpies= -3056.611399
Sum of electronic and thermal Free Energies= -3056.740538
Single Point Energy Calculations with extended basis set: HF = -3059.92615359
N 0.051425 -2.348747 0.177200
C -0.541584 -3.532213 0.177836
C -1.925246 -3.695979 0.167284
C -2.762293 -2.588124 0.159178
C -2.141628 -1.304099 0.202755
C -0.726652 -1.241066 0.193506
N 1.283023 0.060208 0.205199
C 1.913864 1.221459 0.226661
C 1.242004 2.445342 0.237663
C -0.145668 2.486846 0.227009
C -0.836661 1.237292 0.236280
C -0.065773 0.050937 0.209657
H 0.118277 -4.401188 0.166462
H -2.352472 -4.695641 0.120747
H 3.005333 1.173250 0.213551
H 1.809439 3.373586 0.214186
C -2.880055 -0.084051 0.316751
C -2.259060 1.125525 0.333963
H -3.961360 -0.141689 0.419659
H -2.844217 2.035225 0.450422
Ag 2.381455 -2.041814 0.175082
C 5.186296 -2.149872 -0.023427
C 6.609950 -2.621774 -0.121410
C 7.505033 -2.099460 -1.058387
C 7.032167 -3.663740 0.707308
C 8.796872 -2.604125 -1.156643
H 7.183086 -1.294115 -1.716813
C 8.330184 -4.153796 0.625021
H 6.316243 -4.085863 1.409843
C 9.216751 -3.626033 -0.309697

H	9.480901	-2.193465	-1.898697
H	8.648660	-4.959652	1.286122
H	10.232472	-4.014550	-0.382393
C	-4.218374	-2.800576	0.098576
C	-4.806269	-3.782679	0.912879
C	-5.028727	-2.122268	-0.821257
C	-6.155974	-4.073015	0.809997
H	-4.188813	-4.301404	1.648003
C	-6.380944	-2.428812	-0.933108
H	-4.582784	-1.381522	-1.486220
C	-6.948816	-3.405479	-0.123141
H	-6.619781	-4.822170	1.450388
H	-7.022186	-1.926396	-1.655387
C	-0.820959	3.796305	0.202558
C	-1.841679	4.087429	-0.711993
C	-0.377364	4.817576	1.058139
C	-2.391952	5.363184	-0.776080
H	-2.174839	3.316508	-1.408226
C	-0.938581	6.082563	1.001788
H	0.402476	4.595969	1.788416
C	-1.942623	6.365195	0.076589
H	-3.176063	5.610944	-1.489601
H	-0.613300	6.872586	1.677397
S	-8.689784	-3.870710	-0.281294
S	-2.588098	8.051736	-0.029540
O	-8.610893	-5.265728	-0.755011
O	-9.203686	-3.726814	1.093084
O	-9.233422	-2.911317	-1.259065
O	-2.903714	8.384486	1.372002
O	-3.753422	7.937341	-0.925033
O	-1.446806	8.801609	-0.587711
O	4.338330	-3.072650	0.221604
N	4.806454	-0.911722	-0.232170
C	5.642573	0.191248	-0.252538
C	6.616830	0.449735	0.730706
C	5.446537	1.169248	-1.245058
C	7.375336	1.612356	0.696010
H	6.764739	-0.280861	1.526086
C	6.207551	2.330372	-1.272814
H	4.674735	0.985444	-1.993270
C	7.183272	2.561787	-0.305537
H	8.123322	1.783684	1.471011
H	6.031706	3.066928	-2.057104
H	7.774684	3.476196	-0.322772

7

Zero-point correction= 0.102093 (Hartree/Particle)
Thermal correction to Energy= 0.109005
Thermal correction to Enthalpy= 0.109949
Thermal correction to Gibbs Free Energy= 0.070256

Sum of electronic and zero-point Energies= -419.873201
Sum of electronic and thermal Energies= -419.866289
Sum of electronic and thermal Enthalpies= -419.865345
Sum of electronic and thermal Free Energies= -419.905038
Single Point Energy Calculations with extended basis set: HF = -420.4701431

C	-1.828110	0.000096	-0.000029
C	-0.280411	0.000004	-0.000020
C	0.432640	-1.198591	-0.000042
C	0.432661	1.198544	0.000035
C	1.824506	-1.204337	-0.000039
H	-0.155515	-2.116461	-0.000055
C	1.824576	1.204281	0.000051
H	-0.155441	2.116470	0.000046
C	2.527411	-0.000015	0.000002
H	2.370100	-2.150692	-0.000099
H	2.370172	2.150643	0.000119
H	3.619139	0.000012	0.000005
O	-2.352927	1.134546	-0.000089
O	-2.353085	-1.134529	0.000119

8

Zero-point correction= 0.207487 (Hartree/Particle)
Thermal correction to Energy= 0.223050
Thermal correction to Enthalpy= 0.223994
Thermal correction to Gibbs Free Energy= 0.162516
Sum of electronic and zero-point Energies= -819.243980
Sum of electronic and thermal Energies= -819.228417
Sum of electronic and thermal Enthalpies= -819.227473
Sum of electronic and thermal Free Energies= -819.288952
Single Point Energy Calculations with extended basis set: HF = -820.4061562

C	2.035070	-1.850895	-0.833717
O	2.226808	-3.006586	-0.751286
N	1.982170	-0.694948	-1.206630
C	1.617463	0.553976	-0.712006
C	1.751110	0.887153	0.637689
C	1.124775	1.496785	-1.617467
C	1.351862	2.143401	1.073540
H	2.080510	0.126056	1.340730
C	0.746530	2.757058	-1.172389
H	1.023479	1.211571	-2.663386
C	0.856230	3.085595	0.176056
H	1.403781	2.366424	2.137905
H	0.349348	3.481783	-1.883184
H	0.539453	4.066729	0.529161
C	-0.210785	-0.948548	1.701001
C	-1.319652	-0.666530	0.679234
C	-1.472756	-1.466096	-0.453772
C	-2.162311	0.432424	0.843201
C	-2.444209	-1.174195	-1.405892
H	-0.804220	-2.320150	-0.562273

C -3.124680 0.741086 -0.113057
H -2.021337 1.034587 1.740427
C -3.269834 -0.063449 -1.241795
H -2.556380 -1.809761 -2.286139
H -3.767116 1.613848 0.018298
H -4.024755 0.175438 -1.992766
O -0.276320 -0.318244 2.773458
O 0.678159 -1.756229 1.315814

TS8-9

Zero-point correction= 0.206606 (Hartree/Particle)
Thermal correction to Energy= 0.221706
Thermal correction to Enthalpy= 0.222650
Thermal correction to Gibbs Free Energy= 0.159704
Sum of electronic and zero-point Energies= -819.229704
Sum of electronic and thermal Energies= -819.214604
Sum of electronic and thermal Enthalpies= -819.213660
Sum of electronic and thermal Free Energies= -819.276606
Single Point Energy Calculations with extended basis set: HF = -820.3916767
C -2.007076 1.385096 -0.937487
C -2.345869 0.083802 -0.195724
C -2.193180 -0.022727 1.186646
C -2.839851 -1.014542 -0.899252
C -2.522383 -1.199206 1.852846
H -1.813661 0.849018 1.720168
C -3.159478 -2.199084 -0.243234
H -2.966467 -0.895030 -1.974840
C -3.002944 -2.294968 1.138432
H -2.402222 -1.266743 2.935623
H -3.537239 -3.053735 -0.807831
H -3.256332 -3.220829 1.657438
O -2.377759 1.447143 -2.121372
O -1.401253 2.257818 -0.253056
C 0.702028 1.832779 0.539808
O 0.726759 2.747166 1.275550
N 0.918069 0.826767 -0.136145
C 2.104359 0.098524 -0.146788
C 2.129911 -1.090446 -0.884621
C 3.261949 0.499577 0.534202
C 3.285104 -1.858003 -0.937994
H 1.218609 -1.385831 -1.401522
C 4.413783 -0.274519 0.473983
H 3.243628 1.425186 1.110046
C 4.435541 -1.457046 -0.261260
H 3.287009 -2.782296 -1.515661
H 5.305876 0.051730 1.009272
H 5.340966 -2.061266 -0.305997
Imaginary Vibrational Frequency = -57.7503 cm^{-1}

9

Zero-point correction= 0.209183 (Hartree/Particle)
Thermal correction to Energy= 0.223648
Thermal correction to Enthalpy= 0.224592
Thermal correction to Gibbs Free Energy= 0.165041
Sum of electronic and zero-point Energies= -819.247317
Sum of electronic and thermal Energies= -819.232852
Sum of electronic and thermal Enthalpies= -819.231908
Sum of electronic and thermal Free Energies= -819.291458
Single Point Energy Calculations with extended basis set: HF = -820.4052823

C	-1.828104	1.443970	-0.683467
C	-2.151450	0.084722	-0.139488
C	-1.884221	-0.270814	1.184177
C	-2.836294	-0.807784	-0.963600
C	-2.286061	-1.510925	1.666352
H	-1.354518	0.426858	1.831639
C	-3.227888	-2.051725	-0.484388
H	-3.052205	-0.497461	-1.984264
C	-2.954180	-2.405612	0.834198
H	-2.071060	-1.783010	2.699291
H	-3.751316	-2.747884	-1.139898
H	-3.262257	-3.379824	1.214394
O	-2.404838	1.878340	-1.657902
O	-1.005886	2.205124	0.046946
C	0.281385	1.658315	0.458455
O	0.668444	2.078756	1.540864
N	0.729769	0.835784	-0.466666
C	1.934895	0.186292	-0.293501
C	2.302450	-0.716376	-1.315787
C	2.839667	0.326413	0.783912
C	3.485607	-1.435983	-1.272073
H	1.606812	-0.825208	-2.147965
C	4.024777	-0.399634	0.817515
H	2.584510	1.015802	1.583450
C	4.366745	-1.287126	-0.200368
H	3.726029	-2.123695	-2.085457
H	4.700012	-0.266149	1.665839
H	5.299883	-1.850079	-0.161256

TS9-10

Zero-point correction= 0.208506 (Hartree/Particle)
Thermal correction to Energy= 0.222165
Thermal correction to Enthalpy= 0.223110
Thermal correction to Gibbs Free Energy= 0.165751
Sum of electronic and zero-point Energies= -819.234670
Sum of electronic and thermal Energies= -819.221010
Sum of electronic and thermal Enthalpies= -819.220066
Sum of electronic and thermal Free Energies= -819.277425
Single Point Energy Calculations with extended basis set: HF = -820.3898554

C	1.089745	1.235705	0.940962
C	1.783337	0.118294	0.192189

C 1.884239 0.059847 -1.198770
C 2.357138 -0.899025 0.953267
C 2.540772 -1.001175 -1.812061
H 1.449231 0.856539 -1.799975
C 3.008617 -1.964747 0.341664
H 2.281415 -0.818348 2.036848
C 3.103619 -2.019533 -1.045741
H 2.613666 -1.034251 -2.899489
H 3.448541 -2.755198 0.950927
H 3.615052 -2.851969 -1.529960
O 1.299163 1.410059 2.130211
O 0.881415 2.404863 0.067303
C -0.391429 2.113140 -0.331024
O -1.014319 2.739102 -1.169099
N -0.652595 1.011259 0.410025
C -1.653465 0.092871 0.231309
C -1.607430 -1.087431 0.998026
C -2.723916 0.258236 -0.671438
C -2.584012 -2.062295 0.864115
H -0.779390 -1.206410 1.697578
C -3.695887 -0.726724 -0.788623
H -2.761340 1.169978 -1.263288
C -3.641594 -1.894682 -0.029687
H -2.520219 -2.968357 1.469025
H -4.516531 -0.577463 -1.493103
H -4.410729 -2.660405 -0.131172
Imaginary Vibrational Frequency = -177.6389 cm^{-1}

10
Zero-point correction= 0.208983 (Hartree/Particle)
Thermal correction to Energy= 0.223789
Thermal correction to Enthalpy= 0.224733
Thermal correction to Gibbs Free Energy= 0.164591
Sum of electronic and zero-point Energies= -819.258092
Sum of electronic and thermal Energies= -819.243286
Sum of electronic and thermal Enthalpies= -819.242342
Sum of electronic and thermal Free Energies= -819.302484
Single Point Energy Calculations with extended basis set: HF = -820.4187239
C -0.426176 -0.840673 -0.253821
C -1.870541 -0.474417 -0.033612
C -2.282709 0.525812 0.849528
C -2.834554 -1.276308 -0.646265
C -3.636819 0.726705 1.096322
H -1.537611 1.154475 1.336108
C -4.187300 -1.064760 -0.413643
H -2.490396 -2.074832 -1.300892
C -4.593148 -0.061626 0.463247
H -3.945954 1.509965 1.788326
H -4.929640 -1.689024 -0.911810
H -5.653893 0.103247 0.655021

O -0.169161 -2.019884 -0.505905
O -0.505834 1.811487 -1.466939
C 0.048451 1.716690 -0.386267
O 0.374923 2.452279 0.534872
N 0.491209 0.155994 -0.090316
C 1.862601 -0.108387 0.017739
C 2.373644 -1.341696 0.463337
C 2.789459 0.905021 -0.283600
C 3.741829 -1.541438 0.591996
H 1.684371 -2.147970 0.686820
C 4.154864 0.690605 -0.154390
H 2.428290 1.878996 -0.601599
C 4.650732 -0.533790 0.283124
H 4.100509 -2.511371 0.940308
H 4.840797 1.502304 -0.400260
H 5.723644 -0.699219 0.381805

TS10-11

Zero-point correction= 0.207604 (Hartree/Particle)
Thermal correction to Energy= 0.222188
Thermal correction to Enthalpy= 0.223132
Thermal correction to Gibbs Free Energy= 0.163414
Sum of electronic and zero-point Energies= -819.258402
Sum of electronic and thermal Energies= -819.243819
Sum of electronic and thermal Enthalpies= -819.242875
Sum of electronic and thermal Free Energies= -819.302592
Single Point Energy Calculations with extended basis set: HF = -820.4164151
C 0.418548 -0.944191 -0.030857
C 1.866021 -0.524335 -0.142075
C 2.277087 0.633672 -0.806027
C 2.838020 -1.390385 0.363278
C 3.631514 0.926297 -0.939670
H 1.524100 1.305568 -1.212896
C 4.189490 -1.093850 0.242446
H 2.496717 -2.305941 0.843171
C 4.591950 0.068692 -0.412020
H 3.937731 1.832784 -1.462472
H 4.935608 -1.773955 0.655171
H 5.652394 0.302008 -0.514486
O 0.194133 -2.160363 0.060552
O 0.186582 1.349334 1.974150
C -0.016233 1.710337 0.854492
O -0.082058 2.617233 0.072964
N -0.469669 0.071208 -0.097605
C -1.846178 -0.146157 -0.146244
C -2.502716 -1.365632 0.123780
C -2.655916 0.955331 -0.495837
C -3.887931 -1.457995 0.046193
H -1.900725 -2.227569 0.386196
C -4.036808 0.848849 -0.565685

H -2.163180 1.899601 -0.718069
C -4.673226 -0.361166 -0.295896
H -4.362572 -2.416882 0.264106
H -4.624573 1.726334 -0.841096
H -5.758802 -0.446828 -0.352994
Imaginary Vibrational Frequency = -223.3777 cm^{-1}

11
Zero-point correction= 0.207363 (Hartree/Particle)
Thermal correction to Energy= 0.223061
Thermal correction to Enthalpy= 0.224006
Thermal correction to Gibbs Free Energy= 0.161488
Sum of electronic and zero-point Energies= -819.265997
Sum of electronic and thermal Energies= -819.250298
Sum of electronic and thermal Enthalpies= -819.249354
Sum of electronic and thermal Free Energies= -819.311872
Single Point Energy Calculations with extended basis set: HF = -820.4232588
C 0.419326 -1.046247 0.014374
C 1.869141 -0.628250 -0.161657
C 2.247590 0.527444 -0.850495
C 2.868619 -1.446927 0.367572
C 3.590922 0.860142 -0.994422
H 1.459833 1.150290 -1.270849
C 4.211949 -1.115304 0.231148
H 2.545794 -2.350177 0.883289
C 4.579784 0.042371 -0.451165
H 3.870065 1.764512 -1.537256
H 4.979733 -1.763263 0.657165
H 5.632910 0.304461 -0.562540
O 0.219936 -2.189109 0.473699
O -0.014603 1.632691 2.040133
C -0.031587 2.212553 1.028609
O -0.029194 2.926586 0.103251
N -0.441267 -0.093691 -0.364401
C -1.804698 -0.282239 -0.298603
C -2.500165 -1.423654 0.173602
C -2.604231 0.793673 -0.755225
C -3.889469 -1.459569 0.182233
H -1.912740 -2.263980 0.528703
C -3.989228 0.745773 -0.741038
H -2.080843 1.673296 -1.132574
C -4.654904 -0.386012 -0.269414
H -4.389248 -2.356674 0.555803
H -4.559382 1.603326 -1.105228
H -5.744652 -0.429818 -0.255474

12
Zero-point correction= 0.194309 (Hartree/Particle)
Thermal correction to Energy= 0.205952
Thermal correction to Enthalpy= 0.206897

Thermal correction to Gibbs Free Energy= 0.155147
Sum of electronic and zero-point Energies= -630.768287
Sum of electronic and thermal Energies= -630.756644
Sum of electronic and thermal Enthalpies= -630.755700
Sum of electronic and thermal Free Energies= -630.807449
Single Point Energy Calculations with extended basis set: HF = -631.739556

C	0.411522	-0.621253	0.000268
C	1.862056	-0.168014	0.000050
C	2.229682	1.179705	-0.000616
C	2.869258	-1.134535	0.000534
C	3.569989	1.550490	-0.000656
H	1.426150	1.914098	-0.001240
C	4.211323	-0.769191	0.000300
H	2.552334	-2.176683	0.001285
C	4.568518	0.577296	-0.000244
H	3.841654	2.607595	-0.001237
H	4.986098	-1.537976	0.000785
H	5.620204	0.867918	-0.000372
O	0.214329	-1.855986	0.000251
N	-0.443072	0.404693	0.000270
C	-1.802875	0.211589	0.000317
C	-2.507345	-1.020032	-0.000543
C	-2.599378	1.383298	0.000823
C	-3.896816	-1.049578	-0.000890
H	-1.924195	-1.935155	-0.000768
C	-3.984018	1.341960	0.000553
H	-2.066441	2.335212	0.001388
C	-4.656971	0.118821	-0.000332
H	-4.401832	-2.018992	-0.001539
H	-4.549679	2.276730	0.000915
H	-5.747089	0.078956	-0.000496

7S

Zero-point correction= 0.102559 (Hartree/Particle)
Thermal correction to Energy= 0.109498
Thermal correction to Enthalpy= 0.110442
Thermal correction to Gibbs Free Energy= 0.070341
Sum of electronic and zero-point Energies= -419.967677
Sum of electronic and thermal Energies= -419.960738
Sum of electronic and thermal Enthalpies= -419.959794
Sum of electronic and thermal Free Energies= -419.999895
Single Point Energy Calculations with extended basis set: HF = -420.5649614

C	-1.810097	0.000052	0.000128
C	-0.279823	0.000219	0.000061
C	0.434251	1.199842	0.000417
C	0.434070	-1.199705	-0.000315
C	1.826011	1.204845	0.000408
H	-0.131460	2.130357	0.000713
C	1.825688	-1.205090	-0.000439
H	-0.132128	-2.129894	-0.000505

C 2.526687 -0.000108 -0.000056
H 2.368830 2.150028 0.000740
H 2.368378 -2.150317 -0.000810
H 3.616193 -0.000071 -0.000105
O -2.364344 -1.126006 0.000882
O -2.364473 1.125952 -0.001040

8S

Zero-point correction= 0.207428 (Hartree/Particle)
Thermal correction to Energy= 0.223235
Thermal correction to Enthalpy= 0.224179
Thermal correction to Gibbs Free Energy= 0.160681
Sum of electronic and zero-point Energies= -819.331023
Sum of electronic and thermal Energies= -819.315216
Sum of electronic and thermal Enthalpies= -819.314272
Sum of electronic and thermal Free Energies= -819.377770
Single Point Energy Calculations with extended basis set: HF = -820.4938544
C 1.935417 -1.859736 -1.001949
O 2.125591 -3.020763 -0.974657
N 1.812428 -0.686675 -1.255051
C 1.576690 0.549929 -0.659846
C 1.811109 0.765459 0.700560
C 1.118310 1.591602 -1.468185
C 1.572712 2.021839 1.243796
H 2.139173 -0.067236 1.318394
C 0.881376 2.843765 -0.912545
H 0.941892 1.400640 -2.525266
C 1.108144 3.064367 0.443918
H 1.746214 2.184292 2.306503
H 0.518363 3.651933 -1.545255
H 0.922607 4.045399 0.877411
C -0.396024 -1.197128 1.678140
C -1.363356 -0.685074 0.615115
C -1.461003 -1.310778 -0.629117
C -2.155761 0.436984 0.863041
C -2.320405 -0.822017 -1.608672
H -0.842975 -2.189257 -0.811818
C -3.004736 0.943580 -0.116825
H -2.074922 0.911746 1.839971
C -3.089454 0.313541 -1.357277
H -2.389527 -1.322829 -2.574280
H -3.605006 1.830656 0.085074
H -3.755264 0.704760 -2.125868
O -0.540314 -0.738699 2.835188
O 0.469014 -2.025711 1.289415

TS8-9S

Zero-point correction= 0.207248 (Hartree/Particle)
Thermal correction to Energy= 0.222047
Thermal correction to Enthalpy= 0.222992

Thermal correction to Gibbs Free Energy= 0.161559
Sum of electronic and zero-point Energies= -819.315096
Sum of electronic and thermal Energies= -819.300297
Sum of electronic and thermal Enthalpies= -819.299352
Sum of electronic and thermal Free Energies= -819.360785
Single Point Energy Calculations with extended basis set: HF = -820.4747196

C	2.007462	-1.436832	-0.796219
C	2.342676	-0.096059	-0.180566
C	2.133095	0.155296	1.177204
C	2.915253	0.903079	-0.970012
C	2.480280	1.382923	1.732784
H	1.700513	-0.628073	1.798099
C	3.250641	2.137167	-0.423468
H	3.091553	0.690196	-2.023083
C	3.034787	2.379241	0.931947
H	2.318826	1.564594	2.794667
H	3.685770	2.912396	-1.053089
H	3.301990	3.342416	1.364653
O	2.526768	-1.720625	-1.886416
O	1.234719	-2.211019	-0.130657
C	-0.498826	-1.561670	0.589801
O	-0.567445	-2.145246	1.620904
N	-0.879769	-0.807239	-0.330846
C	-2.125202	-0.154512	-0.243504
C	-2.462906	0.706566	-1.294169
C	-3.029244	-0.317626	0.814801
C	-3.672800	1.389791	-1.288364
H	-1.753172	0.825840	-2.111614
C	-4.238520	0.369280	0.813443
H	-2.780544	-0.985152	1.638486
C	-4.569078	1.225911	-0.234128
H	-3.916990	2.055901	-2.114790
H	-4.930459	0.231704	1.643521
H	-5.517155	1.760641	-0.228876

Imaginary Vibrational Frequency = -225.3387 cm^{-1}

9S

Zero-point correction= 0.209319 (Hartree/Particle)
Thermal correction to Energy= 0.223771
Thermal correction to Enthalpy= 0.224715
Thermal correction to Gibbs Free Energy= 0.165269
Sum of electronic and zero-point Energies= -819.328062
Sum of electronic and thermal Energies= -819.313610
Sum of electronic and thermal Enthalpies= -819.312666
Sum of electronic and thermal Free Energies= -819.372112
Single Point Energy Calculations with extended basis set: HF = -820.483798

C	1.709545	-1.396372	-0.770595
C	2.202975	-0.125189	-0.177401
C	2.084448	0.145008	1.188899
C	2.856032	0.788723	-1.007492

C 2.604246 1.322357 1.713258
H 1.587976 -0.573350 1.839244
C 3.367099 1.969723 -0.484074
H 2.951768 0.558298 -2.066858
C 3.242080 2.237259 0.877820
H 2.513518 1.527317 2.778412
H 3.866942 2.682904 -1.137055
H 3.646149 3.160220 1.290422
O 2.066325 -1.794119 -1.859404
O 0.942823 -2.170058 0.031931
C -0.340600 -1.646629 0.439386
O -0.759890 -2.140481 1.482985
N -0.776589 -0.770148 -0.439339
C -1.986771 -0.117582 -0.251367
C -2.349735 0.803275 -1.257026
C -2.884884 -0.270185 0.827181
C -3.529499 1.530167 -1.197577
H -1.661906 0.927539 -2.093965
C -4.066943 0.463223 0.879915
H -2.638706 -0.973537 1.616854
C -4.405134 1.368062 -0.123422
H -3.769145 2.231437 -1.997311
H -4.738416 0.321049 1.727820
H -5.333273 1.935391 -0.071302

TS9-10S

Zero-point correction= 0.208728 (Hartree/Particle)
Thermal correction to Energy= 0.222338
Thermal correction to Enthalpy= 0.223282
Thermal correction to Gibbs Free Energy= 0.166339
Sum of electronic and zero-point Energies= -819.315056
Sum of electronic and thermal Energies= -819.301446
Sum of electronic and thermal Enthalpies= -819.300502
Sum of electronic and thermal Free Energies= -819.357445
Single Point Energy Calculations with extended basis set: HF = -820.4692292
C -1.253515 1.286691 -0.846081
C -1.722494 0.037437 -0.152340
C -1.698042 -0.129689 1.234817
C -2.191900 -1.004635 -0.952345
C -2.136664 -1.318935 1.806683
H -1.339103 0.676660 1.872905
C -2.625075 -2.197511 -0.381839
H -2.213585 -0.859237 -2.031198
C -2.599900 -2.357532 1.000856
H -2.118385 -1.435654 2.889313
H -2.986521 -3.003682 -1.018728
H -2.941136 -3.288302 1.451280
O -1.573448 1.544286 -1.998237
O -1.066553 2.400652 0.085389
C 0.249433 2.177932 0.393488

O 0.834516 2.773921 1.284437
N 0.592347 1.214359 -0.483110
C 1.581050 0.265089 -0.303596
C 1.672895 -0.753087 -1.269537
C 2.467107 0.229798 0.788783
C 2.611608 -1.768399 -1.150151
H 0.980218 -0.724982 -2.111787
C 3.408841 -0.788934 0.892751
H 2.406884 1.013925 1.540088
C 3.491479 -1.794690 -0.068195
H 2.658997 -2.547322 -1.910903
H 4.089088 -0.796548 1.744706
H 4.232060 -2.587443 0.023619
Imaginary Vibrational Frequency = -221.4459 cm^{-1}

10S
Zero-point correction= 0.209249 (Hartree/Particle)
Thermal correction to Energy= 0.223955
Thermal correction to Enthalpy= 0.224900
Thermal correction to Gibbs Free Energy= 0.165026
Sum of electronic and zero-point Energies= -819.344727
Sum of electronic and thermal Energies= -819.330020
Sum of electronic and thermal Enthalpies= -819.329076
Sum of electronic and thermal Free Energies= -819.388949
Single Point Energy Calculations with extended basis set: HF = -820.5068298
C -0.425163 -0.663894 -0.439938
C -1.870804 -0.429074 -0.140239
C -2.288772 0.247146 1.008417
C -2.822270 -1.041908 -0.956081
C -3.639863 0.323078 1.324129
H -1.547797 0.702912 1.663943
C -4.176735 -0.944620 -0.655857
H -2.484868 -1.595379 -1.830899
C -4.587905 -0.263599 0.487284
H -3.956587 0.842425 2.227234
H -4.912924 -1.410411 -1.309069
H -5.646951 -0.195920 0.731319
O -0.078125 -1.755704 -0.888945
O -0.843143 2.093574 -0.844240
C 0.147515 1.812110 -0.161969
O 0.944411 2.508061 0.476405
N 0.475067 0.323129 -0.109930
C 1.841580 -0.049638 0.016642
C 2.225573 -0.984338 0.979093
C 2.813392 0.517802 -0.808203
C 3.560809 -1.350102 1.111638
H 1.464508 -1.422312 1.624045
C 4.149766 0.159528 -0.667722
H 2.512889 1.247371 -1.558567
C 4.529536 -0.777511 0.290593

H 3.846477 -2.081084 1.866752
H 4.898949 0.612168 -1.315780
H 5.575730 -1.058989 0.398050

TS10-11S

Zero-point correction= 0.207128 (Hartree/Particle)
Thermal correction to Energy= 0.222017
Thermal correction to Enthalpy= 0.222961
Thermal correction to Gibbs Free Energy= 0.162072
Sum of electronic and zero-point Energies= -819.335008
Sum of electronic and thermal Energies= -819.320120
Sum of electronic and thermal Enthalpies= -819.319176
Sum of electronic and thermal Free Energies= -819.380064
Single Point Energy Calculations with extended basis set: HF = -820.4921947
C -0.392943 -0.927547 -0.207257
C -1.848873 -0.588526 -0.020821
C -2.289809 0.363897 0.901411
C -2.799050 -1.309499 -0.747823
C -3.649679 0.601913 1.079290
H -1.557739 0.911676 1.493427
C -4.157692 -1.062497 -0.586649
H -2.447521 -2.070383 -1.442721
C -4.587465 -0.105150 0.330432
H -3.979519 1.340251 1.809075
H -4.885786 -1.622041 -1.172615
H -5.651296 0.084688 0.465756
O -0.109521 -2.090347 -0.556138
O -0.493159 2.142087 -1.306228
C -0.012618 2.095143 -0.221884
O 0.364896 2.580934 0.793803
N 0.465199 0.081513 0.014979
C 1.836086 -0.170957 0.033041
C 2.404541 -1.259416 0.722966
C 2.718601 0.728396 -0.589330
C 3.781614 -1.429238 0.785272
H 1.743492 -1.973181 1.209759
C 4.097115 0.554952 -0.524977
H 2.305772 1.568759 -1.148598
C 4.643006 -0.525193 0.163692
H 4.189649 -2.279972 1.331663
H 4.749822 1.272235 -1.022543
H 5.722012 -0.661681 0.216256
Imaginary Vibrational Frequency = -251.2261 cm^{-1}

11S

Zero-point correction= 0.207608 (Hartree/Particle)
Thermal correction to Energy= 0.223341
Thermal correction to Enthalpy= 0.224285
Thermal correction to Gibbs Free Energy= 0.161371
Sum of electronic and zero-point Energies= -819.342150

Sum of electronic and thermal Energies= -819.326417
Sum of electronic and thermal Enthalpies= -819.325473
Sum of electronic and thermal Free Energies= -819.388387
Single Point Energy Calculations with extended basis set: HF = -820.4974704

C	0.443311	-1.009149	-0.011808
C	1.891153	-0.596054	-0.191469
C	2.267768	0.557060	-0.888176
C	2.895449	-1.399270	0.355451
C	3.609173	0.897611	-1.030418
H	1.484493	1.179542	-1.315186
C	4.238272	-1.062216	0.218691
H	2.592615	-2.296798	0.892009
C	4.600729	0.089602	-0.476280
H	3.884638	1.798734	-1.577920
H	5.006707	-1.700051	0.654813
H	5.651137	0.356319	-0.586865
O	0.234667	-2.105013	0.562510
O	-0.202626	1.379145	2.127395
C	-0.109108	2.091311	1.208721
O	-0.009557	2.877806	0.353705
N	-0.423732	-0.118027	-0.497874
C	-1.791733	-0.289077	-0.390886
C	-2.492567	-1.367603	0.202671
C	-2.586615	0.749600	-0.932879
C	-3.884157	-1.384347	0.242400
H	-1.915880	-2.181831	0.627649
C	-3.972365	0.724422	-0.889569
H	-2.064857	1.586992	-1.398162
C	-4.642055	-0.347896	-0.297691
H	-4.387452	-2.232845	0.709293
H	-4.538308	1.550471	-1.322027
H	-5.730371	-0.373813	-0.259920

13

Zero-point correction= 0.276065 (Hartree/Particle)
Thermal correction to Energy= 0.296218
Thermal correction to Enthalpy= 0.297162
Thermal correction to Gibbs Free Energy= 0.222202
Sum of electronic and zero-point Energies= -1137.929805
Sum of electronic and thermal Energies= -1137.909652
Sum of electronic and thermal Enthalpies= -1137.908708
Sum of electronic and thermal Free Energies= -1137.983668
Single Point Energy Calculations with extended basis set: HF = -1139.4202588

N	-1.257207	1.186513	0.003986
C	-0.832552	2.438101	-0.000368
C	-1.707543	3.536831	-0.022146
C	-3.062661	3.298683	-0.039157
C	-3.540544	1.973200	-0.033988
C	-2.581818	0.936001	-0.011740
N	-2.106807	-1.432269	0.018087

C -2.519500 -2.691495 0.025946
C -3.873896 -3.054580 0.012181
C -4.821329 -2.057647 -0.010895
C -4.415361 -0.709386 -0.019707
C -3.028084 -0.440153 -0.004214
H 0.250809 2.567744 0.015238
H -1.310480 4.548421 -0.025092
H -1.743167 -3.455424 0.043903
H -4.152549 -4.104605 0.019607
C -4.935619 1.659695 -0.049922
C -5.355781 0.368633 -0.043110
H -5.651229 2.480524 -0.067312
H -6.417311 0.126011 -0.055072
H -3.777577 4.120425 -0.056222
H -5.884760 -2.293299 -0.022381
Ag 0.121291 -0.797969 0.025928
C 2.830621 0.019478 0.045824
C 4.335773 0.045615 0.008129
C 5.080602 -1.132151 -0.088385
C 5.004031 1.270512 0.067658
C 6.470340 -1.085379 -0.125308
H 4.555385 -2.083803 -0.134449
C 6.392804 1.320417 0.031114
H 4.412808 2.180876 0.142647
C 7.128743 0.141077 -0.065823
H 7.043168 -2.008460 -0.201068
H 6.904484 2.280576 0.077927
H 8.216743 0.177811 -0.095049
O 2.211787 1.096586 0.127266
O 2.287183 -1.138672 -0.011308

14

Zero-point correction= 0.276136 (Hartree/Particle)
Thermal correction to Energy= 0.296142
Thermal correction to Enthalpy= 0.297086
Thermal correction to Gibbs Free Energy= 0.223735
Sum of electronic and zero-point Energies= -1137.923251
Sum of electronic and thermal Energies= -1137.903245
Sum of electronic and thermal Enthalpies= -1137.902301
Sum of electronic and thermal Free Energies= -1137.975651
Single Point Energy Calculations with extended basis set: HF = -1139.420599
N -1.907607 -1.356713 0.133814
C -2.631178 -2.439138 0.382299
C -4.024596 -2.410275 0.532392
C -4.672206 -1.202293 0.419373
C -3.931069 -0.034186 0.157025
C -2.530380 -0.159768 0.016904
N -0.406952 0.898177 -0.397458
C 0.320590 1.975600 -0.638629
C -0.233200 3.260193 -0.758848

C -1.594402 3.403776 -0.622294
C -2.394453 2.273113 -0.364560
C -1.743242 1.023534 -0.256003
H -2.085219 -3.377657 0.467999
H -4.566139 -3.330047 0.734444
H 1.397080 1.821087 -0.738730
H 0.411013 4.112878 -0.956072
C -4.553186 1.248149 0.034834
C -3.813909 2.359040 -0.213960
H -5.634330 1.309408 0.149153
H -4.286119 3.336145 -0.304625
H -5.753475 -1.132052 0.530273
H -2.067876 4.380949 -0.709257
Ag 0.369101 -1.386746 -0.112155
C 3.334895 -1.505814 -0.565493
C 3.347530 -0.161730 0.132198
C 4.026865 0.904999 -0.461449
C 2.728532 0.037647 1.370256
C 4.056312 2.155792 0.147690
H 4.531566 0.734601 -1.410902
C 2.776416 1.281352 1.994315
H 2.222562 -0.795789 1.859539
C 3.431047 2.346039 1.378890
H 4.574530 2.983278 -0.334471
H 2.302959 1.419195 2.965241
H 3.460808 3.321366 1.861910
O 2.329644 -2.277712 -0.340595
O 4.288435 -1.788877 -1.297825

TS14-15

Zero-point correction= 0.272901 (Hartree/Particle)
Thermal correction to Energy= 0.293309
Thermal correction to Enthalpy= 0.294253
Thermal correction to Gibbs Free Energy= 0.220204
Sum of electronic and zero-point Energies= -1137.878758
Sum of electronic and thermal Energies= -1137.858350
Sum of electronic and thermal Enthalpies= -1137.857406
Sum of electronic and thermal Free Energies= -1137.931455
Single Point Energy Calculations with extended basis set: HF = -1139.3706281
N -1.159923 -1.466726 0.073299
C -1.128567 -2.788339 0.167795
C -2.283604 -3.582628 0.178642
C -3.507703 -2.962089 0.086674
C -3.574103 -1.559286 -0.014946
C -2.356618 -0.841304 -0.017578
N -1.222605 1.279731 -0.117659
C -1.247218 2.598549 -0.207175
C -2.437223 3.337614 -0.306495
C -3.633856 2.659692 -0.309670
C -3.639784 1.253992 -0.213367

C -2.389942 0.601153 -0.118489
H -0.141823 -3.244746 0.239050
H -2.197403 -4.662556 0.258610
H -0.277131 3.098782 -0.199377
H -2.398831 4.421202 -0.378462
C -4.818630 -0.861165 -0.113098
C -4.850319 0.492515 -0.208953
H -5.738633 -1.443731 -0.108988
H -5.797106 1.025432 -0.283761
C 2.212817 1.859373 0.930217
C 2.922925 -0.001826 -0.021407
C 3.480097 0.237541 -1.289652
C 3.673782 -0.796879 0.861866
C 4.703860 -0.309696 -1.671844
H 2.951484 0.890483 -1.988187
C 4.899916 -1.348806 0.494256
H 3.297279 -0.969812 1.872788
C 5.414877 -1.108593 -0.778387
H 5.110744 -0.105698 -2.662402
H 5.460288 -1.960206 1.201775
H 6.376600 -1.530753 -1.067838
O 2.109734 2.633883 0.026152
H -4.581538 3.191560 -0.385042
H -4.431479 -3.539050 0.091246
Ag 0.759776 -0.195633 0.042979
O 2.226710 1.622853 2.100197
Imaginary Vibrational Frequency = -364.2992 cm^{-1}

15
Zero-point correction= 0.273805 (Hartree/Particle)
Thermal correction to Energy= 0.295274
Thermal correction to Enthalpy= 0.296218
Thermal correction to Gibbs Free Energy= 0.217531
Sum of electronic and zero-point Energies= -1137.894217
Sum of electronic and thermal Energies= -1137.872748
Sum of electronic and thermal Enthalpies= -1137.871804
Sum of electronic and thermal Free Energies= -1137.950490
Single Point Energy Calculations with extended basis set: HF = -1139.3868367
N -1.197081 -1.197137 -0.099383
C -1.045225 -2.513758 -0.138341
C -2.122495 -3.410595 -0.108447
C -3.398803 -2.903202 -0.034485
C -3.593721 -1.509246 0.008935
C -2.447418 -0.683313 -0.026667
N -1.511241 1.529486 -0.018762
C -1.656344 2.842149 0.018750
C -2.906625 3.477658 0.093101
C -4.037865 2.695761 0.128962
C -3.917219 1.292747 0.090573
C -2.613184 0.752332 0.015388

H -0.019961 -2.880044 -0.195264
H -1.936568 -4.480390 -0.143389
H -0.738436 3.431403 -0.011323
H -2.965213 4.562410 0.121150
C -4.896817 -0.923698 0.086059
C -5.052921 0.424263 0.125176
H -5.759744 -1.587469 0.112466
H -6.044549 0.870651 0.183711
H -4.265137 -3.562946 -0.008917
H -5.029489 3.143099 0.186654
Ag 0.645589 0.184909 -0.150847
C 3.267584 -2.400596 0.619652
C 2.674647 0.750378 -0.198079
C 3.570310 0.279979 -1.179048
C 3.235761 1.583179 0.789793
C 4.928502 0.602902 -1.171814
H 3.204340 -0.371450 -1.977169
C 4.591614 1.913189 0.811382
H 2.598482 1.987327 1.580720
C 5.447323 1.420038 -0.170633
H 5.585016 0.211830 -1.950467
H 4.982381 2.557941 1.599987
H 6.507394 1.672316 -0.157247
O 2.596908 -2.874684 -0.208449
O 3.944899 -1.964422 1.460248

16

Zero-point correction= 0.260924 (Hartree/Particle)
Thermal correction to Energy= 0.278230
Thermal correction to Enthalpy= 0.279174
Thermal correction to Gibbs Free Energy= 0.211738
Sum of electronic and zero-point Energies= -949.399966
Sum of electronic and thermal Energies= -949.382660
Sum of electronic and thermal Enthalpies= -949.381716
Sum of electronic and thermal Free Energies= -949.449151
Single Point Energy Calculations with extended basis set: HF = -950.7063158
N 1.055650 -1.352119 -0.042257
C 1.149673 -2.673881 -0.096507
C 2.373552 -3.355959 -0.134209
C 3.535709 -2.620499 -0.114690
C 3.470587 -1.215397 -0.057204
C 2.191367 -0.615052 -0.021533
N 0.867551 1.388492 0.074947
C 0.772714 2.704840 0.132142
C 1.888003 3.558314 0.158187
C 3.143237 2.996675 0.122290
C 3.278742 1.595849 0.061196
C 2.093068 0.826107 0.039706
H 0.209426 -3.224275 -0.111300
H 2.386898 -4.441339 -0.178014

H -0.237622 3.116182 0.159573
H 1.749079 4.635045 0.205740
C 4.646592 -0.401365 -0.034686
C 4.554851 0.951836 0.021977
H 5.616240 -0.896032 -0.064294
H 5.449647 1.572467 0.038913
C -3.101876 -0.096536 -0.009022
C -3.769805 0.503044 -1.095137
C -3.921051 -0.488251 1.068242
C -5.151734 0.698825 -1.111043
H -3.196965 0.832766 -1.965758
C -5.303769 -0.298046 1.067180
H -3.470910 -0.962153 1.944249
C -5.927402 0.297760 -0.026305
H -5.624785 1.167448 -1.975262
H -5.897291 -0.618327 1.924741
H -7.006749 0.447960 -0.032902
H 4.037988 3.617715 0.140649
H 4.509727 -3.107354 -0.142985
Ag -1.011103 -0.353283 0.000092

17

Zero-point correction= 0.365525 (Hartree/Particle)
Thermal correction to Energy= 0.392034
Thermal correction to Enthalpy= 0.392978
Thermal correction to Gibbs Free Energy= 0.301370
Sum of electronic and zero-point Energies= -1348.763496
Sum of electronic and thermal Energies= -1348.736987
Sum of electronic and thermal Enthalpies= -1348.736043
Sum of electronic and thermal Free Energies= -1348.827651
Single Point Energy Calculations with extended basis set: HF = -1350.6372096
N -2.627290 -1.417765 0.321609
C -2.925604 -2.657034 0.667446
C -4.187763 -3.040472 1.149967
C -5.163106 -2.077622 1.268790
C -4.876721 -0.746041 0.908394
C -3.574810 -0.464713 0.433610
N -1.995203 1.160825 -0.402124
C -1.691468 2.405565 -0.747348
C -2.603754 3.466714 -0.663952
C -3.873723 3.208319 -0.203705
C -4.226491 1.897729 0.170734
C -3.241573 0.890645 0.054280
H -2.127650 -3.394147 0.560210
H -4.376645 -4.076116 1.419729
H -0.675792 2.572087 -1.107762
H -2.298419 4.466232 -0.960743
C -5.846277 0.300083 1.009934
C -5.532456 1.572231 0.655318
H -6.840510 0.051393 1.378443

H -6.267469 2.372134 0.732056
C 2.493613 2.150493 -1.030406
C 1.394245 -1.495457 -0.940282
C 2.290255 -1.123068 -1.962406
C 1.806077 -2.572985 -0.130834
C 3.511304 -1.768995 -2.161797
H 2.036448 -0.290279 -2.623181
C 3.026110 -3.226737 -0.315900
H 1.159197 -2.915977 0.681494
C 3.887297 -2.824142 -1.333955
H 4.174599 -1.443841 -2.964550
H 3.305715 -4.053446 0.338786
H 4.841738 -3.328911 -1.481251
O 1.611474 2.263011 -1.808019
N 3.414024 2.175671 -0.267892
C 4.230732 1.522028 0.651741
C 4.036879 0.172457 0.955179
C 5.250129 2.250287 1.266142
C 4.873365 -0.440661 1.880402
H 3.240193 -0.383790 0.460932
C 6.077996 1.623247 2.190125
H 5.380491 3.300260 1.012315
C 5.893231 0.277978 2.500572
H 4.722565 -1.493886 2.113447
H 6.872787 2.191293 2.669790
H 6.543633 -0.209783 3.224026
H -6.157139 -2.326670 1.638409
H -4.615250 4.002140 -0.123111
Ag -0.415232 -0.476021 -0.589327

TS17-18

Zero-point correction= 0.364463 (Hartree/Particle)
Thermal correction to Energy= 0.389906
Thermal correction to Enthalpy= 0.390850
Thermal correction to Gibbs Free Energy= 0.303763
Sum of electronic and zero-point Energies= -1348.738928
Sum of electronic and thermal Energies= -1348.713485
Sum of electronic and thermal Enthalpies= -1348.712541
Sum of electronic and thermal Free Energies= -1348.799628
Single Point Energy Calculations with extended basis set: HF = -1350.6125243
N -2.245777 -1.340226 0.465641
C -2.730095 -2.408337 1.082801
C -4.060373 -2.506371 1.514029
C -4.903278 -1.442939 1.289265
C -4.418412 -0.293256 0.636609
C -3.063419 -0.286786 0.234487
N -1.242295 0.872918 -0.830456
C -0.755865 1.937477 -1.445751
C -1.518700 3.084808 -1.715755
C -2.837786 3.102307 -1.326739

C -3.386490 1.982388 -0.671906
C -2.534864 0.878112 -0.440561
H -2.032912 -3.229442 1.247065
H -4.402102 -3.407799 2.014847
H 0.291211 1.883547 -1.750503
H -1.065011 3.931408 -2.223889
C -5.248463 0.843084 0.380220
C -4.751460 1.938975 -0.247794
H -6.287692 0.806542 0.703360
H -5.381095 2.805982 -0.442190
C 2.157647 0.193260 -0.666271
C 1.940777 -2.085063 -0.271349
C 2.293300 -2.796425 -1.429943
C 2.550990 -2.484673 0.928590
C 3.184884 -3.867935 -1.394187
H 1.878268 -2.487987 -2.392879
C 3.446025 -3.552505 0.979630
H 2.339363 -1.928886 1.845322
C 3.761575 -4.250728 -0.184685
H 3.438647 -4.400259 -2.311310
H 3.905376 -3.837116 1.926712
H 4.466260 -5.081029 -0.151898
O 2.178415 0.246330 -1.859512
N 2.295895 0.656188 0.489939
C 2.731342 1.988090 0.681812
C 3.094353 2.853571 -0.358368
C 2.794623 2.446257 2.002145
C 3.507224 4.150876 -0.072381
H 3.056223 2.507685 -1.390357
C 3.207003 3.743963 2.278609
H 2.513615 1.763336 2.802667
C 3.565678 4.604428 1.243027
H 3.786761 4.813325 -0.890469
H 3.248892 4.085056 3.311945
H 3.889008 5.620885 1.459436
H -3.469329 3.969215 -1.517263
H -5.943991 -1.474067 1.609141
Ag -0.031295 -1.197205 -0.170270
Imaginary Vibrational Frequency = -301.6489 cm^{-1}

18

Zero-point correction= 0.367861 (Hartree/Particle)
Thermal correction to Energy= 0.392863
Thermal correction to Enthalpy= 0.393807
Thermal correction to Gibbs Free Energy= 0.307774
Sum of electronic and zero-point Energies= -1348.810446
Sum of electronic and thermal Energies= -1348.785444
Sum of electronic and thermal Enthalpies= -1348.784499
Sum of electronic and thermal Free Energies= -1348.870533
Single Point Energy Calculations with extended basis set: HF = -1350.689201

N	-1.445463	1.804273	0.306226
C	-1.296762	3.072213	0.657937
C	-2.375937	3.953992	0.816493
C	-3.649109	3.480413	0.598596
C	-3.839677	2.136364	0.223647
C	-2.690900	1.325460	0.085732
N	-1.744385	-0.824021	-0.437533
C	-1.879000	-2.093125	-0.786511
C	-3.126388	-2.691172	-1.024189
C	-4.260404	-1.923471	-0.892077
C	-4.147627	-0.568431	-0.523115
C	-2.848617	-0.058946	-0.301079
H	-0.274387	3.412514	0.824275
H	-2.194932	4.985204	1.106564
H	-0.957809	-2.671529	-0.878783
H	-3.179898	-3.739241	-1.306195
C	-5.138100	1.584931	-0.013274
C	-5.286552	0.283553	-0.370688
H	-6.004010	2.235044	0.102201
H	-6.275055	-0.137178	-0.548928
C	2.875377	-1.353699	-0.139126
C	1.897220	-2.424562	0.271908
C	1.807662	-3.579047	-0.510111
C	1.132275	-2.340580	1.440555
C	0.942044	-4.610260	-0.159013
H	2.431237	-3.655687	-1.399531
C	0.282118	-3.381578	1.806513
H	1.222802	-1.462494	2.080765
C	0.176616	-4.513905	1.001977
H	0.870126	-5.496339	-0.787841
H	-0.296442	-3.309244	2.726298
H	-0.493746	-5.324192	1.283906
O	3.958828	-1.713390	-0.624440
N	2.448298	-0.082325	0.047906
C	3.331735	0.988599	-0.154413
C	4.694651	0.945066	0.192418
C	2.830469	2.203533	-0.649923
C	5.502702	2.066687	0.047469
H	5.112875	0.019648	0.578063
C	3.643381	3.321778	-0.798193
H	1.772731	2.256367	-0.923843
C	4.990295	3.263676	-0.450163
H	6.552869	2.003059	0.332419
H	3.216990	4.245315	-1.188845
H	5.630568	4.136907	-0.562592
H	-5.248593	-2.346619	-1.068091
H	-4.516419	4.129516	0.711671
Ag	0.313755	0.289695	0.048289

19

Zero-point correction= 0.377274 (Hartree/Particle)
Thermal correction to Energy= 0.403618
Thermal correction to Enthalpy= 0.404562
Thermal correction to Gibbs Free Energy= 0.313992
Sum of electronic and zero-point Energies= -1369.848209
Sum of electronic and thermal Energies= -1369.821866
Sum of electronic and thermal Enthalpies= -1369.820922
Sum of electronic and thermal Free Energies= -1369.911492
Single Point Energy Calculations with extended basis set: HF = -1371.7508753

N	1.265439	-1.244450	-0.473452
C	0.426719	-2.198540	-0.857842
C	0.806502	-3.542434	-0.985069
C	2.105419	-3.890667	-0.698136
C	3.018499	-2.900376	-0.288194
C	2.549089	-1.571174	-0.189046
N	3.008897	0.734085	0.314890
C	3.841175	1.687684	0.692791
C	5.188890	1.452565	1.011166
C	5.666724	0.165607	0.924615
C	4.804384	-0.873985	0.524080
C	3.465376	-0.532359	0.226467
H	-0.594339	-1.882324	-1.076148
H	0.076855	-4.281414	-1.304321
H	3.428152	2.696421	0.748716
H	5.828476	2.276356	1.316406
C	4.381094	-3.205817	0.022454
C	5.241226	-2.231218	0.413658
H	4.709144	-4.240660	-0.063392
H	6.278765	-2.462851	0.650323
C	-0.612847	2.685128	-0.270240
C	-1.615778	2.977838	-1.214788
C	-0.291287	3.724878	0.625049
C	-2.252417	4.218658	-1.270191
H	-1.925348	2.207762	-1.926740
C	-0.919343	4.969778	0.582014
H	0.476960	3.563246	1.385982
C	-1.904676	5.222015	-0.369892
H	-3.025189	4.401307	-2.017938
H	-0.639110	5.746557	1.294575
H	-2.399364	6.192188	-0.407258
H	6.704803	-0.065723	1.160325
H	2.443193	-4.922816	-0.782782
Ag	0.541022	0.909493	-0.283056
C	-3.030083	-0.424076	-0.171721
C	-4.200417	-1.218169	0.270775
C	-4.810011	-1.012634	1.511838
C	-4.695779	-2.196866	-0.594729
C	-5.905703	-1.783903	1.880535
H	-4.423854	-0.248590	2.182368
C	-5.789705	-2.966668	-0.223428

H -4.209111 -2.340543 -1.557148
C -6.394928 -2.759987 1.014960
H -6.380470 -1.623493 2.846484
H -6.173117 -3.729030 -0.898648
H -7.253076 -3.362739 1.307086
O -2.487727 -0.570186 -1.255714
O -2.620676 0.467397 0.730205
H -1.837280 0.953404 0.357009

TS19-20

Zero-point correction= 0.371956 (Hartree/Particle)
Thermal correction to Energy= 0.397813
Thermal correction to Enthalpy= 0.398757
Thermal correction to Gibbs Free Energy= 0.309230
Sum of electronic and zero-point Energies= -1369.843012
Sum of electronic and thermal Energies= -1369.817155
Sum of electronic and thermal Enthalpies= -1369.816211
Sum of electronic and thermal Free Energies= -1369.905739
Single Point Energy Calculations with extended basis set: HF = -1371.7406247
N 0.699886 -1.288550 -0.658673
C -0.245089 -2.071434 -1.159624
C -0.053989 -3.442540 -1.389759
C 1.167355 -3.998674 -1.088665
C 2.191152 -3.189485 -0.558142
C 1.905184 -1.821092 -0.354184
N 2.647511 0.342248 0.398062
C 3.579395 1.131857 0.904841
C 4.863435 0.680012 1.247177
C 5.166231 -0.647169 1.048256
C 4.193458 -1.513344 0.511915
C 2.930686 -0.962987 0.197191
H -1.194069 -1.583977 -1.390289
H -0.865229 -4.039127 -1.798585
H 3.301363 2.176668 1.050749
H 5.591324 1.373104 1.659907
C 3.482239 -3.709246 -0.227403
C 4.446270 -2.902886 0.286260
H 3.671928 -4.768009 -0.397877
H 5.429558 -3.297169 0.538430
C -0.713438 2.874979 0.010117
C -1.048036 3.438450 -1.237850
C -0.129953 3.746242 0.954138
C -0.816153 4.780804 -1.532929
H -1.528159 2.802295 -1.985782
C 0.106728 5.090601 0.674197
H 0.140132 3.363206 1.941653
C -0.235586 5.608545 -0.574161
H -1.092358 5.187121 -2.506097
H 0.556644 5.738327 1.426716
H -0.056014 6.659979 -0.796461

H 6.149332 -1.042879 1.300234
H 1.358766 -5.058272 -1.253510
Ag 0.391568 0.979024 -0.175669
C -2.864391 0.261828 -0.128237
C -3.750347 -0.857073 0.327863
C -4.175691 -0.956680 1.654844
C -4.158964 -1.820637 -0.597674
C -4.992253 -2.010317 2.051142
H -3.859390 -0.201047 2.370629
C -4.975901 -2.873220 -0.203044
H -3.828089 -1.725625 -1.630551
C -5.392826 -2.969366 1.123285
H -5.318624 -2.084184 3.087147
H -5.290536 -3.620373 -0.929715
H -6.032689 -3.793630 1.434332
O -2.448311 0.293472 -1.292628
O -2.573627 1.142138 0.781509
H -1.670932 1.835696 0.411435
Imaginary Vibrational Frequency = -803.4679 cm^{-1}

20

Zero-point correction= 0.377270 (Hartree/Particle)
Thermal correction to Energy= 0.403791
Thermal correction to Enthalpy= 0.404735
Thermal correction to Gibbs Free Energy= 0.314041
Sum of electronic and zero-point Energies= -1369.890513
Sum of electronic and thermal Energies= -1369.863993
Sum of electronic and thermal Enthalpies= -1369.863049
Sum of electronic and thermal Free Energies= -1369.953742
Single Point Energy Calculations with extended basis set: HF = -1371.790162
N 2.049097 -1.915905 0.063307
C 2.142366 -3.224304 -0.109783
C 3.354138 -3.878998 -0.378543
C 4.501264 -3.125184 -0.466934
C 4.434775 -1.729666 -0.289178
C 3.167874 -1.162236 -0.022537
N 1.852364 0.811037 0.417927
C 1.753351 2.120292 0.586267
C 2.854261 2.986613 0.507886
C 4.094658 2.451604 0.249781
C 4.231249 1.060859 0.070065
C 3.064332 0.269037 0.162413
H 1.214059 -3.790477 -0.033324
H 3.370647 -4.957234 -0.511432
H 0.753958 2.509408 0.787701
H 2.710757 4.054945 0.649061
C 5.593028 -0.895039 -0.372429
C 5.494936 0.447923 -0.200003
H 6.553853 -1.364126 -0.578963
H 6.375089 1.085985 -0.264308

C -1.910679 2.397179 0.259187
C -1.475088 2.051482 -1.020976
C -1.627458 3.661706 0.773777
C -0.754508 2.970801 -1.781880
H -1.699259 1.059886 -1.416703
C -0.906807 4.579880 0.011110
H -1.969186 3.932774 1.771700
C -0.469464 4.233644 -1.266151
H -0.414649 2.702097 -2.781192
H -0.685821 5.567441 0.413438
H 0.094075 4.950810 -1.861239
H 4.977894 3.085342 0.180318
H 5.464670 -3.589568 -0.673761
Ag 0.042134 -0.670037 0.475095
C -2.649038 -1.106623 0.010692
C -4.150885 -1.104462 -0.027867
C -4.895308 -0.777248 1.108171
C -4.817959 -1.422375 -1.213066
C -6.285113 -0.767028 1.059589
H -4.368028 -0.529184 2.027238
C -6.207271 -1.416781 -1.262875
H -4.227467 -1.673501 -2.091824
C -6.943070 -1.088144 -0.125910
H -6.858260 -0.508260 1.948567
H -6.719546 -1.667635 -2.190451
H -8.031348 -1.081528 -0.164188
O -2.015868 -1.313657 -1.050270
O -2.100251 -0.864774 1.134543
H -2.464522 1.668506 0.852233

21

Zero-point correction= 0.381151 (Hartree/Particle)
Thermal correction to Energy= 0.410056
Thermal correction to Enthalpy= 0.411000
Thermal correction to Gibbs Free Energy= 0.315827
Sum of electronic and zero-point Energies= -1537.295740
Sum of electronic and thermal Energies= -1537.266835
Sum of electronic and thermal Enthalpies= -1537.265891
Sum of electronic and thermal Free Energies= -1537.361064
Single Point Energy Calculations with extended basis set: HF = -1539.3546779
N -2.343440 1.499995 -0.013972
C -2.149239 2.794963 0.167570
C -3.177651 3.674455 0.542148
C -4.442022 3.165307 0.729869
C -4.676245 1.787877 0.547004
C -3.576858 0.984583 0.169442
N -2.716318 -1.202538 -0.379327
C -2.891748 -2.504552 -0.548234
C -4.132991 -3.135877 -0.378716
C -5.217560 -2.370009 -0.019201

C	-5.060875	-0.983327	0.171419
C	-3.772820	-0.436056	-0.022994
H	-1.129557	3.150426	0.012438
H	-2.966298	4.731651	0.677937
H	-2.007193	-3.077151	-0.826727
H	-4.219919	-4.208084	-0.531220
C	-5.965608	1.196550	0.730675
C	-6.149979	-0.136377	0.549753
H	-6.794535	1.840950	1.019866
H	-7.130549	-0.588808	0.690140
C	1.379463	-2.819851	-0.267786
O	0.456911	-3.112863	-0.940220
N	2.371655	-2.679507	0.397943
C	2.977447	-1.757674	1.253782
C	2.237737	-0.737522	1.856286
C	4.343980	-1.879057	1.501519
C	2.877173	0.167537	2.694039
H	1.169717	-0.657045	1.654584
C	4.973435	-0.968195	2.342841
H	4.900362	-2.681052	1.020149
C	4.244612	0.057200	2.940426
H	2.300206	0.966745	3.156582
H	6.041411	-1.061675	2.531177
H	4.740259	0.769444	3.597198
H	-5.269719	3.811019	1.020701
H	-6.199772	-2.819023	0.122634
Ag	-0.693262	-0.103758	-0.701417
C	1.939518	0.939827	-0.830326
C	3.428690	1.081491	-0.993543
C	4.199992	0.044444	-1.523837
C	4.059029	2.260663	-0.589930
C	5.578262	0.184216	-1.648249
H	3.705129	-0.877005	-1.825206
C	5.436996	2.401986	-0.709686
H	3.447708	3.059402	-0.174190
C	6.199279	1.362651	-1.239708
H	6.171960	-0.630502	-2.060507
H	5.919660	3.324019	-0.388849
H	7.278856	1.471233	-1.333760
O	1.290686	1.881868	-0.337727
O	1.436176	-0.172138	-1.219082

TS21-22

Zero-point correction= 0.380427 (Hartree/Particle)
Thermal correction to Energy= 0.408428
Thermal correction to Enthalpy= 0.409372
Thermal correction to Gibbs Free Energy= 0.313788
Sum of electronic and zero-point Energies= -1537.264082
Sum of electronic and thermal Energies= -1537.236081
Sum of electronic and thermal Enthalpies= -1537.235137

Sum of electronic and thermal Free Energies= -1537.330722
Single Point Energy Calculations with extended basis set: HF = -1539.3224095

N	2.786309	1.132356	-0.626208
C	2.724660	2.310856	-1.222734
C	3.860018	2.977751	-1.709378
C	5.089680	2.380073	-1.555315
C	5.184178	1.125515	-0.920768
C	3.985111	0.531570	-0.467214
N	2.892437	-1.327013	0.623065
C	2.943158	-2.507365	1.221668
C	4.140136	-3.205510	1.435192
C	5.316411	-2.638721	1.002934
C	5.294403	-1.385710	0.360554
C	4.040515	-0.757156	0.189290
H	1.729484	2.747689	-1.316664
H	3.756094	3.945018	-2.193470
H	1.991915	-2.924734	1.550915
H	4.122750	-4.170851	1.933196
C	6.433772	0.457283	-0.727771
C	6.486393	-0.750734	-0.110633
H	7.340500	0.941709	-1.086880
H	7.436259	-1.261682	0.039022
H	5.997181	2.862573	-1.915994
H	6.270111	-3.143716	1.148671
Ag	0.962265	-0.081914	0.297242
C	-1.507811	1.544812	0.224647
C	-2.821280	2.102927	0.636196
C	-3.515054	1.598771	1.739582
C	-3.349519	3.179786	-0.078552
C	-4.727682	2.160559	2.116473
H	-3.097055	0.765985	2.301148
C	-4.573153	3.729274	0.286946
H	-2.794010	3.570558	-0.928987
C	-5.262675	3.220122	1.385125
H	-5.261426	1.769682	2.980813
H	-4.988498	4.558408	-0.282884
H	-6.218537	3.653028	1.675558
O	-0.708075	2.199407	-0.435250
O	-1.196563	0.328780	0.659442
C	-2.145008	-1.080741	0.300950
O	-1.524172	-2.001289	0.763885
N	-3.153482	-0.670588	-0.341021
C	-4.170891	-1.551521	-0.732061
C	-5.379823	-0.963779	-1.131897
C	-4.059911	-2.949190	-0.759932
C	-6.449639	-1.747211	-1.544891
H	-5.453715	0.124028	-1.097375
C	-5.134679	-3.727358	-1.179063
H	-3.128276	-3.419602	-0.449732
C	-6.333295	-3.136262	-1.572946

H -7.381653 -1.270460 -1.846796
H -5.032119 -4.812010 -1.197004
H -7.169914 -3.752391 -1.897771
Imaginary Vibrational Frequency = -318.1512 cm^{-1}

22
Zero-point correction= 0.382376 (Hartree/Particle)
Thermal correction to Energy= 0.410239
Thermal correction to Enthalpy= 0.411183
Thermal correction to Gibbs Free Energy= 0.316614
Sum of electronic and zero-point Energies= -1537.274433
Sum of electronic and thermal Energies= -1537.246570
Sum of electronic and thermal Enthalpies= -1537.245626
Sum of electronic and thermal Free Energies= -1537.340194
Single Point Energy Calculations with extended basis set: HF = -1539.3340709
N 2.236301 0.654296 -0.861843
C 1.930365 1.722512 -1.578692
C 2.880697 2.679723 -1.967780
C 4.189401 2.498811 -1.585543
C 4.544700 1.369797 -0.821545
C 3.516814 0.461666 -0.479675
N 2.864884 -1.583370 0.634419
C 3.168607 -2.654922 1.352793
C 4.468682 -2.936322 1.794881
C 5.476916 -2.059783 1.468251
C 5.185644 -0.912183 0.706076
C 3.845614 -0.709985 0.304287
H 0.882029 1.831377 -1.861424
H 2.575443 3.539820 -2.557438
H 2.345490 -3.326489 1.592832
H 4.659157 -3.830647 2.381399
C 5.888412 1.129301 -0.395841
C 6.196454 0.030815 0.339351
H 6.656942 1.848154 -0.675966
H 7.218470 -0.155748 0.665428
H 4.960517 3.215977 -1.864138
H 6.501995 -2.238021 1.790348
Ag 0.748045 -1.097893 -0.097078
C -1.812784 1.975474 -0.877550
C -2.288358 2.392475 0.460099
C -1.939855 1.696248 1.621631
C -3.057755 3.555294 0.551378
C -2.367994 2.156795 2.860315
H -1.322696 0.800828 1.557477
C -3.494954 4.006268 1.789802
H -3.310200 4.092056 -0.360942
C -3.149571 3.307351 2.944892
H -2.090300 1.617488 3.763737
H -4.103254 4.906022 1.856768
H -3.487639 3.663180 3.916473

O -1.779327 2.703856 -1.840923
O -1.255605 0.724581 -0.960120
C -2.071832 -0.397170 -0.696465
O -1.409800 -1.418810 -0.370582
N -3.336267 -0.168244 -0.845545
C -4.278333 -1.179085 -0.651199
C -5.557572 -0.780529 -0.228756
C -4.068602 -2.544543 -0.911619
C -6.579670 -1.704159 -0.052076
H -5.724773 0.280256 -0.041086
C -5.099077 -3.463904 -0.742187
H -3.091681 -2.875577 -1.255122
C -6.358237 -3.056574 -0.307442
H -7.559275 -1.364428 0.283159
H -4.912701 -4.516560 -0.955120
H -7.158472 -3.782765 -0.174275

TS22-23

Zero-point correction= 0.381876 (Hartree/Particle)
Thermal correction to Energy= 0.408902
Thermal correction to Enthalpy= 0.409846
Thermal correction to Gibbs Free Energy= 0.318460
Sum of electronic and zero-point Energies= -1537.257230
Sum of electronic and thermal Energies= -1537.230203
Sum of electronic and thermal Enthalpies= -1537.229259
Sum of electronic and thermal Free Energies= -1537.320646
Single Point Energy Calculations with extended basis set: HF = -1539.3130672
N 2.162189 0.781971 -0.662096
C 1.528621 1.726477 -1.337987
C 2.199847 2.765857 -2.002874
C 3.573081 2.806176 -1.945590
C 4.272265 1.814302 -1.229838
C 3.510561 0.805801 -0.596390
N 3.478171 -1.202553 0.758239
C 4.111922 -2.145975 1.440835
C 5.506684 -2.192469 1.567380
C 6.253360 -1.214387 0.953477
C 5.609361 -0.198594 0.221436
C 4.197571 -0.229551 0.148293
H 0.437699 1.665584 -1.352480
H 1.633102 3.517350 -2.546032
H 3.488552 -2.904506 1.911921
H 5.971834 -2.989989 2.139710
C 5.698706 1.808690 -1.133607
C 6.342091 0.839838 -0.434363
H 6.254475 2.600410 -1.633946
H 7.428251 0.831836 -0.357683
H 4.134158 3.595239 -2.444805
H 7.340266 -1.210991 1.023711
Ag 1.216140 -1.136759 0.502369

C -2.340211 1.290501 -0.373501
C -3.272835 1.844272 0.661816
C -3.280955 1.426164 1.994078
C -4.172855 2.826069 0.246928
C -4.178649 1.985984 2.895953
H -2.579267 0.665303 2.330939
C -5.076131 3.381009 1.147628
H -4.149061 3.147691 -0.792772
C -5.079921 2.962337 2.475133
H -4.175083 1.658624 3.934300
H -5.775898 4.144903 0.812691
H -5.783236 3.396799 3.183598
O -2.140283 1.842326 -1.443510
O -1.158704 0.594528 0.250183
C -1.613660 -0.664779 0.076124
O -0.946900 -1.668132 0.401110
N -2.802232 -0.493153 -0.473279
C -3.787024 -1.403349 -0.817954
C -4.966573 -0.890275 -1.377166
C -3.665083 -2.789408 -0.633872
C -5.999720 -1.742023 -1.744698
H -5.049731 0.188289 -1.515455
C -4.706985 -3.630888 -1.009176
H -2.752795 -3.191280 -0.198627
C -5.877700 -3.119014 -1.564545
H -6.908871 -1.326214 -2.177186
H -4.600006 -4.705207 -0.862625
H -6.687361 -3.786370 -1.854013
Imaginary Vibrational Frequency = -222.8327 cm^{-1}

23

Zero-point correction= 0.382198 (Hartree/Particle)
Thermal correction to Energy= 0.410320
Thermal correction to Enthalpy= 0.411264
Thermal correction to Gibbs Free Energy= 0.317430
Sum of electronic and zero-point Energies= -1537.293315
Sum of electronic and thermal Energies= -1537.265194
Sum of electronic and thermal Enthalpies= -1537.264250
Sum of electronic and thermal Free Energies= -1537.358084
Single Point Energy Calculations with extended basis set: HF = -1539.3599022
N -2.348379 -1.552836 -0.156984
C -2.488333 -2.684606 -0.827953
C -3.734101 -3.181963 -1.238724
C -4.862812 -2.458108 -0.931223
C -4.744504 -1.244952 -0.225732
C -3.446354 -0.824873 0.143565
N -2.045338 0.833438 1.198664
C -1.896084 1.987785 1.828793
C -2.974178 2.815666 2.174728
C -4.245704 2.410662 1.841013

C	-4.435282	1.191537	1.161857
C	-3.287449	0.425733	0.854864
H	-1.571421	-3.228771	-1.056172
H	-3.790846	-4.118767	-1.786038
H	-0.873883	2.277419	2.073163
H	-2.793639	3.752503	2.694405
C	-5.881445	-0.445919	0.111917
C	-5.732677	0.726359	0.779783
H	-6.867918	-0.800260	-0.183286
H	-6.596566	1.338275	1.034802
H	-5.851449	-2.806059	-1.227929
H	-5.113030	3.020476	2.090501
Ag	-0.301268	-0.558753	0.474104
C	2.795798	-0.323486	0.177210
C	4.192872	-0.636682	0.578848
C	5.245960	-0.571862	-0.337807
C	4.432733	-1.103324	1.873043
C	6.525642	-0.957027	0.042747
H	5.058546	-0.227772	-1.354412
C	5.716857	-1.469462	2.257767
H	3.604604	-1.167251	2.576327
C	6.764391	-1.399430	1.342133
H	7.339994	-0.913847	-0.678030
H	5.900521	-1.816355	3.272950
H	7.768776	-1.695168	1.640251
O	1.881314	-1.027867	0.668308
O	4.063072	2.300110	0.085186
C	3.618250	1.845288	-0.962922
O	3.741420	2.107740	-2.154673
N	2.594598	0.652718	-0.729354
C	1.342369	0.806849	-1.378377
C	0.790410	-0.230467	-2.142066
C	0.679927	2.037339	-1.310897
C	-0.407183	-0.030784	-2.827325
H	1.318657	-1.180793	-2.212946
C	-0.506923	2.232877	-2.008414
H	1.113741	2.840127	-0.714992
C	-1.055878	1.200079	-2.766800
H	-0.826428	-0.843738	-3.418092
H	-1.006968	3.198451	-1.956379
H	-1.983502	1.356427	-3.314032

24

Zero-point correction= 0.380734 (Hartree/Particle)
Thermal correction to Energy= 0.409840
Thermal correction to Enthalpy= 0.410784
Thermal correction to Gibbs Free Energy= 0.313919
Sum of electronic and zero-point Energies= -1537.301566
Sum of electronic and thermal Energies= -1537.272460
Sum of electronic and thermal Enthalpies= -1537.271515

Sum of electronic and thermal Free Energies= -1537.368381
Single Point Energy Calculations with extended basis set: HF = -1539.3602601

N	2.394032	-1.530384	0.379128
C	2.498633	-2.561188	1.201508
C	3.722102	-2.997407	1.732324
C	4.867601	-2.321574	1.380287
C	4.786984	-1.215044	0.512869
C	3.507930	-0.848313	0.035469
N	2.159955	0.659217	-1.280846
C	2.044536	1.719347	-2.064995
C	3.141071	2.491227	-2.476583
C	4.395952	2.132076	-2.042249
C	4.550058	1.013664	-1.200442
C	3.385683	0.297783	-0.840040
H	1.569503	-3.071590	1.458260
H	3.749647	-3.851611	2.403260
H	1.034516	1.976184	-2.385467
H	2.987317	3.350840	-3.123005
C	5.941942	-0.469581	0.118229
C	5.828020	0.601727	-0.707505
H	6.913316	-0.781575	0.499039
H	6.705411	1.172634	-1.007759
H	5.840340	-2.625529	1.764928
H	5.276606	2.702118	-2.335420
Ag	0.357300	-0.584917	-0.420704
C	-2.709056	-0.539278	-0.103483
C	-4.095094	-1.010087	-0.435103
C	-5.185249	-0.681580	0.376092
C	-4.311109	-1.802325	-1.564959
C	-6.463190	-1.128626	0.061025
H	-5.012051	-0.078144	1.265799
C	-5.590389	-2.244229	-1.887511
H	-3.459878	-2.065618	-2.189380
C	-6.670552	-1.908831	-1.075309
H	-7.302042	-0.869935	0.705665
H	-5.744831	-2.854941	-2.775986
H	-7.671750	-2.257532	-1.324098
O	-1.757787	-1.126383	-0.732169
O	-4.379468	2.611321	-0.521177
C	-4.398951	2.620193	0.644426
O	-4.461967	2.693889	1.806187
N	-2.626920	0.432478	0.771348
C	-1.392974	0.892230	1.213457
C	-0.576003	0.127628	2.075256
C	-0.965576	2.198038	0.903453
C	0.590685	0.662669	2.622093
H	-0.901223	-0.878553	2.346183
C	0.200035	2.723299	1.450292
H	-1.578802	2.798371	0.230346
C	0.984725	1.963442	2.318328

H 1.192302 0.050827 3.294533
H 0.496169 3.741611 1.199754
H 1.889771 2.382155 2.754705

13b

Zero-point correction= 0.184873 (Hartree/Particle)
Thermal correction to Energy= 0.201095
Thermal correction to Enthalpy= 0.202039
Thermal correction to Gibbs Free Energy= 0.136687
Sum of electronic and zero-point Energies= -1119.880631
Sum of electronic and thermal Energies= -1119.864409
Sum of electronic and thermal Enthalpies= -1119.863465
Sum of electronic and thermal Free Energies= -1119.928817
Single Point Energy Calculations with extended basis set: HF = -1120.8593992
Ag -0.989241 -0.778957 0.108033
O 0.968831 1.141605 0.081116
O 1.151516 -1.085195 0.013819
C 1.645350 0.097570 0.028913
O -3.155854 -0.672578 0.230277
S -3.820491 0.493486 -0.545984
C -5.564277 0.282316 -0.153369
C -3.516302 1.957679 0.461593
H -5.904292 -0.634286 -0.642916
H -6.125600 1.140290 -0.537234
H -5.669912 0.197490 0.933847
H -3.817986 1.750188 1.494410
H -4.080937 2.800456 0.048554
H -2.443672 2.172635 0.413364
C 3.144072 0.189303 -0.019787
C 3.936083 -0.960559 -0.064482
C 3.759489 1.443132 -0.019635
C 5.322226 -0.858035 -0.107173
H 3.451230 -1.934427 -0.064570
C 5.145028 1.547845 -0.062948
H 3.131533 2.331092 0.015093
C 5.928687 0.396417 -0.106500
H 5.932818 -1.758970 -0.141104
H 5.616803 2.529222 -0.062623
H 7.014147 0.476862 -0.139986

14b

Zero-point correction= 0.184397 (Hartree/Particle)
Thermal correction to Energy= 0.200612
Thermal correction to Enthalpy= 0.201556
Thermal correction to Gibbs Free Energy= 0.137139
Sum of electronic and zero-point Energies= -1119.876745
Sum of electronic and thermal Energies= -1119.860530
Sum of electronic and thermal Enthalpies= -1119.859586
Sum of electronic and thermal Free Energies= -1119.924003
Single Point Energy Calculations with extended basis set: HF = -1120.8609086

Ag 0.541531 1.394691 -0.059743
O -1.468663 2.032622 -0.374873
O -3.510728 1.605800 0.423790
C -2.415544 1.236586 -0.004614
O 2.557081 0.766410 0.413696
S 2.997244 -0.713311 0.471015
C 1.638888 -1.602859 1.252916
C 2.779801 -1.357271 -1.198263
H 1.563392 -1.246882 2.284483
H 1.864344 -2.675368 1.245220
H 0.706708 -1.401788 0.705014
H 1.753974 -1.167197 -1.537894
H 2.990475 -2.432245 -1.191813
H 3.496540 -0.844417 -1.845620
C -2.148887 -0.247349 -0.118106
C -2.691469 -1.111547 0.834257
C -1.390311 -0.781889 -1.165637
C -2.443584 -2.479493 0.771421
H -3.306328 -0.693124 1.629578
C -1.170504 -2.154693 -1.250321
H -0.989248 -0.117769 -1.932651
C -1.684868 -3.004467 -0.272944
H -2.852664 -3.140837 1.533510
H -0.596016 -2.562576 -2.081232
H -1.501677 -4.076060 -0.330079

TS14b-15b

Zero-point correction= 0.181575 (Hartree/Particle)
Thermal correction to Energy= 0.198069
Thermal correction to Enthalpy= 0.199013
Thermal correction to Gibbs Free Energy= 0.134095
Sum of electronic and zero-point Energies= -1119.830837
Sum of electronic and thermal Energies= -1119.814343
Sum of electronic and thermal Enthalpies= -1119.813399
Sum of electronic and thermal Free Energies= -1119.878317
Single Point Energy Calculations with extended basis set: HF = -1120.8109882
Ag 0.167587 -0.483109 0.004475
O -0.837219 2.088518 -1.496006
O -0.725933 2.397446 0.787984
C -0.886801 1.946948 -0.309107
O 2.241923 -1.123555 0.097989
S 3.299216 -0.110259 -0.413247
C 3.329699 1.201422 0.824309
C 4.850274 -0.905991 0.034536
H 2.389689 1.757750 0.742050
H 4.173607 1.868084 0.616547
H 3.420291 0.750680 1.819154
H 4.806796 -1.185447 1.092959
H 5.676752 -0.213805 -0.155832
H 4.957561 -1.795911 -0.591617

C -1.903426 0.073187 -0.012606
C -2.551045 0.010003 1.233543
C -2.636804 -0.334492 -1.140894
C -3.856955 -0.459896 1.355352
H -2.026028 0.363355 2.123356
C -3.942882 -0.806117 -1.031367
H -2.179923 -0.254164 -2.129297
C -4.552918 -0.871686 0.220302
H -4.338477 -0.495824 2.332282
H -4.491599 -1.113769 -1.921225
H -5.577703 -1.230202 0.309122
Imaginary Vibrational Frequency = -379.8990 cm^{-1}

15b

Zero-point correction= 0.182433 (Hartree/Particle)
Thermal correction to Energy= 0.200028
Thermal correction to Enthalpy= 0.200972
Thermal correction to Gibbs Free Energy= 0.131344
Sum of electronic and zero-point Energies= -1119.850938
Sum of electronic and thermal Energies= -1119.833343
Sum of electronic and thermal Enthalpies= -1119.832399
Sum of electronic and thermal Free Energies= -1119.902027
Single Point Energy Calculations with extended basis set: HF = -1120.8321356
Ag 0.119285 -0.811874 -0.169248
O -0.228503 2.544090 -1.149970
O -0.404827 2.477326 1.173389
C -0.324113 2.495811 0.010509
O 2.280037 -1.113706 -0.256717
S 3.154816 0.164575 -0.249995
C 3.165340 0.713261 1.468475
C 4.828580 -0.495304 -0.306661
H 2.158555 1.074788 1.703865
H 3.888640 1.528154 1.580827
H 3.424673 -0.134698 2.112412
H 4.932617 -1.253098 0.477793
H 5.541159 0.323015 -0.160314
H 4.974118 -0.944156 -1.292891
C -1.941280 -0.524362 -0.046184
C -2.669418 -0.899182 1.098269
C -2.681139 0.066084 -1.087361
C -4.046924 -0.700075 1.200772
H -2.152111 -1.361823 1.941908
C -4.058794 0.269826 -0.996532
H -2.172942 0.383538 -2.000730
C -4.748593 -0.113252 0.150820
H -4.574101 -1.004802 2.105677
H -4.595620 0.730657 -1.826636
H -5.824053 0.044755 0.226391

16b

Zero-point correction= 0.169694 (Hartree/Particle)
Thermal correction to Energy= 0.183085
Thermal correction to Enthalpy= 0.184030
Thermal correction to Gibbs Free Energy= 0.126216
Sum of electronic and zero-point Energies= -931.356583
Sum of electronic and thermal Energies= -931.343191
Sum of electronic and thermal Enthalpies= -931.342247
Sum of electronic and thermal Free Energies= -931.400061
Single Point Energy Calculations with extended basis set: HF = -932.1516029

Ag	-0.057173	-0.143288	-0.384936
O	-2.208401	-0.231156	-0.749213
S	-3.111399	-0.277117	0.508304
C	-3.146703	1.419943	1.117568
C	-4.770003	-0.320509	-0.190060
H	-2.148306	1.647632	1.504988
H	-3.884967	1.498150	1.922871
H	-3.395700	2.091893	0.288479
H	-4.864617	0.491057	-0.919969
H	-5.501237	-0.210266	0.617485
H	-4.898157	-1.290175	-0.678602
C	1.995653	-0.031044	-0.053720
C	2.739953	1.114746	-0.391018
C	2.717336	-1.092845	0.522380
C	4.115230	1.199297	-0.169818
H	2.237412	1.973726	-0.841494
C	4.092400	-1.019907	0.748950
H	2.197029	-2.010353	0.806478
C	4.798318	0.129445	0.402784
H	4.655376	2.105746	-0.445947
H	4.614781	-1.865520	1.198052
H	5.872009	0.191007	0.578102

17b

Zero-point correction= 0.274758 (Hartree/Particle)
Thermal correction to Energy= 0.297068
Thermal correction to Enthalpy= 0.298012
Thermal correction to Gibbs Free Energy= 0.218262
Sum of electronic and zero-point Energies= -1330.721268
Sum of electronic and thermal Energies= -1330.698958
Sum of electronic and thermal Enthalpies= -1330.698014
Sum of electronic and thermal Free Energies= -1330.777763
Single Point Energy Calculations with extended basis set: HF = -1332.0833749

C	-0.223222	1.313562	1.547233
N	0.537539	1.996394	0.923128
C	0.828068	-1.891259	-0.152313
C	1.803448	-2.068121	-1.150584
C	1.226498	-2.186849	1.164908
C	3.097320	-2.500562	-0.857364
H	1.555710	-1.856076	-2.193186
C	2.518009	-2.619778	1.471376

H 0.515388 -2.069022 1.986184
C 3.462151 -2.774242 0.458606
H 3.825817 -2.619839 -1.660347
H 2.788307 -2.834988 2.505882
H 4.472301 -3.108865 0.692892
O -1.066250 0.754644 2.157525
C 1.813594 2.127073 0.374625
C 2.741385 1.084584 0.444552
C 2.143280 3.332508 -0.245801
C 4.002836 1.262499 -0.111561
H 2.464048 0.142028 0.917660
C 3.408908 3.495582 -0.796663
H 1.402794 4.128811 -0.285895
C 4.341965 2.463385 -0.730972
H 4.724036 0.448374 -0.059848
H 3.666327 4.436319 -1.279499
H 5.332013 2.594060 -1.163336
O -3.001689 -0.228727 -1.011153
S -3.462555 0.913059 -0.069736
C -4.976548 1.485418 -0.858232
H -5.614434 0.618100 -1.061439
H -5.480594 2.196615 -0.195818
H -4.696184 1.980097 -1.792134
C -4.214880 0.071834 1.335012
H -4.949669 -0.652362 0.965972
H -3.407396 -0.436037 1.871146
H -4.686159 0.813690 1.988632
Ag -1.054629 -1.109484 -0.576827

TS17b-18b

Zero-point correction= 0.273145 (Hartree/Particle)
Thermal correction to Energy= 0.294730
Thermal correction to Enthalpy= 0.295674
Thermal correction to Gibbs Free Energy= 0.217000
Sum of electronic and zero-point Energies= -1330.689885
Sum of electronic and thermal Energies= -1330.668299
Sum of electronic and thermal Enthalpies= -1330.667355
Sum of electronic and thermal Free Energies= -1330.746030
Single Point Energy Calculations with extended basis set: HF = -1332.0516184
C -1.438318 0.379977 0.822300
N -1.981870 -0.073893 -0.215794
C 0.056693 1.853032 -0.010357
C -0.278768 2.326374 -1.289461
C 0.366959 2.811095 0.968702
C -0.285684 3.687670 -1.585797
H -0.570256 1.612348 -2.062772
C 0.364289 4.175127 0.684361
H 0.586559 2.481505 1.986734
C 0.039635 4.614906 -0.597312
H -0.552752 4.029268 -2.586397

H 0.605679 4.898020 1.463657
H 0.027328 5.681138 -0.822497
O -1.345654 0.535976 2.003177
C -3.197199 -0.790786 -0.129185
C -3.711610 -1.303155 -1.325745
C -3.904014 -1.005147 1.061472
C -4.904128 -2.016036 -1.333885
H -3.155946 -1.127865 -2.246017
C -5.098156 -1.718274 1.044181
H -3.517558 -0.609620 1.999180
C -5.605591 -2.227728 -0.148682
H -5.288786 -2.407996 -2.274386
H -5.637562 -1.876323 1.977217
H -6.540420 -2.785296 -0.154391
O 2.351254 -1.788774 0.099393
S 3.748287 -1.674307 -0.563164
C 4.463555 -3.298068 -0.260111
H 5.516474 -3.287283 -0.560349
H 4.360794 -3.532647 0.805203
H 3.910801 -4.021412 -0.865794
C 4.745692 -0.741835 0.614874
H 4.362510 0.283779 0.626308
H 4.647101 -1.197123 1.606892
H 5.789310 -0.744394 0.282524
Ag 1.098560 -0.011712 0.073051
Imaginary Vibrational Frequency = -343.9728 cm^{-1}

18b
Zero-point correction= 0.277119 (Hartree/Particle)
Thermal correction to Energy= 0.298027
Thermal correction to Enthalpy= 0.298972
Thermal correction to Gibbs Free Energy= 0.222955
Sum of electronic and zero-point Energies= -1330.758389
Sum of electronic and thermal Energies= -1330.737480
Sum of electronic and thermal Enthalpies= -1330.736536
Sum of electronic and thermal Free Energies= -1330.812553
Single Point Energy Calculations with extended basis set: HF = -1332.1251331
C 1.605980 1.729884 0.062656
N 1.533431 0.378204 0.096374
C 0.273996 2.433307 0.132745
C -0.722680 2.079711 1.050154
C 0.056624 3.524471 -0.711414
C -1.924015 2.783708 1.095959
H -0.543030 1.266023 1.754183
C -1.150996 4.214155 -0.682749
H 0.849359 3.822036 -1.396432
C -2.145922 3.843533 0.219826
H -2.684875 2.507195 1.824567
H -1.314584 5.049772 -1.361462
H -3.087604 4.389015 0.249904

O 2.622252 2.436234 -0.021703
C 2.671061 -0.444998 0.128621
C 2.463479 -1.811456 0.398042
C 3.998417 -0.029600 -0.094503
C 3.511785 -2.719668 0.440312
H 1.441443 -2.152794 0.584078
C 5.044611 -0.947599 -0.051361
H 4.192578 1.016051 -0.299902
C 4.819651 -2.294739 0.213844
H 3.303381 -3.767621 0.653593
H 6.059437 -0.593833 -0.234127
H 5.646724 -3.001996 0.243683
O -2.253477 -1.393199 -0.930598
S -2.967742 -2.273061 0.128960
C -4.551976 -2.615694 -0.652753
H -5.199788 -3.131199 0.063681
H -4.996980 -1.668044 -0.975456
H -4.361259 -3.261761 -1.513975
C -3.554403 -1.113832 1.379522
H -2.679323 -0.754347 1.931215
H -4.061144 -0.279594 0.880686
H -4.232354 -1.635549 2.063561
Ag -0.359702 -0.515174 -0.365123

19b

Zero-point correction= 0.285604 (Hartree/Particle)
Thermal correction to Energy= 0.308335
Thermal correction to Enthalpy= 0.309279
Thermal correction to Gibbs Free Energy= 0.225735
Sum of electronic and zero-point Energies= -1351.801991
Sum of electronic and thermal Energies= -1351.779260
Sum of electronic and thermal Enthalpies= -1351.778316
Sum of electronic and thermal Free Energies= -1351.861860
Single Point Energy Calculations with extended basis set: HF = -1353.1917944
Ag 1.396101 0.162418 -0.152500
O 2.140740 -1.900127 -0.245268
S 3.680101 -2.044199 -0.320884
C 4.266763 -1.695465 1.348863
C 3.923940 -3.828293 -0.294686
H 4.106736 -0.628183 1.534989
H 5.335332 -1.927336 1.409344
H 3.692411 -2.297046 2.062664
H 3.365793 -4.247989 0.549360
H 4.994111 -4.041440 -0.203086
H 3.544348 -4.227552 -1.239005
C 0.877756 2.196908 -0.043840
C 0.625788 2.833344 1.186927
C 0.823341 3.015229 -1.188521
C 0.345940 4.197570 1.275010
H 0.643397 2.249244 2.110124

C 0.544740 4.380097 -1.113462
H 1.002585 2.578363 -2.173513
C 0.306134 4.977196 0.121957
H 0.156374 4.652807 2.247643
H 0.511955 4.979775 -2.023694
H 0.087188 6.042603 0.185130
O -1.162315 -1.221624 0.083354
C -2.103438 -0.446270 0.020733
O -1.951417 0.874949 -0.063223
H -0.982699 1.079104 -0.066130
C -3.521476 -0.875328 0.031096
C -3.798542 -2.243113 0.101427
C -4.570846 0.046208 -0.026190
C -5.113958 -2.687247 0.114188
H -2.969059 -2.945914 0.144850
C -5.886336 -0.401282 -0.012876
H -4.352137 1.109911 -0.081048
C -6.158174 -1.765965 0.057132
H -5.327748 -3.752844 0.168237
H -6.703034 0.316545 -0.056886
H -7.189739 -2.113600 0.067226

TS19b-20b

Zero-point correction= 0.280234 (Hartree/Particle)
Thermal correction to Energy= 0.302504
Thermal correction to Enthalpy= 0.303448
Thermal correction to Gibbs Free Energy= 0.221474
Sum of electronic and zero-point Energies= -1351.793773
Sum of electronic and thermal Energies= -1351.771503
Sum of electronic and thermal Enthalpies= -1351.770559
Sum of electronic and thermal Free Energies= -1351.852533
Single Point Energy Calculations with extended basis set: HF = -1353.1782547
Ag 1.003393 -0.130678 -0.017129
O 1.978411 -2.113514 -0.079243
S 3.476602 -2.150797 -0.460886
C 4.344747 -1.437801 0.950838
C 3.923418 -3.871485 -0.169659
H 4.110177 -0.368277 0.975918
H 5.422846 -1.577541 0.816633
H 3.995923 -1.925813 1.868111
H 3.595708 -4.151762 0.837612
H 5.006839 -3.986220 -0.276450
H 3.408845 -4.477819 -0.920041
C 0.571003 2.025876 -0.010013
C 0.997006 2.669098 1.170372
C 0.902922 2.661314 -1.224504
C 1.699992 3.871831 1.146557
H 0.754507 2.223192 2.138043
C 1.604804 3.864082 -1.264226
H 0.584890 2.208832 -2.166936

C 2.004260 4.470337 -0.074687
H 2.008553 4.347523 2.077313
H 1.838806 4.333732 -2.219459
H 2.548579 5.413728 -0.099130
O -1.356106 -1.015692 0.104906
C -2.198802 -0.102979 0.068449
O -1.921576 1.158076 0.046235
H -0.735519 1.383335 0.029749
C -3.658237 -0.436264 0.046369
C -4.057474 -1.774199 0.076450
C -4.625807 0.569986 -0.005056
C -5.407364 -2.103595 0.055273
H -3.293098 -2.547650 0.116633
C -5.976277 0.241152 -0.026752
H -4.307535 1.609840 -0.027713
C -6.368290 -1.095567 0.003223
H -5.713044 -3.148198 0.078926
H -6.726625 1.028875 -0.067200
H -7.426189 -1.352829 -0.013759
Imaginary Vibrational Frequency = -940.2298 cm^{-1}

20b
Zero-point correction= 0.285269 (Hartree/Particle)
Thermal correction to Energy= 0.308090
Thermal correction to Enthalpy= 0.309034
Thermal correction to Gibbs Free Energy= 0.226273
Sum of electronic and zero-point Energies= -1351.843933
Sum of electronic and thermal Energies= -1351.821112
Sum of electronic and thermal Enthalpies= -1351.820168
Sum of electronic and thermal Free Energies= -1351.902929
Single Point Energy Calculations with extended basis set: HF = -1353.2287442
Ag 0.542277 -0.179272 -0.805221
O 2.594971 -1.027090 -1.025620
S 3.537472 -1.243146 0.176448
C 2.475675 -1.706051 1.560706
C 4.235713 -2.879543 -0.126380
H 1.931852 -0.808479 1.877810
H 3.097955 -2.070245 2.385837
H 1.775200 -2.481385 1.225649
H 3.417534 -3.592042 -0.280023
H 4.855955 -3.171529 0.727464
H 4.853203 -2.810717 -1.026269
C 1.118233 2.595887 -0.524440
C 0.547925 2.237266 0.701359
C 2.506172 2.667604 -0.652992
C 1.367643 1.947031 1.792894
H -0.535760 2.199968 0.805179
C 3.321285 2.377186 0.438330
H 2.949119 2.954413 -1.605200
C 2.752999 2.015361 1.659304

H 0.922411 1.671793 2.748176
H 4.404077 2.434139 0.339095
H 3.393094 1.789190 2.511195
O -1.404976 -0.879491 0.723551
C -2.119433 -0.340508 -0.154471
O -1.660573 0.181262 -1.221403
H 0.475656 2.839920 -1.370436
C -3.607131 -0.293503 0.049982
C -4.168876 -0.844555 1.204067
C -4.442762 0.297941 -0.900393
C -5.543667 -0.805627 1.406675
H -3.508547 -1.302288 1.937752
C -5.818276 0.338193 -0.699793
H -3.998565 0.724952 -1.797127
C -6.370756 -0.213547 0.454296
H -5.972989 -1.237361 2.309469
H -6.462828 0.801396 -1.445264
H -7.447803 -0.181878 0.611825

CO_2 (in gas phase)
Zero-point correction= 0.012010 (Hartree/Particle)
Thermal correction to Energy= 0.014622
Thermal correction to Enthalpy= 0.015566
Thermal correction to Gibbs Free Energy= -0.008686
Sum of electronic and zero-point Energies= -188.486058
Sum of electronic and thermal Energies= -188.483446
Sum of electronic and thermal Enthalpies= -188.482502
Sum of electronic and thermal Free Energies= -188.506755
Single Point Energy Calculations with extended basis set: HF = -188.672328
C 0.000000 0.000000 0.000000
O 0.000000 -0.000000 1.164710
O 0.000000 0.000000 -1.164710

$PhCO_2^-$ (in gas phase)
Zero-point correction= 0.102093 (Hartree/Particle)
Thermal correction to Energy= 0.109005
Thermal correction to Enthalpy= 0.109949
Thermal correction to Gibbs Free Energy= 0.070256
Sum of electronic and zero-point Energies= -419.873201
Sum of electronic and thermal Energies= -419.866289
Sum of electronic and thermal Enthalpies= -419.865345
Sum of electronic and thermal Free Energies= -419.905038
Single Point Energy Calculations with extended basis set: HF = -420.4701431
C -1.828110 0.000096 -0.000029
C -0.280411 0.000004 -0.000020
C 0.432640 -1.198591 -0.000042
C 0.432661 1.198544 0.000035
C 1.824506 -1.204337 -0.000039
H -0.155515 -2.116461 -0.000055
C 1.824576 1.204281 0.000051

H -0.155441 2.116470 0.000046
C 2.527411 -0.000015 0.000002
H 2.370100 -2.150692 -0.000099
H 2.370172 2.150643 0.000119
H 3.619139 0.000012 0.000005
O -2.352927 1.134546 -0.000089
O -2.353085 -1.134529 0.000119

PhNCO (in gas phase)
Zero-point correction= 0.104018 (Hartree/Particle)
Thermal correction to Energy= 0.111121
Thermal correction to Enthalpy= 0.112065
Thermal correction to Gibbs Free Energy= 0.071608
Sum of electronic and zero-point Energies= -399.349290
Sum of electronic and thermal Energies= -399.342188
Sum of electronic and thermal Enthalpies= -399.341243
Sum of electronic and thermal Free Energies= -399.381701
Single Point Energy Calculations with extended basis set: HF = -399.916889139
C -2.541147 -0.073517 0.000090
O -3.658401 0.287834 0.000492
N -1.443022 -0.568608 -0.000502
C -0.087307 -0.245990 -0.000361
C 0.346172 1.082184 -0.000349
C 0.840719 -1.286819 -0.000054
C 1.706788 1.359402 0.000020
H -0.388535 1.886280 -0.000618
C 2.199227 -0.996974 0.000232
H 0.479435 -2.312901 -0.000077
C 2.637660 0.323963 0.000283
H 2.041141 2.395389 0.000138
H 2.920933 -1.811818 0.000409
H 3.702711 0.547143 0.000557

Ag(O_2CPh) (in gas phase)
Zero-point correction= 0.104186 (Hartree/Particle)
Thermal correction to Energy= 0.112976
Thermal correction to Enthalpy= 0.113920
Thermal correction to Gibbs Free Energy= 0.067894
Sum of electronic and zero-point Energies= -566.843574
Sum of electronic and thermal Energies= -566.834784
Sum of electronic and thermal Enthalpies= -566.833840
Sum of electronic and thermal Free Energies= -566.879867
Single Point Energy Calculations with extended basis set: HF = -567.468900756
Ag -2.500514 0.000013 0.000004
C 0.102003 -0.000019 -0.000026
C 1.594228 -0.000023 -0.000011
C 2.294072 1.207886 -0.000165
C 2.294084 -1.207891 0.000166
C 3.683259 1.206790 -0.000137
H 1.729798 2.137818 -0.000091

C 3.683278 -1.206741 0.000146
H 1.729854 -2.137850 0.000121
C 4.378442 0.000024 -0.000002
H 4.227427 2.149975 -0.000425
H 4.227456 -2.149921 0.000468
H 5.467700 0.000028 0.000026
O -0.502129 -1.114023 -0.000391
O -0.502155 1.113922 0.000374

Ag((Ph)NC(O)Ph) (in gas phase)
Zero-point correction= 0.196115 (Hartree/Particle)
Thermal correction to Energy= 0.209871
Thermal correction to Enthalpy= 0.210815
Thermal correction to Gibbs Free Energy= 0.152514
Sum of electronic and zero-point Energies= -777.720276
Sum of electronic and thermal Energies= -777.706520
Sum of electronic and thermal Enthalpies= -777.705576
Sum of electronic and thermal Free Energies= -777.763877
Single Point Energy Calculations with extended basis set: HF = -778.731688676
Ag 2.651189 -0.835923 0.012296
C -0.010149 -1.036556 0.004994
C -1.499806 -1.119336 0.095289
C -2.147358 -2.134051 -0.612997
C -2.247846 -0.269819 0.914415
C -3.526722 -2.277332 -0.531350
H -1.548415 -2.809098 -1.220717
C -3.624795 -0.429306 1.012356
H -1.749831 0.512382 1.484795
C -4.267754 -1.425494 0.282794
H -4.024548 -3.063678 -1.096595
H -4.198974 0.229560 1.661653
H -5.348146 -1.542156 0.354857
O 0.623944 -2.117792 -0.120653
N 0.660630 0.115788 0.117063
C 0.146285 1.405457 -0.044624
C -0.711662 1.747270 -1.100809
C 0.555207 2.413999 0.837271
C -1.170106 3.050456 -1.241628
H -1.018002 0.975018 -1.805609
C 0.101596 3.718071 0.684997
H 1.234461 2.147866 1.647848
C -0.768783 4.043957 -0.351963
H -1.841766 3.294418 -2.063833
H 0.429259 4.486264 1.384465
H -1.124552 5.065731 -0.471476

$[BSP]^{2-}$ (in gas phase)
Zero-point correction= 0.338168 (Hartree/Particle)
Thermal correction to Energy= 0.364826
Thermal correction to Enthalpy= 0.365770

Thermal correction to Gibbs Free Energy= 0.276822
Sum of electronic and zero-point Energies= -2278.860821
Sum of electronic and thermal Energies= -2278.834163
Sum of electronic and thermal Enthalpies= -2278.833219
Sum of electronic and thermal Free Energies= -2278.922167
Single Point Energy Calculations with extended basis set: HF = -2281.12236351

N	-1.335637	4.306734	-0.206874
C	-2.642562	4.303389	-0.370472
C	-3.434366	3.150456	-0.382319
C	-2.843553	1.906665	-0.228216
C	-1.423411	1.874377	-0.109518
C	-0.723602	3.110460	-0.082394
N	1.335688	4.306763	0.206866
C	2.642618	4.303441	0.370430
C	3.434442	3.150519	0.382277
C	2.843637	1.906720	0.228215
C	1.423504	1.874413	0.109515
C	0.723670	3.110477	0.082406
H	-3.118500	5.282656	-0.482686
H	-4.517508	3.226560	-0.468484
H	3.118543	5.282716	0.482634
H	4.517584	3.226635	0.468434
C	-0.677720	0.654984	-0.048168
C	0.677859	0.655002	0.048078
H	-1.218409	-0.288146	-0.095974
H	1.218590	-0.288111	0.095797
C	-3.709354	0.710581	-0.174123
C	-4.732445	0.545815	-1.120269
C	-3.611718	-0.220180	0.867423
C	-5.628423	-0.507457	-1.022554
H	-4.804993	1.253495	-1.947979
C	-4.519865	-1.269330	0.970429
H	-2.839048	-0.093156	1.626993
C	-5.535510	-1.413625	0.032225
H	-6.413516	-0.649184	-1.764429
H	-4.464652	-1.992429	1.782505
C	3.709419	0.710623	0.174146
C	4.732611	0.545925	1.120192
C	3.611601	-0.220261	-0.867269
C	5.628547	-0.507383	1.022477
H	4.805283	1.253696	1.947815
C	4.519701	-1.269451	-0.970273
H	2.838806	-0.093316	-1.626727
C	5.535471	-1.413664	-0.032191
H	6.413729	-0.649056	1.764268
H	4.464346	-1.992652	-1.782248
S	-6.791434	-2.704386	0.193758
S	6.791339	-2.704477	-0.193755
O	-7.988507	-1.947711	0.610903
O	-6.881701	-3.273516	-1.164383

O -6.249318 -3.615324 1.219138
O 6.248997 -3.615593 -1.218858
O 6.881887 -3.273371 1.164467
O 7.988341 -1.947905 -0.611290

[(BPS)Ag]$^-$ (in gas phase)
Zero-point correction= 0.339827 (Hartree/Particle)
Thermal correction to Energy= 0.368504
Thermal correction to Enthalpy= 0.369448
Thermal correction to Gibbs Free Energy= 0.275154
Sum of electronic and zero-point Energies= -2425.815277
Sum of electronic and thermal Energies= -2425.786600
Sum of electronic and thermal Enthalpies= -2425.785656
Sum of electronic and thermal Free Energies= -2425.879950
Single Point Energy Calculations with extended basis set: HF = -2428.1223461
N 1.389979 3.401016 -0.028514
C 2.719091 3.400508 0.000975
C 3.477436 2.243796 0.087721
C 2.856336 0.998956 0.145972
C 1.424571 0.988546 0.184244
C 0.727485 2.216331 0.070393
N -1.390095 3.401029 -0.028064
C -2.719215 3.400500 0.001541
C -3.477545 2.243777 0.088068
C -2.856421 0.998916 0.146077
C -1.424670 0.988518 0.184315
C -0.727592 2.216327 0.070521
H 3.206809 4.372330 -0.076340
H 4.562246 2.306134 0.048224
H -3.206978 4.372332 -0.075428
H -4.562356 2.306105 0.048649
C 0.679334 -0.207266 0.409947
C -0.679392 -0.207285 0.409954
H 1.223828 -1.124526 0.619098
H -1.223848 -1.124568 0.619095
Ag -0.000244 5.146404 -0.236790
C 3.683678 -0.205599 0.151914
C 4.870266 -0.224917 0.909621
C 3.385501 -1.311550 -0.661038
C 5.718389 -1.314289 0.861370
H 5.096591 0.615031 1.568249
C 4.254415 -2.391781 -0.724922
H 2.495582 -1.294319 -1.291183
C 5.422483 -2.397441 0.031610
H 6.623560 -1.353568 1.465446
H 4.055714 -3.249904 -1.364821
C -3.683755 -0.205641 0.151860
C -3.385440 -1.311561 -0.661085
C -4.870474 -0.224994 0.909363
C -4.254291 -2.391835 -0.725076

H -2.495460 -1.294277 -1.291141
C -5.718560 -1.314386 0.860972
H -5.096942 0.614938 1.567963
C -5.422452 -2.397560 0.031308
H -4.055519 -3.249941 -1.364976
H -6.623873 -1.353597 1.464838
S 6.615378 -3.752534 -0.088138
S -6.615003 -3.752975 -0.088143
O 7.734593 -3.105108 -0.795599
O 6.886939 -4.074987 1.322636
O 5.901631 -4.787288 -0.852541
O -6.885101 -4.076163 1.322747
O -5.901485 -4.787044 -0.853688
O -7.735095 -3.105628 -0.794273

[(Phen)Ag(DMSO)]$^{+}$ (in solution phase)
Zero-point correction= 0.253404 (Hartree/Particle)
Thermal correction to Energy= 0.271755
Thermal correction to Enthalpy= 0.272699
Thermal correction to Gibbs Free Energy= 0.204205
Sum of electronic and zero-point Energies= -1270.915384
Sum of electronic and thermal Energies= -1270.897033
Sum of electronic and thermal Enthalpies= -1270.896089
Sum of electronic and thermal Free Energies= -1270.964583
Single Point Energy Calculations with extended basis set: HF = -1272.1801939
N 0.475679 1.230453 -0.047469
C 0.158657 2.515944 -0.057544
C 1.115974 3.540342 -0.032720
C 2.446536 3.194052 0.003873
C 2.815122 1.834734 0.014528
C 1.779909 0.873073 -0.012615
N 1.134161 -1.451500 -0.028757
C 1.448221 -2.737393 -0.022167
C 2.771246 -3.202125 0.010576
C 3.790521 -2.279316 0.037917
C 3.488138 -0.903768 0.031369
C 2.125044 -0.532029 -0.003450
H -0.904457 2.754215 -0.086769
H 0.798317 4.579168 -0.042271
H 0.616044 -3.440252 -0.043431
H 2.970976 -4.269961 0.014418
C 4.182521 1.417735 0.051164
C 4.506568 0.099814 0.058907
H 4.955214 2.184588 0.072261
H 5.547006 -0.220400 0.086216
H 3.224951 3.955562 0.024450
H 4.832787 -2.594071 0.064597
Ag -1.039097 -0.535205 -0.049445
S -4.354466 -0.332374 0.076820
O -3.119925 -1.253375 0.014260

C -4.028601 0.835692 1.409418
H -4.823267 1.589360 1.428494
H -4.028731 0.273517 2.347613
H -3.049417 1.307258 1.250923
C -4.181240 0.815209 -1.301484
H -4.971550 1.571371 -1.240050
H -3.189470 1.285089 -1.263690
H -4.290595 0.239710 -2.225098

Benzene (in solution phase)
Zero-point correction= 0.100213 (Hartree/Particle)
Thermal correction to Energy= 0.104631
Thermal correction to Enthalpy= 0.105575
Thermal correction to Gibbs Free Energy= 0.072742
Sum of electronic and zero-point Energies= -231.950432
Sum of electronic and thermal Energies= -231.946014
Sum of electronic and thermal Enthalpies= -231.945069
Sum of electronic and thermal Free Energies= -231.977903
Single Point Energy Calculations with extended basis set: HF = -232.3594514
C -1.328845 0.418016 0.000023
C -1.026448 -0.941778 -0.000005
C -0.302386 1.359807 -0.000054
C 0.302427 -1.359818 -0.000026
H -1.828845 -1.678035 0.000080
C 1.026449 0.941808 -0.000027
H -0.539309 2.422775 0.000096
C 1.328869 -0.418025 0.000089
H 0.539047 -2.422838 -0.000183
H 1.828736 1.678220 -0.000029
H 2.367797 -0.744493 0.000001
H -2.367815 0.744313 0.000039

CO_2 (in solution phase)
Zero-point correction= 0.011915 (Hartree/Particle)
Thermal correction to Energy= 0.014534
Thermal correction to Enthalpy= 0.015478
Thermal correction to Gibbs Free Energy= -0.009439
Sum of electronic and zero-point Energies= -188.488736
Sum of electronic and thermal Energies= -188.486117
Sum of electronic and thermal Enthalpies= -188.485173
Sum of electronic and thermal Free Energies= -188.510090
Single Point Energy Calculations with extended basis set: HF = -188.6748051
C 0.000000 0.000000 -0.000066
O 0.000000 0.000000 -1.164450
O -0.000000 -0.000000 1.164499

DMSO (in solution phase)
Zero-point correction= 0.079322 (Hartree/Particle)
Thermal correction to Energy= 0.084951
Thermal correction to Enthalpy= 0.085895

Thermal correction to Gibbs Free Energy= 0.051014
Sum of electronic and zero-point Energies= -552.975994
Sum of electronic and thermal Energies= -552.970365
Sum of electronic and thermal Enthalpies= -552.969421
Sum of electronic and thermal Free Energies= -553.004301
Single Point Energy Calculations with extended basis set: HF = -553.3353211

S	-0.000057	0.233789	-0.446680
O	-0.000552	1.493402	0.388812
C	-1.343795	-0.806902	0.183890
H	-1.309196	-1.789244	-0.299845
H	-1.240852	-0.906029	1.271105
H	-2.289233	-0.311288	-0.056470
C	1.344343	-0.806037	0.183913
H	1.241404	-0.905587	1.271093
H	1.310441	-1.788294	-0.300074
H	2.289473	-0.309760	-0.056242

PhNCO (in solution phase)

Zero-point correction= 0.103865 (Hartree/Particle)
Thermal correction to Energy= 0.110983
Thermal correction to Enthalpy= 0.111928
Thermal correction to Gibbs Free Energy= 0.071438
Sum of electronic and zero-point Energies= -399.353897
Sum of electronic and thermal Energies= -399.346779
Sum of electronic and thermal Enthalpies= -399.345834
Sum of electronic and thermal Free Energies= -399.386324
Single Point Energy Calculations with extended basis set: HF = -399.9211716

C	-2.548648	-0.067238	-0.000028
O	-3.676037	0.270820	-0.000322
N	-1.444733	-0.541227	0.000440
C	-0.084165	-0.233605	0.000168
C	0.360004	1.091338	0.000131
C	0.831891	-1.285513	-0.000014
C	1.724245	1.354221	-0.000017
H	-0.365884	1.902785	0.000122
C	2.194220	-1.009068	-0.000179
H	0.463185	-2.309136	0.000045
C	2.645032	0.308483	-0.000109
H	2.068997	2.386583	0.000066
H	2.907515	-1.831029	-0.000357
H	3.712140	0.521114	-0.000108