

SUPPORTING INFORMATION FOR

**INSIGHTS INTO MECHANISM AND SELECTIVITY IN RUTHENIUM(II)-CATALYSED
ORTHO-ARYLATION REACTIONS DIRECTED BY LEWIS BASIC GROUPS**

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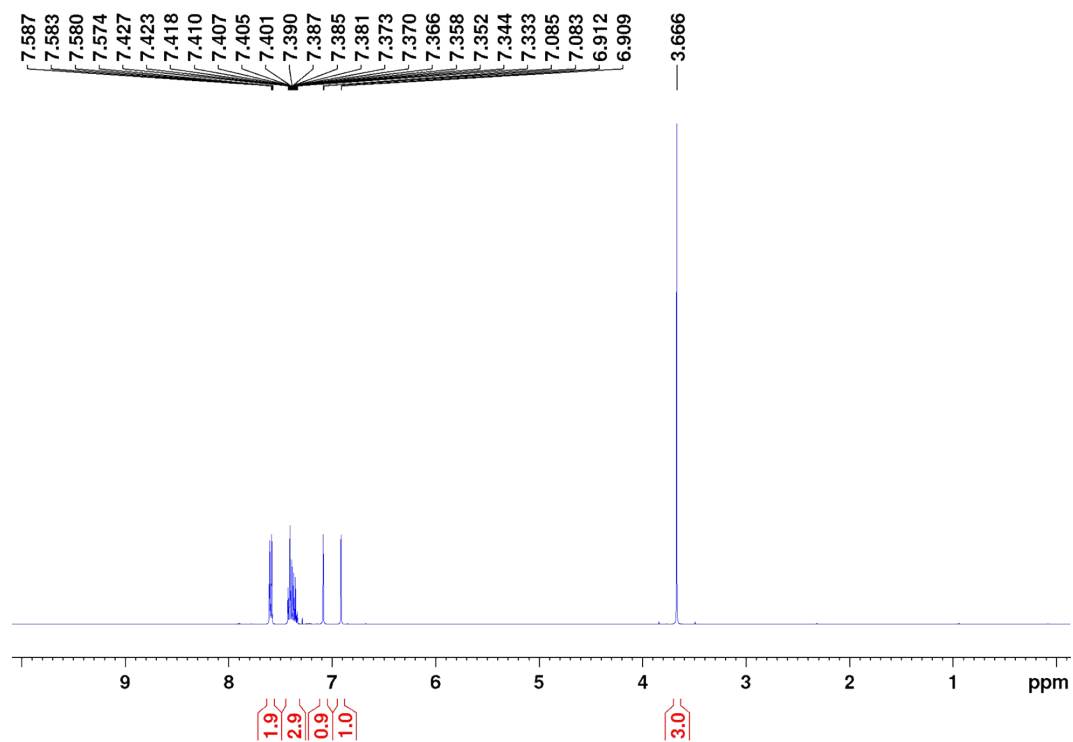
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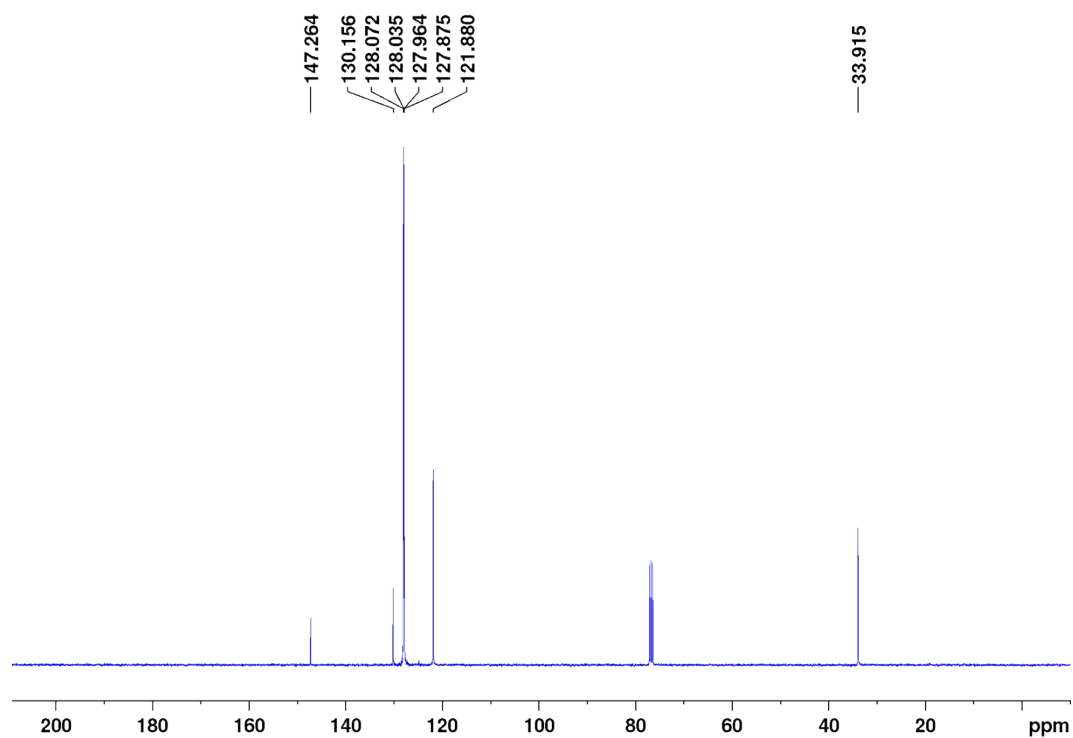
NMR Spectra

Compound 5

^1H NMR Spectrum (D229144)

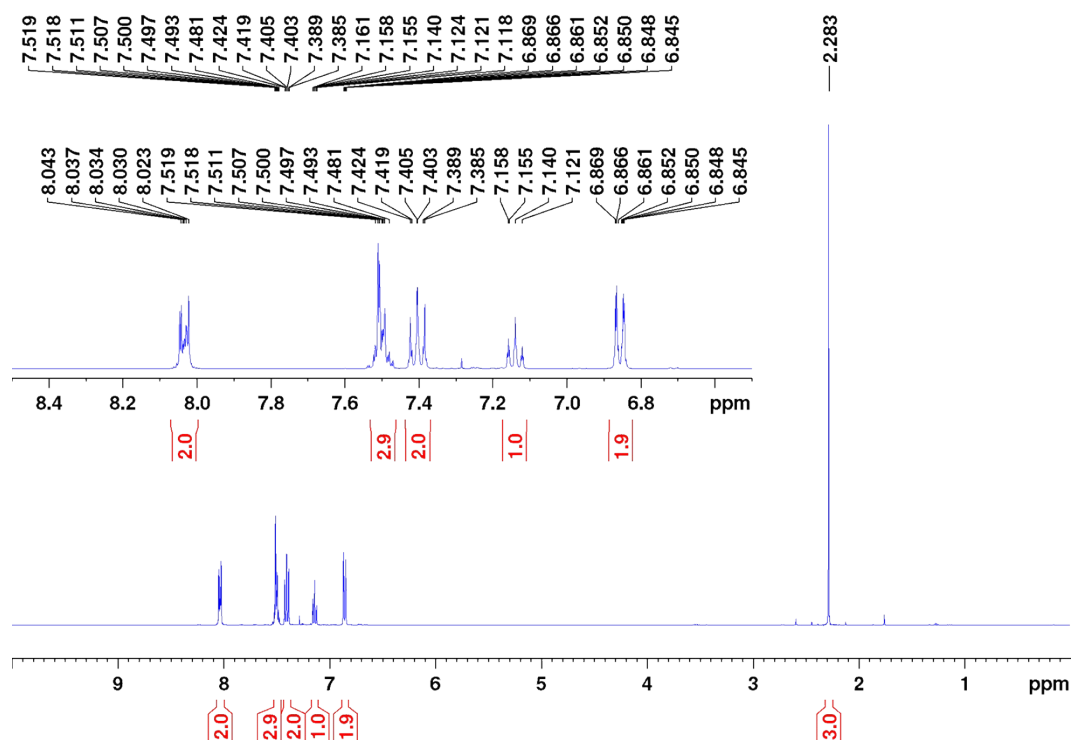


$^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum (D229144)

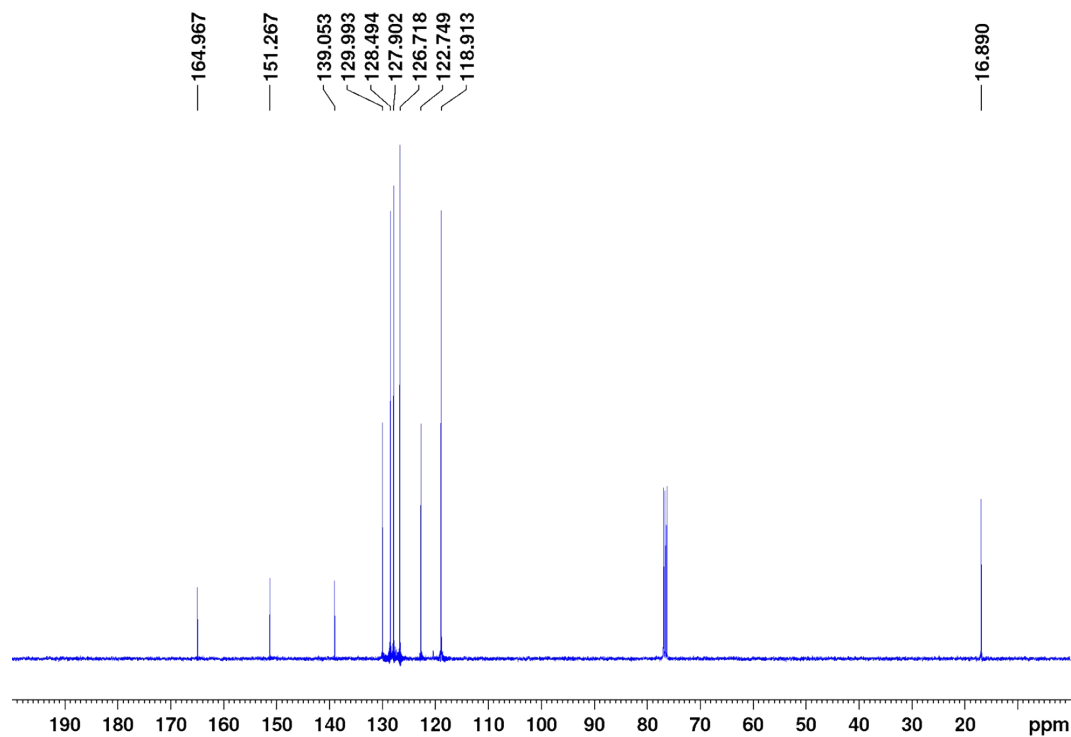


Compound 6

¹H NMR Spectrum (D229390)

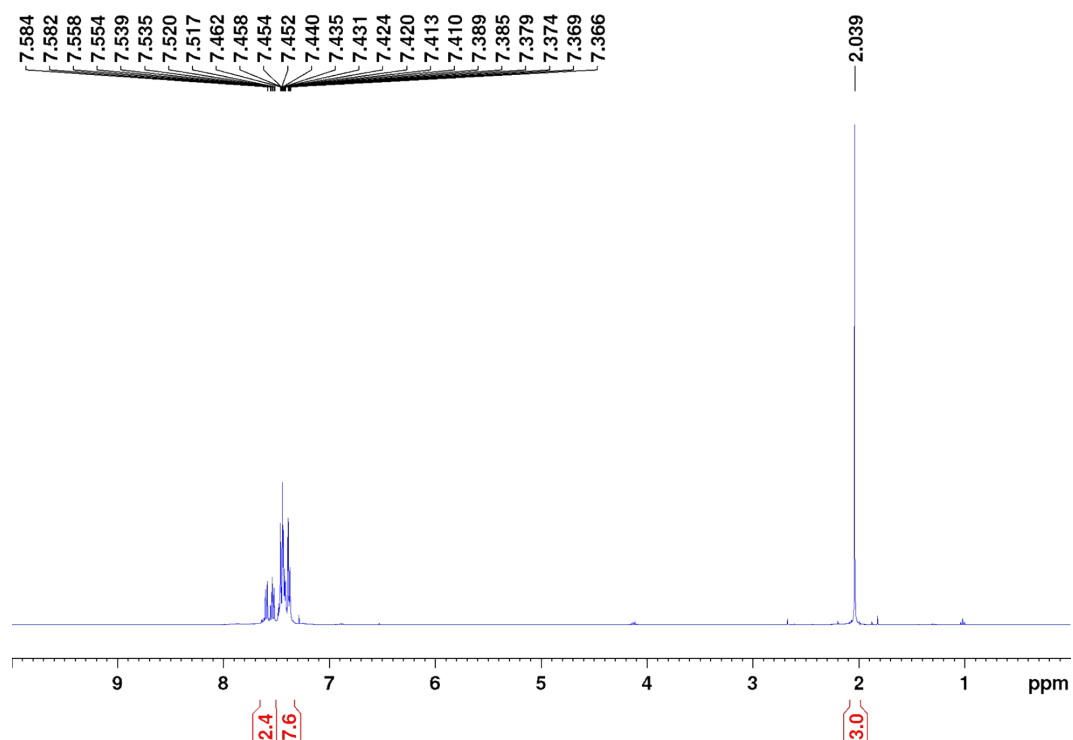


¹³C{¹H} NMR Spectrum (D229398)

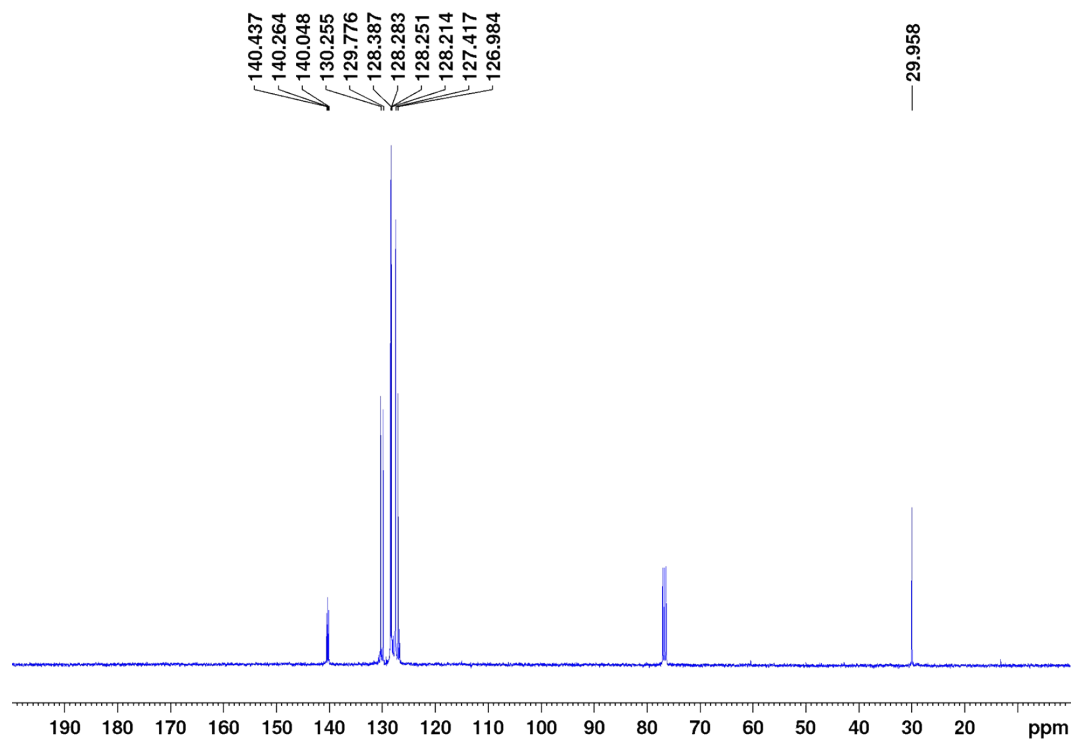


Compound 12

^1H NMR Spectrum (D234106)

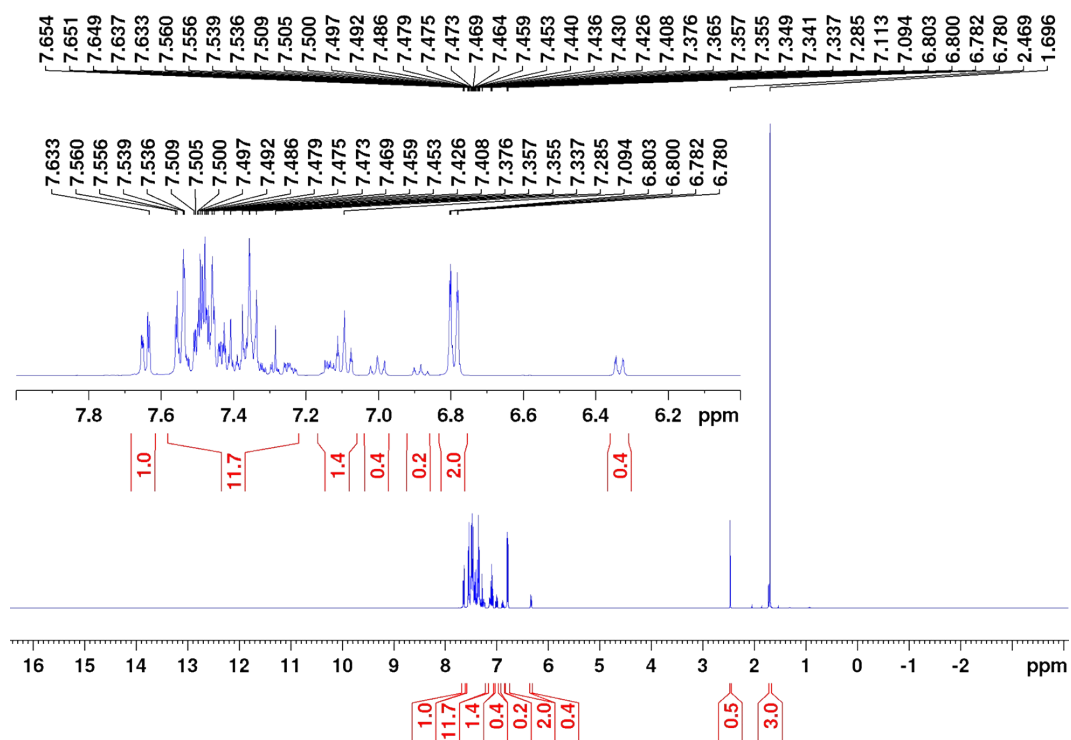


$^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum (D234106)

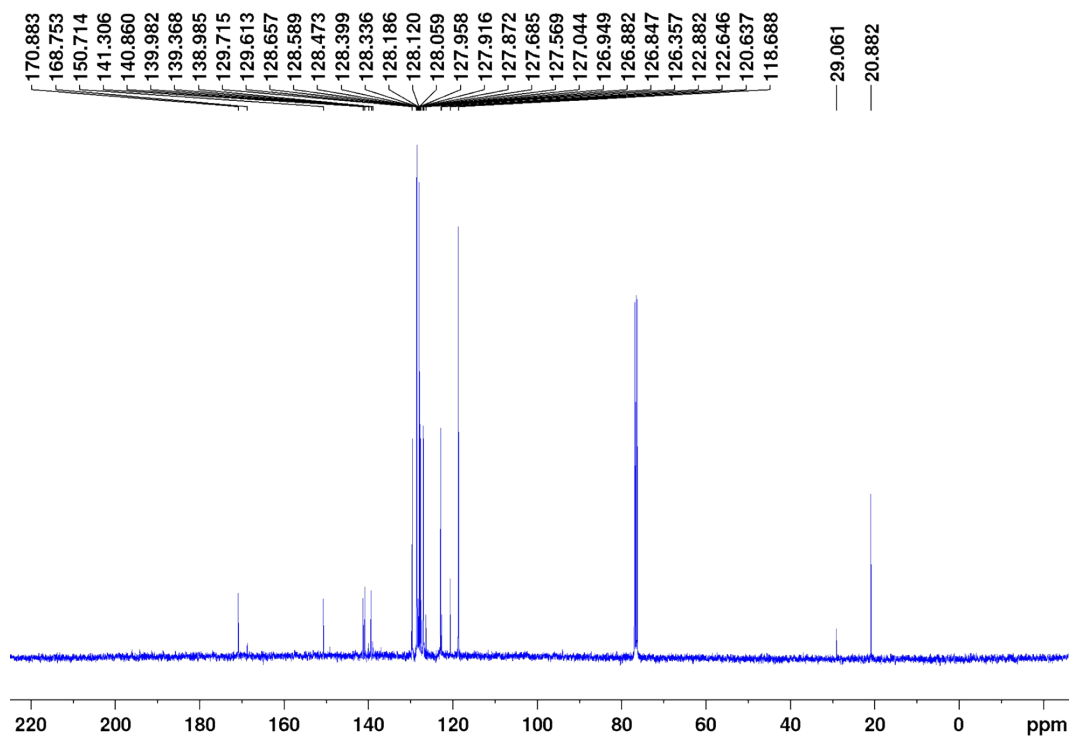


Compound 11

¹H NMR Spectrum (D234841)



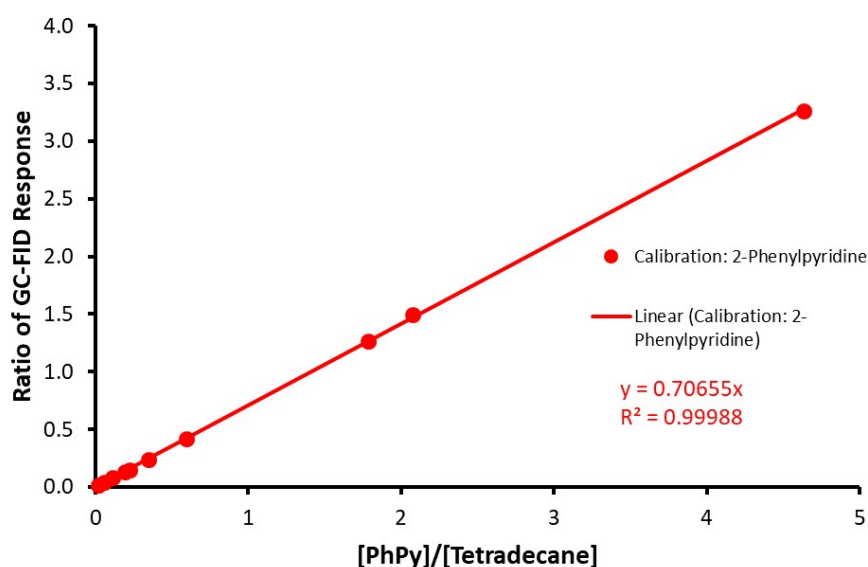
¹³C{¹H} NMR Spectrum (D229398)



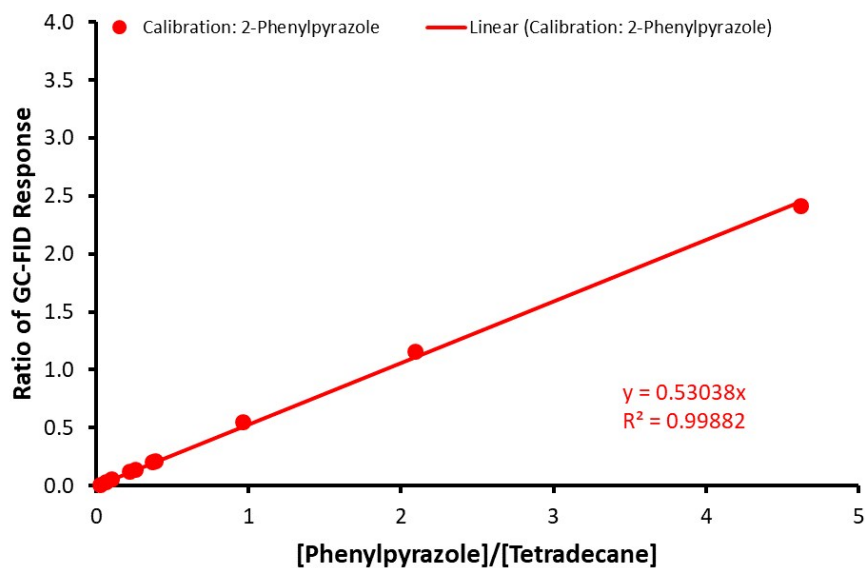
GC Calibration

All calibration carried out by analysing known ratios of analyte to tetradecane. A plot of the GC-FID response *versus* the ratio of concentrations gives a straight line in each case, where the gradient is the response factor.

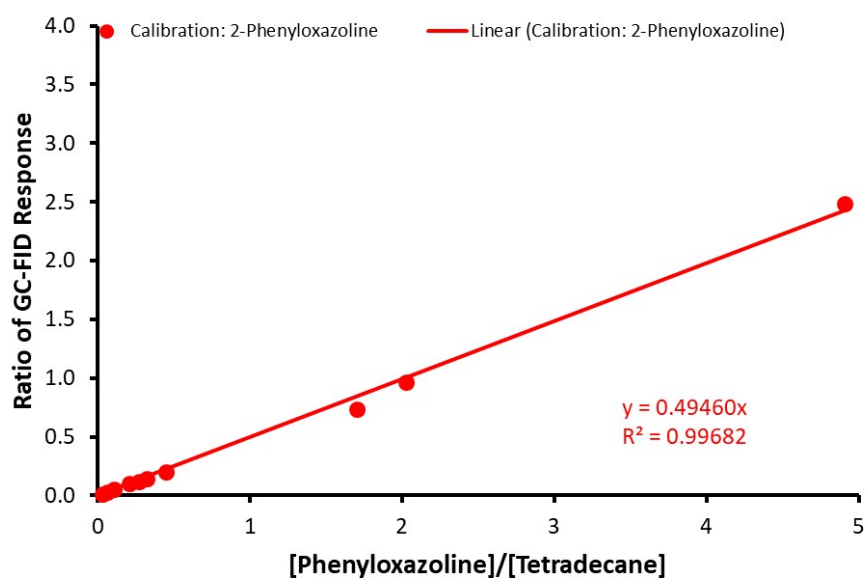
2-phenylpyridine (2)



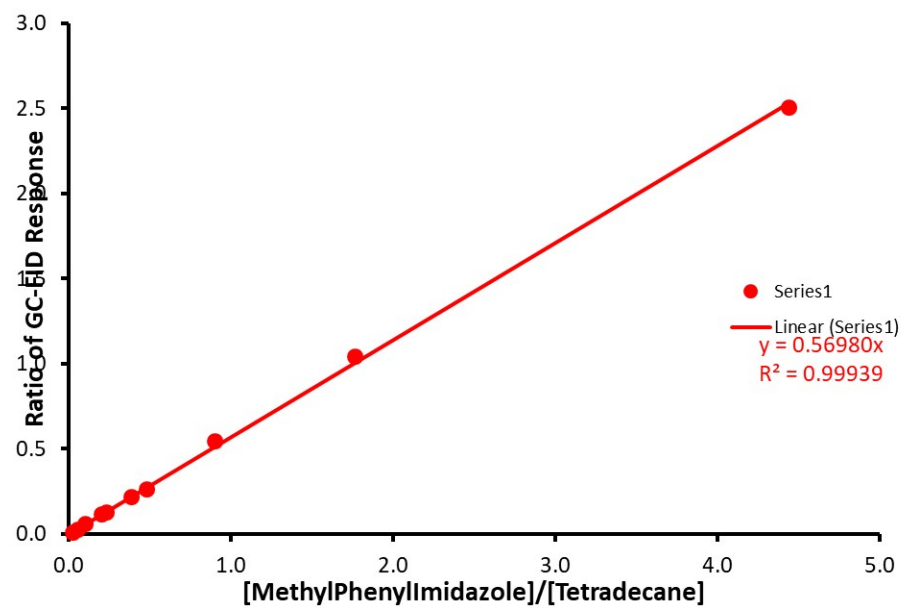
1-phenylpyrazole (3)



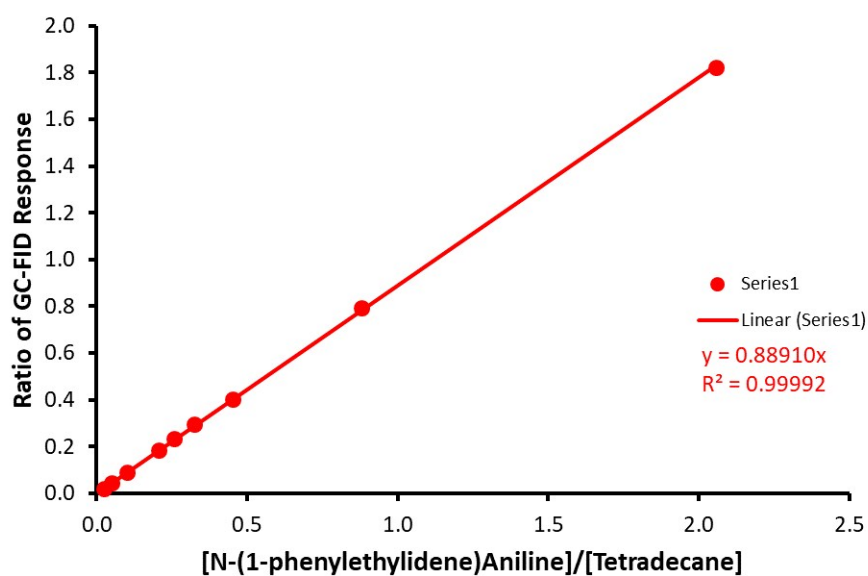
2-phenyloxazoline (4)



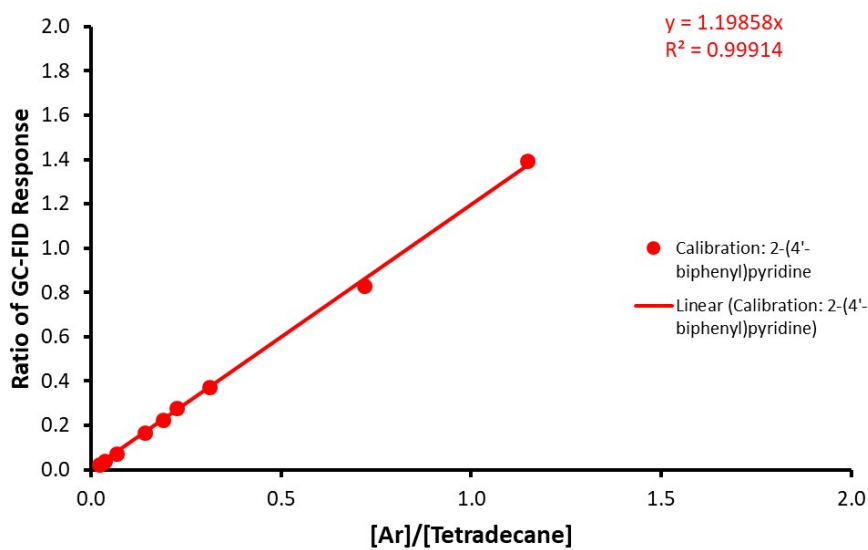
N-methyl-2-phenylimidazole (5)



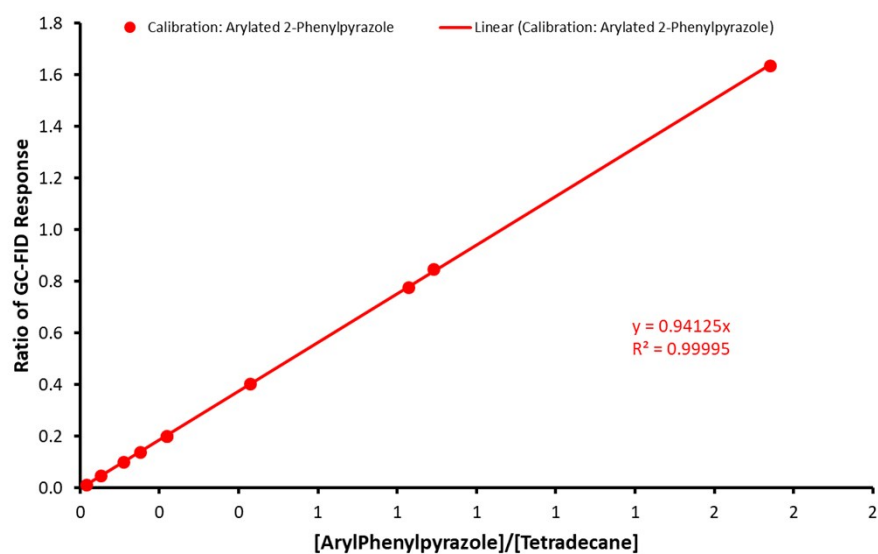
***N*-(1-phenylethylidene)aniline (6)**



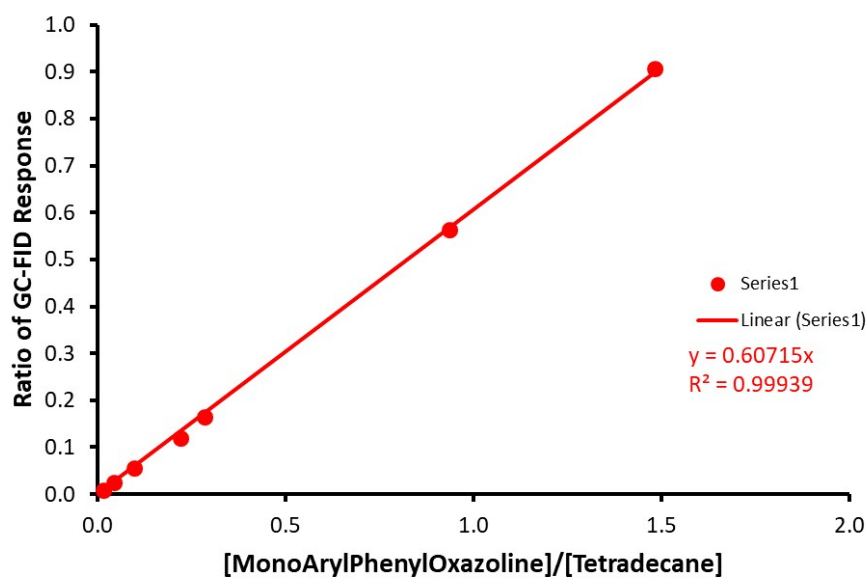
2-([1,1'-biphenyl]-2-yl)pyridine (7)



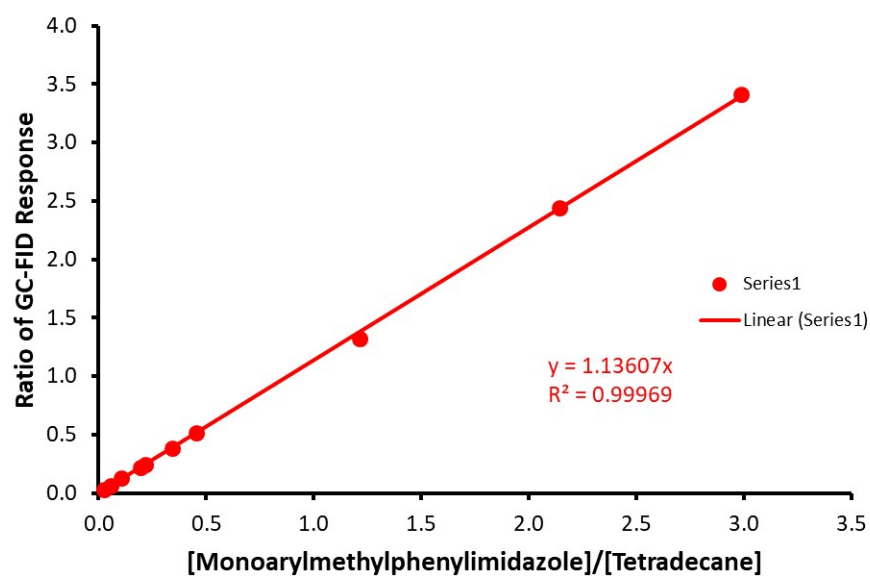
1-([1,1'-biphenyl]-2-yl)pyrazole (8)



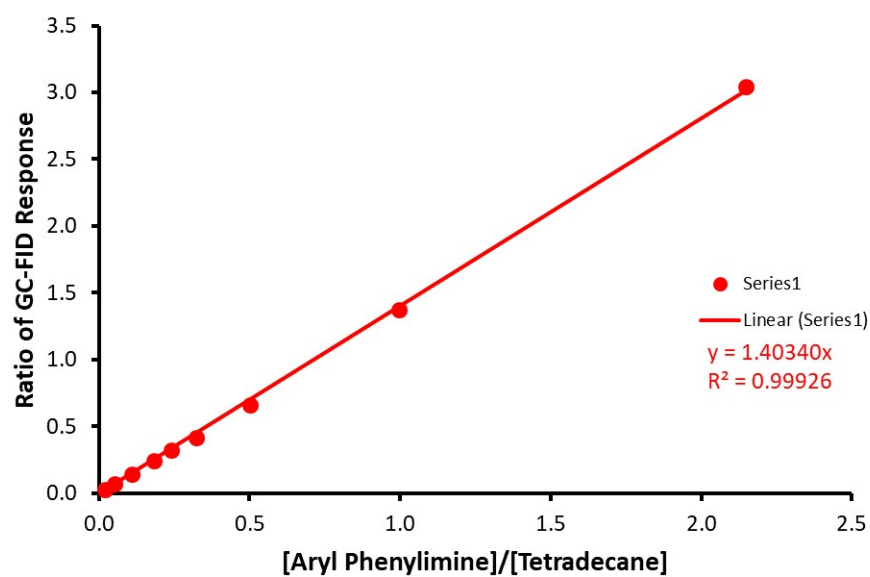
2-([1,1'-biphenyl]-2-yl)oxazoline (9)



2-([1,1'-biphenyl]-2-yl)-1-methyl-imidazole (10)



1-([1,1'-biphenyl]-2-yl)-*N*-phenylethan-1-imine (11)



Results from Competition Experiments

	Experimental Data and Calculations													
	GC Peak Areas				GC Peak Areas Corrected for Calibration				Competition Constants		Calculated from Solver		Errors	
2 vs 3	Substrate 2	Product 2	Substrate 3	Product 3	Substrate 2	Product 2	Substrate 3	Product 3	κ_{23} (expt'l)	$\log \kappa_{23}$ (expt'l)	$\log \kappa_{13}$ (calc'd)	κ_{13} (calc'd)	Δ (expt'l - calc'd)	$(\Delta \text{ (expt'l - calc'd)})^2$
	216.4	191.7	346.4	161.4	306.2	159.9	653.1	171.5	1.803	0.256	0.406	2.547	-0.744	0.554
2 vs 4	Substrate 2	Product 2	Substrate 4	Product 4	Substrate 2	Product 2	Substrate 4	Product 4	κ_{24} (expt'l)	$\log \kappa_{24}$ (expt'l)	$\log \kappa_{14}$ (calc'd)	κ_{14} (calc'd)	Δ (expt'l - calc'd)	$(\Delta \text{ (expt'l - calc'd)})^2$
	385.7	599.7	772.8	21.3	545.8	500.4	869.2	15.2	37.513	1.574	1.531	33.996	3.517	12.368
3 vs 6	Substrate 3	Product 3	Substrate 6	Product 6	Substrate 3	Product 3	Substrate 6	Product 6	κ_{36} (expt'l)	$\log \kappa_{36}$ (expt'l)	$\log \kappa_{34}$ (calc'd)	κ_{34} (calc'd)	Δ (expt'l - calc'd)	$(\Delta \text{ (expt'l - calc'd)})^2$
	297.0	408.5	468.8	36.3	560.0	434.0	527.3	25.9	11.976	1.078	1.125	13.349	-1.374	1.887
2 vs 3	Substrate 2	Product 2	Substrate 3	Product 3	Substrate 2	Product 2	Substrate 3	Product 3	κ_{23} (expt'l)	$\log \kappa_{23}$ (expt'l)	$\log \kappa_{13}$ (calc'd)	κ_{13} (calc'd)	Δ (expt'l - calc'd)	$(\Delta \text{ (expt'l - calc'd)})^2$
	85.5	106.6	103.9	52.1	121.1	88.9	195.9	55.3	2.214	0.345	0.406	2.547	-0.333	0.111
2 vs 6	Substrate 2	Product 2	Substrate 6	Product 6	Substrate 2	Product 2	Substrate 6	Product 6	κ_{26} (expt'l)	$\log \kappa_{26}$ (expt'l)	$\log \kappa_{14}$ (calc'd)	κ_{14} (calc'd)	Δ (expt'l - calc'd)	$(\Delta \text{ (expt'l - calc'd)})^2$
	410.9	862.5	1365.6	54.9	581.6	719.6	1536.0	39.1	32.027	1.506	1.531	33.996	-1.969	3.877
3 vs 6	Substrate 3	Product 3	Substrate 6	Product 6	Substrate 3	Product 3	Substrate 6	Product 6	κ_{36} (expt'l)	$\log \kappa_{36}$ (expt'l)	$\log \kappa_{34}$ (calc'd)	κ_{34} (calc'd)	Δ (expt'l - calc'd)	$(\Delta \text{ (expt'l - calc'd)})^2$
	108.0	142.7	259.2	15.9	203.6	151.6	291.5	11.3	14.592	1.164	1.125	13.349	1.243	1.546
4 vs 6	Substrate 4	Product 4	Substrate 6	Product 6	Substrate 4	Product 4	Substrate 6	Product 6	κ_{46} (expt'l)	$\log \kappa_{46}$ (expt'l)	$\log \kappa_{24}$ (calc'd)	κ_{24} (calc'd)	Δ (expt'l - calc'd)	$(\Delta \text{ (expt'l - calc'd)})^2$
	70.6	38.2	428.2	81.5	142.8	62.8	481.6	58.1	3.201	0.505	0.761	5.771	-2.570	6.603
3 vs 5	Substrate 3	Product 3	Substrate 5	Product 5	Substrate 3	Product 3	Substrate 5	Product 5	κ_{35} (expt'l)	$\log \kappa_{35}$ (expt'l)	$\log \kappa_{35}$ (calc'd)	κ_{35} (calc'd)	Δ (expt'l - calc'd)	$(\Delta \text{ (expt'l - calc'd)})^2$
	110.8	74.3	99.8	77.6	208.8	78.9	175.1	68.3	0.974	-0.012	0.160	1.447	-0.474	0.224
5 vs 6	Substrate 5	Product 5	Substrate 6	Product 6	Substrate 5	Product 5	Substrate 6	Product 6	κ_{56} (expt'l)	$\log \kappa_{56}$ (expt'l)	$\log \kappa_{54}$ (calc'd)	κ_{54} (calc'd)	Δ (expt'l - calc'd)	$(\Delta \text{ (expt'l - calc'd)})^2$
	304.7	397.0	610.4	54.6	534.8	349.5	686.5	38.9	9.125	0.960	0.965	9.225	-0.100	0.010
3 vs 5	Substrate 3	Product 3	Substrate 5	Product 5	Substrate 3	Product 3	Substrate 5	Product 5	κ_{35} (expt'l)	$\log \kappa_{35}$ (expt'l)	$\log \kappa_{35}$ (calc'd)	κ_{35} (calc'd)	Δ (expt'l - calc'd)	$(\Delta \text{ (expt'l - calc'd)})^2$
	395.0	221.8	415.2	200.3	744.8	235.6	728.6	176.3	1.269	0.103	0.160	1.447	-0.178	0.032
5 vs 6	Substrate 5	Product 5	Substrate 6	Product 6	Substrate 5	Product 5	Substrate 6	Product 6	κ_{56} (expt'l)	$\log \kappa_{56}$ (expt'l)	$\log \kappa_{54}$ (calc'd)	κ_{54} (calc'd)	Δ (expt'l - calc'd)	$(\Delta \text{ (expt'l - calc'd)})^2$
	140.1	142.3	230.9	18.7	245.8	125.3	259.6	13.3	8.226	0.915	0.965	9.225	-0.999	0.998
4 vs 5	Substrate 4	Product 4	Substrate 5	Product 5	Substrate 4	Product 4	Substrate 5	Product 5	κ_{45} (expt'l)	$\log \kappa_{45}$ (expt'l)	$\log \kappa_{xy}$ (calc'd)	κ_{xy} (calc'd)	Δ (expt'l - calc'd)	$(\Delta \text{ (expt'l - calc'd)})^2$
	56.7	14.7	263.3	266.9	114.7	24.2	462.1	235.0	0.466	-0.332	-0.204	0.626	-0.160	0.025
2 vs 4	Substrate 2	Product 2	Substrate 4	Product 4	Substrate 2	Product 2	Substrate 4	Product 4	κ_{24} (expt'l)	$\log \kappa_{24}$ (expt'l)	$\log \kappa_{12}$ (calc'd)	κ_{12} (calc'd)	Δ (expt'l - calc'd)	$(\Delta \text{ (expt'l - calc'd)})^2$
	299.7	380.0	30.1	18.8	424.1	317.0	60.8	30.9	1.357	0.133	0.770	5.891	-4.534	20.557
4 vs 3	Substrate 4	Product 4	Substrate 3	Product 3	Substrate 4	Product 4	Substrate 3	Product 3	κ_{43} (expt'l)	$\log \kappa_{43}$ (expt'l)	$\log \kappa_{xy}$ (calc'd)	κ_{xy} (calc'd)	Δ (expt'l - calc'd)	$(\Delta \text{ (expt'l - calc'd)})^2$
	81.3	24.0	385.9	321.8	164.4	39.5	727.7	341.9	0.559	-0.253	-0.364	0.432	0.127	0.016
4 vs 3	Substrate 4	Product 4	Substrate 3	Product 3	Substrate 4	Product 4	Substrate 3	Product 3	κ_{43} (expt'l)	$\log \kappa_{43}$ (expt'l)	$\log \kappa_{xy}$ (calc'd)	κ_{xy} (calc'd)	Δ (expt'l - calc'd)	$(\Delta \text{ (expt'l - calc'd)})^2$
	84.5	23.5	319.4	334.2	170.8	38.8	602.2	355.0	0.441	-0.355	-0.364	0.432	0.009	0.000
2 vs 4	Substrate 2	Product 2	Substrate 4	Product 4	Substrate 2	Product 2	Substrate 4	Product 4	κ_{24} (expt'l)	$\log \kappa_{24}$ (expt'l)	$\log \kappa_{12}$ (calc'd)	κ_{12} (calc'd)	Δ (expt'l - calc'd)	$(\Delta \text{ (expt'l - calc'd)})^2$
	43.7	71.8	28.2	7.4	61.8	59.9	56.9	12.2	3.484	0.542	0.770	5.891	-2.407	5.792
2 vs 5	Substrate 2	Product 2	Substrate 5	Product 5	Substrate 2	Product 2	Substrate 5	Product 5	κ_{25} (expt'l)	$\log \kappa_{25}$ (expt'l)	$\log \kappa_{xy}$ (calc'd)	κ_{xy} (calc'd)	Δ (expt'l - calc'd)	$(\Delta \text{ (expt'l - calc'd)})^2$
	131.3	140.9	145.4	65.3	185.9	117.5	255.2	57.5	2.412	0.382	0.566	3.685	-1.274	1.622
4 vs 5	Substrate 4	Product 4	Substrate 5	Product 5	Substrate 4	Product 4	Substrate 5	Product 5	κ_{45} (expt'l)	$\log \kappa_{45}$ (expt'l)	$\log \kappa_{xy}$ (calc'd)	κ_{xy} (calc'd)	Δ (expt'l - calc'd)	$(\Delta \text{ (expt'l - calc'd)})^2$
	62.9	17.1	402.8	444.5	127.2	28.1	706.8	391.3	0.454	-0.343	-0.204	0.626	-0.172	0.030
2 vs 5	Substrate 2	Product 2	Substrate 5	Product 5	Substrate 2	Product 2	Substrate 5	Product 5	κ_{25} (expt'l)	$\log \kappa_{25}$ (expt'l)	$\log \kappa_{xy}$ (calc'd)	κ_{xy} (calc'd)	Δ (expt'l - calc'd)	$(\Delta \text{ (expt'l - calc'd)})^2$
	276.1	358.3	344.5	173.8	390.8	298.9	604.6	152.9	2.519	0.401	0.566	3.685	-1.166	1.359
4 vs 6	Substrate 4	Product 4	Substrate 6	Product 6	Substrate 4	Product 4	Substrate 6	Product 6	κ_{46} (expt'l)	$\log \kappa_{46}$ (expt'l)	$\log \kappa_{xy}$ (calc'd)	κ_{xy} (calc'd)	Δ (expt'l - calc'd)	$(\Delta \text{ (expt'l - calc'd)})^2$
	191.2	43.0	934.0	206.6	386.6	70.7	1050.5	147.2	1.282	0.108	0.761	5.771	-4.489	20.154

Table S1: Coordinate data sets and absolute energies (in a.u.) for DFT optimized complexes with selected distances (in Å).

A	B
Zero-point correction= 0.307941 (Hartree/Particle) Thermal correction to Energy= 0.330104 Thermal correction to Enthalpy= 0.331048 Thermal correction to Gibbs Free Energy= 0.256082 Sum of electronic and zero-point Energies= -940.691754 Sum of electronic and thermal Energies= -940.669591 Sum of electronic and thermal Enthalpies= -940.668647 Sum of electronic and thermal Free Energies= -940.743614 Solvent Energy = -1420.286397	Zero-point correction= 0.475601 (Hartree/Particle) Thermal correction to Energy= 0.507851 Thermal correction to Enthalpy= 0.508795 Thermal correction to Gibbs Free Energy= 0.412837 Sum of electronic and zero-point Energies= -1419.566528 Sum of electronic and thermal Energies= -1419.534277 Sum of electronic and thermal Enthalpies= -1419.533333 Sum of electronic and thermal Free Energies= -1419.629291 Solvent Energy = -1420.286397
C 1.846838 -1.523994 1.258112 Ru 0.179887 -0.273039 -0.170438 C -1.973381 0.130783 -0.046386 C -1.748176 -1.285520 -0.264713 C -0.945595 -1.754081 -1.344063 C -0.285842 -0.813610 -2.224399 C -0.540654 0.586072 -2.046991 C -1.377320 1.043562 -0.969716 H -2.118549 -2.013164 0.473169 H -0.719815 -2.828621 -1.428255 H 0.012266 1.333269 -2.632629 H -1.429760 2.125866 -0.782035 C 0.697200 -1.299699 -3.256872 H 1.405822 -0.496754 -3.537740 H 1.280446 -2.159353 -2.871596 H 0.158325 -1.626568 -4.172509 C -2.787312 0.643728 1.133392 C -2.459908 1.694236 1.297578 C -2.534811 -0.134198 2.436723 H -1.451405 -0.207851 2.658680 H -3.039743 0.371059 3.285447 H -2.944771 -1.165509 2.385999 C -4.283532 0.658571 0.753828 H -4.893143 1.080264 1.580074 H -4.467867 1.265238 -0.156689 H -4.648857 -0.372124 0.555439 O 0.904928 2.882248 -0.931837 O 1.412776 1.199027 0.523180 C 1.530703 2.415797 0.024674 C 2.585538 3.228680 0.778315 H 2.594702 4.272002 0.412617 H 2.382680 3.204737 1.868006 H 3.584467 2.771542 0.622214 C 2.926628 -2.094263 2.134886 H 3.555373 -2.804356 1.565107 H 3.569641 -1.258271 2.481233 H 2.486541 -2.585020 3.023596 O 0.739309 -1.106627 1.750006 O 2.013841 -1.399384 -0.007493	C -0.785443 -1.143208 2.526340 Ru -0.454416 0.018271 -0.251390 C 0.381210 -0.493310 -2.247192 C -0.843923 0.238786 -2.413711 C -2.026855 -0.206196 -1.750378 C -2.059007 -1.386939 -0.932934 C -0.811098 -2.078416 -0.750509 C 0.387990 -1.672825 -1.424035 H -0.861358 1.189496 -2.965313 H -2.916515 0.436374 -1.814318 H -0.774931 -2.901708 -0.021800 H 1.331692 -2.207834 -1.242654 C -3.358842 -1.870225 -0.307431 H -3.081784 -2.643375 0.435309 C 1.637583 0.004053 -2.915151 H 2.531139 -0.539182 -2.558150 C -0.464529 -0.940856 4.009660 H -0.825508 -1.803102 4.601059 H 0.620662 -0.783889 4.171921 H -0.983749 -0.022948 4.356075 O -0.077628 -0.341270 1.762328 O -1.627479 -1.967126 2.153886 C 2.465022 1.121687 0.351055 C 0.802744 2.701209 -0.152305 N 1.162883 1.399089 0.020128 C -4.108252 -0.762150 0.450402 H -4.430679 0.060106 -0.224118 H -5.021154 -1.176370 0.925897 H -3.457452 -0.335157 1.236881 C -4.232918 -2.511655 -1.407098 H -3.697645 -3.332030 -1.929881 H -5.162656 -2.932883 -0.970282 H -4.529344 -1.760652 -2.171416 H 1.784173 1.087577 -2.728588 H 1.553157 -0.138882 -4.013301 O -1.635194 1.425179 0.747867 O -2.374296 2.335620 0.164219 O -2.321333 2.663224 -1.034536 C -3.341787 3.003515 1.140571 H -2.789165 3.391176 2.020008 H -3.889814 3.823473 0.640699 H -4.059335 2.245582 1.516981 C 3.037377 -0.260668 0.305136 C 4.144649 -0.466012 -0.555006 C 2.575829 -1.343524 1.082834 C 4.741834 -1.731687 -0.672533 H 4.520887 0.372974 -1.162379 C 3.182872 -2.605339 0.973185 H 1.722704 -1.175827 1.752174 C 4.257434 -2.809769 0.089317 H 5.587752 -1.874597 -1.363377 H 2.806531 -3.438635 1.587607 H 4.723335 -3.804036 0.000156 C 1.667513 3.775871 0.079938 C 3.367958 2.174969 0.628483 C 2.972900 3.512394 0.515655 H 4.391380 1.913206 0.933905 H 3.677212 4.327751 0.743141 H 1.299771 4.800150 -0.078589 H -0.217872 2.873699 -0.524824

2 Pyridine:

TS-B-C	C
Zero-point correction= 0.473280 (Hartree/Particle) Thermal correction to Energy= 0.504666 Thermal correction to Enthalpy= 0.505611 Thermal correction to Gibbs Free Energy= 0.412923 Sum of electronic and zero-point Energies= -1419.529860 Sum of electronic and thermal Energies= -1419.498473 Sum of electronic and thermal Enthalpies= -1419.497529 Sum of electronic and thermal Free Energies= -1419.590217 Solvent Energy = -1420.2549957	Zero-point correction= 0.475077 (Hartree/Particle) Thermal correction to Energy= 0.507417 Thermal correction to Enthalpy= 0.508361 Thermal correction to Gibbs Free Energy= 0.411533 Sum of electronic and zero-point Energies= -1419.589096 Sum of electronic and thermal Energies= -1419.556755 Sum of electronic and thermal Enthalpies= -1419.555811 Sum of electronic and thermal Free Energies= -1419.652639 Solvent Energy = -1420.2989727
C -2.633790 2.041057 -1.430357 Ru 0.057068 -0.308341 0.398148 C 0.714558 -0.175413 2.483823 C 0.063641 -1.446280 2.216310 C -1.258949 -1.490585 1.674120 C -1.991061 -0.283344 1.365214 C -1.327489 0.958199 1.587996 C -0.011310 1.014380 2.176780 H 0.614896 -2.389175 2.360188 H -1.663742 -2.470880 1.386654 H -1.792593 1.868076 1.139363 H 0.493527 1.989237 2.259170 C -3.401232 -0.330205 0.798326 H -3.658774 0.716407 0.533862 C 2.137362 -0.124413 2.977092 H 2.633441 0.812872 2.656141 C -3.918421 2.056509 -2.281085 H -4.580565 1.235368 -1.929268 H -4.467386 3.011019 -2.161127 H -3.690544 1.864321 -3.348259 O -1.709089 1.253930 -1.801829 O -2.622636 2.780530 -0.389915 C 2.835431 0.095009 -0.665318 C 3.608057 -2.579899 -0.707960 C 2.334593 -2.182143 -0.285206 H 1.556144 -2.904171 0.011468	C -2.108215 -2.866796 0.719795 Ru 0.068484 0.642564 -0.420841 C 0.554549 2.127291 -1.945656 C -0.055413 2.900151 -0.876562 C -1.302188 2.531474 -0.343953 C -2.035690 1.394617 -0.874605 C -1.501945 0.710545 -2.002305 C -0.207232 1.061447 -2.530265 H 0.509357 3.726494 -0.416810 H -1.677889 3.051587 -0.547594 H -2.056019 -0.142207 -2.421261 H 0.231460 0.458871 -3.340660 C -3.420579 1.044126 -0.346554 H -3.680039 0.051633 -0.767896 C 1.935839 2.470743 -2.443754 H 2.397350 1.608473 -2.963754 C -2.346280 -4.358580 0.575467 H -3.330624 -4.546061 0.109079 H -1.549136 -4.762425 -0.084744 H -2.263857 -4.876385 1.551000 O -1.131124 -2.593414 1.585292 O -2.721071 -2.021235 0.070834 C 3.755726 1.698074 1.636631 C 2.467019 1.703505 1.093440 H 1.769320 2.536653 1.252399 N 1.977620 0.658127 0.383335

N	1.968324	-0.876922	-0.248764
C	-3.523281	-1.187443	-0.472806
H	-3.236358	-2.245135	-0.289365
H	-4.575099	-1.186556	-0.825939
H	-2.876004	-0.767935	-1.268314
C	-4.359213	-0.802391	1.913789
H	-4.284346	-0.164265	2.818963
H	-5.409294	-0.768094	1.556519
H	-4.140119	-1.850615	2.213249
H	2.723850	-0.979619	2.585042
H	2.165023	-0.171882	4.086575
O	-0.419490	-1.348613	-1.316496
C	-0.672759	-2.633693	-1.364884
C	-0.537735	-3.439132	-0.427256
C	-1.184931	-3.061423	-2.735589
H	-0.556332	-2.627916	-3.537972
H	-1.211743	-4.164220	-2.808636
H	-2.207940	-2.653606	-2.871652
H	3.863734	-3.649348	-0.713864
C	2.335007	1.475312	-0.579666
C	3.210652	2.555248	-0.322849
C	0.931537	1.716255	-0.638090
C	2.705748	3.847943	-0.117582
H	4.293857	2.374173	-0.238289
C	0.431312	3.018934	-0.424589
C	0.129876	1.050029	-1.136213
C	1.315717	4.075616	-0.160440
H	3.399624	4.677204	0.093053
H	-0.670077	3.163036	-0.452835
H	0.917351	5.088726	0.009609
C	4.125801	-0.255748	-1.117960
C	4.520881	-1.598305	-1.131825
H	5.525046	-1.878530	-1.485966
H	4.799717	0.534164	-1.478817

C	-3.501491	0.913127	1.181861
H	-3.124429	1.814058	1.709325
H	-4.555393	0.756740	1.491467
H	-2.912577	0.037254	1.505857
C	-4.415665	2.096340	-0.886524
H	-4.375915	2.167853	-1.993627
H	-5.453740	1.832642	-0.594978
H	-4.195020	3.104548	-0.473881
H	2.599772	2.757021	-1.602443
H	1.897522	3.326725	-3.151658
O	-0.434867	-0.106338	1.489436
C	-0.467503	0.700003	2.538772
O	-0.236111	1.911373	2.501684
C	-0.858402	-0.024884	3.822911
H	-0.236529	-0.930940	3.965291
H	-0.757001	0.653149	4.689745
H	-1.911865	-0.364898	3.742630
H	4.109560	2.574103	2.199029
C	2.045221	-1.545475	-0.498984
C	2.629301	-2.798089	-0.804877
C	0.699212	-1.238530	-0.872535
C	1.889292	-3.766951	-1.491048
H	3.666858	-3.018461	-0.505518
C	-0.026985	-2.242547	-1.555259
H	-0.896135	-1.592077	1.542071
C	0.558309	-3.482423	-1.863357
H	2.340599	-4.741539	-1.733679
H	-1.080959	-2.073425	-1.817887
H	-0.033588	-4.242266	-2.400832
C	2.732255	-0.481088	0.225594
C	4.558513	0.554698	1.461748
C	4.037377	-0.538908	0.764140
H	5.576389	0.513655	1.879943
H	4.631145	-1.454791	0.635164

D	TS-D-E
Zero-point correction= 0.413130 (Hartree/Particle) Thermal correction to Energy= 0.439738 Thermal correction to Enthalpy= 0.440682 Thermal correction to Gibbs Free Energy= 0.356739 Sum of electronic and zero-point Energies= -1190.688392 Sum of electronic and thermal Energies= -1190.661785 Sum of electronic and thermal Enthalpies= -1190.660840 Sum of electronic and thermal Free Energies= -1190.744784 Solvent Energy = -1191.2333422	Zero-point correction= 0.501486 (Hartree/Particle) Thermal correction to Energy= 0.535164 Thermal correction to Enthalpy= 0.536108 Thermal correction to Gibbs Free Energy= 0.436136 Sum of electronic and zero-point Energies= -1882.146605 Sum of electronic and thermal Energies= -1882.112927 Sum of electronic and thermal Enthalpies= -1882.111983 Sum of electronic and thermal Free Energies= -1882.211955 Solvent Energy = -1882.9292131
Ru 0.288475 -0.126622 -0.326423 C 0.481167 -1.241036 -2.233738 C 1.305759 -1.969660 -1.297812 C 2.240086 -1.269891 -0.500135 C 2.491535 0.147583 -0.668348 C 1.740360 0.824318 -1.679315 C 0.750350 0.149779 -2.470956 H 1.108763 -3.031908 -1.095610 H 2.731808 -1.814510 0.319032 H 1.878708 1.909624 -1.810101 H 0.144391 0.714750 -3.195147 C 3.544986 0.883982 0.148205 H 3.339654 1.970932 0.017805 C -0.608575 -1.941718 -3.006364 H -1.452046 -1.254323 -3.215461 C -2.628319 0.238785 0.006199 N -1.670604 -0.745964 -0.075972 C 3.477550 0.577687 1.654551 H 3.722197 -0.484874 1.866567 H 4.214445 1.198475 2.205048 H 2.462201 0.772853 2.052238 C 4.944920 0.593019 -0.434358 H 5.003501 0.859951 -1.510073 H 5.726929 1.164697 0.108254 H 5.189520 -0.486988 -0.340904 H -1.004563 -2.812460 -2.448247 H -0.212909 -2.310830 -3.976822 O 0.340361 -0.221800 1.764538 C 0.466610 -1.394511 2.340387 O 0.545855 -2.491818 1.766194 C 0.545259 -1.277425 3.864235 H -0.275380 -0.638922 4.247582 H 0.504167 -2.279569 4.330018 H 1.500069 -0.783024 4.141334 C -2.076302 1.591680 0.021219 C -2.851846 2.767675 0.152083 C -0.647770 1.646944 -0.020022 C -2.221210 4.011988 0.275671 H -3.952660 2.712881 0.170922 C -0.039503 2.910397 0.150845 C -0.812070 4.077037 0.291003 H -2.821557 4.929534 0.376799 H 1.059592 2.989932 0.185202 H -0.311288 5.051666 0.415537 C -3.990074 -0.117500 0.126459 C -2.019416 -2.048194 0.055290 C -3.352918 -2.450651 0.183541 C -4.358210 -1.464828 0.200417 H -1.179637 -2.756700 0.098078 H -3.589144 -3.520171 0.280259 H -5.418823 -1.746287 0.293458 H -4.750551 0.674586 0.178452	Ru -0.067522 0.561269 -0.699079 C 0.733737 0.643702 -2.675012 C 1.924318 0.694543 -1.849311 C 2.024628 1.623003 -0.798747 C 0.974651 2.591603 -0.556532 C -0.136303 2.651861 -1.452595 C -0.279370 1.665653 -2.488567 H 2.698515 -0.087954 -1.900798 H 2.859992 1.474951 -0.097662 H -0.929903 3.397994 -1.293951 H -1.187025 1.653891 -3.112790 C 1.065774 3.630044 0.559473 C 0.042532 3.721007 0.991016 C 0.569808 -0.425359 -3.722722 H -0.499187 -0.604360 -3.951692 C -1.376792 -2.112405 -0.702240 N -0.140045 -1.512380 -0.672881 C 2.042279 3.269351 1.688148 H 3.093044 3.279465 1.330762 H 1.966248 4.012543 2.507923 H 1.845243 2.264145 2.107351 C 1.438718 4.996334 -0.063448 H 0.710187 5.315655 -0.836516 H 1.476425 5.781961 0.719585 H 2.439701 4.943177 -0.541321 H 1.022281 -1.378663 -3.385093 H 1.081854 -0.118821 -4.660545 C -2.482508 -1.150513 -0.707387 C -3.848899 -1.502689 -0.705751 C -2.072338 0.218054 -0.637186 C -4.831987 -0.505327 -0.627949 H -4.151285 -2.561225 -0.756360 C -3.084837 1.200085 -0.551430 C -4.446671 0.846493 -0.542937 H -5.898299 -0.780394 -0.629013 H -2.809669 2.263444 -0.466838 H -5.215071 1.633553 -0.469659 C -1.465360 -3.514917 -0.651370 C 0.991448 -2.241753 -0.551972 C 0.951377 -3.641623 -0.476293 C -0.293819 -4.285914 -0.544614 H 1.964540 -1.690813 -0.437828 H 1.921140 -4.143799 -0.331981 H -0.362487 -5.384861 -0.502375 H -2.454082 -3.995663 -0.675265 C -0.519338 -0.163832 2.384937 C -1.086684 1.111766 2.567663 C -1.307428 -1.326814 2.406457 C -2.475940 1.216315 2.745573 H -0.445359 2.003606 2.564022 C -2.695441 -1.199319 2.575871 H -0.837047 -2.308678 2.251787 C -3.283464 0.066680 2.741113 H -2.930214 2.211372 2.872175 H -3.324484 -2.102466 2.557507 H -4.374457 0.157336 2.849580 O 3.796913 -3.001172 0.488593 C 4.145465 -1.798139 0.552775 O 3.491926 -0.785497 0.100681 C 5.483625 -1.455739 1.249034 H 6.012319 -2.370630 1.579282 H 6.129378 -0.875162 0.557339 H 5.285088 -0.803845 2.126169 Cl 1.209339 -0.313497 2.047101

E	TS-E-F
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Zero-point correction= 0.502510 (Hartree/Particle) Thermal correction to Energy= 0.536347 Thermal correction to Enthalpy= 0.537292 Thermal correction to Gibbs Free Energy= 0.438009 Sum of electronic and zero-point Energies= -1882.173915 Sum of electronic and thermal Energies= -1882.140078 Sum of electronic and thermal Enthalpies= -1882.139134 Sum of electronic and thermal Free Energies= -1882.238417 Solvent Energy = -1882.9471578	Zero-point correction= 0.500728 (Hartree/Particle) Thermal correction to Energy= 0.534276 Thermal correction to Enthalpy= 0.535220 Thermal correction to Gibbs Free Energy= 0.437360 Sum of electronic and zero-point Energies= -1882.126186 Sum of electronic and thermal Energies= -1882.092638 Sum of electronic and thermal Enthalpies= -1882.091694 Sum of electronic and thermal Free Energies= -1882.189555 Solvent Energy = -1882.8889116
Ru -0.776675 -0.762770 -0.317520	Ru -0.048789 -0.090854 -0.467413
C -1.640924 -1.563723 -2.129978	C -0.406307 0.604851 -2.539847
C -2.238738 -0.250108 -1.973191	C -1.684132 0.788573 -1.882335
C -2.888222 0.130631 -0.781897	C -2.350624 -0.286407 -1.274171
C -2.945651 -0.788243 0.332712	C -1.746446 -1.599201 -1.210126
C -2.463890 -2.128172 0.167983	C -0.526415 -1.820124 -1.920226
C -1.799593 -2.504407 -1.049935	C 0.118876 -0.729846 -2.585227
H -2.095060 0.514181 -2.752817	H -2.145962 1.784027 -1.763431
H -3.136834 1.199595 -0.673279	H -3.260050 -0.047587 -0.654500
H -2.526531 -2.843418 1.001946	H -0.053274 -2.810413 -1.944655
H -1.336675 -3.500954 -1.129620	H 1.083596 -0.906489 -3.086298
C -3.554827 -0.380005 1.672577	C -2.458610 -2.706303 -0.434324
H -2.857863 -0.753414 2.457764	C -2.246401 -2.498645 0.641564
C -0.870160 -1.921791 -3.374723	C 0.318078 1.754397 -3.187344
H -0.117113 -2.705764 -3.161494	H 1.414330 1.589789 -3.180631
C 2.052549 -0.420329 -1.174887	C 1.875210 2.124272 -0.024093
N 0.814487 0.175522 -1.276480	N 0.539938 1.811444 0.090659
C -3.713223 1.138360 1.846208	C -3.992159 -2.610431 -0.600354
H -4.496029 1.541652 1.170662	H -4.280574 -2.663404 -1.672152
H -4.017043 1.372890 2.886492	H -4.474033 -3.461440 -0.076704
H -2.780994 1.692024 1.625317	H -4.391036 -1.673918 -0.163062
C -4.912132 -1.096550 1.857129	C -1.949200 -4.117355 -0.773612
H -4.814589 -2.200432 1.807374	H -0.866422 -4.253801 -0.570466
H -5.355569 -0.835683 2.840245	H -2.488687 -4.870748 -0.165264
H -5.626997 -0.782316 1.067431	H -2.124897 -4.359768 -1.843633
H -0.338648 -1.034413 -3.773080	H 0.100739 2.700869 -2.654194
H -1.553546 -2.295856 -4.167319	H -0.009973 1.874902 -4.241782
C 2.049217 -1.637457 -0.358389	C 2.706528 0.988200 -0.407587
C 3.198327 -2.404300 -0.064855	C 4.117003 1.018943 -0.512346
C 0.787156 -1.954211 0.229806	C 1.990866 -0.227049 -0.602775
C 3.116694 -3.479937 0.830356	C 4.823815 -0.153507 -0.802671
H 4.168683 -2.147094 -0.518592	H 4.665386 1.960860 -0.351726
C 0.733401 -0.033869 1.138431	C 2.722286 -1.399309 -0.882295
C 1.883423 -3.787379 1.439963	C 4.122392 -1.364353 -0.980834
H 4.013947 -4.074889 1.061879	H 5.921865 -0.131963 -0.878749
H -0.218537 -3.283671 1.634554	H 2.193868 -2.359573 -0.988199
H 1.817828 -4.622944 2.156239	H 4.675859 -2.293968 -1.190455
C 3.169803 0.189485 -1.768112	C 2.316189 3.434637 0.248313
C 0.662329 1.368464 -1.895662	C -0.363564 2.751577 0.461178
C 1.757922 2.022172 -2.481500	C 0.036222 4.065662 0.738972
C 3.020668 1.417944 -2.434223	C 1.393094 4.414873 0.632709
H -0.345851 1.839093 -1.860786	H -1.448380 2.471425 0.494734
H 1.590311 3.014833 -2.921209	H -0.735710 4.793738 1.027431
H 3.896707 1.908867 -2.886610	H 1.730380 5.441903 0.843449
H 4.156881 -0.284964 -1.678064	H 3.385246 3.672435 0.154474
C 1.541195 1.043568 1.668838	C 0.731781 -1.159082 1.494730
C 2.377635 0.078215 2.245150	C 0.690833 -2.568673 1.436151
C 1.998152 2.227352 1.079747	C 1.753956 -0.507936 2.227378
C 3.762279 0.316277 2.219135	C 1.743906 -3.310166 1.996718
H 1.963357 -0.850388 2.662201	H -0.142315 -3.077722 0.939029
C 3.389628 2.436765 1.072831	C 2.791940 -1.265246 2.783582
H 1.293250 2.943616 0.598163	H 1.739741 0.586109 2.330495
C 4.267651 1.490514 1.632005	C 2.805110 -2.669081 2.661623
H 4.443617 -0.434473 2.648428	H 1.723682 -4.409041 1.912502
H 3.783342 3.353118 0.605521	H 3.601009 -0.746642 3.322257
H 5.354868 1.666512 1.608542	H 3.624436 -3.258375 3.100599
O 0.054614 3.781746 -0.528035	O -3.211479 2.326979 0.172974
C -1.184938 3.559940 -0.371430	C -3.846619 1.578782 0.990009
O -1.897083 2.783849 -1.086190	O -4.273610 0.410449 0.749749
C -1.861996 4.259818 0.826176	C -4.051445 2.136052 2.412208
H -1.528340 3.753787 1.758602	H -3.080069 2.075366 2.950977
H -1.526762 5.314265 0.896763	H -4.340066 3.206127 2.374246
H -2.967093 4.210715 0.768146	H -4.802939 1.551579 2.977633
Cl -0.223123 0.715285 1.628532	Cl -1.106875 -0.204005 1.772109

F_{py}	TS-F-G
Zero-point correction= 0.501831 (Hartree/Particle) Thermal correction to Energy= 0.535872 Thermal correction to Enthalpy= 0.536816 Thermal correction to Gibbs Free Energy= 0.437204 Sum of electronic and zero-point Energies= -1882.149857 Sum of electronic and thermal Energies= -1882.115817 Sum of electronic and thermal Enthalpies= -1882.114872 Sum of electronic and thermal Free Energies= -1882.214484 Solvent Energy = -1882.920619	Zero-point correction= 0.500827 (Hartree/Particle) Thermal correction to Energy= 0.534372 Thermal correction to Enthalpy= 0.535316 Thermal correction to Gibbs Free Energy= 0.436700 Sum of electronic and zero-point Energies= -1882.144618 Sum of electronic and thermal Energies= -1882.111073 Sum of electronic and thermal Enthalpies= -1882.110128 Sum of electronic and thermal Free Energies= -1882.208745 Solvent Energy = -1882.9169761
Ru 0.063936 0.157750 -0.319286	Ru 0.026912 -0.207292 -0.325662
C 0.339104 -0.641372 -2.442781	C -0.221216 0.461155 -2.451996
C 1.625396 -0.635393 -1.806467	C -1.508120 0.639251 -1.825451
C 2.137259 0.541149 -1.221330	C -2.135780 -0.433835 -1.166376
C 1.394557 1.785333 -1.205496	C -1.564402 -1.769617 -1.122386
C 0.168504 1.805882 -1.938188	C -0.341961 -1.971398 -1.813273
C -0.329768 0.620958 -2.555221	C 0.303622 -0.872493 -2.469177
H 2.239835 -1.544467 -1.631086	H -2.011695 1.619838 -1.709868
H 3.128745 0.408791 -0.686485	H -3.100591 -0.187569 -0.614519
H -0.422192 2.727907 -2.025883	H 0.141515 -2.958021 -1.836195
H -1.299781 0.661598 -3.073716	H 1.278803 -1.043201 -2.949573
C 1.937575 3.002759 -0.461561	C -2.311140 -2.841097 -0.353196
H 1.513279 2.922032 0.567950	H -2.336386 -2.458143 0.694713
C -0.264933 -1.897518 -3.008410	C 0.516504 1.605191 -3.093672
H -1.370844 -1.874510 -2.932269	H 1.610424 1.429207 -3.089520
C -1.623185 -2.323020 0.260063	C 1.734841 2.159837 0.217932
N -0.355817 -1.797975 0.334020	N 0.432629 1.727433 0.289970
C 3.471223 2.957543 -0.319115	C -3.777030 -2.920542 -0.842703
H 3.965391 2.952690 -1.314552	H -3.827262 -3.203621 -1.916255
H 3.818005 3.858038 0.227367	H -4.317563 -3.695729 -0.261713
H 3.821822 2.063420 0.233024	H -4.310046 -1.959413 -0.694156
C 1.470703 4.335176 -1.076412	C -1.623063 -2.211245 -0.356822
H 0.369314 4.469374 -1.048682	H -0.602560 -4.164789 0.075173
H 1.906642 5.183023 -0.510902	H -2.203561 -4.926791 0.259516
H 1.800908 4.428308 -2.133319	H -1.556819 -4.637581 -1.381616
H 0.110373 -2.786652 -2.465520	H 0.310084 2.548875 -2.551434
H 0.008285 -2.010257 -4.079109	H 0.184643 1.737917 -4.145334
C -2.615278 -1.394083 -0.265081	C 2.664798 1.182639 -0.335393
C -3.983154 -1.712614 -0.452845	C 3.967583 1.524515 -0.770957
C -2.127143 -0.101595 -0.596452	C 2.173880 -0.155937 -0.489060
C -4.864885 -0.764247 -0.977243	C 4.786932 0.584772 -1.400790

H	-4.356320	-2.713868	-0.186774	H	4.324514	2.558999	-0.648808
C	-3.035170	0.845699	-1.115772	C	3.023717	-1.084535	-1.152112
C	-4.383808	0.518750	-1.313462	C	4.295334	-0.724094	-1.603063
H	-5.926899	-1.015403	-1.120699	H	5.794194	0.864185	-1.744323
H	-2.694014	1.868651	-1.335824	H	2.691187	-2.125570	-1.276972
H	-5.071471	1.278199	-1.718587	H	4.921107	-1.478544	-2.106096
C	-1.858538	-3.658751	0.642623	C	2.065161	3.464134	0.641802
C	0.689776	-2.579312	0.701009	C	-0.554975	2.562198	0.695236
C	0.502391	-3.918856	1.064840	C	-0.271314	3.875988	1.092083
C	-0.791435	-4.463587	1.058916	C	1.057867	4.327850	1.088629
H	1.720362	-2.164140	0.642914	H	-1.610003	2.210836	0.634807
H	1.390694	-4.506545	1.337322	H	-1.111569	4.518059	1.392413
H	-0.967712	-5.509243	1.355980	H	1.309454	5.347540	1.420026
H	-2.880846	-4.059073	0.595745	C	3.115129	3.787494	0.619803
C	-1.191879	1.291330	1.088571	C	1.455840	-1.085720	1.078078
C	-1.310986	2.688117	0.958546	C	1.545686	-2.500529	1.074637
C	-1.778765	0.668025	2.210595	C	1.829655	-0.402741	2.261608
C	-2.006961	3.443369	1.924588	C	1.984456	-3.201391	2.206664
H	-0.865766	3.221150	0.108573	H	1.266284	-3.069638	0.177436
C	-2.472500	1.419564	3.170794	C	2.280340	-1.104010	3.387689
H	-1.684542	-0.420007	2.346419	H	1.760325	0.692725	2.310901
C	-2.594495	2.815177	3.032353	C	2.359101	-2.508187	3.371772
H	-2.080010	4.536510	1.801585	H	2.025294	-4.302192	2.177023
H	-2.919151	0.907121	4.038354	H	2.562086	-0.543008	4.292989
H	-3.138603	3.405679	3.786060	H	2.705476	-3.058069	4.260578
O	3.439334	-2.142031	-0.078729	O	-3.307612	2.262252	-0.129369
C	4.252082	-1.347620	0.506335	C	-4.249237	1.569798	0.387050
O	4.522278	-0.161729	0.150180	O	-4.535342	0.367358	0.106029
C	4.911780	-1.864177	1.795975	C	-5.076321	2.248255	1.494430
H	4.195485	-1.699984	2.630572	H	-4.505943	2.173195	2.445784
H	5.111864	-2.952467	1.730835	H	-5.219445	3.325366	1.274449
H	5.841358	-1.308321	2.027399	H	-6.052758	1.745398	1.637237
Cl	1.314236	0.301601	1.647993	Cl	-1.245163	-0.309712	1.719558

G	H
Zero-point correction= 0.504987 (Hartree/Particle)	Zero-point correction= 0.259344 (Hartree/Particle)
Thermal correction to Energy= 0.538701	Thermal correction to Energy= 0.277868
Thermal correction to Enthalpy= 0.539645	Thermal correction to Enthalpy= 0.278812
Thermal correction to Gibbs Free Energy= 0.439933	Thermal correction to Gibbs Free Energy= 0.212554
Sum of electronic and zero-point Energies= -1882.226432	Sum of electronic and zero-point Energies= -1172.535890
Sum of electronic and thermal Energies= -1882.192718	Sum of electronic and thermal Energies= -1172.517366
Sum of electronic and thermal Enthalpies= -1882.191774	Sum of electronic and thermal Enthalpies= -1172.516422
Sum of electronic and thermal Free Energies= -1882.291486	Sum of electronic and thermal Free Energies= -1172.582680
Solvent Energy = -1883.008261	Solvent Energy = -1172.945173
Ru -0.950822 0.407892 -0.423374	Ru -0.335774 0.107697 0.109748
C -0.639515 0.713232 -2.615689	C -0.249665 2.271939 0.112414
C -2.025511 0.771515 -2.288706	C 0.036016 1.822174 -1.229191
C -2.669707 -0.304187 -1.581536	C 1.006437 0.796161 -1.440659
C -1.940506 -1.446105 -1.132511	C 1.800811 0.248629 -0.357223
C -0.530278 -1.507264 -1.453325	C 1.565567 0.778349 0.950850
C 0.086715 -0.466142 -2.199564	C 0.559450 1.773615 1.195714
H -2.596016 1.689492 -2.499000	H -0.601952 2.153089 -2.063390
H -3.704157 -0.174420 -1.236622	H 1.093822 0.342814 -2.441874
H 0.092555 -2.332841 -1.086881	H 2.053268 0.310406 1.818085
H 1.155256 -0.540940 -2.431088	H 0.323039 2.062351 2.230706
C -2.674184 -2.496444 -0.309593	C 2.783376 -0.879213 -0.636893
H -3.214311 -1.916945 0.472789	H 2.325149 -1.483541 -1.452263
C 0.044061 1.844620 -3.337300	C -1.405144 3.200883 0.376961
H 1.078221 1.982943 -2.970528	H -1.792295 3.067217 1.405710
C 2.075214 1.555028 0.098410	C 4.110372 -0.288962 -1.161859
N 0.732953 1.660016 0.342004	H 4.593538 0.338551 -0.382750
C -3.712186 -3.216748 -1.198362	H 4.818462 -1.098965 -1.434605
H -3.214016 -3.779072 -2.017761	H 3.954092 0.345920 -2.058969
H -4.295821 -3.942916 -0.595150	C 3.003712 -1.812058 0.564124
H -4.429796 -2.507386 -1.659029	H 2.036434 -2.150972 0.989773
C -1.747100 -3.497608 0.389973	H 3.588064 -2.701806 0.252620
H -1.027343 -2.966378 1.042214	H 3.581953 -1.311311 1.370150
H -2.343288 -4.184590 1.025031	H -2.235871 3.007234 -0.329587
H -1.190410 -4.124963 -0.340953	H -1.081016 4.257338 0.257667
H -0.507084 2.795090 -3.195109	O -2.487480 0.008391 -0.080930
H 0.099657 1.634784 -4.427832	O -2.392408 -1.051527 -0.796483
C 2.669889 0.463580 -0.733674	O -1.212391 -1.428657 -1.127709
C 3.252256 0.854708 -1.961254	C -3.605604 -1.849116 -1.181089
C 2.757579 -0.898038 -0.311536	H -3.789038 -2.598238 -0.382482
C 3.821824 -0.079992 -2.837941	H -4.494412 -1.194436 -1.255365
H 3.225016 1.920358 -2.239210	H -3.432155 -2.388783 -2.131219
C 3.337149 -1.822915 -1.217293	Cl -0.579152 -1.435216 1.886352
C 3.841586 -1.435126 -2.467079	
H 4.244864 0.247844 -3.799979	
H 3.431207 -2.874486 -0.906181	
H 4.282761 -2.189957 -3.136799	
C 2.992329 2.497353 0.620466	
C 0.331571 2.641430 1.194818	
C 1.195590 3.576981 1.772860	
C 2.560703 3.525113 1.464500	
H -0.755589 2.668050 1.368505	
H 0.780599 4.339170 2.448904	
H 3.275669 4.250731 1.883036	
H 4.057568 2.370737 0.377079	
C 2.327886 -1.385170 1.028283	
C 1.756629 -2.672359 1.170018	
C 2.538931 -0.624062 2.201691	
C 1.391742 -3.171018 2.427534	
H 1.565325 -3.287867 0.277401	
C 2.177120 -1.123147 3.460795	
H 3.009168 0.366287 2.135376	
C 1.596225 -2.395557 3.580636	
H 0.924090 -4.165009 2.503306	
H 2.345188 -0.505264 4.356654	
H 1.296748 -2.779542 4.568266	
O -2.161474 1.881170 0.444466	
C -3.361804 1.656131 0.951602	
C -4.063524 0.656075 0.788296	
C -3.817305 2.814572 1.843199	
H -3.340387 2.685411 2.837950	
H -3.493142 3.792832 1.436061	
H -4.915804 2.791221 1.971680	
Cl -0.891334 -0.433059 1.814920	

TS-E-F'

F'

Zero-point correction= 0.500931 (Hartree/Particle) Thermal correction to Energy= 0.534575 Thermal correction to Enthalpy= 0.535519 Thermal correction to Gibbs Free Energy= 0.437207 Sum of electronic and zero-point Energies= -1882.170174 Sum of electronic and thermal Energies= -1882.136530 Sum of electronic and thermal Enthalpies= -1882.135586 Sum of electronic and thermal Free Energies= -1882.233898 Solvent Energy = -1882.9140033	Zero-point correction= 0.502078 (Hartree/Particle) Thermal correction to Energy= 0.536595 Thermal correction to Enthalpy= 0.537539 Thermal correction to Gibbs Free Energy= 0.436466 Sum of electronic and zero-point Energies= -1882.171688 Sum of electronic and thermal Energies= -1882.137171 Sum of electronic and thermal Enthalpies= -1882.136227 Sum of electronic and thermal Free Energies= -1882.237300 Solvent Energy = -1882.920338
Ru 0.089692 0.333152 -0.182567 C -1.178438 -2.468570 1.371137 C -2.482472 -2.548275 0.869866 C -3.329866 -1.417203 0.821440 C -2.897809 -0.155090 1.242893 C -1.560380 -0.048674 1.730165 C -0.723037 -1.194163 1.811353 H -2.865753 -3.519812 0.515825 H -4.353814 -1.539851 0.434253 H -1.244143 0.889183 2.211891 H 0.231492 -1.128558 2.354621 C -3.812052 1.062320 1.214839 C -3.193121 1.932621 1.523035 C -0.280711 -3.675732 1.500805 H -0.677069 -4.546647 0.941751 C 2.481993 -1.257946 0.371985 N 1.354209 -1.236542 -0.424598 C -4.339151 1.357799 -0.203156 H -5.017108 0.551246 -0.557222 H -4.923134 2.301853 -0.208465 H -3.509446 1.464123 -0.929494 C -4.966115 0.910103 2.227789 H -4.585801 0.730179 3.254781 H -5.595739 1.824726 2.246686 H -5.623406 0.055645 1.957594 H -0.173693 -3.979530 2.565521 H 0.741202 -3.462245 1.125387 C 2.539724 -0.173494 1.347517 C 3.544716 -0.043231 2.336045 C 1.444859 0.747086 1.282589 C 3.470893 0.990904 3.276864 H 4.383479 -0.756948 2.379772 C 1.394738 1.777872 2.249380 C 2.388933 1.896703 3.235134 H 4.251055 1.092611 4.047292 H 0.572929 2.511748 2.208433 H 2.328298 2.709478 3.977880 C 3.427950 -2.294051 0.211681 C 1.152433 -2.206510 -1.351839 C 2.066259 -3.244663 -1.546193 C 3.227539 -3.289118 -0.749938 H 0.206042 -2.123474 -1.906461 H 1.860897 -4.009075 -2.309605 H 3.966347 -4.095295 -0.877939 H 4.321330 -2.307097 0.852151 C 1.011896 1.900368 -0.953424 C 2.216895 2.624739 -0.755686 C 0.680818 1.229344 -2.155030 C 3.213457 2.413058 -1.700923 H 2.385831 3.219833 0.152162 C 1.764861 0.983336 -3.066634 H -0.380157 1.132874 -2.536264 C 3.005125 1.561967 -2.834991 H 4.199709 2.882759 -1.553198 H 1.560918 0.433519 -3.999558 H 3.824202 1.426460 -3.558956 Cl -0.990584 2.644853 -0.108938 O -1.383356 -0.776291 -1.304471 C -2.127727 -0.430027 -2.310534 O -2.001296 0.607017 -2.994056 C -3.257691 -1.409704 -2.633171 H -3.447004 -1.433585 -3.723678 H -3.039140 -2.422381 -2.244003 H -4.179820 -1.040464 -2.138664	Ru -0.100763 0.114597 0.349920 C -0.209376 -2.416205 -1.736325 C 0.965465 -3.115977 -1.430550 C 2.218401 -2.470652 -1.406500 C 2.349349 -1.097391 -1.668433 C 1.161439 -0.357498 -1.913668 C -0.102472 -1.011008 -1.959591 H 0.912502 -4.196282 -1.219401 H 3.115359 -3.068524 -1.179844 H 1.230303 0.700020 -2.214940 H -0.972616 -0.468866 -2.357235 C 3.715796 -0.424423 -1.684934 C 3.539754 0.666963 -1.815209 C -1.534738 -3.121629 -1.890451 H -2.389756 -2.433219 -1.739490 C -3.032822 -0.251600 -0.069653 N -1.904952 -0.812434 0.466547 C 4.467702 -0.628059 -0.353369 H 4.747227 -1.692603 -0.208666 H 5.402567 -0.030414 -0.333150 H 3.837229 -0.334165 0.509582 C 4.556389 -0.902446 -2.887544 H 4.030858 -0.718738 -3.847154 H 5.535112 -0.376000 -2.919759 H 4.761648 -1.991975 -2.818722 H -1.635602 -3.958314 -1.170471 H -1.633083 -3.549909 -2.912481 C -2.752411 0.961929 -0.812512 C -3.711034 1.656000 -1.590449 C -1.373280 1.335552 -0.791286 C -3.306845 2.712459 -2.410439 H -4.770097 1.352544 -1.567621 C -0.997777 2.390461 -1.660872 C -1.939570 3.059660 -2.458140 H -4.043441 3.257476 -3.020777 H 0.051888 2.720776 -1.700692 H -1.605571 3.878314 -3.116518 C -4.272610 -0.910455 0.085105 C -1.948488 -1.979764 1.156000 C -3.153350 -2.669281 1.314593 C -4.334796 -2.122749 0.777579 H -0.992622 -2.361393 1.570209 H -3.150581 -3.619313 1.867423 H -5.298733 -2.640038 0.902957 H -5.176127 -0.456839 -0.345856 C 0.565892 2.029251 0.658508 C 1.948216 2.058208 0.391627 C -0.081672 3.175878 1.147324 C 2.677007 3.246841 0.619945 H 2.483717 1.173346 0.026554 C 0.649667 4.355276 1.360672 H -1.160620 3.140080 1.356096 C 2.032218 4.398085 1.095247 H 3.759553 3.253193 0.411801 H 0.130980 5.249947 1.741399 H 2.602580 5.325738 1.259785 O 0.741094 -2.817636 2.416383 C 1.440220 -1.827708 2.187203 O 1.324923 -1.135280 1.058465 C 2.488529 -1.299894 3.142732 H 2.106684 -0.333801 3.535845 H 2.651267 -2.007623 3.976549 H 3.440481 -1.095702 2.613323 Cl -0.657615 0.485073 2.646146

B'	TS-B'-C'
Zero-point correction= 0.266320 (Hartree/Particle) Thermal correction to Energy= 0.286937 Thermal correction to Enthalpy= 0.287882 Thermal correction to Gibbs Free Energy= 0.216084 Sum of electronic and zero-point Energies= -1030.509448 Sum of electronic and thermal Energies= -1030.488830 Sum of electronic and thermal Enthalpies= -1030.487886 Sum of electronic and thermal Free Energies= -1030.559684 Solvent Energy = -1030.943242	Zero-point correction= 0.265262 (Hartree/Particle) Thermal correction to Energy= 0.285310 Thermal correction to Enthalpy= 0.286254 Thermal correction to Gibbs Free Energy= 0.215774 Sum of electronic and zero-point Energies= -1030.476024 Sum of electronic and thermal Energies= -1030.455976 Sum of electronic and thermal Enthalpies= -1030.455032 Sum of electronic and thermal Free Energies= -1030.525512 Solvent Energy = -1030.916333
C -2.703358 -0.561110 -0.981928 Ru -0.354163 -0.345695 -0.135303 C -4.089103 -0.822157 -1.508960 H -4.843019 -0.362470 -0.842042 H -4.191386 -0.438865 -2.541776 H -4.264154 -1.918482 -1.524642 O -1.700148 -0.469061 -1.788140 O -2.472022 -0.456497 0.270862 C 1.890481 1.036090 -0.282036 C 2.481339 -1.009609 -1.310618 N 1.547722 -0.199449 -0.763786 O -0.267646 -2.443810 0.220564 C 0.236643 -2.237056 1.384805 O 0.461609 -1.016541 1.718536 C 0.504236 -3.370551 2.334532 H 0.786547 -4.282760 1.775011 H 1.294980 -3.091348 3.055969 H -0.426310 -3.588017 2.900228 C 0.630479 1.634690 0.247018 C 0.532289 2.218807 1.558860 C -0.464227 1.805277 -0.698819 C -0.628681 2.863353 1.947744 H 1.381322 2.109123 2.250457 C -1.633079 2.517814 -0.251102 H -0.273775 1.741577 -1.783159 C -1.728094 3.001346 1.041892 H -0.709063 3.277918 2.965093 H -2.451224 2.684131 -0.969744 H -2.640548 3.522061 1.371790 C 3.822664 -0.595136 -1.382613 C 3.206597 1.496709 -0.303505	C 3.051732 -0.432338 -0.557637 Ru 0.343835 0.342046 -0.005931 C 4.523563 -0.656876 -0.221698 H 5.120867 -0.735340 -1.149254 H 4.910916 0.156751 0.422795 H 4.622114 -1.605034 0.348396 O 2.597156 -0.681896 -1.691446 O 2.331988 -0.013014 0.448522 C -2.306969 -0.516806 -0.129479 C -3.712005 1.802689 -0.682836 C -2.311609 1.788719 -0.637075 H -1.700305 2.685434 -0.821119 N -1.624192 0.655311 -0.347595 O 0.933370 2.250157 -0.586634 C 0.885787 2.655631 0.634340 O 0.459105 1.781659 1.477097 C 1.323276 4.025858 1.045734 H 0.752168 4.360974 1.932452 H 2.398882 3.986362 1.318561 H 1.201638 4.736193 0.206141 H -4.235052 2.741981 -0.916566 C -1.379227 -1.642785 0.114903 C -1.681500 -2.709066 1.000308 C -0.117751 -1.665806 -0.594116 C -0.792784 -3.776576 1.154382 H -2.618392 -2.677051 1.578468 C 0.751622 -2.784440 -0.453072 H 0.060878 -0.998281 -1.510680 C 0.422433 -3.815517 0.426028 H -1.037397 -4.591443 1.853735 H 1.684690 -2.780931 -1.035331

C	4.194648	0.659312	-0.868841
H	3.447481	2.486599	0.111141
H	5.244927	0.986712	-0.907041
H	4.569839	-1.266775	-1.831357
H	2.132147	-1.992103	-1.663227

H	1.112730	-4.663124	0.559721
C	-3.707960	-0.562957	-0.150250
C	-4.424837	0.616963	-0.425853
H	-5.525017	0.607638	-0.450184
H	-4.223675	-1.516750	0.034602

C'	D'
Zero-point correction= 0.266269 (Hartree/Particle) Thermal correction to Energy= 0.287606 Thermal correction to Enthalpy= 0.288550 Thermal correction to Gibbs Free Energy= 0.213352 Sum of electronic and zero-point Energies= -1030.470370 Sum of electronic and thermal Energies= -1030.449034 Sum of electronic and thermal Enthalpies= -1030.448089 Sum of electronic and thermal Free Energies= -1030.523287 Solvent Energy = -1030.9146003	Zero-point correction= 0.204710 (Hartree/Particle) Thermal correction to Energy= 0.220055 Thermal correction to Enthalpy= 0.220999 Thermal correction to Gibbs Free Energy= 0.160449 Sum of electronic and zero-point Energies= -801.582156 Sum of electronic and thermal Energies= -801.566811 Sum of electronic and thermal Enthalpies= -801.565866 Sum of electronic and thermal Free Energies= -801.626416 Solvent Energy = -801.856988
C -0.978229 -1.064671 2.221754 Ru 0.968093 -0.242256 -1.148977 C -2.428189 -1.248149 2.622354 H -2.784605 -0.350872 3.158432 H -3.035987 -1.403062 1.706967 H -2.545461 -2.152276 3.253040 O -0.469815 -2.193433 1.676031 O -0.344715 -0.029054 2.351761 C -3.051013 -1.836628 -1.281673 C -1.659990 -1.709662 -1.350185 H -1.017767 -2.554288 -1.646294 N -1.013966 -0.548950 -1.064787 O 1.705977 -1.533482 0.238411 C 2.924474 -1.044862 0.199375 O 3.132949 -0.154683 -0.673719 C 3.940684 -1.508810 1.196569 H 3.808417 -2.586033 1.415211 H 4.961753 -1.303998 0.825349 H 3.783929 -0.947488 2.142503 H -3.518460 -2.801197 -1.527413 C -0.913288 1.674619 -0.233427 C -1.386924 2.931141 0.199903 C 0.498109 1.396884 -0.236240 C -0.485703 3.899875 0.663751 H -2.466074 3.155412 0.181274 C 1.389502 2.375691 0.266034 H 0.438976 -1.972662 1.322837 C 0.897802 3.616426 0.701165 H -0.857919 4.878397 1.004821 H 2.469317 2.160015 0.299182 H 1.600784 4.380174 1.072911 C -1.753785 0.548647 -0.637697 C -3.818524 -0.718833 -0.901356 C -3.156682 0.473409 -0.572136 H -4.916105 -0.781041 -0.847538 H -3.723751 1.355597 -0.241787	Ru -0.695904 0.619388 0.638403 C 3.103076 2.488174 -0.270410 C 1.755764 2.276166 0.039803 H 1.067972 3.117313 0.225138 N 1.208939 1.034964 0.139271 O -2.858521 0.244462 0.670413 C -2.909486 0.784906 -0.480196 O -1.784261 1.237471 -0.958604 C -4.162100 0.868898 -1.301908 H -5.048095 0.907828 -0.640606 H -4.130099 1.749353 -1.971488 H -4.236464 -0.042066 -1.933119 C 3.488792 3.516281 -0.333416 C 1.264327 -1.333650 -0.060833 C 1.818746 -2.617750 -0.254067 C -0.149734 -1.180177 0.167189 C 0.990649 -3.749930 -0.258270 H 2.904404 -2.738152 -0.404232 C -0.971386 -2.335328 0.132268 C -0.401853 -3.603168 -0.070721 H 1.426095 -4.749719 -0.410567 H -2.057656 -2.230722 0.285037 H -1.049717 -4.495554 -0.077458 C 2.010146 -0.075026 -0.108408 C 3.934036 1.372880 -0.489069 C 3.374447 0.089179 -0.409164 H 5.001143 1.502889 -0.725582 H 3.993303 -0.801796 -0.590093

E'	TS-E'-F'
Zero-point correction= 0.294677 (Hartree/Particle) Thermal correction to Energy= 0.316757 Thermal correction to Enthalpy= 0.317701 Thermal correction to Gibbs Free Energy= 0.243117 Sum of electronic and zero-point Energies= -1493.149025 Sum of electronic and thermal Energies= -1493.126945 Sum of electronic and thermal Enthalpies= -1493.126001 Sum of electronic and thermal Free Energies= -1493.200585 Solvent Energy = -1493.633218	Zero-point correction= 0.293767 (Hartree/Particle) Thermal correction to Energy= 0.315523 Thermal correction to Enthalpy= 0.316467 Thermal correction to Gibbs Free Energy= 0.242509 Sum of electronic and zero-point Energies= -1493.133576 Sum of electronic and thermal Energies= -1493.111821 Sum of electronic and thermal Enthalpies= -1493.110877 Sum of electronic and thermal Free Energies= -1493.184835 Solvent Energy = -1493.620176
Ru 0.758811 -0.404180 -0.146043 C -1.811359 0.683072 -0.990385 N -1.067200 -0.481034 -1.026886 C -1.120445 1.784291 -0.336577 C -1.645967 3.086289 -0.154438 C 0.202646 1.465854 0.106899 C -0.864827 4.078632 0.447351 H -2.668705 3.325012 -0.489495 C 0.982562 2.487615 0.697079 C 0.452330 3.776472 0.863748 H -1.272443 5.091331 0.591239 H 2.005605 2.259472 1.036473 H 1.069212 4.562462 1.330680 C -3.091962 0.716665 -1.585544 C -1.561436 -1.576828 -1.656701 C -2.814138 -1.586421 -2.272638 C -3.600365 -0.415693 -2.227813 H -0.916730 -2.469562 -1.632709 H -3.167425 -2.500749 -2.771146 H -4.597267 -0.391337 -2.694403 H -3.675825 1.647417 -1.543880 C -0.092397 -1.701952 1.299045 C 0.698463 -0.729451 2.027665 C -1.512914 -1.809551 1.518730 C -0.014447 0.201008 2.869556 H 1.766933 -0.916805 2.221402 C -2.142478 -0.849919 2.288702 H -2.077852 -2.618457 1.034334 C -1.393651 0.173378 2.955946 H 0.567599 0.935760 3.446201 H -3.236906 -0.887553 2.406875 H -1.922315 0.912431 3.577041 O 2.893932 -0.020362 0.062494 C 2.962921 0.191395 -1.198464 O 1.877596 0.064434 -1.885112 C 4.242030 0.619190 -1.861297 H 4.276140 1.729073 -1.879456 H 5.114865 0.252106 -1.289315 H 4.274431 0.258508 -2.906985 Cl 0.771986 -3.173810 0.647825	Ru 0.774486 -0.012950 0.092847 C -1.790353 -0.744598 -1.109156 N -0.634527 -1.300290 -0.602077 C -1.804169 0.712327 -1.062713 C -2.887168 1.528797 -1.464430 C -0.580547 1.295631 -0.598732 C -2.755731 2.922591 -1.427996 H -3.833613 1.078742 -1.805952 C -0.464865 2.703807 -0.593918 C -1.542792 3.507826 -0.999249 H -3.597198 3.562035 -1.737597 H 0.479310 3.164272 -0.261323 H -1.445933 4.605981 -0.979474 C -2.782790 -1.588813 -1.654526 C -0.421571 -2.638880 -0.657551 C -1.371097 -3.506208 -1.203358 C -2.578088 -2.971074 -1.698926 H 0.538873 -2.973980 -0.229630 H -1.164633 -4.585929 -1.229715 H -3.348581 -3.631569 -2.126244 H -3.704109 -1.143604 -2.056612 C 0.088438 -0.536145 1.825440 C 0.637252 0.668756 2.335393 C -1.084826 -1.130786 2.329326 C -0.197283 1.447742 3.193090 H 1.703694 0.923972 2.216516 C -1.847893 -0.363750 3.212526 H -1.433327 -2.107951 1.962556 C -1.424099 0.935882 3.612889 H 0.179482 2.402716 3.592302 H -2.812836 -0.755230 3.573647 H -2.054706 1.517678 4.303163 O 2.406039 1.351373 -0.306932 C 2.641557 0.725086 -1.401300 O 1.834553 -0.228120 -1.722398 C 3.829899 1.044675 -2.255812 H 4.675293 0.410795 -1.914589 H 3.620329 0.805619 -3.315592 H 4.115410 2.106898 -2.138123 Cl 2.502287 -1.692462 0.954387

F'	TS-F'G'
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Zero-point correction= 0.294283 (Hartree/Particle) Thermal correction to Energy= 0.317017 Thermal correction to Enthalpy= 0.317961 Thermal correction to Gibbs Free Energy= 0.240611 Sum of electronic and zero-point Energies= -1493.138391 Sum of electronic and thermal Energies= -1493.115657 Sum of electronic and thermal Enthalpies= -1493.114713 Sum of electronic and thermal Free Energies= -1493.192062 Solvent Energy = -1493.624839	Zero-point correction= 0.293727 (Hartree/Particle) Thermal correction to Energy= 0.315624 Thermal correction to Enthalpy= 0.316568 Thermal correction to Gibbs Free Energy= 0.242211 Sum of electronic and zero-point Energies= -1493.130342 Sum of electronic and thermal Energies= -1493.108445 Sum of electronic and thermal Enthalpies= -1493.107501 Sum of electronic and thermal Free Energies= -1493.181858 Solvent Energy = -1493.620421
Ru -0.074789 -0.829804 0.043882 C -1.605098 1.654294 0.282186 N -1.606951 0.317692 0.622179 C -0.533774 2.004637 -0.626822 C -0.360082 3.273375 -1.236353 C 0.306502 0.910184 -0.972369 C 0.623800 3.444681 -2.211486 H -1.010555 4.117155 -0.955932 C 1.278294 1.095627 -1.978979 C 1.427202 2.345314 -2.594425 H 0.765441 4.426784 -2.688393 H 1.927380 0.259668 -2.277264 H 2.188016 2.472011 -3.381715 C -2.636287 2.496280 0.753481 C -2.639972 -0.209935 1.336528 C -3.687319 0.586924 1.797079 C -3.677083 1.969465 1.520060 H -2.589161 -1.287942 1.533142 H -4.494575 0.119472 2.378801 H -4.483766 2.621791 1.888101 H -2.612934 3.562072 0.485851 C 1.757443 -0.146777 0.617898 C 2.758026 -0.943753 0.025931 C 2.096476 0.830947 1.566222 C 4.102090 -0.779712 0.416887 H 2.507792 -1.695795 -0.745601 C 3.442263 1.005372 1.933366 H 1.306267 1.451410 2.017072 C 4.446412 0.198829 1.365057 H 4.880748 -1.412683 -0.038803 H 3.707758 1.775376 2.675951 H 5.499236 0.337353 1.657144 O -0.063471 -1.534337 -1.913475 C -1.110269 -2.308077 -1.796311 O -1.746413 -2.276126 -0.707505 C -1.503874 -3.166980 -2.966185 H -2.008821 -2.530678 -3.722896 H -0.604587 -3.603173 -3.443303 H -2.199427 -3.961620 -2.639800 Cl -0.039346 -1.614361 2.267579	Ru 0.312621 -0.871790 0.242606 C 0.809238 1.746761 -0.862485 N 1.204465 0.423421 -0.935457 C -0.116206 2.016856 0.222304 C -0.347879 3.313790 0.739259 C -0.670570 0.853740 0.876142 C -1.032033 3.487512 1.943591 H 0.070547 4.190845 0.220081 C -1.270580 1.063682 2.155438 C -1.450429 2.345674 2.670294 H -1.203353 4.497544 2.345722 H -1.636723 0.198833 2.727547 H -1.933969 2.467497 3.652863 C 1.362129 2.684204 -1.763469 C 2.140919 0.028086 -1.841188 C 2.708885 0.930415 -2.742187 C 2.308762 2.281731 -2.709208 H 2.400654 -1.038795 -1.823425 H 3.447742 0.563733 -3.469151 H 2.733134 3.010341 -3.416745 H 1.033329 3.731548 -1.705484 C -1.712379 -0.306906 -0.085544 C -2.557139 -1.187877 0.646557 C -2.206019 0.244539 -1.294636 C -3.837404 -1.508824 0.179044 H -2.200493 -1.644249 1.587165 C -3.495401 -0.063017 -1.746608 H -1.564847 0.919000 -1.882355 C -4.319332 -0.939240 -1.015658 H -4.465508 -2.209367 0.752216 H -3.857809 0.378517 -2.688830 H -5.331118 -1.181541 -1.376156 O 1.351439 -0.575006 2.100120 C 2.314334 -1.344467 1.724385 O 2.215272 -1.871255 0.561777 C 3.508705 -1.576509 2.604505 C 3.985294 -2.544087 2.359197 H 4.246233 -0.765413 2.427449 H 3.211906 -1.541473 3.670106 Cl -0.145935 -2.264056 -1.588532

G' Zero-point correction= 0.296172 (Hartree/Particle) Thermal correction to Energy= 0.318101 Thermal correction to Enthalpy= 0.319045 Thermal correction to Gibbs Free Energy= 0.245231 Sum of electronic and zero-point Energies= -1493.160688 Sum of electronic and thermal Energies= -1493.138759 Sum of electronic and thermal Enthalpies= -1493.137814 Sum of electronic and thermal Free Energies= -1493.211629 Solvent Energy = -1493.6582797	I' Zero-point correction= 0.463648 (Hartree/Particle) Thermal correction to Energy= 0.495670 Thermal correction to Enthalpy= 0.496614 Thermal correction to Gibbs Free Energy= 0.400350 Sum of electronic and zero-point Energies= -1972.064844 Sum of electronic and thermal Energies= -1972.032822 Sum of electronic and thermal Enthalpies= -1972.031877 Sum of electronic and thermal Free Energies= -1972.128141 Solvent Energy = -1972.809415
Ru 0.886595 -0.338844 -0.646150 C -1.409024 -0.535265 1.298960 N -0.242986 -1.086571 0.805586 C -1.996220 0.652225 0.638228 C -3.398280 0.746310 0.484987 C -1.167254 1.672654 0.098910 C -3.978189 1.823989 -0.200309 H -4.040868 -0.063284 0.865069 C -1.763299 2.748016 -0.589315 C -3.156535 2.825997 -0.744835 H -5.071294 1.870970 -0.324099 H -1.116314 3.542274 -0.993236 H -3.601791 3.674073 -1.288688 C -2.050783 -1.138449 2.402980 C 0.216342 -2.261356 1.334338 C -0.412664 -2.900005 2.402956 C -1.562725 -2.321781 2.967089 H 1.134630 -2.655317 0.877450 H 0.018562 -3.834914 2.789313 H -2.067625 -2.781978 3.829985 H -2.942902 -0.646342 2.816132 C 0.313589 1.622475 0.286145 C 1.200455 1.880863 -0.828068 C 0.861032 1.763418 1.616798 C 2.541125 2.323850 -0.589925 H 0.760867 2.021485 -1.832657 C 2.180779 2.144066 1.814348 H 0.196208 1.589648 2.477931 C 3.026348 2.435962 0.708560 H 3.190142 2.548038 -1.450469 H 2.576479 2.225651 2.838647 H 4.068339 2.743994 0.883923 O -0.789459 -0.454855 -2.022069 C -0.499791 -1.680112 -2.257150 O 0.525052 -2.174099 -1.646387 C -1.333753 -2.528711 -3.175498 H -0.709024 -3.305670 -3.655494 H -2.119038 -3.037461 -2.577440 H -1.830664 -1.896554 -3.935254 Cl 2.981963 -0.828985 0.282519	Ru -0.378390 -0.447241 -0.169595 C 1.932392 -1.372751 0.825554 N 0.840028 -2.000956 0.299672 C 1.592561 0.070638 0.975029 C 0.386511 0.330392 1.760185 C 2.514452 1.155158 0.693454 C 0.096263 1.684753 2.149204 H -0.025594 -0.474586 2.392208 C 2.146440 2.448127 1.066105 C 0.933009 2.717218 1.768058 H -0.800533 1.879505 2.757314 H 2.819967 3.282508 0.815130 H 0.687620 3.756546 2.036608 C 3.102704 -2.080470 1.125398 C 0.846019 -3.327309 0.056954 C 1.983280 -0.496253 0.346935 C 3.122027 -3.467195 0.883383 H -0.062207 -3.741428 -0.406745 H 1.975852 -5.176116 0.137244 H 4.026876 -4.053510 1.106084 H 3.976833 -1.546763 1.523356 C 3.860991 0.906977 0.106565 C 4.046077 0.099368 -1.040745 C 5.001387 1.478760 0.723017 C 5.333444 -0.122359 -1.553706 H 3.160160 -0.323231 -1.540981 C 6.288691 1.251561 0.208561 H 4.872903 2.087478 1.632493 C 6.459878 0.447588 -0.932373 H 5.455488 -0.744764 -2.454691 H 7.163386 1.698609 0.707855 H 7.468967 0.266172 -1.335952 O -1.910895 -1.288784 1.119159 C -2.335209 -2.004018 0.143675 O -1.794427 -1.795922 -1.005821 C -3.367523 -3.074986 0.345902 H -4.176099 -2.693101 0.997507 H -3.784757 -3.397009 -0.625182 H -2.894560 -3.943414 0.851560 Cl 0.821251 -0.214541 -2.218054 C -2.577646 1.822948 -0.196967 C -0.442305 2.408635 -0.939269 N -1.315656 1.435226 -0.563204 C -3.683653 0.834355 -0.088250 C -4.509761 0.777706 1.055575 C -0.019950 0.060614 -1.221748 C -5.655128 -0.033669 1.066036 H -4.239524 1.368827 1.944706 C -5.174180 -0.739435 -1.213274 H -3.370255 0.097516 -2.108440 C -5.996266 -0.786272 -0.073453 H -6.286498 -0.078238 1.967600 H -5.430318 -1.331165 -2.106129 H -6.901001 -1.414772 -0.069737 C -0.734562 3.774591 -0.884325

	C	-2.904356	3.188300	-0.046098
	C	-1.977760	4.183788	-0.381422
	H	-3.923523	3.446464	0.277997
	H	-2.234289	5.249871	-0.280965
	H	0.032414	4.495677	-1.202851
	H	0.541617	2.050826	-1.276635

J'				
Zero-point correction= 0.216214 (Hartree/Particle)				
Thermal correction to Energy= 0.232627				
Thermal correction to Enthalpy= 0.233571				
Thermal correction to Gibbs Free Energy= 0.171132				
Sum of electronic and zero-point Energies= -1262.336291				
Sum of electronic and thermal Energies= -1262.319878				
Sum of electronic and thermal Enthalpies= -1262.318934				
Sum of electronic and thermal Free Energies= -1262.381372				
Solvent Energy = -1262.713552				
Ru	0.649592	-0.751391	-0.420072	
C	-1.041086	1.533362	0.052543	
N	0.270159	1.147728	-0.174965	
C	-1.986984	0.422046	0.078893	
C	-3.301379	0.497024	0.584677	
C	-1.461373	-0.842436	-0.363500	
C	-4.102555	-0.651463	0.651113	
H	-3.692384	1.455072	0.962684	
C	-2.295423	-1.989254	-0.305732	
C	-3.593956	-1.893176	0.210729	
H	-5.124546	-0.585280	1.054566	
H	-1.909822	-2.954041	-0.671850	
H	-4.224886	-2.794600	0.266855	
C	-1.340199	2.899368	0.228982	
C	1.262506	2.078529	-0.237815	
C	0.998491	3.439130	-0.070423	
C	-0.324408	3.860277	0.171427	
H	2.270418	1.681911	-0.426529	
H	1.829309	4.156512	-0.136182	
H	-0.558861	4.927204	0.304560	
H	-2.384915	3.195194	0.401834	
O	0.650227	-1.059751	1.710213	
C	1.923248	-0.892761	1.744273	
O	2.515008	-0.665538	0.624192	
C	2.692040	-0.946289	3.033821	
H	3.571412	-1.610535	2.918139	
H	3.071877	0.068550	3.273257	
H	2.044335	-1.300858	3.856294	
Cl	1.499951	-0.685404	-2.591819	
H	-0.759687	-0.843987	-1.383931	

3 Pyrazole:

B'					TS-B'-C'				
Zero-point correction= 0.248809 (Hartree/Particle)					Zero-point correction= 0.247586 (Hartree/Particle)				
Thermal correction to Energy= 0.268635					Thermal correction to Energy= 0.267080				
Thermal correction to Enthalpy= 0.269579					Thermal correction to Enthalpy= 0.268024				
Thermal correction to Gibbs Free Energy= 0.199778					Thermal correction to Gibbs Free Energy= 0.198330				
Sum of electronic and zero-point Energies= -1008.447564					Sum of electronic and zero-point Energies= -1008.414644				
Sum of electronic and thermal Energies= -1008.427738					Sum of electronic and thermal Energies= -1008.395151				
Sum of electronic and thermal Enthalpies= -1008.426794					Sum of electronic and thermal Enthalpies= -1008.394206				
Sum of electronic and thermal Free Energies= -1008.496595					Sum of electronic and thermal Free Energies= -1008.463901				
Solvent Energy = -1008.872699					Solvent Energy = -1008.843111				
C	-2.675901	-0.341129	-0.815913		C	-2.279692	1.926896	-0.560162	
Ru	-0.258027	-0.347059	-0.185885		Ru	-0.480999	-0.139175	0.044585	
C	-4.126127	-0.472201	-1.194503		C	-3.490645	2.836240	-0.402618	
H	-4.763015	0.036233	-0.445725		H	-3.464060	3.645047	-1.156561	
H	-4.301642	-0.059906	-2.205931		H	-4.412082	2.236413	-0.557504	
H	-4.396598	-1.548977	-1.202815		H	-3.537440	3.257500	0.621085	
O	-1.756996	-0.285772	-1.716540		O	-1.595506	1.918794	-1.606231	
O	-2.306223	-0.313393	0.410589		O	-2.028713	1.157729	0.463083	
C	2.731643	-0.811924	-1.557645		C	2.578459	-3.058855	-0.754839	
N	1.648354	-0.275951	-0.966323		C	1.199414	-2.756225	-0.601307	
O	-0.314253	-2.455839	0.063487		H	0.319782	-3.406750	-0.659582	
C	0.311560	-2.352816	1.181339		N	1.036476	-1.438158	-0.365929	
O	0.663988	-1.171975	1.545625		O	-1.887417	-1.524406	-0.600583	
C	0.574593	-3.553202	2.045951		C	-2.062699	-1.934372	0.608685	
H	0.739846	-4.449289	1.417627		O	-1.291195	-1.387952	1.480581	
H	1.443855	-3.371055	2.705428		C	-3.108504	-2.941354	0.971685	
H	-0.316920	-3.738627	2.681605		H	-3.298655	-3.620716	0.118984	
C	0.879305	1.489014	0.222130		H	-2.796844	-3.511228	1.867655	
C	0.967514	2.003363	1.559696		H	-4.052358	-2.406657	1.208719	
C	-0.236462	1.829516	-0.644549		H	3.023236	-4.035482	-0.973173	
C	-0.090055	2.737205	2.066103		C	2.528185	0.485845	-0.070034	
H	1.853139	1.762734	2.165833		C	3.318602	1.063544	0.732297	
C	-1.292059	2.618588	-0.062017		C	1.181748	1.232499	-0.512636	
H	-0.108982	1.828662	-1.739504		C	3.182019	2.411005	1.119841	
C	-1.236666	3.029278	1.258630		H	4.158633	0.452080	1.095495	
H	-0.052414	3.099004	3.105527		C	1.067359	2.584368	-0.085385	
H	-2.139674	2.911391	-0.701518		H	0.615629	0.932673	-1.446646	
H	-2.063134	3.616204	1.688226		C	2.045815	3.154741	0.741642	
C	3.838571	0.064529	-1.383010		H	3.954622	2.869945	1.756016	
H	4.860205	-0.078269	-1.751160		H	0.205621	3.160640	-0.451805	
H	2.664627	-1.779409	-2.067671		H	1.936648	4.196980	1.079271	
C	3.356995	1.157203	-0.651661		C	3.253473	-1.848622	-0.603275	
H	3.836912	2.073026	-0.290462		H	4.314435	-1.585495	-0.669345	
N	2.035558	0.904548	-0.426980		N	2.297560	-0.891675	-0.375853	

C'					D'				
Zero-point correction= 0.249303 (Hartree/Particle)					Zero-point correction= 0.187419 (Hartree/Particle)				
Thermal correction to Energy= 0.269470					Thermal correction to Energy= 0.201924				
Thermal correction to Enthalpy= 0.270414					Thermal correction to Enthalpy= 0.202868				
Thermal correction to Gibbs Free Energy= 0.199533					Thermal correction to Gibbs Free Energy= 0.144579				
Sum of electronic and zero-point Energies= -1008.422465					Sum of electronic and zero-point Energies= -779.527735				
Sum of electronic and thermal Energies= -1008.402299					Sum of electronic and thermal Energies= -779.513230				
Sum of electronic and thermal Enthalpies= -1008.401354					Sum of electronic and thermal Enthalpies= -779.512286				

Sum of electronic and thermal Free Energies= Solvent Energy = -1008.853224	-1008.472235	Sum of electronic and thermal Free Energies= Solvent Energy = -779.7922984	-779.570574
C 1.138923 1.954040 1.608946		Ru -0.673697 -0.710294 -0.608538	
Ru 0.241491 -1.422413 -0.673672		C 1.806222 -2.544900 0.074106	
C 0.373742 3.244658 1.791531		H 1.275585 -3.488175 -0.098843	
H 1.068403 4.102621 1.743304		N 1.153089 -1.369295 -0.089462	
H -0.346925 3.325088 0.950099		O -2.720059 0.041812 -0.724474	
H -0.201078 3.247710 2.737498		C -2.844337 -0.252594 0.508784	
O 0.473061 0.891683 2.104564		O -1.811918 -0.806489 1.074860	
O 2.222265 1.872392 1.042872		C -4.074101 0.053174 1.311779	
C -2.332473 -2.276705 0.946785		H -4.965267 0.053120 0.656272	
H -1.982487 -3.294605 1.153085		H -4.190887 -0.674241 2.137432	
N -1.560409 -1.436856 0.217776		H -3.966195 1.065519 1.755825	
O 1.578847 -1.233249 0.846883		C 1.569036 0.942592 0.104357	
C 2.614240 -1.088372 0.043928		C 2.347731 2.081832 0.350898	
O 2.354809 -1.192088 -1.191311		C 0.189923 1.006602 -0.276193	
C 3.955207 -0.769951 0.612558		C 1.746418 3.348316 0.232114	
H 4.136187 -1.358188 1.533265		H 3.408876 1.993458 0.633014	
H 4.746648 -0.949206 -0.137582		C -0.382215 2.298814 -0.376948	
H 3.922229 0.305854 0.890106		C 0.388141 3.450418 -0.129182	
C -1.593269 0.784096 -0.566501		H 2.341888 4.254278 0.422884	
C -2.167221 2.038190 -0.816970		H -1.443580 2.392181 -0.658274	
C -0.278036 0.426728 -1.006457		H -0.077995 4.445155 -0.220214	
C -1.406733 3.000102 -1.508391		C 3.141322 -2.309937 0.480286	
H -3.189859 2.270839 -0.481028		C 3.270877 -0.921213 0.554623	
C 0.466029 1.428587 -1.675314		H 3.914119 -3.055722 0.693229	
H 0.958302 0.070089 1.799611		H 4.121449 -0.285985 0.822581	
C -0.095591 2.693745 -1.926690		N 2.064967 -0.380399 0.206737	
H -1.839084 3.991183 -1.714435			
H 1.496804 1.207156 -1.992015			
H 0.500696 3.455401 -2.454209			
C -3.525838 -1.624847 1.340184			
H -4.345050 -2.038739 1.936996			
C -3.441351 -0.336890 0.807952			
H -4.128358 0.514140 0.857703			
N -2.253824 -0.250766 0.137332			

E'		TS-E'-F'	
Zero-point correction=	0.276975 (Hartree/Particle)	Zero-point correction=	0.276195 (Hartree/Particle)
Thermal correction to Energy=	0.298422	Thermal correction to Energy=	0.297234
Thermal correction to Enthalpy=	0.299366	Thermal correction to Enthalpy=	0.298179
Thermal correction to Gibbs Free Energy=	0.225019	Thermal correction to Gibbs Free Energy=	0.225580
Sum of electronic and zero-point Energies=	-1471.092705	Sum of electronic and zero-point Energies=	-1471.076805
Sum of electronic and thermal Energies=	-1471.071258	Sum of electronic and thermal Energies=	-1471.055766
Sum of electronic and thermal Enthalpies=	-1471.070314	Sum of electronic and thermal Enthalpies=	-1471.054822
Sum of electronic and thermal Free Energies=	-1471.144661	Sum of electronic and thermal Free Energies=	-1471.127420
Solvent Energy = -1471.564931		Solvent Energy = -1471.550625	
Ru -0.818517 -0.092118 0.134480		Ru -0.727728 -0.071424 -0.052421	
N 0.673942 -0.736905 1.332038		N 0.403555 -0.302943 1.591736	
C 1.781449 1.138128 0.450338		C 1.878161 1.139986 0.460372	
C 2.863626 2.016606 0.275417		C 3.075951 1.852546 0.288693	
C 0.530150 1.313034 -0.204144		C 0.834230 1.127922 -0.508312	
C 2.697955 3.125118 -0.570969		C 3.241769 2.599340 -0.890199	
H 3.821666 1.845669 0.791031		H 3.868763 1.831390 1.052604	
C 0.393434 2.443337 -1.038453		C 1.032885 1.899820 -1.672373	
C 1.464058 3.338085 -1.218982		C 2.223944 2.624721 -1.864972	
H 3.533958 3.825207 -0.722371		H 4.172716 3.166097 -1.046562	
H -0.563842 2.608576 -1.558038		H 0.236993 1.925554 -2.434076	
H 1.338183 4.211976 -1.878839		H 2.364431 3.216201 -2.784101	
C 0.878121 -1.731188 2.221155		C 0.248860 -0.906912 2.784964	
C 2.179718 -1.625687 2.766610		C 1.369190 -0.617554 3.599435	
H 0.083089 -2.462478 2.404820		H -0.659068 -1.498363 2.957467	
H 2.641902 -2.275340 3.517077		H 1.547485 -0.951461 4.626903	
C -0.441208 -1.868257 -0.957493		C -0.129525 -1.858010 -0.463856	
C -0.614991 -0.806644 -1.930199		C -0.456355 -1.568848 -1.815205	
C 0.799390 -2.597554 -0.871160		C 0.924991 -2.708987 -0.075906	
C 0.547464 -0.428573 -2.699146		C 0.522644 -1.913199 -2.799151	
H -1.615565 -0.571880 -2.327662		H -1.471272 -1.270299 -2.125300	
C 1.888510 -2.144533 -1.590461		C 1.828513 -3.071135 -1.076408	
H 0.872493 -3.467075 -0.203170		H 1.084091 -2.979505 0.978259	
C 1.769572 -1.041538 -2.498142		C 1.648946 -2.642358 -2.424586	
H 0.436801 0.360162 -3.458724		H 0.325234 -1.688542 -3.859344	
H 2.857720 -2.655955 -1.479541		H 2.717372 -3.666693 -0.811512	
H 2.650444 -0.716299 -3.072535		H 2.386816 -2.942311 -3.185003	
O -2.504901 1.077501 -0.540104		O -2.094513 1.071266 -1.254222	
C -2.648547 1.550627 0.643966		C -2.452345 1.734386 -0.213639	
O -1.816075 1.158626 1.545015		O -1.832408 1.486035 0.886755	
C -3.764701 2.498610 0.984031		C -3.576214 2.724320 -0.260218	
H -4.610907 1.921440 1.413016		H -4.514297 2.190336 -0.000080	
H -3.427715 3.227081 1.746080		H -3.415109 3.526426 0.484874	
H -4.117992 3.018493 0.074063		H -3.679162 3.144586 -1.278264	
Cl -1.942654 -2.679247 -0.314027		Cl -2.659472 -1.536801 0.694358	
C 2.755284 -0.510252 2.152915		C 2.204230 0.195999 2.825963	
N 1.825439 0.003431 1.292172		N 1.596423 0.368627 1.614690	
H 3.736067 -0.039816 2.275691		H 3.162337 0.674421 3.053722	

F'		TS-F'G'	
Zero-point correction=	0.276667 (Hartree/Particle)	Zero-point correction=	0.276268 (Hartree/Particle)
Thermal correction to Energy=	0.298361	Thermal correction to Energy=	0.297408
Thermal correction to Enthalpy=	0.299305	Thermal correction to Enthalpy=	0.298352
Thermal correction to Gibbs Free Energy=	0.225291	Thermal correction to Gibbs Free Energy=	0.225674
Sum of electronic and zero-point Energies=	-1471.087286	Sum of electronic and zero-point Energies=	-1471.069497
Sum of electronic and thermal Energies=	-1471.065591	Sum of electronic and thermal Energies=	-1471.048358
Sum of electronic and thermal Enthalpies=	-1471.064647	Sum of electronic and thermal Enthalpies=	-1471.047414
Sum of electronic and thermal Free Energies=	-1471.138662	Sum of electronic and thermal Free Energies=	-1471.120091
Solvent Energy = -1471.562207		Solvent Energy = -1471.549028	
Ru 0.713491 0.314228 -0.195209		Ru -0.499680 -0.744850 -0.339378	
N -0.387638 0.045892 1.512144		N -0.980808 0.137379 1.325303	
C -1.393491 -1.666041 0.251215		C 0.169588 1.987806 0.455396	
C -2.246934 -2.766044 0.054258		C 0.330050 3.378052 0.356277	
C -0.489947 -1.218949 -0.746502		C 0.515547 1.074653 -0.601230	
C -2.195060 -3.437401 -1.177681		C 0.791178 3.929520 -0.846626	
H -2.932954 -3.102300 0.846797		H 0.043297 4.029030 1.196562	
C -0.449752 -1.914564 -1.967578		C 0.879139 1.694531 -1.834720	
C -1.297904 -3.016855 -2.180624		C 1.023148 3.078501 -1.950224	
H -2.855874 -4.300590 -1.352295		H 0.926841 5.017448 -0.938679	
H 0.253614 -1.574541 -2.743136		H 1.099446 1.059489 -2.704952	
H -1.261023 -3.554915 -3.141265		H 1.331194 3.506507 -2.917195	
C -2.020731 -1.001992 2.643855		C -1.637862 -0.254971 2.436924	
C -0.456642 0.600209 2.737210		C -1.551422 0.773806 3.405959	

C	-1.477307	-0.030382	3.488484	C	1.598140	-0.342033	-0.247233
H	0.231327	1.411189	3.000389	C	2.244425	-0.952695	-1.358640
H	-1.783526	0.193626	4.515584	C	2.326196	-0.224285	0.965763
H	-2.826700	-1.726953	2.796791	C	3.558402	-1.426683	-1.256768
C	-0.727172	1.294803	-1.073192	H	1.705680	-1.072565	-2.315444
C	-2.128836	1.219132	-1.197731	C	3.649046	-0.674188	1.052987
C	-0.066829	2.503830	-0.721929	H	1.843322	0.218758	1.849808
C	-2.884774	2.319352	-0.780152	C	4.274792	-1.278537	-0.053717
H	-2.607724	0.288918	-1.543103	H	4.027781	-1.915573	-2.125380
C	-0.861381	3.579255	-0.229698	H	4.193798	-0.568655	2.004945
H	1.004323	2.669281	-0.942433	H	5.311881	-1.640315	0.022644
C	-2.254296	3.482424	-0.260588	O	-1.887834	0.204985	-1.687392
H	-3.985232	2.272424	-0.824642	C	-2.811679	-0.635613	-1.370814
H	-0.371186	4.519169	0.071280	O	-2.507226	-1.540744	-0.517442
H	-2.872412	4.332062	0.069658	C	-4.191021	-0.526683	-1.955116
Cl	2.101163	0.573282	-2.139896	H	-4.784515	0.183488	-1.341436
O	2.409877	0.649565	1.119352	H	-4.139868	-0.127040	-2.985983
C	2.811081	-0.557543	0.943659	H	-4.695057	-1.511166	-1.938347
O	2.069066	-1.318672	0.228156	Cl	0.165506	-2.651490	0.845532
C	4.111674	-1.047910	1.507364	H	-2.091381	-1.250788	2.469217
H	4.084187	-2.144747	1.649536	H	-1.967804	0.759874	4.418419
H	4.913666	-0.808280	0.777921	C	-0.803827	1.798254	2.822310
H	4.339625	-0.531059	2.459058	H	-0.486255	2.775008	3.200508
N	-1.341682	-0.933060	1.459995	N	-0.471847	1.387575	1.557472

G'				I'			
Zero-point correction=	0.278563 (Hartree/Particle)			Zero-point correction=	0.428772 (Hartree/Particle)		
Thermal correction to Energy=	0.299822			Thermal correction to Energy=	0.459224		
Thermal correction to Enthalpy=	0.300766			Thermal correction to Enthalpy=	0.460168		
Thermal correction to Gibbs Free Energy=	0.228232			Thermal correction to Gibbs Free Energy=	0.367474		
Sum of electronic and zero-point Energies=	-1471.105278			Sum of electronic and zero-point Energies=	-1927.954719		
Sum of electronic and thermal Energies=	-1471.084019			Sum of electronic and thermal Energies=	-1927.924268		
Sum of electronic and thermal Enthalpies=	-1471.083075			Sum of electronic and thermal Enthalpies=	-1927.923324		
Sum of electronic and thermal Free Energies=	-1471.155608			Sum of electronic and thermal Free Energies=	-1928.016018		
Solvent Energy = -1471.592384				Solvent Energy = -1928.677222			
Ru	-0.858621	0.556226	-0.488807	Ru	0.362385	-0.474368	0.308204
N	0.132397	0.807304	1.194242	N	-0.817312	-2.067339	-0.291583
C	2.005220	-0.671852	0.658467	C	-1.436552	0.026685	-0.938383
C	3.409532	-0.622182	0.610406	C	-0.195510	0.329156	-1.649748
C	1.262804	-1.516375	-0.204009	C	-2.416930	1.057773	-0.655956
C	4.101930	-1.436219	-0.299299	C	0.083897	1.713907	-1.932837
H	3.953746	0.079128	1.260624	H	0.244354	-0.439019	-2.308849
C	1.982784	-2.302246	-1.126177	C	-2.029264	2.375117	-0.896995
C	3.385994	-2.269048	-1.176370	C	-0.780229	2.705240	-1.507528
H	5.201425	-1.398285	-0.337476	H	0.990628	1.965921	-2.503553
H	1.419488	-2.965592	-1.800558	H	-2.723530	3.184999	-0.624833
H	3.923048	-2.898900	-1.902495	H	-0.536185	3.764223	-1.683912
C	1.670815	0.576502	2.817686	C	-2.805177	-2.193526	-1.334594
C	-0.229715	1.597491	2.227414	C	-1.191267	-3.357348	-0.276745
C	0.716541	1.482080	3.272297	C	-2.447894	-3.484802	-0.928503
H	-1.162244	2.168256	2.152851	H	-0.559368	-4.112358	0.203836
H	0.688787	1.980271	4.246691	H	-3.025724	-4.402430	-1.081425
H	2.559619	0.150234	3.294354	H	-3.689900	-1.797156	-1.842479
C	-0.228935	-1.578203	-0.128542	C	-3.807470	0.741424	-0.229834
C	-1.027704	-1.523493	-1.334410	C	-4.103326	-0.220333	0.767300
C	-0.849639	-2.121102	1.058909	C	-4.886262	1.412619	-0.859396
C	-2.357182	-2.057447	-1.335161	C	-5.433603	-0.485182	1.127206
H	-0.517737	-1.352852	-2.300485	H	-3.272654	-0.721816	1.286885
C	-2.158217	-2.581446	1.037107	C	-6.215899	1.143375	-0.496882
H	-0.253083	-2.183815	1.983063	H	-4.674259	2.137984	-1.661126
C	-2.917505	-2.558100	-0.165220	C	-6.495361	0.191525	0.499549
H	-2.937937	-2.039395	-2.270263	H	-5.640729	-1.226344	1.915668
H	-2.612645	-2.971638	1.960921	H	-7.038101	1.674339	-1.003029
H	-3.952688	-2.931780	-0.164719	H	-7.537761	-0.023211	0.784679
O	0.907902	1.141894	-1.620179	O	1.999542	-1.386120	-0.803323
C	0.564949	2.368709	-1.482649	C	2.387671	-1.983132	0.262579
O	-0.525968	2.610363	-0.835777	O	1.799124	-1.668711	1.359602
C	1.404449	3.494609	-2.018420	C	3.432482	-3.063845	0.219837
H	0.757691	4.327842	-2.354276	H	4.123740	-2.891656	-0.625493
H	2.055597	3.876855	-1.204138	H	3.989733	-3.097480	1.174508
H	2.046174	3.136744	-2.845053	H	2.928403	-4.043331	0.076199
Cl	-2.995879	0.700001	0.454702	Cl	-1.043025	-0.213675	2.211300
N	1.305863	0.184244	1.553472	C	0.512256	2.410937	1.325526
				N	1.208117	1.369352	0.820589
				C	3.511488	1.081572	-0.017469
				C	3.894763	1.090760	-1.367547
				C	4.228057	0.338331	0.937587
				C	5.013917	0.345058	-1.770603
				H	3.302746	1.670715	-2.089793
				C	5.347274	-0.401967	0.526117
				H	3.889612	0.338703	1.983611
				C	5.741208	-0.398615	-0.824787
				H	5.314724	0.339847	-2.829687
				H	5.914143	-0.988143	1.265843
				H	6.619145	-0.982977	-1.142271
				C	2.472283	3.234091	0.661643
				C	1.265555	3.604063	1.247542
				H	3.386317	3.792322	0.430619
				H	0.964860	4.603359	1.578731
				H	-0.502122	2.227408	1.698086
				N	-1.791774	-1.376460	-0.930064
				N	2.408458	1.887608	0.411347

J'	B
Zero-point correction= 0.198657 (Hartree/Particle)	Zero-point correction= 0.457903 (Hartree/Particle)
Thermal correction to Energy= 0.215196	Thermal correction to Energy= 0.489496
Thermal correction to Enthalpy= 0.216140	Thermal correction to Enthalpy= 0.490441
Thermal correction to Gibbs Free Energy= 0.152698	Thermal correction to Gibbs Free Energy= 0.395031
Sum of electronic and zero-point Energies= -1240.275343	Sum of electronic and zero-point Energies= -1397.518667
Sum of electronic and thermal Energies= -1240.258803	Sum of electronic and thermal Energies= -1397.487073
Sum of electronic and thermal Enthalpies= -1240.257859	Sum of electronic and thermal Enthalpies= -1397.486129
Sum of electronic and thermal Free Energies= -1240.321302	Sum of electronic and thermal Free Energies= -1397.581539
Solvent Energy = -1240.641081	Solvent Energy = -1398.2265183
Ru 0.716121 -0.625429 -0.340889	C -0.705898 -1.596904 2.304250
N 0.204001 1.247361 -0.335546	Ru -0.440897 0.081509 -0.216181
C -1.989410 0.457194 0.049580	C 0.456666 -0.081487 -2.238596
C -3.290606 0.589392 0.551348	C -0.780923 0.645718 -2.324121
C -1.393814 -0.822813 -0.202719	C -1.968992 0.084647 -1.768148
C -4.046593 -0.569617 0.799400	C -1.993296 -1.214884 -1.150337
H -3.704413 1.583887 0.777434	C -0.738014 -1.912726 -1.060889

C	-2.187950	-1.969919	0.056485
C	-3.490448	-1.842587	0.561050
H	-5.069998	-0.476200	1.193129
H	-1.765853	-2.965208	-0.153583
H	-4.084802	-2.746953	0.764859
C	0.870113	2.409867	-0.489941
C	-0.049017	3.486004	-0.412846
H	1.951796	2.390656	-0.660621
H	0.175795	4.552740	-0.513998
O	0.823103	-0.544423	1.807699
C	2.085738	-0.317010	1.741201
O	2.611693	-0.271496	0.567582
C	2.913654	-0.094601	2.974778
H	3.871572	-0.644318	2.890854
H	3.153677	0.985884	3.059604
H	2.358103	-0.413837	3.875725
Cl	1.462750	-0.921323	-2.531309
H	-0.713907	-0.945018	-1.229513
N	-1.124858	1.552947	-0.153101
C	-1.302166	2.912212	-0.203738
H	-2.297432	3.356177	-0.101841
C	0.469901	-1.379877	-1.618600
H	-0.799835	1.674860	-2.710158
H	-2.868414	0.716746	-1.743203
H	-0.703462	-2.842892	-0.475035
H	1.422918	-1.915737	-1.491743
C	-3.288560	-1.816302	-0.627120
H	-2.999917	-2.696449	-0.019813
C	1.717311	0.544484	-2.778884
H	2.615646	-0.034391	-2.496522
C	-0.383052	-1.661790	3.799681
H	-0.688237	-2.640161	4.215807
H	0.692996	-1.476293	3.990693
H	-0.949769	-0.858076	4.314404
O	-0.059307	-0.617982	1.709786
O	-1.498185	-2.386250	1.779784
C	2.084721	3.500420	0.589004
C	0.879771	2.806798	0.330604
H	-0.130617	3.190801	0.141345
N	1.098750	1.479006	0.264036
C	-4.060629	-0.863124	0.300254
H	-4.386427	0.059695	-0.226585
H	-4.973104	-1.363173	0.685514
H	-3.424957	-0.566503	1.156112
C	-4.147250	-2.282429	-1.822131
H	-3.594110	-2.992139	-2.472548
H	-5.067420	-2.790743	-1.465049
H	-4.461314	-1.421110	-2.451184
H	1.832438	1.584005	-2.409424
H	1.661691	0.586983	-3.887273
O	-1.660573	1.270332	0.973611
C	-2.352064	2.295679	0.542003
O	-2.248541	2.835350	-0.572822
C	-3.340100	2.800605	1.594367
H	-2.817316	2.982642	2.554791
H	-3.834232	3.726040	1.245171
H	-4.102551	2.016671	1.783451
H	2.218239	4.579757	0.713646
C	3.151581	0.062239	0.306838
C	4.303146	0.053552	-0.508955
C	2.726182	-1.108406	0.957022
C	5.025164	-1.138616	-0.678709
H	4.613534	0.972707	-1.028769
C	3.445975	-2.298579	0.762308
H	1.819220	-1.067621	1.579804
C	4.592985	-2.321142	-0.051274
H	5.921117	-1.144235	-1.318895
H	3.105233	-3.217942	1.264020
H	5.153333	-3.258233	-0.194975
N	2.447395	1.300480	0.464826
C	3.058949	2.512453	0.667592
H	4.133191	2.558417	0.876501

4 Oxazoline:

B'	TS-B'-C'
Zero-point correction= 0.259582 (Hartree/Particle)	Zero-point correction= 0.258070 (Hartree/Particle)
Thermal correction to Energy= 0.279819	Thermal correction to Energy= 0.278449
Thermal correction to Enthalpy= 0.280763	Thermal correction to Enthalpy= 0.279393
Thermal correction to Gibbs Free Energy= 0.210420	Thermal correction to Gibbs Free Energy= 0.206890
Sum of electronic and zero-point Energies= -1029.500437	Sum of electronic and zero-point Energies= -1029.467835
Sum of electronic and thermal Energies= -1029.480200	Sum of electronic and thermal Energies= -1029.447456
Sum of electronic and thermal Enthalpies= -1029.479256	Sum of electronic and thermal Enthalpies= -1029.446512
Sum of electronic and thermal Free Energies= -1029.549599	Sum of electronic and thermal Free Energies= -1029.519015
Solvent Energy = -1029.971876	Solvent Energy = -1029.937848
C	-2.183939
Ru	-0.104772
C	-3.375594
H	-4.071247
H	-3.885229
H	-3.027226
O	-1.567406
O	-1.726116
C	1.192395
C	2.572715
N	1.172432
O	1.023594
C	1.458369
O	1.112315
C	2.284577
H	2.946028
H	2.875599
H	1.605797
C	-0.041462
C	-0.075562
C	-1.277344
C	-1.293595
H	0.874910
C	-2.511722
H	-1.287244
C	-2.520395
H	-1.320586
H	-3.456668
H	-3.474224
C	3.323564
H	3.504577
H	2.635469
O	2.400595
H	2.950358
H	4.276729
C	-2.373618
Ru	-0.551602
C	-3.534466
H	-3.281657
H	-3.740925
H	-4.438215
O	-1.658307
O	-2.160300
C	2.248253
C	2.713604
C	1.190815
H	0.847675
N	1.043932
O	-1.883449
C	-1.998467
O	-1.244704
C	-2.960503
H	-2.599838
H	-3.941653
H	-3.105039
H	2.944097
C	2.331299
C	3.352648
C	1.121743
C	3.164881
H	4.260595
C	0.965346
H	0.532795
C	1.961588
H	3.954785
H	0.066908
H	1.819947
O	3.294536
H	0.558618
H	3.203922
C	1.893936
O	-0.119136
C	2.865168
C	3.621097
C	3.376722
C	2.328587
C	1.879362
O	1.107029
C	-0.779909
C	-2.953538
C	-2.771470
C	-3.217543
C	-1.310132
O	-1.589892
C	-2.030933
O	-1.446743
C	-3.116534
H	-3.660922
H	-2.657137
C	-3.808579
C	-2.253066
C	0.644373
C	1.268837
C	1.362519
C	2.583554
H	0.702177
C	2.688355
H	0.863302
C	0.10432
H	-1.391548
C	3.274085
H	3.066948
H	3.245346
C	4.293370
O	-1.628988
H	-3.182712
C	-3.662549

C'	D'
Zero-point correction= 0.260176 (Hartree/Particle)	Zero-point correction= 0.198139 (Hartree/Particle)
Thermal correction to Energy= 0.280943	Thermal correction to Energy= 0.213303
Thermal correction to Enthalpy= 0.281887	Thermal correction to Enthalpy= 0.214247
Thermal correction to Gibbs Free Energy= 0.209487	Thermal correction to Gibbs Free Energy= 0.154258
Sum of electronic and zero-point Energies= -1029.474822	Sum of electronic and zero-point Energies= -800.579797
Sum of electronic and thermal Energies= -1029.454055	Sum of electronic and thermal Energies= -800.564634
Sum of electronic and thermal Enthalpies= -1029.453110	Sum of electronic and thermal Enthalpies= -800.563689
Sum of electronic and thermal Free Energies= -1029.525510	Sum of electronic and thermal Free Energies= -800.623678
Solvent Energy = -1029.948915	Solvent Energy = -800.8877654

C	1.271686	1.823911	1.697922
Ru	0.155950	-1.439749	-0.677447
C	0.562500	3.145601	1.883358
H	1.296605	3.971287	1.871269
H	-0.130947	3.273494	1.024903
H	-0.038792	3.158406	2.812774
O	0.530805	0.782924	2.129172
O	2.375262	1.702073	1.180251
C	-2.545075	-2.012334	1.056472
H	-2.741123	-3.031762	0.665753
N	-1.690708	-1.240931	0.141445
O	1.507807	-1.360538	0.841830
C	2.556776	-1.307994	0.045185
O	2.296867	-1.409343	-1.188976
C	3.911742	-1.072295	0.622331
H	4.062990	-1.695055	1.525878
H	4.694981	-1.269754	-0.131690
H	3.929906	-0.005003	0.933595
C	-1.450523	0.962368	-0.692897
C	-1.854573	2.281409	-0.978917
C	-0.134133	0.467192	-1.020170
C	-0.937340	3.158705	-1.577897
H	-2.875701	2.608120	-0.724973
C	0.773944	1.388067	-1.596744
H	0.980296	-0.052580	1.803215
C	0.369369	2.706712	-1.873862
H	-1.230281	4.194496	-1.808584
H	1.800443	1.067400	-1.830266
H	1.091474	3.402878	-2.331500
C	-2.231544	-0.043930	-0.013249
C	-3.827504	-1.142316	1.127244
H	-4.203065	-0.968322	2.154136
O	-3.431736	0.148691	0.567614
H	-4.652653	-1.544223	0.500480
H	-2.034962	-2.114924	2.040758

Ru	-0.639508	-0.765397	-0.568788
C	2.045750	-2.432098	0.271913
H	1.933303	-3.221670	-0.498832
N	1.276374	-1.227290	-0.074357
O	-2.729960	-0.158517	-0.793805
C	-2.900257	-0.455129	0.432579
O	-1.861797	-0.929650	1.054956
C	-4.190142	-0.233250	1.166979
H	-5.042772	-0.292299	0.464507
H	-4.303102	-0.968099	1.986689
H	-4.174994	0.783180	1.614678
C	1.455552	1.133274	0.044420
C	2.106340	2.367454	0.244989
C	0.039463	1.036785	-0.225596
C	1.351949	3.548728	0.204831
H	3.191791	2.388660	0.433735
C	-0.692479	2.250693	-0.246363
C	-0.039615	3.479231	-0.037405
H	1.838615	4.523762	0.361140
H	-1.775005	2.228738	-0.450486
H	-0.627748	4.411933	-0.070688
C	2.058187	-0.174924	0.120280
C	3.494165	-1.887310	0.361753
H	4.057069	-2.229939	1.251509
O	3.337734	-0.437860	0.456083
H	4.089158	-2.104972	-0.551831
H	1.676116	-2.843286	1.238602

E'		TS-E'-F'	
Zero-point correction=	0.287815 (Hartree/Particle)	Zero-point correction=	0.286734 (Hartree/Particle)
Thermal correction to Energy=	0.309767	Thermal correction to Energy=	0.308497
Thermal correction to Enthalpy=	0.310711	Thermal correction to Enthalpy=	0.309441
Thermal correction to Gibbs Free Energy=	0.236073	Thermal correction to Gibbs Free Energy=	0.234850
Sum of electronic and zero-point Energies=	-1492.148248	Sum of electronic and zero-point Energies=	-1492.132436
Sum of electronic and thermal Energies=	-1492.126296	Sum of electronic and thermal Energies=	-1492.110673
Sum of electronic and thermal Enthalpies=	-1492.125352	Sum of electronic and thermal Enthalpies=	-1492.109729
Sum of electronic and thermal Free Energies=	-1492.199990	Sum of electronic and thermal Free Energies=	-1492.184321
Solvent Energy = -1492.663288		Solvent Energy = -1492.647777	
Ru	0.769506	-0.388606	-0.123699
N	-0.902221	-0.537217	-1.271111
C	-1.273850	1.650568	-0.476815
C	-1.965748	2.378989	-0.332911
C	-0.012037	1.403541	0.163467
C	-1.396669	3.886484	0.446793
H	-2.933253	3.016770	-0.840107
C	0.542745	2.542913	0.933103
C	-0.143044	3.671226	1.068722
H	-1.917179	4.848518	0.572604
H	1.513301	2.302524	1.431916
H	0.302834	4.476350	1.676720
C	-1.447585	-1.532221	-2.198046
C	-2.842460	-0.937956	-2.528787
H	-1.499792	-2.532505	-1.721427
H	-3.665483	-1.458392	-1.993115
C	-0.220778	-1.803764	1.090413
C	0.525241	-0.927795	1.977942
C	-1.658746	-1.883523	1.179946
C	-0.240727	-0.065828	2.848795
H	1.561998	-1.177987	2.257176
C	-2.333367	-0.986447	1.985450
H	-2.196661	-2.635906	0.584546
C	-1.621715	-0.059293	2.816227
H	0.303474	0.586921	3.548432
H	-3.434524	-1.002482	2.009349
H	-2.185899	0.629752	3.463064
O	2.786692	0.225191	0.393942
C	2.999551	0.534670	-0.831394
O	2.043912	0.328126	-1.671298
C	4.293259	1.158762	-1.273433
H	4.210363	2.260651	-1.162831
H	5.127140	0.808978	-0.635647
H	4.488817	0.931510	-2.338418
Cl	0.661733	-3.255057	0.414622
H	-0.785846	-1.618970	-3.088262
H	-3.075700	-0.904519	-3.610604
C	-1.688538	0.519302	-1.263729
O	-2.792973	0.438703	-2.034630

Ru	-0.731768	0.004822	-0.072182
N	0.477112	-0.422026	1.487533
C	1.970266	1.048548	0.401294
C	3.184594	1.742926	0.213597
C	0.874997	1.142033	-0.524346
C	3.323794	2.556846	-0.917642
H	3.997573	1.643030	0.950167
C	1.047266	1.983897	-1.645782
C	2.257306	2.673694	-1.839803
H	4.261242	3.108793	-1.088493
H	0.223209	2.093519	-2.369132
H	2.379470	3.318936	-2.725771
C	0.236597	-1.065779	2.782709
C	1.639964	-0.981501	3.435149
H	-0.141061	-2.099203	2.652753
H	1.633315	-0.627361	4.483544
C	-0.348989	-1.805178	-0.623519
C	-0.638476	-1.363776	-1.944881
C	0.619069	-2.787417	-0.324708
C	0.301521	-1.720551	-2.961904
H	-1.619002	-0.945546	-2.223830
C	1.482626	-3.149573	-1.358521
H	0.745457	-3.173900	0.696871
C	1.350368	-2.586580	-2.662192
H	0.130622	-1.383551	-3.996658
H	2.305454	-3.853796	-1.153641
H	2.057437	-2.887877	-3.450717
O	-2.105578	1.327957	-1.090326
C	-2.369270	1.894337	0.028664
O	-1.711122	1.497923	1.065313
C	-3.429979	2.947482	0.150771
H	-3.565106	3.471754	-0.813762
H	-4.384744	2.448459	0.419412
H	-3.173457	3.661644	0.956150
Cl	-2.642988	-1.565215	0.618224
C	1.640631	0.193225	1.516436
O	2.370130	0.008643	2.632113
H	2.201461	-1.938666	3.374884
H	-0.544227	-0.497557	3.332954

F'		TS-F'G'	
Zero-point correction=	0.287906 (Hartree/Particle)	Zero-point correction=	0.286718 (Hartree/Particle)
Thermal correction to Energy=	0.310486	Thermal correction to Energy=	0.308620
Thermal correction to Enthalpy=	0.311430	Thermal correction to Enthalpy=	0.309564
Thermal correction to Gibbs Free Energy=	0.234709	Thermal correction to Gibbs Free Energy=	0.234499
Sum of electronic and zero-point Energies=	-1492.157145	Sum of electronic and zero-point Energies=	-1492.129594
Sum of electronic and thermal Energies=	-1492.134565	Sum of electronic and thermal Energies=	-1492.107692
Sum of electronic and thermal Enthalpies=	-1492.133621	Sum of electronic and thermal Enthalpies=	-1492.106748
Sum of electronic and thermal Free Energies=	-1492.210342	Sum of electronic and thermal Free Energies=	-1492.181813
Solvent Energy = -1492.668052		Solvent Energy = -1492.648756	
Ru	0.077859	-0.717453	-0.203161
N	-0.123636	0.672540	1.322112
C	-1.757688	1.601963	-0.059641
C	-2.757683	2.503191	-0.472160
C	-1.403802	0.451322	-0.839991
C	-3.436680	2.248773	-1.672411
H	-2.996833	3.380423	0.148915
C	-2.135582	0.191187	-2.022517
C	-3.126497	1.099543	-2.434386
H	-4.223263	2.938616	-2.015607
H	-1.911243	-0.703423	-2.620202
H	-3.675530	0.904701	-3.369933
C	0.694537	0.957889	2.500186
C	-0.061022	2.156732	3.135008

Ru	-0.429817	-0.794580	-0.175222
C	-0.704910	1.716269	1.120881
N	-1.167356	0.481038	1.112407
C	0.202930	2.084817	0.078493
C	0.484952	3.421353	-0.285346
C	0.602791	0.949129	-0.742000
C	1.076531	3.689788	-1.520106
H	0.175610	4.234330	0.390381
C	1.092963	1.290255	-2.043686
C	1.326894	2.614290	-2.411569
H	1.302333	4.724301	-1.820018
H	1.343542	0.486874	-2.751400
H	1.728237	2.823689	-3.416336
C	-2.093473	0.281062	2.229860

H	0.751237	0.069102	3.158799	C	-2.276669	1.736603	2.734978
H	-0.671818	1.863983	4.015289	H	-3.031947	-0.191386	1.878816
C	1.820383	0.233684	-0.463724	H	-3.246574	2.180332	2.423753
C	1.921990	1.626581	-0.700433	C	1.641131	-0.351701	-0.054948
C	3.006308	-0.540676	-0.401708	C	2.277036	-1.244843	-0.966132
C	3.181108	2.228662	-0.875462	C	2.340453	0.019866	1.121467
H	1.011570	2.243755	-0.770439	C	3.547256	-1.764877	-0.690333
C	4.261799	0.073003	-0.548743	H	1.760864	-1.547866	-1.895437
H	2.948970	-1.629422	-0.239837	C	3.624203	-0.478943	1.374923
C	4.354534	1.457597	-0.788956	H	1.864461	0.708778	1.835677
H	3.244046	3.310464	-1.078335	C	4.234243	-1.374700	0.476496
H	5.176297	-0.539486	-0.489652	H	4.009687	-2.474546	-1.394792
H	5.340322	1.932610	-0.915951	H	4.151320	-0.175471	2.293684
Cl	0.439399	-2.132449	-1.999476	H	5.241278	-1.768816	0.683535
O	0.120348	-1.935534	1.431580	O	-1.488855	-0.442180	-1.991819
C	-1.015904	-2.581107	1.282261	C	-2.491329	-1.149895	-1.592731
O	-1.805917	-2.204172	0.394292	O	-2.413809	-1.646764	-0.415706
C	-1.249882	-3.769785	2.180489	C	-3.663981	-1.409041	-2.495060
H	-2.334261	-3.972413	2.257119	H	-3.844846	-0.536852	-3.151847
H	-0.756225	-4.653967	1.725641	H	-3.436261	-2.284246	-3.139844
H	-0.807438	-3.607790	3.182132	H	-4.563708	-1.644331	-1.896012
O	-0.985854	2.614334	2.088969	Cl	0.057463	-2.230712	1.625002
C	-0.974225	1.653723	1.147518	O	-1.208916	2.508997	2.088653
H	1.726396	1.213619	2.169048	H	-2.159086	1.848463	3.830041
H	0.588844	3.010299	3.407685	H	-1.621848	-0.403898	2.967518

G'	I'
Zero-point correction= 0.289733 (Hartree/Particle) Thermal correction to Energy= 0.311472 Thermal correction to Enthalpy= 0.312416 Thermal correction to Gibbs Free Energy= 0.237736 Sum of electronic and zero-point Energies= -1492.169756 Sum of electronic and thermal Energies= -1492.148017 Sum of electronic and thermal Enthalpies= -1492.147073 Sum of electronic and thermal Free Energies= -1492.221753 Solvent Energy = -1492.694656	Zero-point correction= 0.450543 (Hartree/Particle) Thermal correction to Energy= 0.482186 Thermal correction to Enthalpy= 0.483130 Thermal correction to Gibbs Free Energy= 0.387552 Sum of electronic and zero-point Energies= -1970.066230 Sum of electronic and thermal Energies= -1970.034586 Sum of electronic and thermal Enthalpies= -1970.033642 Sum of electronic and thermal Free Energies= -1970.129221 Solvent Energy = -1970.873265
Ru 1.033531 0.301168 0.038412 N 0.137349 -1.403184 0.422843 C -2.248508 -0.934312 -0.167040 C -3.465882 -1.611101 -0.442356 C -2.165288 0.476245 -0.348135 C -4.589637 -0.915440 -0.900457 H -3.511593 -2.698304 -0.286924 C -3.317841 1.152170 -0.805634 C -4.516403 0.476677 -1.083743 H -5.523075 -1.459200 -1.113420 H -3.256469 2.243597 -0.943378 H -5.392934 1.038501 -1.443423 C 0.848514 -2.479145 1.160249 C -0.164819 -3.630856 1.110936 H 1.055313 -2.094599 2.182522 H -0.283730 -4.174675 2.067669 C -0.953709 1.327307 -0.070793 C -0.049067 1.616350 -1.180495 C -1.105958 2.350625 0.957351 C 0.819564 2.767138 -1.057778 H -0.209882 1.144577 -2.164780 C -0.284477 3.459593 1.007692 H -1.896855 2.210501 1.710417 C 0.722125 3.637556 0.007488 H 1.526331 2.974840 -1.894643 H -0.386930 4.191936 1.821698 H 1.405901 4.498957 0.073563 O 1.736427 -0.481166 -1.866803 C 2.815960 -0.902248 -1.314603 O 2.945061 -0.722919 -0.049883 C 3.909376 -1.543098 -2.126759 H 4.655412 -0.767486 -2.400873 H 4.430384 -2.315414 -1.528925 H 3.497938 -1.976764 -3.057652 Cl 1.106697 0.773247 2.343249 C -1.131433 -1.730225 0.340166 O -1.426611 -2.974091 0.804828 H 1.816952 -2.708774 0.681157 H 0.048480 -4.360010 0.298041	Ru 0.389147 -0.395771 -0.135131 N -0.945323 -1.880629 -0.545485 C -1.909769 0.125384 -1.062309 C -0.797855 0.496325 -1.923800 C -2.824552 1.123296 -0.586426 C -0.642177 1.873283 -2.280058 H -0.373402 -0.259306 -2.604572 C -2.594615 2.459628 -0.940561 C -1.509209 2.832449 -1.774059 H 0.162000 2.150752 -2.979560 H -3.278239 3.232811 -0.556614 H -1.373255 3.894081 -2.036677 C -3.164680 -2.358755 -1.058516 C -2.440442 -3.585967 -0.456630 H -2.739919 -3.749673 0.602037 H -4.102678 -2.109056 -0.525091 C -4.027344 0.742855 0.203103 C -3.929554 -0.114054 1.325412 C -5.302536 1.226964 -0.175925 C -5.082148 -0.481093 2.038819 H -2.929826 -0.450688 1.651356 C -6.452622 0.856299 0.540561 H -5.390528 1.879996 -1.059211 C -6.347053 -0.003112 1.648903 H -4.987319 -1.138457 2.918205 H -7.438499 1.234460 0.225531 H -7.249077 -0.295911 2.209887 O 1.782707 -0.991740 -1.711015 C 2.386555 -1.734009 -0.859811 O 1.921845 -1.730515 0.342435 C 3.615067 -2.520930 -1.203990 H 4.502431 -1.886311 -0.993813 H 3.682297 -3.425019 -0.570011 H 3.614385 -2.789135 -2.277215 Cl -0.543753 -0.215007 2.046001 N 1.417295 1.292483 0.243325 C 3.829889 0.820356 0.510153 C 5.007957 1.017473 -0.250039 C 3.826286 -0.151146 1.540152 C 6.152114 0.243406 -0.001339 H 5.018098 1.773731 -1.051099 C 4.974704 -0.919312 1.786645 H 2.915706 -0.289042 2.140743 C 6.137852 -0.726784 1.019206 H 7.059427 0.396631 -0.606703 H 4.957777 -1.674450 2.587821 H 7.036967 -1.331689 1.217064 C 2.742853 3.206153 0.480852 C 1.306006 3.588668 0.117742 H 3.015207 3.453366 1.532457 H 0.866444 4.404035 0.724146 C 2.664100 1.700878 0.329124 C -2.084094 -1.328479 -0.861283 O -1.010188 -3.261343 -0.469265 O 0.541792 2.397610 0.388986 H 1.211078 3.839253 -0.965829 H 3.507799 3.665810 -0.177187 H -2.565466 -4.524610 -1.029948 H -3.401511 -2.466257 -2.141527

J'	B
Zero-point correction= 0.209326 (Hartree/Particle) Thermal correction to Energy= 0.225701 Thermal correction to Enthalpy= 0.226646 Thermal correction to Gibbs Free Energy= 0.163832 Sum of electronic and zero-point Energies= -1261.333190 Sum of electronic and thermal Energies= -1261.316814 Sum of electronic and thermal Enthalpies= -1261.315870 Sum of electronic and thermal Free Energies= -1261.378683 Solvent Energy = -1261.741639	Zero-point correction= 0.468987 (Hartree/Particle) Thermal correction to Energy= 0.501043 Thermal correction to Enthalpy= 0.501987 Thermal correction to Gibbs Free Energy= 0.405799 Sum of electronic and zero-point Energies= -1418.581648 Sum of electronic and thermal Energies= -1418.549592 Sum of electronic and thermal Enthalpies= -1418.548648 Sum of electronic and thermal Free Energies= -1418.644836 Solvent Energy = -1419.3309505
Ru -0.715868 -0.578611 0.472422 C 1.101061 1.509178 -0.177803 N -0.171507 1.247823 0.056400 C 2.024515 0.406339 -0.127092	C -0.759411 -1.442599 2.417768 Ru -0.477503 0.016997 -0.215978 C 0.403556 -0.345417 -2.217785 C -0.799187 0.432167 -2.364128

C	3.346411	0.410597	-0.613499
C	1.403258	-0.802367	0.369177
C	4.079635	-0.783199	-0.625430
H	3.775713	1.346961	-1.002766
C	2.179538	-1.991478	0.350031
C	3.487168	-1.978267	-0.155180
H	5.111905	-0.793204	-1.007230
H	1.746586	-2.924151	0.745095
H	4.066559	-2.915364	-0.173020
C	-0.935468	2.500881	0.083125
C	0.102209	3.501730	-0.489266
H	-1.853347	2.413956	-0.530920
H	0.191471	4.440190	0.090341
O	-0.814594	-1.103839	-1.607970
C	-2.070641	-0.834672	-1.628976
O	-2.600566	-0.432104	-0.528460
C	-2.888799	-0.977111	-2.881630
H	-3.772267	-1.615661	-2.680027
H	-3.267136	0.019413	-3.189816
H	-2.279536	-1.412259	-3.694713
Cl	-1.482475	-0.205327	2.650559
H	0.721708	-0.717271	1.401643
H	-0.083961	3.745023	-1.557294
H	-1.239962	2.713280	1.130744
O	1.391379	2.803944	-0.412776

C	-2.012604	-0.030319	-1.775271
C	-2.100561	-1.275369	-1.059677
C	-0.882498	-2.019640	-0.910088
C	0.348434	-1.594750	-1.510800
H	-0.773328	1.425302	-2.834743
H	-2.883256	0.640205	-1.808854
H	-0.892972	-2.905751	-0.258029
H	1.270384	-2.173463	-1.355478
C	-3.424249	-1.778053	-0.504590
H	-3.178100	-2.620257	0.171964
C	1.698776	0.158175	-2.801462
H	2.576525	-0.348013	-2.357649
C	-0.313358	-1.508277	3.881042
H	-0.703274	-2.426718	4.358676
H	0.790187	-1.460315	3.970152
O	-0.726859	-0.625970	4.412977
O	-0.025842	-0.599624	1.722218
O	-1.711319	-2.109618	2.000836
C	2.124697	3.486914	0.289600
C	0.760941	2.794368	0.422229
H	0.006880	3.129216	-0.315515
N	1.091823	1.366562	0.201707
C	-4.163210	-0.726047	0.337842
H	-4.429132	0.174232	-0.257101
H	-5.108453	-1.151551	0.733810
H	-3.527824	-0.412214	1.187528
C	-4.290210	-2.300891	-1.670894
H	-3.759692	-3.079148	-2.258898
H	-5.233233	-2.744329	-1.287905
H	-4.563418	-1.478516	-2.367482
H	1.807364	1.250598	-2.645911
H	1.705806	-0.027178	-3.896957
O	-1.652032	1.321198	0.902264
C	-2.341376	2.313451	0.393340
O	-2.253218	2.753876	-0.764446
C	-3.312041	2.913373	1.411721
H	-2.793319	3.120805	2.369137
H	-3.768929	3.837440	1.011640
H	-4.107067	2.170169	1.629621
H	2.328602	4.257496	1.057307
C	3.223178	0.026063	0.245254
C	4.510631	0.125138	-0.336268
C	2.771487	-1.216067	0.745082
C	5.316135	-1.016243	-0.459411
H	4.862674	1.100326	-0.703823
C	3.590463	-2.349771	0.626219
H	1.784243	-1.264153	1.233030
C	4.855001	-2.258144	0.015726
H	6.310345	-0.936475	-0.926354
H	3.237206	-3.315278	1.021712
H	5.489457	-3.153769	-0.079386
O	3.078439	2.400198	0.470804
C	2.387840	1.239370	0.311552
H	0.309421	2.887516	1.432222
H	2.294306	3.923141	-0.720017

5 Imidazole:

B'	TS-B'-C'
Zero-point correction= 0.276161 (Hartree/Particle)	Zero-point correction= 0.275355 (Hartree/Particle)
Thermal correction to Energy= 0.297996	Thermal correction to Energy= 0.296656
Thermal correction to Enthalpy= 0.298940	Thermal correction to Enthalpy= 0.297600
Thermal correction to Gibbs Free Energy= 0.224327	Thermal correction to Gibbs Free Energy= 0.223846
Sum of electronic and zero-point Energies= -1047.723047	Sum of electronic and zero-point Energies= -1047.693226
Sum of electronic and thermal Energies= -1047.701212	Sum of electronic and thermal Energies= -1047.671925
Sum of electronic and thermal Enthalpies= -1047.700268	Sum of electronic and thermal Enthalpies= -1047.670981
Sum of electronic and thermal Free Energies= -1047.774881	Sum of electronic and thermal Free Energies= -1047.744735
Solvent Energy = -1048.193617	Solvent Energy = -1048.162873
C	2.911500
Ru	0.529206
C	4.371901
H	4.860228
H	4.496294
H	4.860694
O	2.046226
O	2.490506
C	-1.964909
C	-2.345790
N	-1.363826
O	1.057114
C	0.371872
O	-0.262497
C	0.354520
H	0.448544
H	-0.571352
H	1.223328
C	-1.004186
C	-1.149677
C	0.045344
C	-0.251040
H	-1.953121
C	0.927409
H	-0.071479
C	0.805838
H	-0.344488
H	1.701962
H	1.507363
C	-3.579386
H	-4.601560
H	-2.122263
N	-3.322960
C	-4.307862
H	-3.789362
H	-4.836036
H	-5.050316
C	-2.823599
Ru	-0.675531
C	-4.198069
H	-4.291874
H	-4.972982
H	-4.382806
O	-2.099294
O	-2.474811
C	2.213388
C	2.885701
C	1.502347
H	0.782847
N	1.098158
O	-1.745923
C	-1.851593
O	-1.236260
C	-2.662125
H	-2.257541
H	-3.706312
H	-2.676566
H	3.584992
C	2.016994
C	2.831190
C	0.726975
C	2.380127
H	3.789990
C	0.298032
C	0.260111
C	1.104904
H	3.017155
H	-0.662678
H	0.751722
N	3.325118
C	4.705216
H	4.738006
H	5.163659
H	5.296068
C	1.446862
C	-0.192408
C	2.098789
C	2.886742
C	1.325807
C	2.516578
C	1.555506
C	0.764463
C	-0.402520
C	-2.492074
C	-2.469476
C	-3.290929
N	-1.168355
O	-1.860347
C	-2.275169
C	-1.559785
C	-3.479151
H	-3.946779
C	-3.159786
C	-4.203053
C	-3.312828
C	1.011283
C	1.821326
C	1.498633
C	3.092702
C	1.435464
C	2.783487
C	1.092853
C	3.555192
H	3.713058
H	3.157938
H	4.539359
N	-1.183973
C	-0.725113
H	0.303814
H	-0.725171
H	-1.388149
C	-0.657495
C	0.056582
C	-0.584297
C	-1.354995
C	-0.771224
C	0.425220
C	-1.672245
C	0.395658
C	-0.274981
C	-0.625753
C	-0.521396
C	-0.602464
N	-0.305535
O	-0.583830
C	0.630866
C	1.504531
C	1.000566
H	1.918336
C	1.202367
C	0.163482
C	-0.817239
C	-0.007082
C	0.806200
C	-0.454873
C	1.208998
H	1.185955
C	-0.025674
C	-1.400023
C	0.824308
H	1.858826
H	-0.407934
H	1.170180
N	-0.472012
C	-0.514389
H	-0.922060
H	0.497137
H	-1.175259

C'	D'
Zero-point correction= 0.276651 (Hartree/Particle)	Zero-point correction= 0.215126 (Hartree/Particle)
Thermal correction to Energy= 0.298890	Thermal correction to Energy= 0.231363
Thermal correction to Enthalpy= 0.299834	Thermal correction to Enthalpy= 0.232307

Thermal correction to Gibbs Free Energy= 0.223602 Sum of electronic and zero-point Energies= -1047.694054 Sum of electronic and thermal Energies= -1047.671816 Sum of electronic and thermal Enthalpies= -1047.670871 Sum of electronic and thermal Free Energies= -1047.747104 Solvent Energy = -1048.16844	Thermal correction to Gibbs Free Energy= 0.170231 Sum of electronic and zero-point Energies= -818.803076 Sum of electronic and thermal Energies= -818.786839 Sum of electronic and thermal Enthalpies= -818.785895 Sum of electronic and thermal Free Energies= -818.847971 Solvent Energy = -819.1074836
Ru -1.901961 -1.794828 1.464026 C 1.230039 -0.265745 -1.167374 C -3.231252 -2.527572 1.489276 H -4.003637 -1.889729 1.955238 H -3.526107 -2.768686 0.447482 H -3.138697 -3.486732 2.036861 O -0.901387 -2.609123 1.086039 O -1.764310 -0.610715 1.740908 C -1.804237 -0.968100 -1.839692 H -1.605613 -1.871516 -2.426062 N -0.788411 -0.167127 -1.357589 O 1.470804 -1.529074 0.406812 C 2.762948 -1.338870 0.511333 O 3.282249 -0.596501 -0.371175 C 3.515375 -1.945822 1.657391 H 3.082500 -2.926967 1.932289 H 4.585845 -2.046903 1.399076 H 3.424842 -1.273043 2.536641 C -0.469067 1.777580 0.008336 C -0.802058 2.946658 0.721367 C 0.905526 1.350522 -0.110079 C 0.208588 3.704623 1.338512 H -1.846670 3.279707 0.803606 C 1.898616 2.125990 0.533579 H -0.045329 -2.095484 1.001995 C 1.551497 3.291668 1.243595 H -0.054452 4.616662 1.896568 H 2.953035 1.810667 0.473409 H 2.342177 3.886487 1.730735 C -1.362992 0.858528 -0.672903 C -3.015320 -0.428997 -1.439946 H -4.046605 -0.750884 -1.616410 C -3.680850 1.471071 0.084559 H -3.406240 1.374352 1.154957 H -3.697569 2.539252 -0.210482 H -4.690077 1.046195 -0.070180 N -2.725425 0.721125 -0.716417	Ru -0.903268 -0.736951 -0.613756 C 1.690088 -2.510912 -0.020937 H 1.210837 -3.488812 -0.139247 N 0.991212 -1.329319 -0.172183 O -2.985761 -0.043420 -0.647878 C -3.054878 -0.364379 0.581952 O -1.987499 -0.897076 1.101334 C -4.263149 -0.108118 1.435787 H -5.178322 -0.124854 0.814288 H -4.328182 -0.851353 2.253114 H -4.169116 0.900158 1.892221 C 1.321143 1.040724 -0.013032 C 2.002195 2.262972 0.174038 C -0.101111 1.015886 -0.291676 C 1.296631 3.476669 0.112400 C 3.084938 2.285217 0.367103 C -0.781758 2.258220 -0.334815 C -0.090661 3.467694 -0.138385 H 1.829487 4.428888 0.259783 H -1.864901 2.269044 -0.538002 H -0.641985 4.421734 -0.186490 C 1.862555 -0.305650 0.047084 C 3.004338 -2.211858 0.293016 H 3.869596 -2.854106 0.486765 N 3.102276 -0.824624 0.332632 C 4.309820 -0.073320 0.636398 H 4.601975 0.568096 -0.220146 H 4.157475 0.568018 1.528369 H 5.132373 -0.782177 0.845706

E'	TS-E'-F'
Zero-point correction= 0.304759 (Hartree/Particle) Thermal correction to Energy= 0.327834 Thermal correction to Enthalpy= 0.328778 Thermal correction to Gibbs Free Energy= 0.251831 Sum of electronic and zero-point Energies= -1510.371513 Sum of electronic and thermal Energies= -1510.348438 Sum of electronic and thermal Enthalpies= -1510.347494 Sum of electronic and thermal Free Energies= -1510.424441 Solvent Energy = -1510.883199	Zero-point correction= 0.303878 (Hartree/Particle) Thermal correction to Energy= 0.326661 Thermal correction to Enthalpy= 0.327606 Thermal correction to Gibbs Free Energy= 0.251234 Sum of electronic and zero-point Energies= -1510.356600 Sum of electronic and thermal Energies= -1510.333816 Sum of electronic and thermal Enthalpies= -1510.332872 Sum of electronic and thermal Free Energies= -1510.409243 Solvent Energy = -1510.869937
Ru 0.943813 -0.121383 -0.241602 C -1.872323 0.001885 -0.851464 N -0.783122 -0.768608 -1.093677 C -1.670578 1.175374 -0.029051 C -2.629209 2.133196 0.378441 C -0.290101 1.301514 0.361769 C -2.233183 3.229418 1.157242 H -3.686094 2.034306 0.090589 C 0.078876 2.424359 1.135942 C -0.879181 3.375029 1.527110 H -2.978746 3.975176 1.474294 H 1.131783 2.543489 1.437692 H -0.569680 4.242057 2.134329 C -1.164728 -1.813263 -1.906663 C -2.514880 -1.679641 -2.177148 H -0.454708 -2.581753 -2.229630 H -3.197010 -2.286005 -2.782004 C 0.761427 -1.857163 0.939922 C 1.257010 -0.805845 1.811322 C -0.501800 -2.500135 1.205509 C 0.371453 -0.353211 2.859801 H 2.341356 -0.644259 1.925396 C -1.325311 -1.977228 2.183522 H -0.808254 -3.361730 0.595410 C -0.894675 -0.885761 3.008144 H 0.732334 0.426352 3.548138 H -2.318959 -2.423803 2.347847 H -1.564643 -0.504137 3.793939 O 2.745940 1.066535 -0.007638 C 2.602010 1.506815 -1.202827 O 1.597644 1.071607 -1.882163 C 3.540767 2.528181 -1.782789 H 3.584701 2.431990 -2.884206 H 3.157285 3.541263 -1.538169 H 4.547960 2.421799 -1.337056 Cl 1.997193 -2.799630 -0.024867 N -2.951420 -0.537911 -1.511374 C -4.304930 -0.007082 -1.538492 H -4.313714 1.022806 -1.950185 H -4.932416 -0.651329 -2.182034 H -4.741970 0.010187 -0.519094	Ru -0.853622 -0.057344 -0.112563 C 1.934354 -0.149904 -0.864699 N 0.742530 0.341530 -1.281637 C 1.943121 -0.851505 0.404231 C 3.054012 -1.400195 1.085204 C 0.612536 -0.956393 0.948929 C 2.856548 -2.068847 2.303067 H 4.073115 -1.310201 0.681248 C 0.451172 -1.647277 2.168584 C 1.559056 -2.194178 2.841292 H 3.719810 -2.496547 2.836779 H -0.561097 -1.753471 2.591041 H 1.414617 -2.723596 3.797567 C 0.901032 0.907301 -2.525620 C 2.229646 0.763774 -2.884317 H 0.048657 1.353970 -3.050139 H 2.772337 1.065485 -3.786249 C -0.794998 1.832142 0.276443 C -1.463216 1.524381 1.492617 C 0.125189 2.892319 0.139068 C -0.945075 2.125470 2.681580 H -2.435935 1.006688 1.514285 C 0.563427 3.495498 1.318634 H 0.546288 3.156470 -0.841890 C 0.060433 3.085615 2.588386 H -1.415350 1.897790 3.651481 H 1.339106 4.272725 1.270450 H 0.436000 3.577937 3.499105 O -2.379029 -1.395496 0.634413 C -2.232723 -2.124296 -0.410451 O -1.307416 -1.791859 -1.244075 C -3.129633 -2.294392 -0.686499 H -3.999316 -2.930614 -1.273107 H -2.597972 -4.056065 -1.287658 H -3.501108 -3.727298 0.261372 Cl -2.587048 1.107866 -1.595431 N 2.869971 0.100927 -1.838596 C 4.272227 -0.287080 -1.813943 H 4.809558 0.223380 -0.988714 H 4.370173 -1.838878 -1.683422 H 4.741822 -0.000847 -2.773145

F'	TS-F'G'
Zero-point correction= 0.304668 (Hartree/Particle) Thermal correction to Energy= 0.328428 Thermal correction to Enthalpy= 0.329372 Thermal correction to Gibbs Free Energy= 0.250152 Sum of electronic and zero-point Energies= -1510.380616 Sum of electronic and thermal Energies= -1510.356857 Sum of electronic and thermal Enthalpies= -1510.355912 Sum of electronic and thermal Free Energies= -1510.435133 Solvent Energy = -1510.890911	Zero-point correction= 0.303833 (Hartree/Particle) Thermal correction to Energy= 0.326745 Thermal correction to Enthalpy= 0.327690 Thermal correction to Gibbs Free Energy= 0.251057 Sum of electronic and zero-point Energies= -1510.351289 Sum of electronic and thermal Energies= -1510.328376 Sum of electronic and thermal Enthalpies= -1510.327432 Sum of electronic and thermal Free Energies= -1510.404065 Solvent Energy = -1510.870781
Ru 0.636390 -0.604639 -0.082438 C -1.840833 0.806705 0.685418 N -0.598529 0.537502 1.138972 C -2.181094 0.213831 -0.584796	Ru 0.258363 -1.052801 0.019700 C 0.888360 1.663181 -0.622494 N 1.139582 0.379002 -0.982933 C 0.126748 1.859063 0.584236

C	-3.385801	0.305696	-1.313414
C	-1.079608	-0.565311	-1.087693
C	-3.511779	-0.387143	-2.528088
H	-4.229500	0.904618	-0.941023
C	-1.248646	-1.291069	-2.289608
C	-2.451234	-1.180949	-3.009867
H	-4.451009	-0.317552	-3.098798
H	-0.428438	-1.919265	-2.664402
H	-2.564197	-1.729266	-3.958851
C	-0.419298	1.199024	2.327932
C	-1.588701	1.884640	2.617616
H	0.519931	1.136811	2.886235
H	-1.864524	2.518729	3.466779
C	1.585179	1.134421	-0.339589
C	0.933247	2.310911	-0.784775
C	2.979904	1.178556	-0.084013
C	1.661591	3.496196	-0.987641
H	-0.148187	2.295192	-0.995534
C	3.694220	2.375899	-0.256224
H	3.510087	0.270425	0.244944
C	3.040974	3.536557	-0.714278
H	1.144641	4.397687	-1.356032
H	4.776269	2.397814	-0.046925
H	3.608434	4.469225	-0.862104
Cl	2.083506	-1.775673	-1.470868
O	1.057732	-1.421218	1.730232
C	0.478728	-2.597041	1.625815
O	-0.242558	-2.829036	0.636388
C	0.778327	-3.598261	2.714598
H	-0.013032	-4.370061	2.740177
H	1.746456	-4.089016	2.481974
H	0.874845	-3.100437	3.698673
N	-2.478383	1.632632	1.579301
C	-3.832688	2.153213	1.466241
H	-4.569779	1.325262	1.433791
H	-4.049906	2.786727	2.345924
H	-3.940769	2.769506	0.550520

C	0.102016	3.035728	1.368608
C	-0.476054	0.621030	1.062126
C	-0.422932	3.012374	2.664237
H	0.554346	3.963516	0.988531
C	-0.894068	0.624881	2.428962
C	-0.876162	1.784672	3.202119
H	-0.438881	3.929063	3.273035
H	-1.284276	-0.303278	2.871468
H	-1.230270	1.740034	4.244544
C	1.937911	0.371184	-2.105839
C	2.174731	1.690033	-2.452005
C	-1.709362	-0.222066	0.044379
C	-2.585491	-1.135385	0.699637
C	-2.243861	0.569396	-1.006177
C	-3.925905	-1.253539	0.313937
H	-2.206664	-1.775692	1.515854
C	-3.591589	0.467011	-1.370588
H	-1.584235	1.267904	-1.543072
C	-4.442645	-0.443092	-0.715840
H	-4.574952	-1.984075	0.822888
H	-3.980532	1.094486	-2.188770
H	-5.500647	-0.526171	-1.009389
O	1.516838	-1.195384	1.755504
C	3.248366	-1.953173	1.127178
O	2.066508	-2.241923	-0.087600
C	3.606260	-2.440152	1.789335
H	3.428767	-2.612005	2.868347
H	3.967153	-3.363188	1.298204
H	4.389346	-1.658756	1.692429
Cl	-0.503287	-1.985905	-1.993150
H	2.242531	-0.562661	-2.586924
H	2.733475	2.123158	-3.287886
N	1.509159	2.491141	-1.528379
C	1.487857	3.945200	-1.527763
H	0.457195	4.309562	-1.347532
H	2.159137	4.360403	-0.746852
H	1.823405	4.310719	-2.516436

G'	I'
Zero-point correction= 0.306383 (Hartree/Particle)	Zero-point correction= 0.484036 (Hartree/Particle)
Thermal correction to Energy= 0.329300	Thermal correction to Energy= 0.517989
Thermal correction to Enthalpy= 0.330244	Thermal correction to Enthalpy= 0.518933
Thermal correction to Gibbs Free Energy= 0.253367	Thermal correction to Gibbs Free Energy= 0.418793
Sum of electronic and zero-point Energies= -1510.389080	Sum of electronic and zero-point Energies= -2006.519936
Sum of electronic and thermal Energies= -1510.366163	Sum of electronic and thermal Energies= -2006.485983
Sum of electronic and thermal Enthalpies= -1510.365219	Sum of electronic and thermal Enthalpies= -2006.485038
Sum of electronic and thermal Free Energies= -1510.442097	Sum of electronic and thermal Free Energies= -2006.585179
Solvent Energy = -1510.915361	Solvent Energy = -2007.321116
Ru 1.182612 -0.386726 -0.330115	Ru 0.259252 -0.494878 0.294037
N -0.320038 -1.043717 0.774041	C -2.082200 -1.393195 -0.523216
C -2.114481 0.532770 0.069434	N -1.151355 -2.047627 0.180116
C -3.464795 0.528970 -0.358348	C -1.642761 -0.048867 -0.948553
C -1.229333 1.541867 -0.410192	C -0.401946 -0.029515 -1.734649
C -3.945944 1.515124 -1.230859	C -2.446609 1.154527 -0.821384
H -4.136369 -0.285438 -0.050431	C 0.000948 1.228235 -2.316085
C -1.731723 2.514930 -1.296992	H -0.081983 -0.954026 -2.246420
C -3.075805 2.512187 -1.704331	C -1.957024 2.339145 -1.367286
H -4.997063 1.490567 -1.558133	C -0.726404 2.381477 -2.093391
H -1.046744 3.297968 -1.658372	H 0.899401 1.251715 -2.953480
H -3.442965 3.288046 -2.394394	H -2.540309 3.264260 -1.237538
C -0.181875 -2.103908 1.652708	C -0.382514 3.341641 -2.509525
C -1.363240 -2.232853 2.353836	C -1.669437 -3.267068 0.540687
H 0.761321 -2.653098 1.729158	C -2.958453 -3.350995 0.027884
H -1.652133 -2.919811 3.155633	H -1.110032 -3.994764 1.138228
C 0.203414 1.625416 0.028303	H -3.708865 -4.146770 0.078870
C 1.246535 1.709784 -0.975829	C -3.801040 1.108060 -0.205153
C 0.498597 2.120529 1.349544	C -4.046485 0.433211 1.015319
C 2.511236 2.299685 -0.632792	C -4.894502 1.710881 -0.874958
H 0.961050 1.620483 -2.040046	C -5.347318 0.359735 1.538413
C 1.745971 2.652689 1.658583	H -3.192263 0.004690 1.564569
H -0.295424 2.081116 2.112581	C -6.194835 1.633979 -0.349584
C 2.753565 2.751488 0.662214	H -4.720575 2.218010 -1.837764
H 3.286487 2.390138 -1.409713	C -6.428382 0.951586 0.858161
H 1.953022 3.000486 2.682023	H -5.515152 -0.161033 2.494925
H 3.735409 3.177033 0.920476	H -7.032426 2.101209 -0.892321
O 0.072897 -0.933575 -2.112227	H -7.448468 0.885503 1.269502
C 0.527057 -2.127247 -2.013223	O 1.631661 -1.855252 -0.713844
O 1.336697 -2.378271 -1.038977	C 2.151947 -2.156998 0.418712
C 0.120891 -3.212904 -2.971740	O 1.713004 -1.527329 1.448356
H 0.982062 -3.875307 -3.185524	C 3.255750 -3.168386 0.539748
H -0.672983 -3.831364 -2.502525	H 4.226918 -2.631403 0.545365
H -0.275968 -2.773041 -3.905617	H 3.163624 -3.726369 1.491443
Cl 2.743602 -0.495840 1.420343	H 3.243256 -3.857735 -0.325051
C -1.571138 -0.537540 0.903317	Cl -0.886067 0.360092 2.201723
N -2.223298 -1.248677 1.890781	C 2.763206 1.438520 0.317070
C -3.540236 -0.976717 2.452231	C 0.852169 2.458149 0.703371
H -4.333766 -1.560291 1.940107	N 1.429336 1.238918 0.382250
H -3.536458 -1.247370 3.525858	C 3.816989 0.498977 -0.110576
H -3.771191 0.100994 2.358851	C 3.746535 -0.106068 -1.385841
	C 4.952339 0.262143 0.700429
	C 4.796579 -0.915794 -1.845300
	H 2.855239 0.063145 -2.004808
	C 6.006546 -0.539816 0.234059
	H 4.995633 0.702069 1.708620
	C 5.932994 -1.126570 -1.043339
	H 4.725885 -1.384931 -2.838978
	H 6.883976 -0.718024 0.875529
	H 6.757853 -1.758542 -1.408762
	C 1.842105 3.406568 0.845771
	H 1.797022 4.470850 1.098692
	H -0.229782 2.550626 0.835657
	N 3.043477 2.762093 0.603418
	N -3.205697 -2.163826 -0.654990
	C -4.430700 -1.814771 -1.360751
	H -5.205483 -1.450831 -0.655214
	H -4.211775 -1.003789 -2.078859
	H -4.805571 -2.698989 -1.912703
	C 4.351057 3.402495 0.604694
	H 4.823618 3.361289 1.608429
	H 5.018524 2.898307 -0.119627
	H 4.236231 4.462823 0.307135

J'	B
Zero-point correction= 0.226497 (Hartree/Particle) Thermal correction to Energy= 0.243870 Thermal correction to Enthalpy= 0.244814 Thermal correction to Gibbs Free Energy= 0.180279 Sum of electronic and zero-point Energies= -1279.557072 Sum of electronic and thermal Energies= -1279.539699 Sum of electronic and thermal Enthalpies= -1279.538755 Sum of electronic and thermal Free Energies= -1279.603290 Solvent Energy = -1279.96349	Zero-point correction= 0.485987 (Hartree/Particle) Thermal correction to Energy= 0.519114 Thermal correction to Enthalpy= 0.520058 Thermal correction to Gibbs Free Energy= 0.421746 Sum of electronic and zero-point Energies= -1436.804464 Sum of electronic and thermal Energies= -1436.771338 Sum of electronic and thermal Enthalpies= -1436.770393 Sum of electronic and thermal Free Energies= -1436.868706 Solvent Energy = -1437.551446
Ru 1.025463 -0.498952 -0.380292 C -1.356064 1.057297 -0.063829 N -0.013523 1.153540 -0.259560 C -1.914362 -0.271538 0.055286 C -3.184924 -0.630757 0.552861 C -0.945572 -1.297770 -0.277498 C -3.522176 -1.982910 0.718830 H -3.908465 0.142260 0.849968 C -1.324818 -2.655390 -0.110821 C -2.588653 -2.989976 0.393889 H -4.513836 -2.254237 1.112158 H -0.610546 -3.446469 -0.389526 H -2.856752 -4.049931 0.529293 C 0.327962 2.485213 -0.352949 C -0.835597 3.224731 -0.222342 H 1.361406 2.803697 -0.520509 H -1.006727 4.305693 -0.251836 O 1.114283 -0.570288 1.769645 C 2.259395 0.010497 1.748954 O 2.748278 0.302575 0.595933 C 2.996870 0.348010 3.014925 H 4.049122 0.009025 2.938298 H 3.012222 1.449959 3.145974 H 2.503211 -0.119266 3.886691 Cl 1.805285 -0.363303 -2.578050 H -0.278572 -1.129935 -1.302999 C -3.285257 2.679208 0.105455 H -3.908002 2.069557 -0.579185 H -3.627463 2.516150 1.148599 H -3.419133 3.746699 -0.150648 N -1.881902 2.327728 -0.048695	C -0.897992 1.232353 -2.494851 Ru -0.596335 -0.011389 0.249441 C 0.195115 0.550481 2.238133 C -0.958691 -0.294124 2.408195 C -2.179494 0.038080 1.750046 C -2.325683 1.222865 0.943982 C -1.153447 2.035283 0.773395 C 0.086151 1.736207 1.433223 H -0.878149 -1.248845 2.947305 H -3.001639 -0.690347 1.802660 H -1.200132 2.865940 0.053572 H 0.979197 2.351043 1.243429 C -3.659470 1.583031 0.306061 H -3.451612 2.401924 -0.410688 C 1.499466 0.165302 2.887673 H 2.343088 0.762325 2.494876 C -0.447299 1.171881 -3.958011 H -0.892879 2.006404 -4.531288 H 0.658137 1.190748 -4.042119 H -0.792581 0.210461 -4.392196 O -0.146623 0.477737 -1.724250 O -1.867130 1.914748 -2.146365 C 2.389760 -1.011690 -0.210135 C 2.189278 -3.239684 -0.113131 C 0.952188 -2.661408 0.085920 H -0.012422 -3.124358 0.322698 N 1.083839 -1.287187 0.007037 C -4.272073 0.425842 -0.500678 H -4.497260 -0.455285 0.137944 H -5.225680 0.749913 -0.966633 H -3.571955 0.108925 -1.296504 C -4.620163 2.096358 1.399790 H -4.185490 2.951114 1.959448 H -5.578681 2.431681 0.950761 H -4.855189 1.295399 2.134271 H 1.718730 -0.909229 2.722730 H 1.430732 0.332184 3.983784 N 3.085315 -2.201494 -0.304636 C 4.492262 -2.380020 -0.645896 H 4.591911 -3.232354 -1.346138 H 4.874500 -1.467465 -1.138770 H 5.105540 -2.583024 0.256528 O -1.642713 -1.454366 -0.822647 C -2.261745 -2.473438 -0.283482 O -2.173273 -2.846360 0.899252 C -3.135688 -3.212665 -1.298170 H -2.529668 -3.508372 -2.178444 H -3.594306 -4.105330 -0.833937 H -3.928580 -2.528933 -1.665556 H 2.502433 -4.288170 -0.149037 C 3.058043 0.305307 -0.200581 C 4.192705 0.501846 0.626895 C 2.564564 1.393143 -0.955554 C 4.816432 1.757031 0.699923 H 4.563842 -0.324145 1.253465 C 3.190015 2.647636 -0.873432 H 1.669520 1.230665 -1.576390 C 4.314358 2.836549 -0.049485 H 5.689544 1.895974 1.356866 H 2.791046 3.488087 -1.463423 H 4.799052 3.823889 0.011706

6 Imine:

B'	TS-B'-C'
Zero-point correction= 0.325418 (Hartree/Particle) Thermal correction to Energy= 0.349994 Thermal correction to Enthalpy= 0.350938 Thermal correction to Gibbs Free Energy= 0.269558 Sum of electronic and zero-point Energies= -1147.091448 Sum of electronic and thermal Energies= -1147.066873 Sum of electronic and thermal Enthalpies= -1147.065929 Sum of electronic and thermal Free Energies= -1147.147309 Solvent Energy = -1147.609204	Zero-point correction= 0.324606 (Hartree/Particle) Thermal correction to Energy= 0.348625 Thermal correction to Enthalpy= 0.349569 Thermal correction to Gibbs Free Energy= 0.269752 Sum of electronic and zero-point Energies= -1147.059847 Sum of electronic and thermal Energies= -1147.035828 Sum of electronic and thermal Enthalpies= -1147.034883 Sum of electronic and thermal Free Energies= -1147.114701 Solvent Energy = -1147.577063
C -2.038465 -2.176911 -0.787168 Ru -0.584280 -0.328636 0.092163 C -2.801781 -3.377165 -1.282081 H -3.837955 -3.356335 -0.894488 H -2.796088 -3.413287 -2.387944 H -2.307881 -4.295537 -0.900634 O -1.072995 -1.681661 -1.487852 O -2.295590 -1.639216 0.341684 C 0.514955 2.015996 -0.439226 N 1.013511 0.799802 -0.424641 O 0.509166 -1.756927 1.233531 C 0.494230 -0.975711 2.253023 O -0.068476 0.171191 2.108224 C 1.080305 -1.402884 3.569684 H 2.014648 -1.972905 3.402269 H 1.268587 -0.523902 4.213831 H 0.359327 -2.073824 4.082316 C -0.957349 1.837285 -0.241941 C -1.726289 2.588501 0.718222 C -1.653351 1.045885 -1.256480 C -3.104743 2.479727 0.745429 H -1.195512 3.217787 1.448887 C -3.093411 1.007779 -1.203650 H -1.159204 0.826606 -2.218586 C -3.795500 1.668789 -0.212141 H -3.681450 3.027556 1.507537 H -3.628763 0.443633 -1.984006 H -4.893980 1.601782 -0.173997 C 2.358764 0.388993 -0.584828 C 3.421862 1.038844 0.080038	C 2.494057 -2.321889 0.474923 Ru 0.497498 -0.459743 -0.096958 C 3.423830 -3.514629 0.301200 H 4.187816 -3.525293 1.101351 H 2.825305 -4.446900 0.376068 H 3.902572 -3.502532 -0.697560 O 2.359395 -1.753597 1.583353 O 1.845713 -1.956057 -0.591582 C -0.283564 2.267470 0.325975 N -0.795204 1.045244 0.334393 O -0.864536 -1.977501 0.299748 C -1.315076 -1.919874 -0.903150 O -0.713249 -1.069054 -1.662919 C -2.516634 -2.688215 -1.348306 H -2.499637 -2.829235 -2.445310 H -2.563675 -3.662847 -0.826620 H -3.419211 -2.098538 -1.075590 C 1.174104 2.246330 0.133586 C 1.872917 3.236453 -0.594279 C 1.897416 1.100824 0.639118 C 3.241622 3.085871 -0.859939 H 1.327405 4.108394 -0.988111 C 3.289173 0.983774 0.373620 H 1.494974 0.513675 1.517680 C 3.944012 1.949155 -0.398132 H 3.768908 3.853477 -1.448158 H 3.821093 0.120467 0.799540 H 5.014798 1.835365 -0.628893 C -2.198284 0.792640 0.393755 C -3.025018 1.149508 -0.692878

C	2.610268	-0.755840	-1.373169
C	4.734204	0.561711	-0.075108
H	3.211553	1.890478	0.743484
C	3.924997	-1.215294	-1.529917
H	1.756576	-1.270006	-1.840849
C	4.991008	-0.557989	-0.885554
H	5.560856	1.065309	0.450669
H	4.119130	-2.102964	-2.152200
H	6.021312	-0.928550	-1.003794
C	1.216019	3.321599	-0.642311
H	1.403928	3.827022	0.331874
H	2.192806	3.189878	-1.149103
H	0.574675	4.001644	-1.239564

C	-2.731992	0.066116	1.477967
C	-4.384308	0.796151	-0.682723
H	-2.582283	1.677446	-1.550815
C	-4.092719	-0.276020	1.483641
C	-2.060346	-0.241451	2.292644
C	-4.922660	0.084377	0.404760
H	-5.024254	1.072363	-1.535608
H	-4.506059	-0.840295	2.334247
H	-5.987943	-0.194692	0.409634
C	-1.069738	3.541238	0.446814
H	-1.236098	4.005584	-0.551167
H	-2.066342	3.358822	0.893446
H	-0.521925	4.282170	1.064111

C'	D'
Zero-point correction= 0.326322 (Hartree/Particle) Thermal correction to Energy= 0.350979 Thermal correction to Enthalpy= 0.351924 Thermal correction to Gibbs Free Energy= 0.271146 Sum of electronic and zero-point Energies= -1147.064558 Sum of electronic and thermal Energies= -1147.039900 Sum of electronic and thermal Enthalpies= -1147.038956 Sum of electronic and thermal Free Energies= -1147.119733 Solvent Energy = -1147.584206	Zero-point correction= 0.264046 (Hartree/Particle) Thermal correction to Energy= 0.283333 Thermal correction to Enthalpy= 0.284277 Thermal correction to Gibbs Free Energy= 0.214287 Sum of electronic and zero-point Energies= -918.168090 Sum of electronic and thermal Energies= -918.148803 Sum of electronic and thermal Enthalpies= -918.147859 Sum of electronic and thermal Free Energies= -918.217849 Solvent Energy = -918.5223355
C 1.873028 -0.057173 2.285653 Ru -0.089022 -0.784836 -1.216475 C 2.453821 1.267471 2.721206 H 3.449039 1.111665 3.175290 H 2.576398 1.888929 1.808283 H 1.777621 1.803063 3.414801 O 0.525194 -0.022371 2.196768 O 2.540603 -1.043282 2.003146 N -1.147321 0.789028 -0.578671 O -0.053848 -1.959537 0.437327 C 0.829487 -2.811421 -0.048398 O 1.160279 -2.623675 -1.254000 C 1.409569 -3.851576 0.850329 H 0.616563 -4.317900 1.467373 H 1.954933 -4.612319 0.263225 H 2.104652 -3.314343 1.531545 C 0.925572 1.829192 -0.694687 C 1.858438 2.889351 -0.642478 C 1.367476 0.473604 -0.930067 C 3.230774 2.620379 -0.771981 H 1.513468 3.924771 -0.486532 C 2.756682 0.223316 -1.010257 H 0.245241 -0.852904 1.707098 C 3.672497 1.289337 -0.943292 H 3.960802 3.443447 -0.727767 H 3.115038 -0.810157 -1.135207 H 4.751720 1.080798 -1.027405 C -0.501384 1.944804 -0.426296 C -1.146086 3.207553 0.063921 H -2.248911 3.125904 0.092866 H -0.788863 3.454490 1.087382 H -0.869642 4.061798 -0.589368 C -2.465447 0.560588 -0.091795 C -3.505310 0.236509 -0.989527 C -2.710198 0.576479 1.299357 C -4.786946 -0.055906 -0.496414 H -3.293634 0.224342 -2.070344 C -3.993897 0.276136 1.782018 H -1.873995 0.797512 1.980379 C -5.034919 -0.037888 0.888984 H -5.598652 -0.299824 -1.199936 H -4.180573 0.280842 2.867710 H -6.039766 -0.274147 1.272624	Ru -0.405723 -0.705736 -0.666186 N 0.860963 0.709576 -0.019927 O -1.815444 -2.380624 -0.869827 C -1.473377 -2.736033 0.302406 O -0.557981 -2.012845 0.883907 C -2.101705 -3.884117 1.036985 H -2.446694 -4.651369 0.318494 H -1.389969 -4.317696 1.764953 H -2.984241 -3.508803 1.597464 C -1.099474 1.936683 0.179938 C -1.911798 3.064215 0.434801 C -1.694093 0.665729 -0.168095 C -3.309846 2.948922 0.381136 H -1.450134 4.036552 0.674058 C -3.105922 0.570285 -0.190218 C -3.898699 1.702574 0.075561 H -3.944251 3.826865 0.579147 H -3.580959 -0.393544 -0.436036 H -4.997531 1.615296 0.038185 C 0.354281 1.905061 0.282864 C 2.243803 0.381355 0.046058 C 3.177581 0.974749 -0.832389 C 2.669303 -0.609484 0.961056 C 4.526972 0.586237 -0.786720 H 2.829659 1.732786 -1.551153 C 4.019986 -0.987008 0.999673 H 1.923729 -1.069877 1.627236 C 4.953239 -0.393109 0.127961 H 5.249993 1.051730 -1.475349 H 4.348069 -1.753236 1.719933 H 6.011366 -0.696292 0.160237 C 1.170295 3.071797 0.759775 H 0.726250 2.495182 1.685123 H 2.219695 2.790441 0.967560 H 1.174218 3.887927 0.004411

E'	TS-E'-F'
Zero-point correction= 0.354047 (Hartree/Particle) Thermal correction to Energy= 0.379963 Thermal correction to Enthalpy= 0.380907 Thermal correction to Gibbs Free Energy= 0.297407 Sum of electronic and zero-point Energies= -1609.736652 Sum of electronic and thermal Energies= -1609.710736 Sum of electronic and thermal Enthalpies= -1609.709792 Sum of electronic and thermal Free Energies= -1609.793292 Solvent Energy = -1610.298882	Zero-point correction= 0.352978 (Hartree/Particle) Thermal correction to Energy= 0.378573 Thermal correction to Enthalpy= 0.379517 Thermal correction to Gibbs Free Energy= 0.296730 Sum of electronic and zero-point Energies= -1609.716701 Sum of electronic and thermal Energies= -1609.691107 Sum of electronic and thermal Enthalpies= -1609.690163 Sum of electronic and thermal Free Energies= -1609.772950 Solvent Energy = -1610.284724
Ru -0.384511 0.761418 0.130203 C 0.050094 -1.740503 -1.272237 N 0.715231 -0.702048 -0.763138 C -1.377537 -1.676256 -1.043648 C -2.318215 -2.662942 -1.438486 C -1.813698 -0.471913 -0.396547 C -3.681953 -2.456704 -1.211936 H -1.976555 -3.591937 -1.923236 C -3.200471 -0.278343 -0.191818 C -4.118983 -1.258079 -0.597600 H -4.414865 -3.220772 -1.514611 H -3.550538 0.645582 0.296122 H -5.197078 -1.095325 -0.431157 C 0.566275 0.242635 1.964786 C -0.852705 0.385469 2.236789 C 1.237741 -1.008947 2.194170 C -1.573782 -0.815243 2.590977 H -1.265129 1.365395 2.526755 C 0.481466 -2.131369 2.476570 H 2.331631 -1.052727 2.104920 C -0.937614 -2.040951 2.653460 H -2.647452 -0.732490 2.817758 H 0.983913 -3.104501 2.597594 H -1.512791 -2.948389 2.893265 O -1.651059 2.539682 0.262895 C -1.410439 2.783207 -0.968527 O -0.624714 1.971784 -1.596728 C -2.046012 3.939956 -1.687627 H -1.386344 4.300729 -2.499551 H -2.996377 3.592604 -2.145257 H -2.278791 4.754508 -0.976230 Cl 1.577761 1.750842 1.968664	Ru -0.256856 0.712623 0.288176 C 0.208288 -1.572242 -1.453646 N 0.857888 -0.724682 -0.657866 C -1.230343 -1.400858 -1.470871 C -2.139587 -2.229494 -2.177188 C -1.689376 -0.264729 -0.728439 C -3.504861 -1.928314 -2.154157 H -1.780042 -3.107055 -2.738578 C -3.070661 0.032351 -0.746593 C -3.966266 -0.795051 -1.442744 H -4.220295 -2.569025 -2.693002 H -3.439141 0.916937 -0.202966 H -5.044264 -0.562773 -1.434601 C -0.154671 -0.479109 1.807030 C -1.180819 0.326180 2.371425 C -0.061961 -1.869404 2.011640 C -2.321301 -0.355268 2.898712 H -1.041559 1.406805 2.550581 C -1.170869 -2.496316 2.583077 H 0.800302 -2.442113 1.642403 C -2.313181 -1.745612 2.986897 H -3.153389 0.230046 3.321241 H -1.179103 -3.593536 2.687757 O -3.175539 -2.273836 3.422760 H -1.388868 2.520417 0.055902 C -0.701582 2.852930 -0.978202 O 0.187172 2.021226 -1.382734 C -0.956313 4.142204 -1.700222 H -1.310591 4.909654 -0.986183 H -0.035283 4.479586 -2.211471 H -1.746205 3.980145 -2.463425 Cl 1.410604 2.153855 1.479804

C	2.122101	-0.531634	-0.886400
C	2.613956	0.698462	-1.378759
C	3.032966	-1.526203	-0.464578
C	3.996538	0.922935	-1.450362
H	1.894637	1.464359	-1.707603
C	4.415698	-1.290447	-0.535116
H	2.644711	-2.470101	-0.055227
C	4.903217	-0.066733	-1.026728
H	4.369511	1.883080	-1.840459
H	5.117173	-2.069074	-0.195492
H	5.987830	0.116898	-1.076814
C	0.687472	-2.832253	-2.089833
H	0.034740	-3.095926	-2.946210
H	1.678364	-2.535455	-2.481542
H	0.822826	-3.755408	-1.485940

C	0.903111	-2.576173	-2.333362
H	0.823972	-3.596206	-1.899808
H	0.416492	-2.605207	-3.328481
H	1.976125	-2.344336	-2.462775
C	2.279394	-0.737112	-0.504703
C	3.020428	0.430227	-0.786787
C	2.939438	-1.892786	-0.031501
C	4.411012	0.425700	-0.606275
H	2.493831	1.326682	-1.139580
C	4.330695	-1.882628	0.155524
H	2.356875	-2.800972	0.186676
C	5.070627	-0.722469	-0.131547
H	4.983256	1.340101	-0.826653
H	4.835709	-2.786359	0.531451
H	6.161399	-0.712035	0.019544

F'	TS-F'G'
Zero-point correction= 0.354382 (Hartree/Particle)	Zero-point correction= 0.353300 (Hartree/Particle)
Thermal correction to Energy= 0.380793	Thermal correction to Energy= 0.378980
Thermal correction to Enthalpy= 0.381738	Thermal correction to Enthalpy= 0.379924
Thermal correction to Gibbs Free Energy= 0.296867	Thermal correction to Gibbs Free Energy= 0.296990
Sum of electronic and zero-point Energies= -1609.746935	Sum of electronic and zero-point Energies= -1609.715813
Sum of electronic and thermal Energies= -1609.720523	Sum of electronic and thermal Energies= -1609.690134
Sum of electronic and thermal Enthalpies= -1609.719579	Sum of electronic and thermal Enthalpies= -1609.689190
Sum of electronic and thermal Free Energies= -1609.804449	Sum of electronic and thermal Free Energies= -1609.772124
Solvent Energy = -1610.304336	Solvent Energy = -1610.283657
Ru -0.489535 -0.349315 0.786628	Ru 0.117279 -0.368260 -0.784830
C -0.555698 1.840438 -1.190113	C -0.319547 1.192083 1.588410
N 0.289881 1.000179 -0.620712	N -0.873453 0.264295 0.800583
C -1.930625 1.659624 -0.762334	C 0.924173 1.717903 1.099437
C -3.027781 2.408951 -1.245170	C 1.533040 2.897257 1.603739
C -2.110698 0.640209 0.240357	C 1.429085 1.076187 -0.095092
C -4.311899 2.163301 -0.741716	C 2.539874 3.530306 0.876478
H -2.877425 3.187986 -2.009573	H 1.167436 3.344374 2.541999
C -3.421390 0.426473 0.742656	C 2.373585 1.816384 -0.867367
C -4.502122 1.173832 0.248831	C 2.916207 3.007379 -0.388583
H -5.170369 2.743196 -1.115114	H 3.008492 4.450538 1.257346
H -3.586775 -0.340118 1.513827	H 2.716845 1.415469 -1.832638
H -5.514796 0.983747 0.640566	H 3.662093 3.541222 -0.999367
C -0.172673 -1.673144 -0.690500	C 2.043522 -0.688962 0.069291
C -0.806373 -1.535648 -1.951236	C 2.970989 -1.138935 -0.909554
C 0.590276 -2.835521 -0.414556	C 2.250277 -1.071920 1.416154
C -0.712629 -2.565803 -2.903080	C 4.055253 -1.949393 -0.550065
H -1.392401 -0.634791 -2.186205	H 2.835837 -0.863754 -1.969918
C 0.696860 -3.845929 -1.383605	C 3.344421 -1.871172 1.773433
H 1.096780 -2.941466 0.554122	H 1.540607 -0.734828 2.187103
C 0.048081 -3.716773 -2.627414	C 4.253766 -2.314669 0.795505
H -1.231445 -2.461948 -3.869978	H 4.752268 -2.299617 -1.328213
H 1.288450 -4.748688 -1.160899	H 3.484782 -2.157377 2.828313
H 0.135299 -4.514839 -3.381951	H 5.112606 -2.942920 1.078713
Cl -1.441027 -1.716483 2.388919	O -0.406724 1.236299 -2.093520
O 1.688514 -1.041763 1.736763	C -1.510081 0.658211 -2.438218
C 1.648407 0.091096 2.258300	O -1.744595 -0.485372 -1.924914
O 0.639821 0.879460 1.969035	C -2.484978 1.337194 -3.355401
C 2.718083 0.650852 3.159581	H -3.274357 1.814484 -2.736876
H 2.289145 1.553543 3.899123	H -1.980392 2.118161 -3.954356
H 3.250426 -0.175858 3.645295	H -2.974431 0.591089 -4.010304
H 3.440521 1.206123 2.524897	Cl -0.018158 -2.672786 -0.363787
C 1.702738 1.106943 -0.782770	C -0.995540 1.690217 2.837294
C 2.428727 0.114973 -1.473874	H -1.458679 2.685979 2.668965
C 2.382962 2.183889 -0.172641	H -1.791077 1.000098 3.174599
C 3.826507 0.210246 -1.555841	H -0.251634 1.804840 3.651595
H 1.891829 -0.725300 -1.934198	C -2.247039 -0.112863 0.947809
C 3.782144 2.266591 -0.257009	C -2.600591 -1.404143 1.380047
H 1.799372 2.930460 0.385564	C -3.244898 0.832166 0.627315
C 4.508578 1.279483 -0.946794	C -3.957802 -1.738101 1.508877
H 4.388925 -0.565990 -2.098003	H -1.806074 -2.135568 1.581947
H 4.307112 3.107410 0.223791	C -4.598685 0.486963 0.752774
H 5.606267 1.342277 -1.008460	H -2.940180 1.830090 0.274443
C -0.145363 2.888094 -2.188108	C -4.957904 -0.799180 1.195731
H -0.260639 3.904070 -1.754527	H -4.236157 -2.747929 1.848726
H 0.905309 2.764384 -2.508907	H -5.377112 1.224214 0.500090
H -0.801086 2.839993 -3.081806	H -6.020519 -1.072738 1.290063

G'	I'
Zero-point correction= 0.355416 (Hartree/Particle)	Zero-point correction= 0.582085 (Hartree/Particle)
Thermal correction to Energy= 0.381248	Thermal correction to Energy= 0.621810
Thermal correction to Enthalpy= 0.382192	Thermal correction to Enthalpy= 0.622755
Thermal correction to Gibbs Free Energy= 0.299421	Thermal correction to Gibbs Free Energy= 0.509644
Sum of electronic and zero-point Energies= -1609.745587	Sum of electronic and zero-point Energies= -2205.228106
Sum of electronic and thermal Energies= -1609.719755	Sum of electronic and thermal Energies= -2205.188381
Sum of electronic and thermal Enthalpies= -1609.718811	Sum of electronic and thermal Enthalpies= -2205.187436
Sum of electronic and thermal Free Energies= -1609.801582	Sum of electronic and thermal Free Energies= -2205.300547
Solvent Energy = -1610.318291	Solvent Energy = -2206.131031
Ru -0.105206 0.628234 0.844747	Ru -0.388201 0.146858 0.157580
N -0.530759 -0.716291 -0.536469	C 1.539402 1.686668 -0.919543
C 1.724868 -1.437192 -1.052542	N 0.525597 1.953736 -0.134195
C 2.513009 -2.598616 -1.235182	C 1.429547 0.251335 -1.314090
C 2.350420 -0.227295 -0.634241	C 0.148674 -0.102982 -1.947563
C 3.887618 -2.585593 -0.959028	C 2.562168 -0.651867 -1.431851
H 2.036983 -3.537635 -1.557140	C 0.058974 -1.373579 -2.624012
C 3.732013 -0.230731 -0.366503	H -0.492049 0.706331 -2.339582
C 4.498026 -1.399676 -0.514210	C 2.382495 -1.872500 -2.081957
H 4.481525 -3.504185 -1.085339	C 1.130742 -2.242343 -2.662054
H 4.213713 0.709767 -0.056518	H -0.873474 -1.614561 -3.155137
H 5.577727 -1.379463 -0.297275	H 3.231612 -2.571157 -2.140953
C 1.568795 1.047096 -0.538472	H 1.040080 -3.215533 -3.170322
C 1.736828 1.921486 0.603953	C 3.914511 -0.277042 -0.935350
C 1.051635 1.643956 -1.754826	C 4.103726 0.282060 0.351038
C 1.494897 3.326861 0.474547	C 5.046021 -0.462965 -1.767690
H 2.325666 1.556953 1.464038	C 5.388507 0.641296 0.787323
C 0.769581 3.000288 -1.828790	H 3.228680 0.397959 1.012932
H 0.925320 1.000318 -2.640404	C 6.329260 -0.098772 -1.328098
C 1.007476 3.854380 -0.715077	H 4.907945 -0.870249 -2.782115
H 1.667571 3.978730 1.344607	C 6.505649 0.456406 -0.047775
H 0.364277 3.422037 -2.762030	H 5.516827 1.065110 1.796324
H 0.794819 4.931132 -0.796390	H 7.195558 -0.240212 -1.994224
O 0.951696 -0.898066 1.907330	H 7.511580 0.745327 0.296673
C -0.125870 -1.261923 2.509583	O -2.114612 1.206558 -0.682909
O -1.202108 -0.620880 2.232011	C -2.504640 1.479345 0.504311

C	-0.129109	-2.416716	3.472642	O	-1.875591	0.903716	1.470838
H	-0.837544	-2.222377	4.300702	C	-3.566151	2.503511	0.774821
H	-0.470123	-3.329994	2.940490	H	-4.145061	2.232859	1.678439
H	0.890199	-2.597137	3.862157	H	-3.059401	3.474799	0.965867
Cl	-1.603496	2.410509	0.706864	H	-4.232333	2.606329	-0.101369
C	0.268079	-1.490550	-1.256432	Cl	1.138446	-0.221313	1.953708
C	-0.303809	-2.447754	-2.278177	C	-2.159792	-2.386747	-0.264874
H	0.424479	-2.629799	-3.091527	N	-1.125921	-1.839387	0.329132
H	-0.549016	-3.427291	-1.812651	C	-3.274868	-1.558137	-0.806988
H	-1.243530	-2.057639	-2.713432	C	-3.587776	-1.509840	-2.181121
C	-1.956875	-0.779784	-0.731207	C	-4.128581	-0.912612	0.115312
C	-2.575109	0.177008	-1.560655	C	-4.698719	-0.779927	-2.632300
C	-2.713214	-1.795005	-0.115943	H	-2.949814	-2.040373	-2.904875
C	-3.957416	0.106368	-1.779957	C	-5.255873	-0.207765	-0.335291
H	-1.959381	0.976572	-1.998339	H	-3.887133	-0.958247	1.187863
C	-4.098684	-1.851348	-0.335704	C	-5.536837	-0.127845	-1.710244
C	-2.209699	-2.517023	0.542125	H	-4.916407	-0.726170	-3.710731
C	-4.722547	-0.904893	-1.167879	H	-5.913883	0.290550	0.393934
H	-4.444030	0.856545	-2.422527	H	-6.415148	0.434793	-2.064141
H	-4.695232	-2.637707	0.152728	C	-0.346132	-2.734115	1.153424
H	-5.810305	-0.949368	-1.333665	C	-0.879205	-3.119768	2.397770
				C	0.919298	-3.193496	0.753555
				C	-0.145537	-3.973043	3.237008
				H	-1.857964	-2.721457	2.706522
				C	1.640779	-4.057367	1.590229
				H	1.333646	-2.847707	-0.199793
				C	1.114129	-4.450200	2.833678
				H	-0.559757	-4.260748	4.216386
				H	2.634304	-4.411148	1.272439
				H	1.689684	-5.118298	3.493530
				C	0.119829	3.214245	0.365161
				C	-0.216936	4.269953	-0.507520
				C	-0.042757	3.357943	1.760058
				C	-0.703386	5.477733	0.019559
				H	-0.122029	4.121787	-1.593807
				C	-0.522508	4.571360	2.274476
				H	0.201931	2.499521	2.404484
				C	-0.856678	5.632011	1.409594
				H	-0.973580	6.299677	-0.662176
				H	-0.646135	4.686664	3.362803
				H	-1.242878	6.578522	1.819543
				C	-2.371486	-3.880593	-0.366118
				H	-1.434289	-4.451837	-0.228193
				H	-3.100088	-4.220750	0.401793
				H	-2.821279	-4.118267	-1.352430
				C	2.556432	2.667800	-1.418076
				H	2.307568	2.962415	-2.461718
				H	2.576250	3.581238	-0.792502
				H	3.564500	2.211783	-1.438820

J'

Zero-point correction=0.276023 (Hartree/Particle)

Thermal correction to Energy=0.296996

Thermal correction to Enthalpy=0.297941

Thermal correction to Gibbs Free Energy=0.225156

Sum of electronic and zero-point Energies=-1378.924345

Sum of electronic and thermal Energies=-1378.903371

Sum of electronic and thermal Enthalpies=-1378.902427

Sum of electronic and thermal Free Energies=-1378.975212

Solvent Energy = -1379.78236

Ru0.352800-1.0931970.152880

C0.6742711.7500260.427677

N-0.2220560.7597200.423784

C2.0397031.3146200.219126

C3.1209832.174439-0.080668

C2.231756-0.1154160.212226

C4.3751741.642188-0.407099

H2.9692063.265461-0.091184

C3.514564-0.629497-0.111367

C4.5641410.241273-0.432459

H5.2118252.315136-0.649966

H3.677254-1.718888-0.094500

H5.551972-0.171924-0.692126

O0.240486-0.699602-1.954401

C-0.926987-1.241059-2.007711

O-1.386251-1.746019-0.922115

C-1.741596-1.224867-3.268201

H-2.314135-2.167232-3.365666

H-2.471584-0.390810-3.194804

H-1.094996-1.062766-4.150484

Cl-0.065930-2.2195752.153057

H1.713299-0.7392931.132810

C0.3004083.1923540.631814

H1.0261643.6798731.314293

H0.3250683.750591-0.329115

H-0.7149583.2978081.057142

C-1.6337730.9841410.416197

C-2.4413920.4359681.432672

C-2.2163231.683954-0.662543

C-3.8307310.6197871.379010

H-1.968540-0.1545322.231837

C-3.6092091.854221-0.709010

H-1.5678062.072851-1.462515

C-4.4187291.3269310.313005

H-4.4627630.1940242.173843

H-4.0639742.398171-1.552063

H-5.5114651.4574950.273431

B

Zero-point correction=0.534310 (Hartree/Particle)

Thermal correction to Energy=0.570656

Thermal correction to Enthalpy=0.571600

Thermal correction to Gibbs Free Energy=0.466399

Sum of electronic and zero-point Energies=-1536.154512

Sum of electronic and thermal Energies=-1536.118166

Sum of electronic and thermal Enthalpies=-1536.117222

Sum of electronic and thermal Free Energies=-1536.222424

Solvent Energy = -1536.951634

Ru1.393440-1.0521782.450941

Ru0.124171-0.481072-0.325821

C0.6095670.192425-2.376422

C-0.146146-0.955380-2.469649

C0.176472-2.148760-1.733045

C1.332646-2.233443-0.900287

C2.193347-1.066700-0.843785

C1.8988470.110739-1.579820

H-1.107502-0.909183-2.997850

H-0.564884-2.960125-1.739859

C3.027351-1.063766-0.128605

H2.5554080.987380-1.485031

C1.640988-3.476679-0.077230

H2.359282-3.1543020.704544

C0.3449591.467533-3.097540

H0.5231562.354126-2.459086

C1.008463-1.3672073.899660

H1.908667-1.3857544.542505

H0.262774-0.6448284.284691

H0.535201-2.3716643.919387

O0.371417-0.6165571.757792

O2.556080-1.2232292.050165

N-0.6613801.4647630.125701

C0.398679-4.0395480.637150

H-0.339823-4.454782-0.081409

H0.691154-4.8641051.319404

H-0.113273-3.2501571.223894

C2.322486-4.532149-0.972600

H3.237395-4.128600-1.454637

H2.614963-5.422007-0.376628

H1.636586-4.872535-1.778501

H-0.7130671.470446-3.422959

H0.9833521.575891-4.000453

O-1.682191-1.1922950.407191

C-2.689448-1.659389-0.293084

O-2.768131-1.745522-1.526161

C-3.841824-2.0884420.617453

H-4.231515-1.1921371.140651

H-4.648344-2.5540670.021440

H-3.477338-2.7919651.392634

C1.4358132.7081810.266369

C2.1232983.606663-0.583932

C2.1806771.8791281.132178

C3.5273663.617975-0.613486

H1.5617844.271632-1.259777

C3.5820371.8975621.110048

H1.6432531.2009961.802249

C4.2599102.7573070.226580

H4.0529074.299381-1.300845

H4.1297351.2121521.774316

H5.3609812.7634340.194982

C-0.0489672.6206090.246471

C-0.8135343.9177890.405158

H-1.7622133.917047-0.165862

H-1.0802104.0580021.474827

H-0.1898604.7839790.111687

	C	-2.093960	1.478850	0.271700
	C	-2.648387	1.520032	1.565105
	C	-2.926801	1.432680	-0.860027
	C	-4.042453	1.555594	1.719679
	H	-1.972552	1.495048	2.432540
	C	-4.320554	1.465659	-0.696424
	H	-2.475620	1.341643	-1.857289
	C	-4.882632	1.536291	0.590583
	H	-4.476242	1.581276	2.731753
	H	-4.970414	1.418664	-1.583765
	H	-5.976484	1.555224	0.714920