

Supporting Information

The annulation of N-hydroxyoximes and 1,3-diyne to synthesize alkynylated isoquinolines regioselectively catalyzed by ruthenium: a theoretical study

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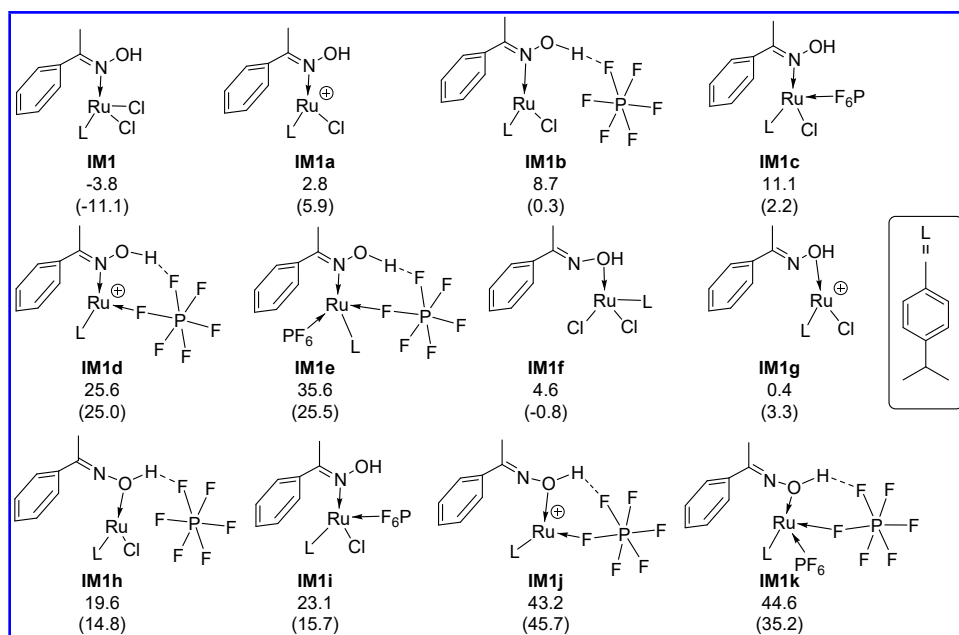


Fig. S1. Other unfavorable coordination isomers in reaction A. The relative free energies and relative enthalpic energies (in parentheses) are given in kcal/mol.

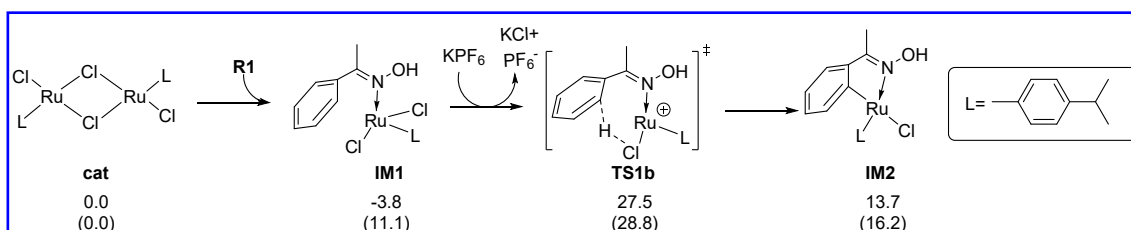


Fig. S2. The unfavorable inner-sphere CMD mechanism in reaction A. The relative free energies and relative enthalpic energies (in parentheses) are given in kcal/mol.

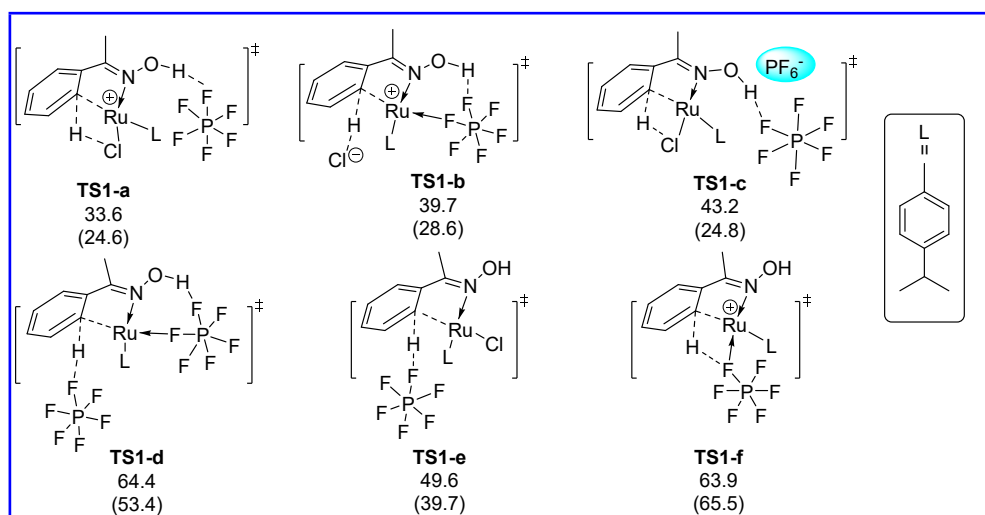


Fig. S3. Other inaccessible C-H activation transition states in reaction A. The relative free energies and relative enthalpic energies (in parentheses) are given in kcal/mol.

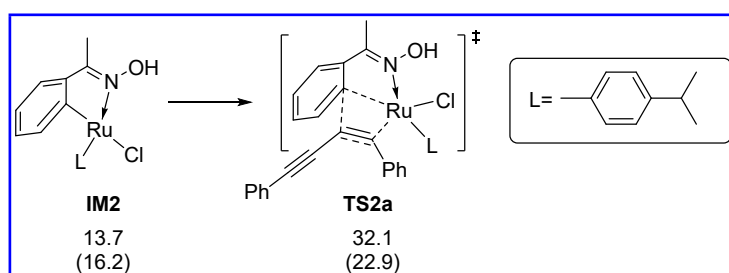


Fig. S4. The inaccessible insertion transition state without the assistant of KPF_6 in reaction A. The relative free energies and relative enthalpic energies (in parentheses) are given in kcal/mol.

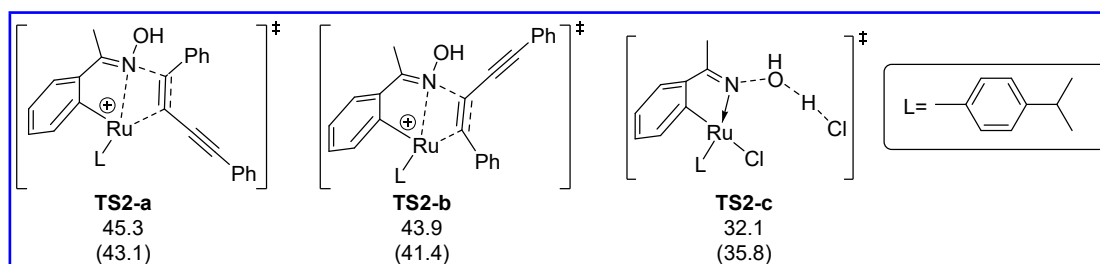


Fig. S5. The infeasible transition states of **R2** inserting into the Ru-N bond and the cleavage of N-O bond in reaction A. The relative free energies and relative enthalpic energies (in parentheses) are given in kcal/mol.

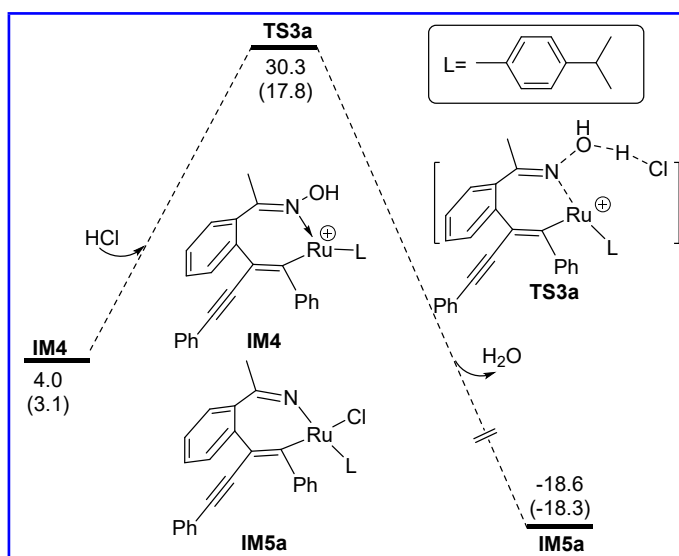


Fig. S6. The infeasible pathway that protodemetalation prior to reductive elimination in reaction A. The relative free energies and relative enthalpic energies (in parentheses) are given in kcal/mol.

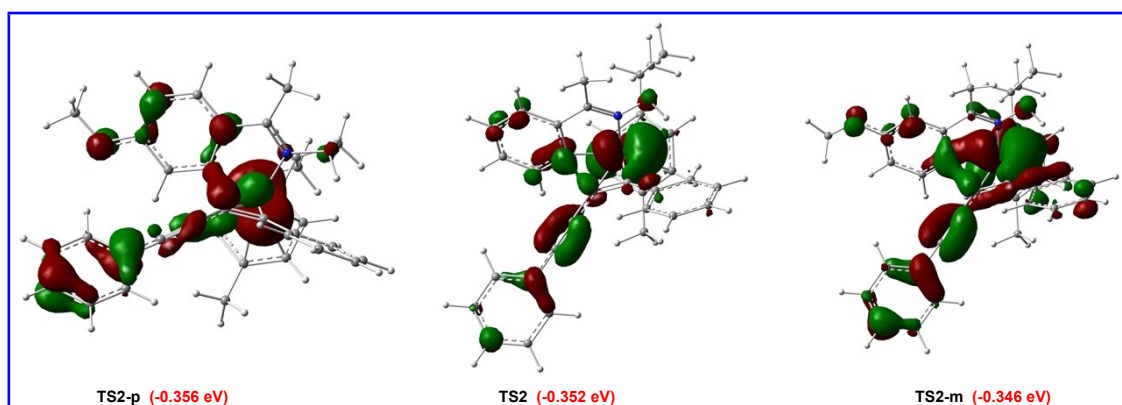


Fig. S7. The MO analysis of the transition states TS2-p, TS2, and TS2-m.

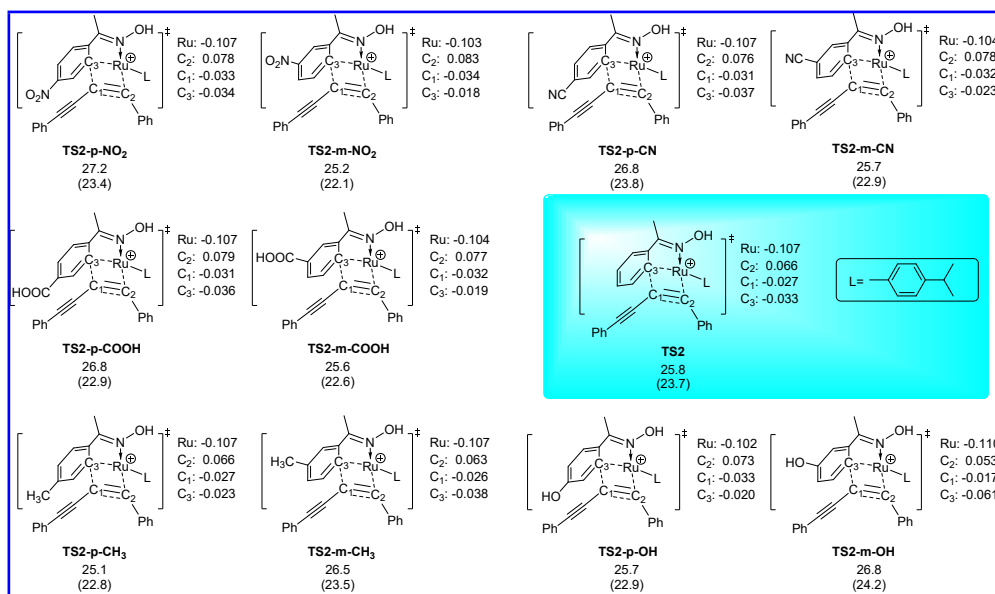


Fig. S8. NBO charges (e) of the 1,3-diyne insertion transition states with different substituted groups. The relative free energies and relative enthalpic energies (in parentheses) are given in kcal/mol.

Cartesian coordinates and sum of electronic and thermal free energies for all of the calculated structures

cat				H	5.05677	-2.71925	1.40756
Sum of electronic and thermal Free Energies =	-2807.400537			H	3.62691	-2.52115	2.43895
Sum of electronic and thermal Enthalpies=	-2807.303312			H	3.46802	-3.30708	0.85895
Cl	0.99255	-2.72729	-0.55652	C	2.79604	2.70344	-1.17856
Cl	-0.13802	-0.2145	1.49542	C	3.83707	3.74556	-0.71368
Cl	-0.72899	2.92789	0.36717	C	2.71228	2.67327	-2.70943
Cl	0.03558	0.31485	-1.74586	H	4.84334	3.48383	-1.06141
C	-3.21398	-1.00907	-0.18328	H	3.58561	4.72925	-1.12228
C	-3.18668	-0.3054	-1.41471	H	3.86827	3.83457	0.37623
C	-3.48485	1.09231	-1.50761	H	2.42058	3.66215	-3.07542
C	-3.782	1.84883	-0.34677	H	3.67922	2.43023	-3.16726
C	-3.72638	1.17616	0.9179	H	1.96335	1.9575	-3.05586
C	-3.44043	-0.21434	0.98636	Ru	-1.78938	0.78563	-0.08819
H	-2.86927	-0.82995	-2.30967	Ru	1.76934	-0.46634	-0.11772
H	-3.41328	1.59096	-2.4674	H	-2.05128	-2.6671	-0.78623
H	-3.84154	1.74574	1.83279	H	1.81332	3.00012	-0.7913
H	-3.32328	-0.66765	1.96319	1cat			
C	-2.93647	-2.5051	-0.15864	Sum of electronic and thermal Free Energies =	-1403.695300		
C	-4.12932	-3.2581	-0.78688	Sum of electronic and thermal Enthalpies =	-1403.633674		
C	-2.61364	-3.06105	1.23327	Cl	-0.86141	2.19276	1.07943
H	-5.03818	-3.12615	-0.18809	Cl	0.04454	-0.25211	-0.99979
H	-4.34318	-2.91322	-1.80364	C	-3.38043	-1.18314	-0.41005
H	-3.9113	-4.32952	-0.83553	C	-3.33229	-0.5116	-1.65537
H	-2.36697	-4.12317	1.14878	C	-3.52335	0.89877	-1.73335
H	-1.75119	-2.55542	1.67239	C	-3.93349	1.67706	-0.5974
H	-3.46979	-2.97793	1.91468	C	-4.03824	1.00211	0.64059
C	-4.05635	3.32355	-0.41476	C	-3.68732	-0.37368	0.74258
H	-5.10855	3.51517	-0.17315	H	-2.98832	-1.03063	-2.53913
H	-3.42529	3.85938	0.29852	H	-3.34162	1.40165	-2.67745
H	-3.8513	3.71808	-1.41182	H	-4.22023	1.56973	1.54589
C	3.23381	-0.06534	1.48444	H	-3.64597	-0.81769	1.72954
C	3.70912	-1.18364	0.75504	C	-3.10685	-2.68515	-0.25624
C	3.82755	-1.02641	-0.66915	C	-2.10973	-2.84139	0.9198
C	3.52802	0.20406	-1.29828	C	-4.39459	-3.46987	0.06036
C	3.11176	1.3578	-0.54261	H	-1.16493	-2.32454	0.72092
C	2.94786	1.18815	0.85059	H	-2.52516	-2.44272	1.8514
H	3.01156	-0.18137	2.53994	H	-1.88465	-3.90134	1.0764
H	4.06334	-1.89146	-1.27886	H	-5.13862	-3.34678	-0.7324
H	3.55455	0.254	-2.3793	H	-4.15679	-4.53489	0.13878
H	2.50627	1.98726	1.43532	H	-4.83806	-3.16864	1.01549
C	3.98045	-2.51046	1.4055	C	-4.1515	3.15968	-0.71021

H	-5.20355	3.36715	-0.94058
H	-3.89424	3.66536	0.22269
H	-3.53917	3.58596	-1.50853
Ru	-1.99804	0.60496	-0.21778
H	-2.67799	-3.09361	-1.14738

RI

Sum of electronic and thermal Free Energies = -440.078615

Sum of electronic and thermal Enthalpies = -440.033529

C	-2.71775	-0.7547	0.04497
C	-1.32931	-0.73799	0.12754
C	-0.62084	0.47652	0.06496
C	-1.34967	1.66714	-0.08581
C	-2.74286	1.64711	-0.17046
C	-3.43305	0.43775	-0.10281
H	-3.24645	-1.702	0.10255
H	-0.77176	-1.6603	0.24436
H	-0.83399	2.61954	-0.15953
H	-3.28589	2.57998	-0.29245
H	-4.51743	0.4222	-0.16282
C	0.86398	0.48314	0.13763
C	1.60818	1.74137	0.53388
H	2.0678	2.23961	-0.32924
H	0.94293	2.45619	1.01718
H	2.40271	1.51656	1.25677
N	1.44688	-0.63156	-0.15117
O	2.8253	-0.67684	-0.10504
H	3.13612	-1.56871	-0.34275

IMI

Sum of electronic and thermal Free Energies = -1843.779007

Sum of electronic and thermal Enthalpies = -1843.697032

C	-1.40247	-1.78844	-0.61228
C	-1.51281	-1.2951	0.68755
C	-2.44894	-0.29082	0.99218
C	-3.31078	0.17459	-0.01234
C	-3.20596	-0.33798	-1.30801
C	-2.24883	-1.30724	-1.61519
H	-0.66593	-2.55388	-0.83873
H	-0.86477	-1.68397	1.4689
H	-4.07108	0.9075	0.22893
H	-3.88896	0.01525	-2.07531
H	-2.17373	-1.7004	-2.62489
C	-2.55673	0.18673	2.39549
C	-2.86152	-0.81595	3.47883
H	-2.97256	-1.81574	3.05976

H	-2.0809	-0.81574	4.24655
H	-3.78916	-0.5247	3.98245
N	-2.40576	1.43569	2.70574
O	-2.54238	1.64746	4.05963
H	-2.63383	2.63075	4.13961
Cl	-2.38829	4.51942	3.51703
C	-1.31261	2.96736	-0.64968
C	-0.44317	2.18319	0.13061
C	0.26451	2.74507	1.2475
C	0.07866	4.12674	1.49971
C	-0.76416	4.93443	0.66815
C	-1.4905	4.3788	-0.40709
H	-1.9096	2.47194	-1.40224
H	-0.38302	1.11793	-0.05612
H	0.52052	4.57212	2.38369
H	-0.93012	5.9632	0.95777
C	1.15747	1.89805	2.11137
Ru	-1.9017	3.20043	1.52263
C	-2.41519	5.24701	-1.27364
C	-3.23643	6.23536	-0.41546
C	-1.48744	6.03493	-2.23516
H	-3.88971	5.71033	0.28341
H	-2.606	6.93021	0.14768
H	-3.86312	6.83979	-1.07825
H	-0.88951	5.36349	-2.86135
H	-2.09512	6.65989	-2.89726
H	-0.80241	6.69131	-1.68827
H	1.23078	2.30484	3.12252
H	0.78673	0.8725	2.17562
H	2.1663	1.86504	1.68256
Cl	-4.01085	3.17017	0.97487
H	-3.09817	4.6581	-1.84951

KPF₆

Sum of electronic and thermal Free Energies = -1540.551810

Sum of electronic and thermal Enthalpies = -1540.509289

P	0.6351	-0.66198	0.03712
F	0.63694	0.94256	-0.04196
F	-1.03573	-0.65878	0.15149
F	0.52948	-0.82357	-1.55782
F	2.23922	-0.74776	0.0235
F	0.64982	-0.58377	1.71039
F	0.54432	-2.32502	0.21477
K	-1.20027	-2.32883	2.10664

KCl

Sum of electronic and thermal Free Energies = -1060.189060

Sum of electronic and thermal Enthalpies = -1060.161894

K	-0.74277	0.33708	0
Cl	-3.53192	0.33708	0

IM1a

Sum of electronic and thermal Free Energies = -1383.328957

Sum of electronic and thermal Enthalpies = -1383.249231

C	-2.84822	-2.63949	2.14156
C	-1.67938	-1.88113	2.23415
C	-1.69552	-0.50809	1.91907
C	-2.90207	0.09228	1.5218
C	-4.05758	-0.67411	1.41367
C	-4.03488	-2.03923	1.72453
H	-2.83622	-3.68829	2.42158
H	-0.77494	-2.32506	2.63773
H	-2.92886	1.14404	1.2564
H	-4.98186	-0.20879	1.08703
H	-4.94598	-2.6249	1.65754
C	-0.4536	0.27667	2.0265
C	-0.43791	1.62515	2.68893
H	-1.44106	2.05108	2.70377
H	-0.1223	1.54195	3.73816
H	0.24367	2.3077	2.17398
N	0.63043	-0.27171	1.56543
O	1.83679	0.39832	1.7975
H	1.8205	0.7273	2.71435
Ru	0.80046	-1.92593	0.23593
Cl	-0.51651	-0.71213	-1.27355
C	1.01339	-3.95331	-0.71028
C	1.14945	-4.11742	0.71176
C	2.15046	-3.36759	1.38692
C	2.92706	-2.41287	0.68428
C	2.77497	-2.21131	-0.72669
C	1.81588	-3.03783	-1.40986
H	0.22056	-4.47884	-1.23213
H	2.25139	-3.45556	2.46337
H	3.58867	-1.76057	1.24106
H	1.62324	-2.85777	-2.46223
C	3.63038	-1.24949	-1.52998
C	4.78021	-2.06057	-2.17748
C	4.17699	-0.0554	-0.73442
H	5.46348	-2.44875	-1.41336
H	4.41237	-2.90691	-2.76803
H	5.35376	-1.40921	-2.8428

H	4.69189	0.62617	-1.41631
H	3.38116	0.50191	-0.23321
H	4.91164	-0.36825	0.01796
C	0.262	-5.08477	1.44369
H	0.66862	-6.09793	1.33406
H	0.21051	-4.86141	2.51173
H	-0.7495	-5.08996	1.02925
H	2.9916	-0.86394	-2.33483

TS1

Sum of electronic and thermal Free Energies = -1843.728635

Sum of electronic and thermal Enthalpies = -1843.647540

Imaginary frequency= -268.8373

C	-2.19154	0.2729	4.50495
C	-2.21986	0.26763	5.89812
C	-1.01977	0.17295	6.60854
C	0.23975	0.14209	5.93399
C	0.22	0.12646	4.52045
C	-0.97437	0.18955	3.81437
H	-3.12318	0.33729	3.95034
H	-3.17208	0.3033	6.41767
H	1.16144	0.12806	3.97884
H	-0.96858	0.1976	2.72835
C	-0.96864	0.02583	8.05737
C	-2.12221	0.33778	8.96046
H	-2.98524	-0.27771	8.68303
H	-1.87435	0.14434	10.00196
H	-2.41054	1.38789	8.84629
N	0.17026	-0.44901	8.47107
O	0.28316	-0.62104	9.85078
H	0.89592	-1.36887	9.92202
Cl	1.53415	2.74466	6.61884
C	3.30843	-2.51642	7.74836
C	3.38278	-2.36532	6.31928
C	3.5042	-1.06196	5.80822
C	3.55841	0.07048	6.68034
C	3.57311	-0.07424	8.09077
C	3.42347	-1.40428	8.60398
H	3.1342	-3.50241	8.16382
H	3.49748	-0.90727	4.73493
H	3.54732	1.07205	6.26236
H	3.37218	-1.55983	9.67635
C	3.77873	1.15056	8.96791
Ru	1.64796	-1.05221	7.16572
C	3.2862	-3.57045	5.4282

H	3.16001	1.94184	8.52638
H	0.96462	1.08692	6.34307
Cl	0.12785	-2.9191	6.70813
H	3.12323	-3.28127	4.38682
H	2.4547	-4.20959	5.74086
H	4.21794	-4.14757	5.4847
C	3.35701	0.9634	10.43092
H	3.98922	0.23415	10.95407
H	3.46161	1.91389	10.9622
H	2.31249	0.65125	10.51444
C	5.25646	1.5932	8.87673
H	5.54797	1.81107	7.84473
H	5.41054	2.5022	9.46653
H	5.93065	0.82021	9.26575

TS1'

Sum of electronic and thermal Free Energies = -1843.733492

Sum of electronic and thermal Enthalpies = -1843.647298

Imaginary frequency= -379.3650

C	-2.47502	-3.82563	-1.92175
C	-1.88033	-2.58791	-2.21082
C	-1.20404	-2.45476	-3.46205
C	-1.11583	-3.5283	-4.35544
C	-1.71333	-4.74704	-4.03574
C	-2.39513	-4.89013	-2.82471
H	-2.99857	-3.96808	-0.98203
H	-0.80482	-2.33831	-1.08934
H	-0.59354	-3.41273	-5.30074
H	-1.64756	-5.58131	-4.72736
H	-2.86613	-5.83794	-2.57844
C	-0.69874	-1.11486	-3.7536
C	0.00553	-0.7306	-5.0167
H	-0.56811	-1.06885	-5.88506
H	0.98972	-1.21051	-5.06267
H	0.13775	0.3486	-5.07051
N	-0.97907	-0.28042	-2.79722
O	-0.63982	1.05724	-2.97819
H	-1.47664	1.50341	-2.74422
Ru	-1.96402	-0.83283	-1.14145
Cl	0.23978	-1.94462	-0.1469
C	-2.55308	-0.66618	1.33786
C	-2.98015	0.66491	1.55275
C	-4.32382	0.95405	1.31097
C	-5.21621	-0.02811	0.86775
C	-4.8034	-1.34013	0.64104

C	-3.44984	-1.6537	0.88534
H	-1.55807	-0.95805	1.65718
H	-4.69574	1.96238	1.47211
H	-6.25335	0.2407	0.68703
H	-3.12471	-2.68911	0.85614
C	-5.75473	-2.37985	0.11116
C	-2.00553	1.71467	2.07088
H	-1.05016	1.20455	2.24947
Cl	-3.82425	0.1703	-2.22452
H	-5.68409	-2.42324	-0.98265
H	-5.52494	-3.3771	0.50027
H	-6.79141	-2.14336	0.36693
C	-1.74894	2.82142	1.02996
H	-2.67326	3.35434	0.7816
H	-1.03102	3.55413	1.41435
H	-1.34238	2.40572	0.10195
C	-2.46691	2.31607	3.41213
H	-2.63256	1.53638	4.16207
H	-1.7133	3.00897	3.80143
H	-3.40201	2.87554	3.29893

IM2

Sum of electronic and thermal Free Energies = -1382.955164

Sum of electronic and thermal Enthalpies = -1382.878652

C	-3.00187	-3.65149	2.44454
C	-2.30964	-2.43718	2.55624
C	-1.47434	-2.2743	3.69511
C	-1.37928	-3.25862	4.69178
C	-2.10697	-4.43747	4.5671
C	-2.90795	-4.63232	3.43616
H	-3.61618	-3.84967	1.57072
H	-0.73359	-3.10704	5.55293
H	-2.04226	-5.20468	5.33277
H	-3.46205	-5.56136	3.32375
C	-0.67205	-1.05882	3.68685
C	0.43685	-0.77184	4.65166
H	0.03554	-0.64167	5.66304
H	1.13066	-1.61783	4.68124
H	0.977	0.12865	4.36484
N	-0.98499	-0.28193	2.69332
O	-0.18737	0.84915	2.48263
H	0.04143	0.74112	1.53889
Ru	-2.39232	-0.82528	1.30017
Cl	-0.37595	-1.53701	0.09357
C	-4.44499	-1.30625	0.3989

C	-3.67553	-0.79366	-0.6593
C	-3.15741	0.5493	-0.53786
C	-3.33673	1.29031	0.62502
C	-4.0002	0.71743	1.76854
C	-4.57769	-0.57324	1.62006
H	-4.87069	-2.30005	0.32072
H	-2.56234	0.95343	-1.34979
H	-2.89774	2.27807	0.7
H	-5.11351	-1.01829	2.4515
C	-4.22847	1.49945	3.05578
C	-5.6565	2.08566	3.06665
C	-3.18968	2.60169	3.31212
H	-5.79258	2.79615	2.24326
H	-6.41569	1.30405	2.96422
H	-5.84311	2.61931	4.0045
H	-3.32102	3.00559	4.32075
H	-2.1663	2.23015	3.21933
H	-3.31461	3.43903	2.61552
C	-3.40827	-1.58477	-1.91064
H	-3.83911	-1.08023	-2.78343
H	-2.32928	-1.68471	-2.06505
H	-3.83852	-2.5871	-1.84556
H	-4.1586	0.77281	3.87538

IM2'

Sum of electronic and thermal Free Energies = -922.504724

Sum of electronic and thermal Enthalpies = -922.430861

C	-3.27675	-3.55325	2.74132
C	-2.4595	-2.42083	2.73286
C	-1.35288	-2.39141	3.62609
C	-1.09023	-3.45903	4.4867
C	-1.92793	-4.58127	4.47666
C	-3.01204	-4.62918	3.60558
H	-4.13359	-3.62361	2.07764
H	-0.24303	-3.43175	5.16473
H	-1.72805	-5.40956	5.1485
H	-3.66375	-5.49787	3.59736
C	-0.51912	-1.18107	3.57558
C	0.6681	-0.94051	4.45037
H	0.33501	-0.62079	5.44542
H	1.24272	-1.86079	4.57519
H	1.30943	-0.16198	4.04006
N	-0.943	-0.31724	2.69856
O	-0.24255	0.88823	2.65813
H	-0.49089	1.27547	1.80606

Ru	-2.56259	-0.81884	1.46213
C	-4.48851	-1.26486	0.37536
C	-3.5616	-0.80043	-0.59159
C	-3.0232	0.52855	-0.45628
C	-3.30068	1.29879	0.67262
C	-4.08902	0.76759	1.75205
C	-4.71722	-0.50889	1.55291
H	-4.93565	-2.24552	0.2616
H	-2.34623	0.90167	-1.21769
H	-2.84235	2.27543	0.78073
H	-5.34343	-0.91474	2.34016
C	-4.41216	1.56927	3.0016
C	-5.76829	2.2837	2.79658
C	-3.32238	2.56781	3.41606
H	-5.70903	3.0158	1.98422
H	-6.5713	1.5788	2.56137
H	-6.04581	2.81779	3.70972
H	-3.5731	2.99697	4.38976
H	-2.33977	2.096	3.49972
H	-3.24905	3.40528	2.71294
C	-3.19744	-1.64008	-1.78514
H	-3.81193	-1.34057	-2.64321
H	-2.15011	-1.50207	-2.06637
H	-3.37324	-2.70163	-1.59959
H	-4.53496	0.84154	3.81337

R2

Sum of electronic and thermal Free Energies = -615.463273

Sum of electronic and thermal Enthalpies = -615.406945

C	-7.09332	0.14581	0.22718
C	-8.59324	0.13194	0.2199
C	-9.31943	1.33973	0.25841
C	-9.29664	-1.08897	0.17477
C	-10.71155	1.32121	0.25148
H	-8.78073	2.28059	0.29341
C	-10.68892	-1.0961	0.16845
H	-8.74046	-2.01979	0.14504
C	-11.40005	0.10608	0.20663
H	-11.26137	2.25699	0.28138
H	-11.22102	-2.04189	0.13337
H	-12.48579	0.09613	0.20146
C	-5.87178	0.15682	0.23315
C	-4.36185	0.14271	0.2309
C	-3.1403	0.13192	0.22917
C	-1.63036	0.12157	0.22168

C	-0.90725	1.3318	0.21419
C	-0.92384	-1.09838	0.22253
C	0.48492	1.31658	0.20765
H	-1.44835	2.27193	0.21388
C	0.46845	-1.10219	0.21579
H	-1.47763	-2.03107	0.2282
C	1.17651	0.10239	0.20835
H	1.03234	2.25423	0.20214
H	1.00297	-2.04726	0.2163
H	2.26227	0.09503	0.20318

IM3

Sum of electronic and thermal Free Energies = -1537.987367

Sum of electronic and thermal Enthalpies = -1537.879748

C	-2.96212	0.35324	4.93246
C	-2.53419	-0.29025	3.76805
C	-1.15182	-0.56484	3.62983
C	-0.23065	-0.1869	4.62142
C	-0.67709	0.47219	5.76153
C	-2.04122	0.74049	5.91255
H	-4.01653	0.54694	5.10133
H	0.82637	-0.40259	4.49882
H	0.02851	0.77282	6.52909
H	-2.39418	1.25419	6.8029
C	-0.77608	-1.2449	2.40065
C	0.62433	-1.63617	2.04666
H	1.20389	-0.74758	1.77083
H	1.11493	-2.09181	2.91064
H	0.63799	-2.32968	1.20807
N	-1.8012	-1.46104	1.62567
O	-1.52236	-2.01363	0.37703
H	-2.17023	-2.73756	0.27603
Ru	-3.69743	-0.80807	2.13978
C	-4.47072	-0.00307	-0.03693
C	-3.77283	1.08411	0.58354
C	-4.22311	1.49349	1.85481
C	-5.30417	0.84083	2.50755
C	-6.01648	-0.20432	1.87105
C	-5.58581	-0.59658	0.57038
H	-4.14536	-0.35689	-1.00807
H	-3.70495	2.29564	2.37005
H	-5.60903	1.1697	3.49446
H	-6.10894	-1.40109	0.06335
C	-7.21156	-0.85061	2.51716
C	-4.03799	-2.92822	2.38777

C	-3.82023	-4.09011	1.55826
C	-3.97313	-4.05376	0.15617
C	-3.44705	-5.30805	2.16731
C	-3.75635	-5.19886	-0.61209
H	-4.29864	-3.13491	-0.32279
C	-3.23773	-6.44527	1.39373
H	-3.32499	-5.34428	3.24489
C	-3.38589	-6.39531	0.00355
H	-3.88538	-5.15717	-1.68925
H	-2.9524	-7.37524	1.87584
H	-3.21611	-7.28512	-0.5942
C	-4.28747	-2.43756	3.53479
C	-4.71873	-2.40972	4.83156
C	-5.11322	-2.36741	5.98832
C	-5.56179	-2.33881	7.33641
C	-4.85811	-1.58821	8.30188
C	-6.71076	-3.05996	7.7236
C	-5.29994	-1.56123	9.62082
H	-3.96931	-1.04154	8.00375
C	-7.14208	-3.02487	9.04597
H	-7.24999	-3.64107	6.98263
C	-6.44065	-2.27682	9.9957
H	-4.75312	-0.98392	10.3599
H	-8.02631	-3.58282	9.33798
H	-6.78095	-2.25351	11.0263
C	-2.65409	1.85069	-0.10981
C	-1.9624	1.07764	-1.24133
C	-3.21015	3.19717	-0.62809
H	-1.6135	0.09368	-0.91792
H	-2.62729	0.94519	-2.1025
H	-1.0984	1.64708	-1.59445
H	-3.64626	3.7974	0.176
H	-2.40539	3.78004	-1.0852
H	-3.98197	3.03594	-1.3883
H	-7.27024	-1.91283	2.26809
H	-7.1787	-0.75379	3.6042
H	-8.13032	-0.37066	2.15999
H	-1.90486	2.07532	0.6600

IM3'

Sum of electronic and thermal Free Energies = -1537.986481

Sum of electronic and thermal Enthalpies = -1537.877867

C	-0.64068	-4.9411	4.71197
C	-1.94522	-4.62416	4.32246
C	-2.98796	-4.82337	5.2613

C	-2.72473	-5.33336	6.5439
C	-1.41981	-5.65831	6.90225
C	-0.38292	-5.4635	5.98471
H	0.19342	-4.76986	4.03857
H	-3.53402	-5.48115	7.25256
H	-1.20952	-6.05802	7.88891
H	0.6378	-5.70998	6.26379
C	-4.31972	-4.47332	4.78838
C	-5.56757	-4.58568	5.60647
H	-5.86092	-5.63739	5.70445
H	-5.39205	-4.1991	6.61373
H	-6.38878	-4.04197	5.14285
N	-4.30634	-4.06388	3.55205
O	-5.54094	-3.79197	2.97182
H	-5.40065	-2.95212	2.49086
Ru	-2.56017	-3.99962	2.45513
C	-3.41373	-4.94131	0.3933
C	-2.91069	-6.03111	1.17639
C	-1.55992	-5.95767	1.57957
C	-0.73258	-4.8548	1.23896
C	-1.22944	-3.80195	0.43578
C	-2.5861	-3.88003	0.00278
H	-4.4532	-4.94168	0.08747
H	-1.15278	-6.74524	2.2054
H	0.29618	-4.82908	1.58069
H	-2.99719	-3.07269	-0.59458
C	-0.34983	-2.66203	0.00204
C	-3.73562	-7.26971	1.49825
H	-3.46242	-7.5707	2.51754
C	-5.07475	-0.66264	1.59989
C	-6.23292	0.0106	1.12048
C	-6.69441	-0.19999	-0.19571
C	-6.93069	0.90015	1.96516
C	-7.82838	0.46458	-0.65147
H	-6.15572	-0.87918	-0.84884
C	-8.06299	1.55917	1.49759
H	-6.57315	1.06512	2.97618
C	-8.51395	1.34318	0.19224
H	-8.17799	0.30008	-1.66583
H	-8.59474	2.24376	2.15081
H	-9.39781	1.86048	-0.16789
C	-4.07268	-1.20235	2.0535
C	-2.96759	-1.8472	2.55019
C	-1.90253	-2.01046	3.21812

C	-0.75606	-1.47734	3.92
C	0.13284	-0.63234	3.22337
C	-0.53245	-1.72819	5.28656
C	1.22135	-0.06304	3.87871
H	-0.04729	-0.41546	2.17562
C	0.55534	-1.14648	5.93431
H	-1.21918	-2.35997	5.83586
C	1.43747	-0.32029	5.23482
H	1.89611	0.58886	3.33236
H	0.71201	-1.33766	6.99146
H	2.28456	0.12756	5.7451
H	0.05552	-2.86764	-0.99575
H	-0.91225	-1.72678	-0.05545
H	0.49108	-2.52401	0.68459
C	-5.25427	-7.04773	1.45342
H	-5.60722	-6.88695	0.42848
H	-5.76335	-7.94072	1.82615
H	-5.57008	-6.1961	2.06151
C	-3.32281	-8.41526	0.54578
H	-2.2535	-8.63736	0.61239
H	-3.87253	-9.32651	0.79861
H	-3.5527	-8.16188	-0.49474

TS2

Sum of electronic and thermal Free Energies = -1537.961739

Sum of electronic and thermal Enthalpies = -1537.855277

Imaginary frequency= -328.6019

C	-3.0884	0.42176	4.91512
C	-2.63823	-0.36301	3.83364
C	-1.22793	-0.51948	3.67701
C	-0.33399	0.04241	4.60193
C	-0.81119	0.81098	5.65732
C	-2.19153	1.01265	5.79798
H	-4.15362	0.53231	5.08839
H	0.73499	-0.0939	4.47112
H	-0.11848	1.2567	6.36347
H	-2.56791	1.62308	6.61373
C	-0.77956	-1.20611	2.47699
C	0.60155	-1.74949	2.27434
H	1.25783	-0.97645	1.85731
H	1.02697	-2.07953	3.22377
H	0.58333	-2.5807	1.56932
N	-1.71779	-1.29453	1.58008
O	-1.35661	-1.92163	0.39069
H	-2.14644	-2.43451	0.14526

Ru	-3.65536	-0.55164	1.92598	H	-3.72478	3.88111	-0.44232
C	-4.34121	0.08823	-0.20486	H	-2.41438	3.78499	-1.62836
C	-3.69468	1.25302	0.33582	H	-3.91711	2.89074	-1.89867
C	-4.18025	1.74968	1.56043	H	-7.16184	-1.72542	2.15298
C	-5.2293	1.08377	2.25119	H	-7.02064	-0.54954	3.4691
C	-5.91771	-0.02555	1.69024	H	-8.0246	-0.18373	2.05921
C	-5.45493	-0.49875	0.42839	H	-1.90424	2.37708	0.36406
H	-3.98582	-0.32991	-1.13927	TS2'			
H	-3.69959	2.60612	2.02099	Sum of electronic and thermal Free Energies = -1537.960585			
H	-5.5329	1.44974	3.22613	Sum of electronic and thermal Enthalpies = -1537.855216			
H	-5.93842	-1.35799	-0.02421	Imaginary frequency= -304.5645			
C	-7.09261	-0.65997	2.38463	C	-0.72454	-4.67112	4.687
C	-3.75254	-2.52797	2.51931	C	-2.02269	-4.33736	4.24344
C	-3.8653	-3.82542	1.90666	C	-3.11959	-4.72758	5.07298
C	-4.12656	-3.97951	0.52782	C	-2.90301	-5.35491	6.31009
C	-3.68419	-4.98879	2.69047	C	-1.61	-5.67293	6.71281
C	-4.20975	-5.24685	-0.04604	C	-0.5249	-5.34853	5.88532
H	-4.29208	-3.09729	-0.0848	H	0.13508	-4.36608	4.09894
C	-3.77118	-6.24924	2.11129	H	-3.74837	-5.62932	6.93361
H	-3.47719	-4.88436	3.75063	H	-1.44331	-6.17689	7.65916
C	-4.03196	-6.38506	0.74286	H	0.4843	-5.60671	6.19269
H	-4.41624	-5.34713	-1.10726	C	-4.44667	-4.52018	4.51589
H	-3.63205	-7.13269	2.72682	C	-5.71934	-4.5707	5.3031
H	-4.09538	-7.37221	0.29616	H	-6.07019	-5.60561	5.39246
C	-3.68536	-1.97323	3.7112	H	-5.56172	-4.18008	6.31052
C	-4.25057	-2.20853	4.95735	H	-6.50016	-3.99839	4.80285
C	-4.74136	-2.42512	6.0547	N	-4.40414	-4.28766	3.23572
C	-5.30224	-2.68452	7.33488	O	-5.62414	-4.08431	2.59953
C	-4.74572	-2.08922	8.48681	H	-5.45797	-3.30753	2.03347
C	-6.41762	-3.53785	7.46971	Ru	-2.60507	-4.20261	2.18405
C	-5.29738	-2.34113	9.73881	C	-3.13544	-5.90508	0.74027
H	-3.88362	-1.43832	8.38306	C	-1.93901	-6.33459	1.35688
C	-6.9583	-3.78607	8.72734	C	-0.85692	-5.4135	1.31193
H	-6.84527	-3.9974	6.58452	C	-0.91298	-4.21872	0.54824
C	-6.40205	-3.18886	9.86224	C	-2.0734	-3.86508	-0.19752
H	-4.86429	-1.88037	10.62122	C	-3.20516	-4.70077	-0.02394
H	-7.81525	-4.44534	8.82466	H	-4.03084	-6.51148	0.83542
H	-6.82778	-3.38505	10.84151	H	0.05301	-5.64282	1.85637
C	-2.58965	1.99461	-0.40274	H	-0.03506	-3.58529	0.52185
C	-1.78024	1.12835	-1.37819	H	-4.14457	-4.44995	-0.49813
C	-3.20303	3.21164	-1.13255	C	-2.05453	-2.68913	-1.18409
H	-1.39446	0.2213	-0.9062	C	-1.26791	-3.18479	-2.42756
H	-2.37672	0.83792	-2.25052	C	-3.47241	-2.2754	-1.62385
H	-0.93047	1.70391	-1.75547	C	-1.34315	-1.45262	-0.59381

H	-1.74298	-4.06162	-2.87902	C	-0.08691	-1.36337	3.9006
H	-1.23647	-2.39273	-3.18218	C	1.07038	-0.58404	4.04883
H	-4.08796	-1.97183	-0.77192	C	1.08907	0.5315	4.87936
H	-3.40371	-1.42126	-2.30305	C	-0.06754	0.87466	5.58469
H	-3.98766	-3.07301	-2.16806	H	-2.08145	0.33387	6.07797
H	-1.32585	-0.65532	-1.3426	H	1.95865	-0.85026	3.4861
H	-1.86994	-1.07695	0.28715	H	1.99328	1.12548	4.97681
H	-0.30327	-1.65517	-0.32165	H	-0.07009	1.74227	6.23726
C	-1.83498	-7.64951	2.07953	C	-0.07504	-2.46422	2.92148
H	-1.4347	-8.41895	1.40896	C	1.07943	-3.40627	2.75159
H	-1.16545	-7.57627	2.94029	H	1.74899	-3.05663	1.95608
H	-2.8132	-7.98833	2.42936	H	1.65251	-3.48025	3.67747
C	-4.7716	-0.57968	1.79413	H	0.7171	-4.39346	2.45585
C	-5.72754	0.33956	1.27636	N	-1.14843	-2.52203	2.20546
C	-5.33005	1.64355	0.91233	O	-1.18512	-3.5351	1.25457
C	-7.07796	-0.03688	1.12263	H	-2.13246	-3.72981	1.16735
C	-6.26446	2.54142	0.4058	Ru	-2.73891	-1.13786	2.47331
H	-4.29278	1.93737	1.03472	C	-3.72545	0.90022	2.45423
C	-8.00373	0.87043	0.61676	C	-4.75828	-0.05314	2.27928
H	-7.39153	-1.03582	1.40988	C	-4.57924	-0.98428	1.21188
C	-7.60041	2.15894	0.25648	C	-3.4333	-0.91038	0.37199
H	-5.95119	3.54322	0.12886	C	-2.48671	0.17288	0.45651
H	-9.04189	0.57358	0.50499	C	-2.65176	1.06723	1.51978
H	-8.32585	2.86396	-0.13741	H	-3.76438	1.55736	3.31736
C	-3.90982	-1.31876	2.2575	H	-5.31955	-1.75809	1.04804
C	-3.00524	-2.22757	2.74999	H	-3.3055	-1.65206	-0.41109
C	-2.076	-2.50217	3.62544	H	-1.92265	1.8472	1.70168
C	-1.01612	-1.71821	4.27155	C	-1.37742	0.27633	-0.5751
C	-0.25642	-0.8251	3.4933	C	-1.90037	1.05818	-1.80305
C	-0.80931	-1.75874	5.6617	C	-0.07771	0.89258	-0.03944
C	0.69498	-0.00141	4.09179	H	-2.80757	0.60841	-2.21917
H	-0.41783	-0.7846	2.421	H	-2.12985	2.0954	-1.53427
C	0.13239	-0.92238	6.25574	H	-1.14058	1.07126	-2.59016
H	-1.40266	-2.4283	6.2742	H	0.29592	0.35013	0.83527
C	0.89149	-0.04793	5.4735	H	0.69266	0.8588	-0.81474
H	1.27955	0.67897	3.48004	H	-0.20797	1.9446	0.23804
H	0.27216	-0.94981	7.332	C	-5.95251	-0.11796	3.19207
H	1.62969	0.59719	5.93991	H	-6.7869	0.44835	2.76166
H	-0.23646	-3.44935	-2.17436	H	-6.28381	-1.14894	3.33819
IM4				H	-5.72638	0.31303	4.17042
Sum of electronic and thermal Free Energies = -1537.989945				C	-3.14536	-2.58269	3.82465
Sum of electronic and thermal Enthalpies = -1537.881516				C	-3.97528	-3.77933	3.81455
C	-1.21161	0.09352	5.47678	C	-4.63788	-4.18225	2.63229
C	-1.2675	-1.0521	4.64806	C	-4.06471	-4.64499	4.93208

C	-5.37228	-5.36318	2.57075	Ru	-2.67134	-4.5225	2.16607
H	-4.55694	-3.56281	1.74752	C	-3.39635	-6.27686	0.80037
C	-4.80252	-5.82148	4.86974	C	-2.18025	-6.74516	1.31874
H	-3.54888	-4.38869	5.84839	C	-1.07568	-5.83386	1.24928
C	-5.46535	-6.18627	3.69388	C	-1.10959	-4.63302	0.49395
H	-5.86726	-5.64438	1.64587	C	-2.32551	-4.20184	-0.10541
H	-4.85498	-6.46388	5.74343	C	-3.48382	-4.9952	0.15491
H	-6.03757	-7.10741	3.65113	H	-4.29964	-6.86698	0.92283
C	-2.44085	-2.00873	4.86619	H	-0.15436	-6.09572	1.76135
C	-2.85955	-2.10033	6.21743	H	-0.21774	-4.0239	0.42437
C	-3.23036	-2.11117	7.38062	H	-4.44406	-4.66549	-0.22979
C	-3.66702	-2.1123	8.73377	C	-2.43354	-2.97534	-0.99257
C	-2.83826	-1.59794	9.75261	C	-2.60207	-3.43735	-2.45993
C	-4.93793	-2.62254	9.07302	C	-1.26233	-1.99302	-0.86102
C	-3.27581	-1.59291	11.07319	H	-3.46195	-4.10243	-2.58781
H	-1.85819	-1.2102	9.49466	H	-2.75018	-2.56737	-3.10668
C	-5.36371	-2.615	10.3975	H	-1.46267	-1.10377	-1.46474
H	-5.57763	-3.01749	8.29063	H	-1.12041	-1.6668	0.17136
C	-4.53657	-2.10037	11.39938	H	-0.32553	-2.42651	-1.22662
H	-2.63235	-1.19497	11.85141	C	-2.04267	-8.08086	1.99838
H	-6.34295	-3.00923	10.6506	H	-1.51322	-8.78681	1.34773
H	-4.87319	-2.09531	12.43148	H	-1.46884	-7.9939	2.92614
H	-1.15534	-0.74843	-0.9023	H	-3.01928	-8.51103	2.23446

IM4'

Sum of electronic and thermal Free Energies = -1537.996447

Sum of electronic and thermal Enthalpies = -1537.888675

C	-0.28085	-4.1	4.67929	C	-3.99431	-0.6167	1.46934
C	-1.65083	-3.82472	4.43894	C	-4.75432	0.47632	0.96614
C	-2.60088	-4.8038	4.881	C	-4.96902	1.60412	1.78861
C	-2.16226	-5.95878	5.55962	C	-5.30141	0.463	-0.33308
C	-0.81093	-6.18346	5.78494	C	-5.7136	2.68159	1.31962
C	0.13419	-5.25107	5.33314	H	-4.54702	1.61545	2.78792
H	0.44772	-3.35366	4.3766	C	-6.04249	1.54765	-0.79321
H	-2.89767	-6.67584	5.9132	H	-5.13984	-0.39943	-0.97252
H	-0.49067	-7.07268	6.32225	C	-6.25129	2.65755	0.02991
H	1.19138	-5.41727	5.5165	H	-5.87516	3.54296	1.9602
C	-4.06599	-4.59887	4.67447	H	-6.45828	1.52918	-1.79575
C	-5.08344	-4.64052	5.77237	H	-6.83173	3.50038	-0.33274
H	-5.47478	-5.65774	5.8966	C	-3.33736	-1.49431	2.01664
H	-4.63601	-4.33157	6.7197	C	-2.68084	-2.52088	2.6968
H	-5.92878	-3.99406	5.52735	C	-2.03599	-2.46883	3.89158
N	-4.33427	-4.40121	3.43189	C	-1.62113	-1.26558	4.64393
O	-5.65865	-4.19299	3.09266	C	-1.2871	-0.06946	3.9785
H	-5.60721	-3.62062	2.309	C	-1.53608	-1.29514	6.04962
				C	-0.89559	1.05851	4.69601
				H	-1.31948	-0.03294	2.89512
				C	-1.1544	-0.16275	6.76501

H	-1.78402	-2.20677	6.58787
C	-0.82802	1.01787	6.09096
H	-0.6261	1.96759	4.16285
H	-1.10761	-0.20216	7.8495
H	-0.51766	1.89739	6.64769
H	-1.70858	-3.96644	-2.80846
H	-3.35039	-2.45009	-0.69246

TS3

Sum of electronic and thermal Free Energies = -1537.858696

Sum of electronic and thermal Enthalpies = -1537.964314

Imaginary frequency= -354.8503

C	-0.31336	-0.3223	5.3795
C	-0.62548	-1.44148	4.5695
C	0.463	-2.11453	3.91229
C	1.7992	-1.67492	4.13669
C	2.06268	-0.58244	4.92933
C	0.99044	0.09771	5.54941
H	-1.12219	0.18818	5.88972
H	2.61562	-2.17964	3.63298
H	3.08215	-0.24118	5.07164
H	1.19528	0.95554	6.18332
C	0.18832	-3.19298	3.03562
C	1.18756	-4.2301	2.62549
H	2.10155	-4.15755	3.21131
H	0.75355	-5.22504	2.76058
H	1.42668	-4.14538	1.55969
N	-1.06878	-3.26776	2.54367
O	-1.25032	-4.35252	1.66889
H	-1.99979	-4.8576	2.03954
Ru	-2.64435	-1.72137	2.35646
C	-4.02416	0.01468	2.26046
C	-4.7952	-1.13687	1.93351
C	-4.32582	-1.93936	0.85197
C	-3.15162	-1.56848	0.14692
C	-2.47136	-0.32527	0.38444
C	-2.92884	0.45826	1.45201
H	-4.29708	0.59397	3.13649
H	-4.85269	-2.8473	0.57834
H	-2.77771	-2.23654	-0.62094
H	-2.4089	1.3721	1.71798
C	-1.3052	0.12001	-0.48268
C	-1.81948	0.5428	-1.8746
C	-0.19044	-0.93325	-0.5959
H	-2.25121	-0.30766	-2.4131

H	-2.58556	1.32034	-1.80065
H	-0.99575	0.93584	-2.47818
H	0.63628	-0.53723	-1.19309
H	0.19916	-1.20201	0.39064
H	-0.53898	-1.8475	-1.08794
C	-6.03401	-1.49198	2.71056
H	-6.91062	-1.0153	2.2554
H	-6.20632	-2.57126	2.7189
H	-5.96309	-1.1445	3.7443
C	-2.44992	-3.08448	3.746
C	-3.00355	-4.36449	4.17833
C	-2.60981	-4.93887	5.40514
C	-3.89728	-5.0719	3.34693
C	-3.1031	-6.18149	5.78759
H	-1.92735	-4.39576	6.05124
C	-4.37686	-6.32475	3.72804
H	-4.23298	-4.60878	2.42302
C	-3.9804	-6.87812	4.94788
H	-2.80344	-6.61373	6.73709
H	-5.06645	-6.86185	3.08447
H	-4.35801	-7.85053	5.24864
C	-1.98937	-1.95246	4.53828
C	-2.91681	-1.53596	5.54002
C	-3.74418	-1.20556	6.37165
C	-4.71879	-0.82836	7.34043
C	-4.40034	0.08889	8.36232
C	-6.01956	-1.3708	7.2869
C	-5.36231	0.45475	9.29926
H	-3.39962	0.50547	8.41133
C	-6.97237	-1.00151	8.23172
H	-6.26624	-2.08508	6.50769
C	-6.64848	-0.08784	9.23801
H	-5.10785	1.1631	10.08142
H	-7.97005	-1.42689	8.18421
H	-7.3948	0.19875	9.97244
H	-0.87549	1.00683	-0.0005

IM5

Sum of electronic and thermal Free Energies = -1537.993747

Sum of electronic and thermal Enthalpies = -1537.890523

C	-0.72794	0.01789	5.26253
C	-0.93911	-1.21296	4.55307
C	0.00989	-1.59705	3.49264
C	1.01639	-0.6255	3.12516
C	1.11711	0.57198	3.77345

C	0.26081	0.87855	4.87837	H	-2.52382	-4.73631	1.64506
H	-1.38055	0.24139	6.09977	C	-4.96404	-6.39049	3.34449
H	1.717	-0.87121	2.33335	H	-5.55699	-5.95459	5.36845
H	1.88113	1.28422	3.47867	H	-4.13333	-6.59729	1.36326
H	0.40613	1.80884	5.41878	H	-5.68245	-7.19436	3.2185
C	0.31157	-3.02277	3.3978	C	-2.05732	-2.10679	4.7706
C	1.6883	-3.58491	3.26743	C	-2.97634	-1.88054	5.82711
H	2.2676	-3.00494	2.54616	C	-3.72955	-1.62702	6.75071
H	2.20686	-3.51273	4.23122	C	-4.62022	-1.36025	7.83175
H	1.66152	-4.63276	2.97037	C	-4.22736	-0.51261	8.88731
N	-0.7122	-3.80883	3.60061	C	-5.90366	-1.94341	7.85888
O	-0.45868	-5.11102	4.00418	C	-5.10019	-0.25754	9.94088
H	-1.22921	-5.61447	3.67483	H	-3.23798	-0.06683	8.87328
Ru	-2.21006	-1.39143	2.7459	C	-6.76838	-1.68177	8.91744
C	-3.45667	0.55192	2.36584	H	-6.21027	-2.59601	7.04751
C	-4.34623	-0.55314	2.46435	C	-6.37043	-0.83964	9.95927
C	-4.1064	-1.65692	1.59756	H	-4.78884	0.39483	10.75079
C	-3.08056	-1.63066	0.60743	H	-7.75481	-2.13497	8.93111
C	-2.2056	-0.52518	0.50039	H	-7.04776	-0.63843	10.78343
C	-2.39586	0.54272	1.43581	H	-0.46575	0.34221	-0.48772
H	-3.56416	1.38977	3.04647	TS4			
H	-4.73376	-2.53811	1.67957	Sum of electronic and thermal Free Energies =	-1998.775247		
H	-2.98003	-2.47676	-0.06069	Sum of electronic and thermal Enthalpies =	-1998.665335		
H	-1.70758	1.37736	1.43895	Imaginary frequency=	-109.3277		
C	-1.1621	-0.45799	-0.62801	C	0.4283	-4.89902	6.67576
C	-1.94021	-0.20939	-1.94665	C	-0.04447	-4.00739	5.66163
C	-0.37465	-1.78084	-0.74528	C	0.92897	-3.22346	4.92244
H	-2.63205	-1.02797	-2.1677	C	2.3178	-3.32169	5.30104
H	-2.51831	0.71879	-1.89766	C	2.71298	-4.16388	6.29829
H	-1.2393	-0.12557	-2.78326	C	1.75632	-4.97012	6.99175
H	0.34835	-1.709	-1.56342	H	-0.29969	-5.49893	7.20915
H	0.17243	-1.99556	0.17758	H	3.05409	-2.73055	4.76932
H	-1.02167	-2.63535	-0.96243	H	3.76263	-4.23174	6.56652
C	-5.48543	-0.56084	3.44614	H	2.09238	-5.63604	7.78026
H	-6.34276	-0.01999	3.02844	C	0.53968	-2.43816	3.84987
H	-5.80705	-1.58055	3.66945	C	1.48343	-1.69656	2.94471
H	-5.20571	-0.07661	4.38509	H	2.17297	-1.0758	3.52635
C	-2.06376	-3.22465	3.79322	H	2.09628	-2.3814	2.3478
C	-3.10439	-4.2958	3.67867	H	0.94058	-1.05134	2.25491
C	-3.96689	-4.66105	4.72387	N	-0.82768	-2.35125	3.50148
C	-3.17846	-5.0164	2.46713	O	-0.96634	-2.8199	2.02827
C	-4.8961	-5.68932	4.54869	Ru	-1.81762	-0.64405	4.2658
H	-3.90647	-4.14983	5.67607	C	-0.33058	0.65987	5.3526
C	-4.0936	-6.05649	2.30405	C	-1.4256	0.50992	6.25498

C	-2.71407	0.83185	5.75094	H	-1.17758	0.95366	9.66326
C	-2.88658	1.32618	4.43091	H	-0.30404	1.86581	8.42198
C	-1.78253	1.59499	3.56787	H	-2.07315	1.93215	8.49001
C	-0.50644	1.20984	4.04844	C	-0.0665	-0.88008	7.93139
H	0.66218	0.35424	5.65959	H	-0.09839	-1.2647	8.95543
H	-3.59004	0.64207	6.36116	H	-0.06665	-1.73619	7.25081
H	-3.89418	1.48957	4.06339	H	0.8839	-0.34587	7.82052
H	0.35611	1.31022	3.39788	IM6			
C	-1.97281	2.23573	2.22065	Sum of electronic and thermal Free Energies =	-1922.505066		
C	-1.26894	0.04269	7.69165	Sum of electronic and thermal Enthalpies =	-1922.400364		
H	-2.18057	-0.5163	7.93887	C	0.60009	-5.49028	6.39038
C	-1.82415	-2.8773	4.4038	C	0.13954	-4.31258	5.75661
C	-3.19691	-2.45058	4.08111	C	1.08332	-3.40482	5.19316
C	-3.45687	-1.72832	2.86973	C	2.46739	-3.71031	5.28895
C	-4.27402	-2.58447	5.02287	C	2.89051	-4.8633	5.91341
C	-4.7459	-1.16723	2.64322	C	1.94977	-5.75992	6.46697
H	-2.79934	-1.8306	2.02166	H	-0.12819	-6.17605	6.80789
C	-5.50774	-2.0412	4.75947	H	3.20059	-3.0333	4.86765
H	-4.10307	-3.10888	5.95202	H	3.95075	-5.08582	5.97835
C	-5.7549	-1.3174	3.56389	H	2.29369	-6.66758	6.95308
H	-4.92876	-0.66286	1.69915	C	0.61839	-2.20894	4.55556
H	-6.30584	-2.16173	5.48616	C	1.59935	-1.24102	3.95501
H	-6.74342	-0.91214	3.37195	H	2.23352	-0.79109	4.72812
C	-1.41768	-3.86793	5.37105	H	2.2613	-1.75972	3.25534
C	-2.36113	-4.72524	5.98042	H	1.08658	-0.46176	3.39779
C	-3.13545	-5.51074	6.50236	N	-0.6862	-1.94373	4.50242
C	-4.083	-6.39793	7.08188	Ru	-1.6887	-0.16147	3.79186
C	-3.71027	-7.27019	8.12576	C	-0.64067	1.2541	5.12115
C	-5.41442	-6.41107	6.61388	C	-1.83199	0.90141	5.82964
C	-4.6501	-8.12935	8.68585	C	-3.04257	1.03904	5.11304
H	-2.68714	-7.26431	8.4871	C	-3.09542	1.65103	3.81668
C	-6.34496	-7.27501	7.18124	C	-1.93561	2.10769	3.16206
H	-5.69984	-5.7458	5.80518	C	-0.68668	1.8137	3.81648
C	-5.96684	-8.13429	8.21714	H	0.32509	1.05732	5.57467
H	-4.35638	-8.79798	9.48901	H	-3.9615	0.65699	5.54421
H	-7.36663	-7.28177	6.8146	H	-4.05648	1.72194	3.32447
H	-6.69607	-8.80758	8.65673	H	0.24516	2.02576	3.30995
Cl	-0.60067	-0.58936	-0.28125	C	-2.01297	2.87894	1.83801
H	-0.65532	-3.74306	2.05114	C	-2.45469	4.3187	2.21913
H	-0.72063	-1.57118	0.56443	C	-0.64923	2.94986	1.12242
H	-1.16477	1.97734	1.53206	H	-3.4425	4.32903	2.69081
H	-1.99049	3.32765	2.33386	H	-1.74351	4.79182	2.90434
H	-2.92094	1.93537	1.7676	H	-2.50702	4.93257	1.31478
C	-1.20644	1.27712	8.61867	H	-0.26412	1.95365	0.89067

H	-0.76929	3.49253	0.18086
H	0.09633	3.49699	1.70929
C	-1.77991	0.35265	7.22749
H	-1.76075	1.17922	7.9474
H	-2.65592	-0.2608	7.44667
H	-0.88144	-0.24861	7.38905
C	-1.61872	-2.82391	5.00401
C	-3.01674	-2.4024	4.74625
C	-3.36346	-2.03947	3.41992
C	-3.99593	-2.34023	5.75463
C	-4.66822	-1.58415	3.13521
H	-2.69882	-2.32894	2.61247
C	-5.28234	-1.90373	5.44983
H	-3.74637	-2.64107	6.766
C	-5.61991	-1.50765	4.14402
H	-4.9282	-1.33662	2.1105
H	-6.03402	-1.86786	6.23331
H	-6.62976	-1.17626	3.92272
C	-1.26095	-4.00394	5.64289
C	-2.24055	-4.89809	6.14408
C	-3.05914	-5.68614	6.58263
C	-4.04592	-6.58016	7.08592
C	-3.68127	-7.65765	7.91879
C	-5.40452	-6.39234	6.75693
C	-4.65524	-8.52181	8.40949
H	-2.63685	-7.80514	8.17373
C	-6.36997	-7.26263	7.25326
H	-5.68507	-5.56685	6.11065
C	-5.99928	-8.32728	8.0795
H	-4.36661	-9.34927	9.05015
H	-7.41371	-7.1136	6.99417
H	-6.75567	-9.00469	8.46372
Cl	-0.9097	-0.73441	1.55666
H	-2.73214	2.45058	1.17152

PI

Sum of electronic and thermal Free Energies = -979.239413

Sum of electronic and thermal Enthalpies = -979.167902

C	0.60009	-5.49028	6.39038
C	0.13954	-4.31258	5.75661
C	1.08332	-3.40482	5.19316
C	2.46739	-3.71031	5.28895
C	2.89051	-4.8633	5.91341
C	1.94977	-5.75992	6.46697
H	-0.12819	-6.17605	6.80789

H	3.20059	-3.0333	4.86765
H	3.95075	-5.08582	5.97835
H	2.29369	-6.66758	6.95308
C	0.61839	-2.20894	4.55556
C	1.59935	-1.24102	3.95501
H	2.23352	-0.79109	4.72812
H	2.2613	-1.75972	3.25534
H	1.08658	-0.46176	3.39779
N	-0.6862	-1.94373	4.50242
C	-1.61872	-2.82391	5.00401
C	-3.01674	-2.4024	4.74625
C	-3.36346	-2.03947	3.41992
C	-3.99593	-2.34023	5.75463
C	-4.66822	-1.58415	3.13521
H	-2.69882	-2.32894	2.61247
C	-5.28234	-1.90373	5.44983
C	-3.74637	-2.64107	6.766
H	-2.69882	-2.32894	2.61247
C	-5.28234	-1.90373	5.44983
H	-3.74637	-2.64107	6.766
C	-5.61991	-1.50765	4.14402
H	-4.9282	-1.33662	2.1105
H	-6.03402	-1.86786	6.23331
H	-6.62976	-1.17626	3.92272
C	-1.26095	-4.00394	5.64289
H	-6.03402	-1.86786	6.23331
H	-6.62976	-1.17626	3.92272
C	-1.26095	-4.00394	5.64289
C	-2.24055	-4.89809	6.14408
C	-3.05914	-5.68614	6.58263
C	-4.04592	-6.58016	7.08592
C	-3.68127	-7.65765	7.91879
C	-5.40452	-6.39234	6.75693
C	-4.65524	-8.52181	8.40949
C	-3.68127	-7.65765	7.91879
C	-5.40452	-6.39234	6.75693
C	-4.65524	-8.52181	8.40949
H	-2.63685	-7.80514	8.17373
C	-6.36997	-7.26263	7.25326
H	-5.68507	-5.56685	6.11065
C	-5.99928	-8.32728	8.0795
H	-4.36661	-9.34927	9.05015
H	-7.41371	-7.1136	6.99417
H	-6.75567	-9.00469	8.46372

IM1a

Sum of electronic and thermal Free Energies = -1383.328957

Sum of electronic and thermal Enthalpies = -1383.249231

C	-2.84822	-2.63949	2.14156
C	-1.67938	-1.88113	2.23415
C	-1.69552	-0.50809	1.91907
C	-2.90207	0.09228	1.5218
C	-4.05758	-0.67411	1.41367
C	-4.03488	-2.03923	1.72453

H	-2.83622	-3.68829	2.42158	C	-1.72431	-0.55608	1.85391
H	-0.77494	-2.32506	2.63773	C	-2.87825	0.13025	1.44743
H	-2.92886	1.14404	1.2564	C	-4.04249	-0.57619	1.16485
H	-4.98186	-0.20879	1.08703	C	-4.08005	-1.96833	1.31336
H	-4.94598	-2.6249	1.65754	H	-2.99015	-3.72426	1.91856
C	-0.4536	0.27667	2.0265	H	-0.92238	-2.44989	2.48692
C	-0.43791	1.62515	2.68893	H	-2.84959	1.2066	1.31114
H	-1.44106	2.05108	2.70377	H	-4.9256	-0.0438	0.82513
H	-0.1223	1.54195	3.73816	H	-4.99694	-2.51032	1.10193
H	0.24367	2.3077	2.17398	C	-0.45766	0.16185	2.09253
N	0.63043	-0.27171	1.56543	C	-0.39941	1.38313	2.95906
O	1.83679	0.39832	1.7975	H	-1.40091	1.76775	3.15362
H	1.8205	0.7273	2.71435	H	0.06086	1.09728	3.91181
Ru	0.80046	-1.92593	0.23593	H	0.23113	2.15239	2.50908
Cl	-0.51651	-0.71213	-1.27355	N	0.60743	-0.35183	1.56377
C	1.01339	-3.95331	-0.71028	O	1.79149	0.32276	1.8639
C	1.14945	-4.11742	0.71176	H	2.20098	-0.21574	2.58858
C	2.15046	-3.36759	1.38692	F	3.31702	-1.48774	5.8363
C	2.92706	-2.41287	0.68428	F	0.80183	-2.27698	3.90791
C	2.77497	-2.21131	-0.72669	F	2.67298	-3.37643	4.65324
C	1.81588	-3.03783	-1.40986	F	1.43559	-0.38355	5.05216
H	0.22056	-4.47884	-1.23213	F	1.20299	-2.40935	6.19078
H	2.25139	-3.45556	2.46337	F	2.90641	-1.35505	3.55345
H	3.58867	-1.76057	1.24106	P	2.05244	-1.89075	4.92952
H	1.62324	-2.85777	-2.46223	Ru	0.71854	-1.99681	0.265
C	3.63038	-1.24949	-1.52998	Cl	-0.61343	-0.78665	-1.28715
C	4.78021	-2.06057	-2.17748	C	0.91918	-4.07313	-0.6022
C	4.17699	-0.0554	-0.73442	C	1.10793	-4.16455	0.81895
H	5.46348	-2.44875	-1.41336	C	2.13584	-3.39443	1.41767
H	4.41237	-2.90691	-2.76803	C	2.86094	-2.46024	0.64361
H	5.35376	-1.40921	-2.8428	C	2.65229	-2.30575	-0.76736
H	4.69189	0.62617	-1.41631	C	1.68214	-3.18177	-1.37287
H	3.38116	0.50191	-0.23321	H	0.11242	-4.62642	-1.07063
H	4.91164	-0.36825	0.01796	H	2.27611	-3.41855	2.49024
C	0.262	-5.08477	1.44369	H	3.52764	-1.79082	1.16929
H	0.66862	-6.09793	1.33406	H	1.43544	-3.06045	-2.41911
H	0.21051	-4.86141	2.51173	C	3.52206	-1.3628	-1.60806
H	-0.7495	-5.08996	1.02925	C	4.75732	-2.19773	-2.03989
H	2.9916	-0.86394	-2.33483	C	3.99675	-0.14372	-0.78937
IM1b				H	5.32077	-2.55964	-1.17367
Sum of electronic and thermal Free Energies = -2324.102922				H	4.46808	-3.06303	-2.64575
Sum of electronic and thermal Enthalpies = -2324.007313				H	5.42715	-1.57459	-2.64127
C	-2.95035	-2.6512	1.75648	H	4.5375	0.54142	-1.44876
C	-1.76907	-1.95212	2.02688	H	3.15919	0.39515	-0.33988

H	4.68799	-0.42583	0.01056
C	0.25954	-5.07629	1.6605
H	0.70395	-6.0794	1.66821
H	0.21739	-4.72105	2.69245
H	-0.75412	-5.16505	1.26113
H	3.01129	-1.01368	-2.48106

IM1c

Sum of electronic and thermal Free Energies = -2324.103093

Sum of electronic and thermal Enthalpies = -2324.008225

F	-3.98524	2.9381	1.23481
F	-6.13352	2.18179	0.8122
F	-5.68105	3.14539	2.84102
F	-5.38738	4.06517	-0.24561
F	-4.92828	5.03329	1.77399
F	-7.1024	4.25557	1.33961
C	-1.61311	-1.45106	-1.08212
C	-1.53604	-1.12924	0.2723
C	-2.48257	-0.26739	0.85593
C	-3.53766	0.22562	0.07423
C	-3.61674	-0.11454	-1.27884
C	-2.65491	-0.9409	-1.86229
H	-0.86924	-2.10741	-1.52432
H	-0.73667	-1.54547	0.88071
H	-4.29733	0.85634	0.51736
H	-4.44442	0.26611	-1.86989
H	-2.72397	-1.20132	-2.91452
C	-2.39516	0.01007	2.31523
C	-2.48708	-1.14737	3.27752
H	-2.62589	-2.08474	2.73949
H	-1.59275	-1.2068	3.90657
H	-3.33007	-0.98736	3.95761
N	-2.24718	1.21282	2.77285
O	-2.18147	1.24297	4.15117
H	-2.32561	2.20178	4.36622
Cl	-2.53232	4.13647	3.913
P	-5.62551	3.64477	1.31361
C	-1.1559	2.95555	-0.33829
C	-0.25151	2.30364	0.52258
C	0.31372	2.97398	1.66095
C	-0.08003	4.32082	1.87107
C	-0.9596	5.00451	0.96973
C	-1.50834	4.33879	-0.14632
H	-1.6385	2.38863	-1.12593
H	-0.05659	1.24728	0.37642

H	0.23373	4.82765	2.77664
H	-1.28103	6.00804	1.21401
C	1.25955	2.27187	2.59648
Ru	-1.90494	3.12009	1.78742
C	-2.47717	4.98693	-1.11726
C	-3.07155	6.31432	-0.63496
C	-1.76756	5.15451	-2.48084
H	-3.60349	6.19258	0.30983
H	-2.30468	7.09151	-0.53218
H	-3.79617	6.66878	-1.37306
H	-1.38222	4.2062	-2.86916
H	-2.47487	5.55372	-3.21352
H	-0.92894	5.85569	-2.40544
H	1.20196	2.69211	3.60298
H	1.03682	1.2039	2.65677
H	2.29041	2.38193	2.23906
H	-3.30806	4.28461	-1.24123

IM1d

Sum of electronic and thermal Free Energies = -1863.646536

Sum of electronic and thermal Enthalpies = -1863.557507

C	-1.14454	-2.20784	0.74754
C	-0.88565	-1.52701	1.95514
C	-1.50683	-0.26889	2.19563
C	-2.3956	0.25888	1.25313
C	-2.62111	-0.42367	0.05938
C	-1.98442	-1.64438	-0.20658
H	-0.71601	-3.19157	0.57886
H	-0.45546	-2.06836	2.79383
H	-2.83582	1.23674	1.40595
H	-3.27874	0.01279	-0.68648
H	-2.16369	-2.15469	-1.14831
C	-1.00963	0.57298	3.29603
C	-1.86952	1.45209	4.14114
H	-2.87794	1.52036	3.7325
H	-1.94056	1.02611	5.14878
H	-1.42896	2.44559	4.23486
N	0.28298	0.52188	3.40139
O	0.85522	1.33138	4.37479
H	1.31069	2.00828	3.83099
Ru	1.43503	-0.53249	2.04445
C	2.6577	-2.13507	0.9912
C	2.38589	-2.57664	2.3314
C	2.73502	-1.71696	3.4046
C	3.37957	-0.46846	3.15605

C	3.69958	-0.04452	1.84002	H	2.3421	1.01248	5.86905
C	3.26643	-0.89343	0.76017	H	2.68216	-0.68223	6.15352
H	2.32521	-2.7358	0.15236	N	3.6273	-0.06106	3.68322
H	2.48833	-2.	4.42164	O	2.26651	-0.33161	3.70864
H	3.58218	0.1874	3.99324	H	2.11332	-0.85511	2.89166
H	3.37189	-0.53352	-0.25746	F	6.22007	-3.78372	3.1473
C	4.48469	1.2132	1.5233	F	6.60774	-2.24596	0.31955
P	0.73759	2.70968	0.62149	F	7.60892	-2.14857	2.36587
F	-0.15556	2.62498	-0.6983	F	5.21101	-3.89154	1.08277
F	0.86994	4.29095	0.62103	F	7.53696	-4.19667	1.23545
F	-0.59425	2.72173	1.55505	F	5.28574	-1.86131	2.249
F	0.62875	0.92119	0.67049	P	6.46289	-3.11254	1.70334
F	1.6386	2.57919	2.02195	Ru	4.42376	-0.00232	1.66847
F	2.09708	2.48604	-0.22417	C	5.62832	0.45612	-0.19105
H	3.91327	1.76032	0.76761	C	6.33525	1.0058	0.93537
C	1.75441	-3.91448	2.59057	C	5.62511	1.86576	1.808
H	1.07388	-4.20884	1.78986	C	4.25443	2.19664	1.56159
H	1.22028	-3.93787	3.54259	C	3.558	1.6776	0.44345
H	2.54642	-4.67145	2.63956	C	4.28601	0.78545	-0.42524
C	4.71687	2.1369	2.72409	H	6.10663	-0.31064	-0.78648
H	5.33485	1.66144	3.49457	H	6.10995	2.22842	2.70691
H	5.24923	3.03232	2.39042	H	3.72106	2.79335	2.29148
H	3.77707	2.46987	3.17033	H	3.73832	0.259	-1.19777
C	5.83532	0.78929	0.89187	C	2.11248	2.0123	0.127
H	5.7042	0.17999	-0.00773	C	2.09196	3.10367	-0.96706
H	6.39196	1.68566	0.60417	C	1.27808	2.42557	1.34554
H	6.44795	0.22489	1.60298	H	2.53368	4.03893	-0.60467
IM1e				H	2.63838	2.79403	-1.86374
Sum of electronic and thermal Free Energies = -2804.420030				H	1.05833	3.30909	-1.26084
Sum of electronic and thermal Enthalpies = -2804.311781				H	0.23435	2.54516	1.04248
C	7.24335	2.02244	5.94592	H	1.30749	1.66645	2.13116
C	5.89879	1.74437	5.70707	H	1.60498	3.38557	1.76316
C	5.52596	0.55829	5.04833	C	7.77599	0.66535	1.16557
C	6.5155	-0.35942	4.66648	H	8.38568	1.30202	0.51118
C	7.85976	-0.08091	4.92297	H	8.06965	0.85043	2.19973
C	8.2272	1.10781	5.55569	H	7.97495	-0.37775	0.92363
H	7.52239	2.94465	6.44707	P	1.40903	-2.03973	0.35348
H	5.13668	2.44999	6.02718	F	2.76373	-1.35467	1.41896
H	6.24251	-1.28803	4.18473	F	2.40116	-3.25075	0.04893
H	8.60941	-0.80527	4.62131	F	2.08205	-1.18875	-0.86571
H	9.27355	1.31829	5.75708	F	0.91396	-2.74252	1.71415
C	4.08741	0.25857	4.85062	F	0.61047	-0.68786	0.7938
C	3.15527	0.29793	6.03392	F	0.2115	-2.58473	-0.53906
H	3.69798	0.55277	6.94352	H	1.66841	1.10448	-0.28823

IM1f

Sum of electronic and thermal Free Energies = -1843.766418

Sum of electronic and thermal Enthalpies = -1843.681268

C	-2.93291	0.08478	-0.00906
N	-2.81289	1.01056	0.88196
O	-3.45306	2.2135	0.47819
H	-3.62202	2.71072	1.31221
Cl	-3.27038	4.84462	1.70008
C	-1.18849	3.96774	-2.31866
C	-0.66556	2.9557	-1.48839
C	-0.13423	3.24906	-0.18058
C	-0.21913	4.58048	0.26932
C	-0.81407	5.60035	-0.54329
C	-1.28397	5.32629	-1.85516
H	-1.63336	3.70387	-3.27128
H	-0.69223	1.92446	-1.82463
H	0.06245	4.81858	1.28853
H	-0.96676	6.5815	-0.11332
C	0.44764	2.15932	0.67653
Ru	-2.30019	4.00223	-0.38328
C	-1.90222	6.37909	-2.75783
C	-2.47124	7.59126	-2.01002
C	-0.86555	6.80699	-3.81903
H	-3.20271	7.28372	-1.25845
H	-1.68486	8.18043	-1.52377
H	-2.97518	8.25266	-2.72072
H	-0.48008	5.95165	-4.38399
H	-1.32487	7.49972	-4.53106
H	-0.01312	7.31701	-3.35563
H	0.4959	2.46624	1.72348
H	-0.14891	1.24665	0.61824
H	1.46564	1.92605	0.34091
Cl	-4.42804	4.29201	-1.48871
C	-3.64412	0.269	-1.32493
H	-4.37545	1.07427	-1.25293
H	-2.928	0.55545	-2.10605
H	-4.13087	-0.65614	-1.64277
C	-2.29677	-1.21683	0.3359
C	-2.07469	-2.19252	-0.64878
C	-1.90294	-1.49485	1.65886
C	-1.4756	-3.41053	-0.32338
H	-2.36256	-2.00483	-1.67754
C	-1.3077	-2.71022	1.97998
H	-2.08055	-0.74988	2.42579

C

-1.09126 -3.67428 0.99052

H

-1.31244 -4.15264 -1.09921

H

-1.01741 -2.91024 3.00727

H

-0.63127 -4.62475 1.24481

H

-2.73875 5.88535 -3.26584

IM1g

Sum of electronic and thermal Free Energies = -1383.3369395

Sum of electronic and thermal Enthalpies = -1383.257613

C	-4.82192	-0.93147	1.23131
C	-3.50839	-0.6459	1.59021
C	-3.06085	0.68631	1.63725
C	-3.95402	1.72856	1.32745
C	-5.26154	1.43481	0.94831
C	-5.69823	0.10798	0.90262
H	-5.17119	-1.95995	1.22308
H	-2.83257	-1.44228	1.87741
H	-3.62389	2.76276	1.35496
H	-5.94167	2.24363	0.69601
H	-6.72253	-0.11659	0.62273
C	-1.67399	1.00566	2.01221
C	-1.34523	2.26011	2.77694
H	-2.22357	2.63251	3.30288
H	-0.54315	2.07078	3.49348
H	-0.99862	3.03931	2.0848
N	-0.74664	0.17941	1.64561
O	0.6	0.50791	2.03458
H	0.84801	1.25993	1.44293
Ru	0.38122	-1.03799	0.32323
Cl	0.54745	1.04096	-0.87064
C	-0.38491	-2.65523	-0.95119
C	-0.45003	-3.19869	0.37444
C	0.72057	-3.13383	1.16745
C	1.9252	-2.58303	0.63989
C	2.0415	-2.16184	-0.72063
C	0.84782	-2.19574	-1.49379
H	-1.28661	-2.59504	-1.55075
H	0.68435	-3.43827	2.20796
H	2.7707	-2.45572	1.30705
H	0.84799	-1.74726	-2.48149
C	3.34031	-1.65198	-1.31901
C	4.16375	-2.85712	-1.82797
C	4.16421	-0.7707	-0.36653
H	4.48001	-3.49796	-0.99639
H	3.59922	-3.47274	-2.53713

H	5.06408	-2.49847	-2.33537
H	5.04516	-0.39367	-0.8927
H	3.58502	0.09118	-0.02231
H	4.52773	-1.32616	0.50595
C	-1.72643	-3.78441	0.90413
H	-1.74002	-4.85879	0.68093
H	-1.80748	-3.67224	1.98808
H	-2.60169	-3.33848	0.42588
H	3.06239	-1.03707	-2.18368

IM1h

Sum of electronic and thermal Free Energies = -2324.092090

Sum of electronic and thermal Enthalpies = -2323.990741

C	-6.68385	-0.998	2.99763
C	-5.48283	-0.39924	2.61864
C	-4.73618	-0.92106	1.55051
C	-5.22077	-2.04749	0.86373
C	-6.42517	-2.63748	1.24026
C	-7.15938	-2.11541	2.30882
H	-7.24769	-0.58899	3.83009
H	-5.11319	0.45924	3.16913
H	-4.65578	-2.4372	0.02225
H	-6.79751	-3.50016	0.69338
H	-8.09973	-2.57504	2.59942
C	-3.44102	-0.29095	1.17559
C	-3.23481	1.18676	1.3452
H	-4.18936	1.7002	1.45432
H	-2.61319	1.37245	2.22494
H	-2.69645	1.58602	0.48485
N	-2.55131	-1.11417	0.73523
O	-1.30818	-0.40018	0.40306
H	-0.80507	-0.36977	1.27069
F	1.7288	0.6954	3.37925
F	-1.46235	0.24306	3.89796
F	0.476	-0.62336	4.7962
F	-0.20995	1.55081	2.48807
F	0.14153	1.69424	4.79439
F	0.11176	-0.73634	2.50535
P	0.14108	0.51513	3.70544
Ru	-0.13165	-1.66903	-0.86854
Cl	-0.8088	-0.37075	-2.66797
C	0.34058	-3.61706	-1.78908
C	-0.42766	-3.81965	-0.58771
C	0.10321	-3.31848	0.64092
C	1.28198	-2.5462	0.65937

C	1.98243	-2.24369	-0.55059
C	1.52439	-2.85271	-1.76959
H	-0.06567	-3.94913	-2.73946
H	-0.49016	-3.3877	1.54589
H	1.55127	-2.04233	1.57933
H	2.01802	-2.60974	-2.70392
C	3.19728	-1.33319	-0.53589
C	4.36533	-2.06767	0.15727
C	2.92067	0.03978	0.1084
H	4.14491	-2.25421	1.21274
H	4.58124	-3.02497	-0.32274
H	5.26844	-1.45256	0.10819
H	3.8374	0.63825	0.08989
H	2.15255	0.58673	-0.45309
H	2.59388	-0.02641	1.15112
C	-1.75005	-4.53133	-0.61972
H	-1.60585	-5.59288	-0.38278
H	-2.43256	-4.102	0.11702
H	-2.21279	-4.46387	-1.60724
H	3.4776	-1.163	-1.58297

IM1i

Sum of electronic and thermal Free Energies = -2324.093259

Sum of electronic and thermal Enthalpies = -2323.996119

F	-4.99092	4.87002	1.17221
F	-6.48888	3.17429	0.60455
F	-6.42304	3.9022	2.77758
F	-6.83949	5.31325	-0.1632
F	-6.77301	6.05497	2.02723
F	-8.29471	4.39145	1.44019
C	-3.53633	-2.4053	5.78714
C	-3.94231	-1.10656	5.47811
C	-4.0498	-0.69554	4.14025
C	-3.7512	-1.61822	3.12163
C	-3.35177	-2.91461	3.43401
C	-3.24325	-3.31307	4.7683
H	-3.45258	-2.70897	6.8265
H	-4.15825	-0.40758	6.28325
H	-3.85684	-1.30733	2.08765
H	-3.137	-3.61995	2.6339
H	-2.9404	-4.32857	5.01161
C	-4.4576	0.68928	3.78301
C	-5.46752	1.44995	4.60629
H	-5.75686	0.88289	5.48879
H	-5.06913	2.42247	4.91732

H	-6.37701	1.63965	4.02639	H	-6.15238	-2.9761	2.12295
N	-3.8914	1.1442	2.71707	C	-1.8256	0.13812	2.78325
O	-4.3331	2.40337	2.2834	C	-1.80009	1.21926	3.83068
H	-5.12542	2.7857	2.74109	H	-2.55837	1.044	4.59287
Cl	-3.05026	4.79993	3.74908	H	-0.81543	1.30291	4.29585
P	-6.7195	4.62553	1.29444	H	-2.03569	2.18519	3.36466
C	-2.64667	3.51265	-0.66254	N	-0.87034	-0.10574	1.94871
C	-2.05467	2.49941	0.11641	O	0.2522	0.84237	2.12271
C	-1.1386	2.80605	1.18531	H	-0.0726	1.73477	1.85586
C	-0.842	4.17854	1.41339	Ru	1.8829	0.41691	0.78676
C	-1.45722	5.21451	0.64851	C	2.34335	-1.29415	-0.52747
C	-2.39551	4.89752	-0.37695	C	1.91538	-1.84348	0.71294
H	-3.41565	3.25156	-1.3811	C	2.5853	-1.36518	1.88721
H	-2.38265	1.47336	-0.01017	C	3.63621	-0.42083	1.81498
H	-0.23651	4.45082	2.27056	C	4.09029	0.089	0.5477
H	-1.29484	6.24404	0.93674	C	3.42223	-0.36203	-0.61791
C	-0.56473	1.71339	2.0429	H	1.78449	-1.52339	-1.42782
Ru	-3.00628	3.92514	1.52493	H	2.20955	-1.65895	2.86226
C	-3.17683	5.95639	-1.13619	H	4.05695	-0.01833	2.73052
C	-3.41661	7.25483	-0.35203	H	3.65806	0.08564	-1.57707
C	-2.46803	6.22598	-2.48415	C	5.13936	1.15922	0.47925
H	-3.93499	7.05651	0.5899	P	1.04118	3.25996	-0.26571
H	-2.48867	7.79889	-0.14196	F	2.2693	3.07391	-1.27566
H	-4.04972	7.91473	-0.95101	F	1.48236	4.70524	0.19174
H	-2.30557	5.30718	-3.05468	F	0.01762	3.68881	-1.38904
H	-3.07969	6.89698	-3.09479	F	0.6579	1.57482	-0.57164
H	-1.49635	6.70445	-2.32324	F	-0.14201	3.19308	0.87586
H	-0.14976	2.11705	2.96775	F	2.0775	2.56659	0.97888
H	-1.34016	0.99007	2.3006	H	4.96976	1.82452	-0.36986
H	0.23343	1.19364	1.50419	H	5.16201	1.75625	1.39361
H	-4.16139	5.51804	-1.34699	H	6.12357	0.69048	0.35756
IM1j				C	0.79494	-2.8577	0.83844
Sum of electronic and thermal Free Energies = -1863.642480				C	-0.17	-2.87341	-0.35303
Sum of electronic and thermal Enthalpies = -1863.548297				C	1.42231	-4.25114	1.07864
C	-4.59205	-1.85536	1.14446	H	0.31294	-3.23125	-1.26911
C	-3.46864	-1.04971	1.31506	H	-0.9959	-3.55695	-0.13968
C	-3.02385	-0.72037	2.60755	H	-0.5983	-1.88387	-0.53621
C	-3.72147	-1.2141	3.72344	H	0.62845	-4.9852	1.2435
C	-4.83456	-2.03372	3.54532	H	2.00754	-4.57607	0.2122
C	-5.27455	-2.35095	2.25781	H	2.0778	-4.26402	1.95595
H	-4.94281	-2.08587	0.14251	H	0.22148	-2.57641	1.72906
H	-2.94864	-0.64343	0.4538	IM1k			
H	-3.38549	-0.98328	4.72974	Sum of electronic and thermal Free Energies = -2804.409140			
H	-5.3618	-2.41992	4.41152	Sum of electronic and thermal Enthalpies = -2804.299730			

C	10.05718	-2.61725	5.6848	H	0.74763	1.24814	3.66077
C	9.13449	-1.87372	4.95011	H	0.49505	0.54021	2.07034
C	7.76095	-2.00203	5.20997	C	5.39073	-0.99617	-2.14591
C	7.32887	-2.88781	6.21023	H	5.12416	-0.43827	-3.05238
C	8.25632	-3.62175	6.94523	H	6.46894	-0.94881	-2.00451
C	9.62259	-3.48653	6.68658	H	5.10344	-2.03959	-2.28834
H	11.11662	-2.5228	5.46604	P	2.91753	-3.86633	2.08793
H	9.47855	-1.23428	4.1451	F	4.37084	-3.01639	1.55446
H	6.26673	-2.98882	6.40468	F	2.14117	-3.12195	0.85642
H	7.91268	-4.29929	7.72132	F	2.59367	-2.48983	3.01577
H	10.34446	-4.06067	7.2603	F	3.34127	-5.06776	1.1253
C	6.77595	-1.208	4.42605	F	3.79067	-4.42717	3.30428
C	7.12585	0.1992	4.02893	F	1.56856	-4.55146	2.59428
H	7.56207	0.72033	4.88548	H	3.02945	1.86168	3.16214
H	7.86701	0.18183	3.2261				
H	6.24758	0.74382	3.68539	TS1b			
N	5.68068	-1.8327	4.17598	Sum of electronic and thermal Free Energies =	-1383.305956		
O	4.70898	-1.01402	3.45484	Sum of electronic and thermal Enthalpies =	-1383.229230		
H	3.91698	-1.60056	3.52105	Imaginary frequency=	-648.4522		
F	9.04426	-0.974	1.66495	C	-2.97835	-3.66542	2.71169
F	7.19675	-2.65411	-0.39866	C	-2.18458	-2.51343	2.60963
F	7.92191	-0.48867	-0.25729	C	-1.27822	-2.22516	3.6706
F	8.34733	-3.15537	1.52819	C	-1.19904	-3.05475	4.79342
F	9.50188	-2.20893	-0.28532	C	-2.01858	-4.18384	4.87722
F	6.76231	-1.44528	1.55933	C	-2.89898	-4.49259	3.83923
P	8.21202	-1.86774	0.58842	H	-3.65208	-3.93661	1.90349
Ru	4.72745	-0.90741	1.23812	H	-1.31989	-2.75392	1.30321
C	3.41782	-0.88499	-0.53401	H	-0.50906	-2.82895	5.60045
C	4.66779	-0.39104	-0.97853	H	-1.95955	-4.828	5.7489
C	5.23646	0.67732	-0.2123	H	-3.5232	-5.3791	3.90342
C	4.54862	1.26699	0.87715	C	-0.44618	-1.03227	3.48846
C	3.2296	0.8346	1.24798	C	0.66791	-0.64213	4.4079
C	2.707	-0.28429	0.55011	H	0.26151	-0.25274	5.34659
H	3.02259	-1.80189	-0.95569	H	1.27614	-1.51531	4.65048
H	6.26612	0.95572	-0.40048	H	1.29598	0.12446	3.9616
H	5.0479	2.0379	1.44928	N	-0.77491	-0.35622	2.42699
H	1.79468	-0.75934	0.8789	O	-0.05197	0.8065	2.19175
C	2.4254	1.56341	2.33084	H	-0.02658	0.87429	1.22376
C	1.86524	2.83194	1.63015	Ru	-2.34899	-0.93581	1.19555
C	1.2462	0.71407	2.84708	Cl	-0.60337	-2.46791	0.06729
H	2.66789	3.49266	1.2868	C	-4.40616	-1.32213	0.26355
H	1.24106	2.574	0.7686	C	-3.63369	-0.70452	-0.74698
H	1.2473	3.3926	2.33866	C	-3.04973	0.57965	-0.47689
H	1.57136	-0.25708	3.22878	C	-3.20282	1.18199	0.77905
				C	-3.95438	0.55442	1.83291

C	-4.54621	-0.70488	1.53962
H	-4.85392	-2.2923	0.07949
H	-2.44784	1.06062	-1.24034
H	-2.70337	2.12429	0.9767
H	-5.09842	-1.21859	2.31943
C	-4.2624	1.25703	3.14573
C	-5.48611	2.17608	2.92699
C	-3.08815	2.03788	3.75288
H	-5.25206	2.98192	2.22404
H	-6.34481	1.62227	2.53655
H	-5.78241	2.63479	3.87515
H	-3.41281	2.51871	4.68147
H	-2.24644	1.3815	3.9865
H	-2.72626	2.83347	3.09096
C	-3.43716	-1.35722	-2.08649
H	-4.15427	-0.93517	-2.80125
H	-2.4326	-1.17677	-2.4761
H	-3.60259	-2.43501	-2.03697
H	-4.55565	0.47866	3.86082

TS1-a

Sum of electronic and thermal Free Energies = -2324.066197

Sum of electronic and thermal Enthalpies = -2323.971414

Imaginary frequency= -662.4019

C	-2.46542	-4.05494	2.58671
C	-1.95978	-2.75342	2.7253
C	-0.95123	-2.53085	3.70567
C	-0.50241	-3.57648	4.52145
C	-1.04322	-4.85522	4.37518
C	-2.01642	-5.09789	3.40522
H	-3.20789	-4.2687	1.8219
H	-1.21525	-2.46073	1.21827
H	0.26265	-3.40451	5.27174
H	-0.69427	-5.6631	5.01118
H	-2.42622	-6.09667	3.28352
C	-0.43642	-1.16164	3.77147
C	0.74854	-0.71366	4.57151
H	0.48726	0.15458	5.18323
H	1.13096	-1.50664	5.21301
H	1.54742	-0.38815	3.89674
N	-1.08411	-0.31959	3.01487
O	-0.57759	0.94649	3.0539
H	-1.04799	1.5425	2.41798
Ru	-2.70028	-0.98521	1.8567
Cl	-0.85807	-1.68851	0.11541

C	-4.03614	0.94892	1.88237
C	-4.35166	0.07936	2.98773
C	-4.7231	-1.26243	2.68961
C	-4.78917	-1.73585	1.34237
C	-4.40662	-0.89467	0.27986
C	-4.04303	0.46815	0.57263
H	-3.6787	1.95674	2.05154
H	-4.94662	-1.94051	3.50615
H	-5.06306	-2.76691	1.14823
H	-3.686	1.12114	-0.21339
C	-4.3818	-1.38584	-1.14173
C	-4.39097	0.56442	4.43061
H	-3.92373	-0.21885	5.04192
P	-1.35897	3.31663	0.37168
F	-1.739	3.01499	2.00708
F	-1.24299	1.67506	0.21094
F	-1.02642	3.52698	-1.18813
F	-2.9706	3.19093	0.04639
F	-1.54051	4.89398	0.6428
F	0.20099	3.3768	0.79039
C	-3.63495	1.87671	4.66654
H	-4.09279	2.70916	4.1233
H	-3.66809	2.1282	5.73084
H	-2.58886	1.80992	4.36105
C	-5.8635	0.70203	4.87836
H	-6.41694	-0.23572	4.76973
H	-5.9085	1.00047	5.93002
H	-6.37807	1.46913	4.28992
H	-4.37049	-2.47703	-1.19246
H	-3.50642	-1.00241	-1.67096
H	-5.27291	-1.02692	-1.66983

TS1-b

Sum of electronic and thermal Free Energies = -2324.055889

Sum of electronic and thermal Enthalpies = -2323.964631

Imaginary frequency= -86.2212

C	-2.52933	-1.51829	5.19322
C	-2.26147	-0.53346	6.14468
C	-0.93593	-0.24059	6.46898
C	0.15174	-0.88882	5.80927
C	-0.16134	-1.89246	4.86875
C	-1.4836	-2.20686	4.56679
H	-3.55896	-1.76217	4.94963
H	-3.07947	-0.041	6.65999
H	0.64104	-2.39625	4.34032

H	-1.70729	-2.97498	3.83238	Sum of electronic and thermal Free Energies =	-3264.740328		
C	-0.57878	0.63243	7.5833	Sum of electronic and thermal Enthalpies =	-3264.626312		
C	-1.50247	1.64383	8.18127	Imaginary frequency=	-478.2259		
H	-2.16386	1.13537	8.89321	C	-2.45908	-3.56541	2.22416
H	-0.93963	2.40484	8.71998	C	-1.85463	-2.30018	2.24253
H	-2.11151	2.11061	7.40394	C	-0.99273	-1.99268	3.3317
N	0.60186	0.36837	8.06055	C	-0.79216	-2.90409	4.37353
O	1.00726	1.102	9.17393	C	-1.43565	-4.14308	4.34438
H	0.88896	0.44426	9.89213	C	-2.2599	-4.47635	3.26853
F	-1.56658	-1.28414	9.64893	H	-3.08777	-3.85069	1.38435
F	0.01317	-2.36291	8.33312	H	-0.99535	-2.16846	0.86554
F	0.6108	-1.30817	10.3771	H	-0.15121	-2.64656	5.2112
F	0.64637	-3.59176	10.19891	H	-1.28646	-4.84801	5.15733
F	-1.56134	-3.59558	9.49405	H	-2.75024	-5.44608	3.24056
F	-0.98582	-2.56079	11.51472	C	-0.35852	-0.67016	3.28365
Cl	1.7607	1.35664	4.63219	C	0.74116	-0.22976	4.19282
C	3.15011	-3.02194	7.23281	H	0.33375	0.2539	5.08526
C	3.4454	-2.21344	6.11855	H	1.35247	-1.08295	4.49231
C	3.61113	-0.80606	6.35898	H	1.36636	0.5076	3.68593
C	3.66082	-0.29264	7.68259	N	-0.84314	0.08326	2.34086
C	3.52112	-1.14789	8.82613	O	-0.32956	1.34913	2.16402
C	3.16677	-2.49064	8.56576	H	-0.48281	1.86436	2.99943
H	2.87594	-4.06185	7.08734	Ru	-2.26508	-0.6216	1.00512
H	3.6399	-0.10276	5.53286	Cl	-0.2246	-1.70747	-0.2749
H	3.7656	0.77837	7.82205	C	-3.24626	1.24579	-0.08548
H	2.85011	-3.12552	9.38617	C	-3.61881	1.2486	1.28014
C	3.64587	-0.62095	10.22819	C	-4.20053	0.05461	1.8198
Ru	1.69888	-1.23287	7.3982	C	-4.46647	-1.06597	0.97673
P	-0.51929	-2.48146	9.98615	C	-4.10141	-1.07152	-0.39357
C	3.58705	-2.83028	4.73501	C	-3.44515	0.09679	-0.88636
C	3.41239	-1.84864	3.5671	H	-2.77193	2.1099	-0.53382
C	4.98053	-3.49915	4.65818	H	-4.45629	0.01454	2.87336
H	4.21401	-1.10473	3.54678	H	-4.90713	-1.95728	1.4138
H	3.45369	-2.39742	2.62123	H	-3.07876	0.1231	-1.90541
H	2.47359	-1.29503	3.60802	C	-4.46314	-2.24955	-1.28714
H	5.11192	-3.97799	3.68279	C	-5.88867	-2.03758	-1.84418
H	5.76961	-2.74894	4.77213	C	-3.46739	-2.48982	-2.43032
H	5.11641	-4.25878	5.4337	H	-6.62594	-1.94407	-1.03892
H	2.99008	-1.16569	10.91033	H	-5.92171	-1.13207	-2.45504
H	3.39898	0.44265	10.27034	H	-6.17648	-2.89058	-2.46924
H	4.67992	-0.74055	10.57434	H	-2.44829	-2.62024	-2.05499
H	1.00239	-0.07432	5.45154	H	-3.75094	-3.39595	-2.97527
H	2.83465	-3.62661	4.65334	H	-3.46888	-1.66059	-3.13944
TS1-c				C	-3.39004	2.44217	2.15874

H	-4.28556	3.07638	2.13217	C	-1.69302	0.18665	3.1844
H	-3.2103	2.1647	3.19749	C	-2.90541	0.69662	3.76681
H	-2.54477	3.03933	1.81016	C	-2.77001	1.78149	4.67632
P	-1.36754	2.80498	5.6497	H	-1.43308	3.16349	5.70234
F	-1.88629	1.34168	5.06839	H	0.42273	0.44416	2.92549
F	-0.60302	3.03402	4.16404	H	-1.73579	-0.58222	2.42523
F	-0.80976	4.24276	6.13247	H	-3.65184	2.22586	5.11946
F	-2.70638	3.49908	5.03458	C	-4.26573	0.02484	3.51579
F	-2.10546	2.53147	7.06154	C	-4.5347	-0.88292	4.74543
F	-0.00351	2.07558	6.18996	C	-4.25212	-0.85005	2.24454
P	-4.11998	1.69108	-4.14528	H	-3.7409	-1.6254	4.87823
F	-3.0285	0.4489	-3.96415	H	-4.61132	-0.29785	5.66779
F	-4.8134	0.88605	-5.37511	H	-5.47855	-1.42068	4.60702
F	-3.09856	2.43707	-5.16218	H	-5.25222	-1.26277	2.08061
F	-5.12087	0.9063	-3.07979	H	-3.97219	-0.27664	1.35573
F	-5.19974	2.89405	-4.27268	H	-3.5706	-1.70099	2.34032
F	-3.41079	2.44704	-2.8645	C	1.03953	2.43932	4.69298
H	-4.47757	-3.14282	-0.64717	H	1.58206	1.82209	5.41913

TS1-d

Sum of electronic and thermal Free Energies = -2804.379400

Sum of electronic and thermal Enthalpies = -2804.272572

Imaginary frequency= -826.0212

C	-3.02115	5.15204	4.10925
C	-2.89848	4.35792	2.9501
C	-4.00547	4.35619	2.04302
C	-5.15399	5.10763	2.29158
C	-5.23878	5.86886	3.46028
C	-4.17583	5.89699	4.36366
H	-2.16773	5.25225	4.76982
H	-5.98905	5.08852	1.59742
H	-6.13459	6.45291	3.65533
H	-4.23285	6.51547	5.25343
C	-3.8849	3.46896	0.88161
C	-4.71141	3.59716	-0.35892
H	-5.66985	3.07662	-0.24226
H	-4.91888	4.64924	-0.56135
H	-4.18736	3.15458	-1.20744
N	-2.98539	2.54663	1.039
O	-2.86308	1.63837	0.01662
H	-1.91328	1.36989	0.03659
Ru	-1.82896	2.45918	2.78689
C	-1.48639	2.3171	5.02787
C	-0.31122	1.83739	4.4265
C	-0.44901	0.75201	3.48893

C	1.62225	2.47417	3.77099
H	0.95274	3.45395	5.08023
P	0.7282	2.27408	0.22734
F	-0.23117	3.12235	1.41684
F	1.65951	3.55904	0.12886
F	1.59549	1.6776	1.47128
F	-0.33481	0.97426	0.44742
F	1.55482	1.42358	-0.84427
F	-0.30145	2.84056	-0.879
H	-1.77065	4.87297	2.36438
P	0.20829	6.56433	2.786
F	-1.08525	7.24059	3.49155
F	0.08085	5.32393	3.86447
F	-1.01822	5.60635	1.79026
F	0.13703	7.65159	1.61128
F	1.32834	5.73919	1.99797
F	1.24838	7.37202	3.68932
H	-5.05865	0.73828	3.43105

TS1-e

Sum of electronic and thermal Free Energies = -2324.050740

Sum of electronic and thermal Enthalpies = -2323.957406

Imaginary frequency= -969.2488

C	-5.00997	-1.67856	3.73579
C	-4.27979	-0.51886	3.40173
C	-3.25678	-0.13957	4.32568
C	-2.96421	-0.90561	5.46219

C	-3.69433	-2.05918	5.73828	H	-5.07754	2.34268	-1.3036
C	-4.72475	-2.43371	4.87668	H	-5.98259	0.83218	-1.47775
H	-5.76675	-2.04639	3.05525	H	-6.8328	2.39475	-1.59007
H	-4.10112	-0.86398	1.95112	H	-7.31327	0.80464	5.02604
H	-2.17851	-0.59015	6.14222	TS1-f			
H	-3.46401	-2.65469	6.61656	Sum of electronic and thermal Free Energies =	-1863.605250		
H	-5.30245	-3.33192	5.077	Sum of electronic and thermal Enthalpies =	-1863.512595		
C	-2.59189	1.13982	4.09274	Imaginary frequency=	-857.6381		
C	-1.32443	1.5635	4.7692	C	0.61708	-1.65469	3.6507
H	-1.50652	1.76332	5.8322	C	-0.0739	-0.77988	2.79709
H	-0.5832	0.7606	4.70519	C	0.67849	-0.0153	1.85689
H	-0.92957	2.46731	4.30723	C	2.06798	-0.11823	1.80047
N	-3.22349	1.87687	3.23493	C	2.72962	-0.98763	2.67803
O	-2.66719	3.10462	2.89784	C	2.01139	-1.76176	3.59004
H	-2.59952	3.00515	1.91876	H	0.06014	-2.29162	4.33151
Ru	-4.83239	1.19569	2.14555	H	-1.08441	-1.5033	2.13925
C	-6.81045	0.68912	1.03264	H	2.64317	0.46579	1.0888
C	-6.28812	1.83757	0.39519	H	3.81118	-1.06804	2.63399
C	-5.98195	2.9804	1.19897	H	2.53271	-2.45167	4.24691
C	-6.20613	2.96546	2.59259	C	-0.10599	0.84933	0.96138
C	-6.76494	1.8287	3.25422	C	0.4458	1.52535	-0.25371
C	-7.01529	0.68915	2.43963	H	0.84641	2.51083	0.00996
H	-6.97378	-0.21734	0.46719	H	1.25408	0.93587	-0.68719
H	-5.52148	3.84724	0.73886	H	-0.33569	1.67513	-0.99823
H	-5.91406	3.83302	3.17486	N	-1.34779	0.95524	1.32727
H	-7.36485	-0.22332	2.90994	O	-2.14051	1.75951	0.52105
P	-4.90524	-2.71743	0.043	H	-3.04068	1.4311	0.66818
F	-5.15829	-1.41144	-0.87745	Ru	-2.05866	0.0324	3.06882
F	-3.84199	-1.60437	1.0901	C	-2.42952	-0.47013	5.27056
F	-4.57495	-3.84553	1.13785	C	-3.68273	-0.63229	4.64909
F	-6.16942	-2.23639	0.9749	C	-4.20231	0.47207	3.88565
F	-3.54871	-3.02963	-0.73991	C	-3.50283	1.68138	3.79119
F	-5.81808	-3.66805	-0.85393	C	-2.21104	1.86028	4.40204
Cl	-3.01346	1.29363	0.47109	C	-1.69315	0.74556	5.12169
C	-6.02653	1.84818	-1.08313	H	-1.99344	-1.29619	5.82102
C	-7.15411	1.84806	4.72381	H	-5.14612	0.35236	3.36425
C	-6.07675	2.43957	5.6461	H	-3.91998	2.47998	3.19018
C	-8.49606	2.59999	4.88131	H	-0.70708	0.80793	5.56311
H	-5.86889	3.49143	5.41541	C	-1.50309	3.22366	4.407
H	-6.41688	2.39758	6.68613	C	-2.0152	3.96003	5.67533
H	-5.14032	1.88002	5.56716	C	-1.85674	4.07128	3.16631
H	-8.83319	2.56658	5.92278	H	-3.10263	4.08531	5.65758
H	-8.38805	3.65461	4.59609	H	-1.74886	3.42137	6.59008
H	-9.28188	2.16169	4.25681	H	-1.56576	4.9562	5.72632

H	-1.2893	5.00529	3.19801	H	-4.84281	-0.22218	-0.15118
H	-1.61462	3.56061	2.23035	H	-5.70771	3.27302	2.18776
H	-2.91486	4.35151	3.14173	H	-6.40345	1.84292	4.06621
C	-4.47041	-1.90421	4.76057	H	-5.51849	-1.64977	1.73275
H	-5.37358	-1.71693	5.34585	C	-2.92879	-2.68997	2.40702
H	-4.77198	-2.27545	3.77807	C	-3.20843	-4.04513	1.98087
H	-3.89693	-2.68453	5.25564	C	-3.42124	-4.33578	0.619
P	-2.36875	-4.09074	1.97122	C	-3.27813	-5.09552	2.92209
F	-2.21465	-3.58574	3.49545	C	-3.70061	-5.63856	0.21255
F	-2.1197	-1.7628	1.68223	H	-3.35832	-3.5292	-0.10499
F	-3.90106	-3.6302	2.03562	C	-3.5565	-6.39358	2.50653
F	-2.45454	-4.02933	0.39235	H	-3.10973	-4.87845	3.97203
F	-2.52642	-5.62994	2.22955	C	-3.7697	-6.67017	1.15195
F	-0.7799	-3.98571	1.85368	H	-3.86205	-5.84976	-0.84062
H	-0.43941	3.12276	4.46447	H	-3.60469	-7.19463	3.23894
TS2a				H	-3.98537	-7.68554	0.8317
Sum of electronic and thermal Free Energies =	-1998.387662			C	-2.80194	-2.01071	3.5372
Sum of electronic and thermal Enthalpies =	-1998.273473			C	-3.10673	-2.24675	4.87231
Imaginary frequency=	-276.0065			C	-3.39468	-2.47997	6.0367
C	-2.57193	0.61474	4.33643	C	-3.74137	-2.76655	7.38473
C	-1.92651	-0.33052	3.5178	C	-3.34531	-1.90397	8.4293
C	-0.50886	-0.46472	3.63783	C	-4.49275	-3.91829	7.70378
C	0.19801	0.28062	4.58918	C	-3.69355	-2.18857	9.74662
C	-0.47032	1.19812	5.39929	H	-2.76566	-1.01838	8.18908
C	-1.84986	1.38151	5.24867	C	-4.83253	-4.19464	9.02472
H	-3.64776	0.72946	4.26459	H	-4.80385	-4.5837	6.90469
H	1.27605	0.17647	4.66939	C	-4.43648	-3.33269	10.05108
H	0.08303	1.77871	6.13111	H	-3.38233	-1.51586	10.54079
H	-2.3681	2.11592	5.85945	H	-5.41094	-5.085	9.25473
C	0.14697	-1.2657	2.60849	H	-4.70517	-3.55096	11.08047
C	1.5657	-1.74788	2.64683	C	-4.79157	2.56976	-0.27181
H	2.18777	-1.17697	1.94864	C	-5.10074	1.97982	-1.6581
H	1.98363	-1.65705	3.6498	C	-3.30945	2.98931	-0.17796
H	1.61514	-2.7941	2.33473	H	-4.44977	1.13017	-1.88506
N	-0.61284	-1.47211	1.57164	H	-6.14074	1.64553	-1.73045
O	-0.04388	-2.18171	0.53949	H	-4.93475	2.73608	-2.43305
H	-0.67734	-2.02323	-0.19889	H	-3.06242	3.70443	-0.9706
Ru	-2.55784	-0.94021	1.54388	H	-3.08882	3.46017	0.78475
C	-5.11695	0.2435	0.78779	H	-2.65556	2.11967	-0.29435
C	-5.17766	1.64977	0.88167	Cl	-2.43892	-0.96984	-0.896
C	-5.63632	2.192	2.08608	H	-5.39705	3.47965	-0.15672
C	-6.03204	1.37953	3.15412	C	-6.4811	-0.90544	4.21773
C	-5.98207	-0.0149	3.06469	H	-5.88223	-0.73191	5.0873
C	-5.50772	-0.57067	1.8615	H	-7.50189	-0.66923	4.43473

H	-6.4059	-1.93392	3.9323
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TS2-a

Sum of electronic and thermal Free Energies = -1537.938283

Sum of electronic and thermal Enthalpies = -1537.831990

Imaginary frequency= -411.6598

C	-3.30651	0.79719	0.34773
C	-2.7591	-0.37889	-0.20136
C	-2.78934	-1.55138	0.6354
C	-3.31788	-1.51157	1.9549
C	-3.82925	-0.33186	2.45046
C	-3.82929	0.82028	1.63594
H	-3.35004	1.70282	-0.24839
H	-3.32041	-2.4026	2.57449
H	-4.2369	-0.28779	3.45481
H	-4.25476	1.74256	2.02285
C	-2.24106	-2.72775	0.0561
C	-1.8913	-3.99215	0.76665
H	-2.44326	-4.09782	1.69991
H	-0.81977	-3.97931	1.00743
H	-2.05979	-4.86095	0.12748
N	-1.97033	-2.59599	-1.26452
O	-1.17282	-3.6398	-1.75704
H	-1.0981	-3.43579	-2.70275
Ru	-1.88417	-0.59974	-2.00564
C	-1.25298	1.56674	-2.24995
C	-0.1203	0.94733	-1.62061
C	0.42413	-0.17597	-2.27237
C	-0.01784	-0.57713	-3.57786
C	-1.07044	0.07498	-4.22619
C	-1.73965	1.11887	-3.49353
H	-1.74606	2.39679	-1.75653
H	1.23057	-0.73103	-1.80802
H	0.48357	-1.40768	-4.06661
H	-2.61364	1.59288	-3.92631
C	-1.50209	-0.29047	-5.62171
C	0.41663	1.51836	-0.31846
H	-0.45741	1.80982	0.27819
C	-3.67814	-2.63734	-2.23377
C	-4.15206	-3.98726	-2.33936
C	-4.64208	-4.70912	-1.22792
C	-4.21116	-4.57628	-3.62442
C	-5.16293	-5.98633	-1.39842
H	-4.63122	-4.25005	-0.24346
C	-4.76493	-5.84286	-3.79064

H	-3.85063	-4.01659	-4.48314
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C	-5.22877	-6.55327	-2.67903
H	-5.53699	-6.53676	-0.53928
H	-4.82923	-6.27801	-4.78474
H	-5.6488	-7.54591	-2.80871
C	-3.70048	-1.39487	-2.65259
C	-4.70387	-0.77032	-3.40125
C	-5.57059	-0.21503	-4.0577
C	-6.63476	0.34578	-4.82026
C	-6.53683	1.64135	-5.36799
C	-7.80963	-0.40486	-5.03897
C	-7.58509	2.16636	-6.1183
H	-5.63723	2.22506	-5.19958
C	-8.8543	0.13099	-5.78549
H	-7.88754	-1.40127	-4.6158
C	-8.74444	1.41464	-6.32833
H	-7.50037	3.16378	-6.53922
H	-9.75549	-0.45275	-5.94621
H	-9.56059	1.82831	-6.91285
C	1.24091	0.52759	0.51358
H	2.17328	0.24768	0.01017
H	1.5159	0.98849	1.46674
H	0.67689	-0.38506	0.73289
C	1.22871	2.79742	-0.6209
H	0.63632	3.53708	-1.16648
H	1.56385	3.25859	0.3114
H	2.11345	2.56619	-1.2207
H	-1.41316	-1.36552	-5.80506
H	-0.85921	0.21976	-6.34985
H	-2.53363	0.01235	-5.81545

TS2-b

Sum of electronic and thermal Free Energies = -1537.942323

Sum of electronic and thermal Enthalpies = -1537.836416

Imaginary frequency= -442.6686

C	-4.06573	0.88673	-0.0218
C	-3.37021	-0.25751	-0.46647
C	-3.48723	-1.43868	0.35447
C	-4.26894	-1.44142	1.54434
C	-4.92879	-0.29753	1.93256
C	-4.82527	0.86743	1.14091
H	-4.03458	1.8003	-0.60695
H	-4.34513	-2.33925	2.14869
H	-5.52713	-0.28774	2.83745
H	-5.36001	1.76358	1.44495

C	-2.76623	-2.57046	-0.09801
C	-2.58481	-3.86873	0.60581
H	-2.94142	-4.68094	-0.03952
H	-3.1134	-3.89809	1.5566
H	-1.52009	-4.05784	0.77997
N	-2.20598	-2.39395	-1.32695
O	-1.21363	-3.34911	-1.60399
H	-0.99052	-3.17329	-2.53137
Ru	-2.2109	-0.43003	-2.09465
C	-1.74013	1.80725	-2.3622
C	-0.67343	1.34045	-1.52355
C	0.08379	0.26057	-2.01045
C	-0.08994	-0.23686	-3.34408
C	-1.07468	0.27371	-4.19277
C	-1.95926	1.26543	-3.64215
H	-2.38105	2.60728	-2.008
H	0.85667	-0.17968	-1.39149
H	0.56978	-1.02356	-3.69892
H	-2.77906	1.63665	-4.24678
C	-1.24051	-0.19051	-5.61392
C	-0.4178	2.01661	-0.18739
H	-1.39762	2.32623	0.19824
C	-3.73181	-1.45582	-3.02282
C	-4.66038	-1.00554	-4.07343
C	-5.28019	0.25453	-3.97638
C	-4.95923	-1.82353	-5.1807
C	-6.18124	0.67773	-4.95155
H	-5.0699	0.88124	-3.1157
C	-5.84634	-1.38736	-6.16328
H	-4.48907	-2.79847	-5.26782
C	-6.46104	-0.13764	-6.05154
H	-6.66515	1.64529	-4.85441
H	-6.06113	-2.02591	-7.01519
H	-7.15505	0.19801	-6.81597
C	-3.65653	-2.6999	-2.57224
C	-4.08634	-3.98618	-2.52678
C	-4.44739	-5.16106	-2.4873
C	-4.90876	-6.49987	-2.45106
C	-6.09478	-6.82327	-1.754
C	-4.19395	-7.52226	-3.11426
C	-6.54986	-8.13658	-1.72666
H	-6.64424	-6.03568	-1.24921
C	-4.6565	-8.83277	-3.07541
H	-3.28523	-7.27169	-3.65229

C	-5.83253	-9.14085	-2.38387
H	-7.46318	-8.38098	-1.19305
H	-4.10458	-9.61588	-3.58458
H	-6.19154	-10.16531	-2.35859
H	-0.67734	-1.10661	-5.80543
H	-0.87407	0.57866	-6.30384
H	-2.29226	-0.37163	-5.85227
C	0.23097	1.10736	0.86445
H	1.25737	0.83625	0.59394
H	0.28115	1.63116	1.82318
H	-0.34432	0.1879	1.01071
C	0.42217	3.29347	-0.41505
H	-0.05411	3.97226	-1.12943
H	0.54918	3.83325	0.52799
H	1.41725	3.04346	-0.79825

TS2-c

Sum of electronic and thermal Free Energies = -1843.712703

Sum of electronic and thermal Enthalpies = -1843.629027

Imaginary frequency= -165.7574

C	-3.29439	-3.2406	3.05322
C	-2.3508	-2.2292	2.8429
C	-1.29649	-2.11404	3.7831
C	-1.21326	-2.93112	4.92026
C	-2.18665	-3.9041	5.12153
C	-3.21583	-4.05829	4.18479
H	-4.09038	-3.41851	2.33659
H	-0.39498	-2.81802	5.62552
H	-2.13878	-4.55115	5.99186
H	-3.9639	-4.83264	4.3342
C	-0.29983	-1.1056	3.39845
C	1.03292	-0.95832	4.0677
H	0.91086	-0.49685	5.05503
H	1.46711	-1.95004	4.21935
H	1.70607	-0.35569	3.46256
N	-0.76517	-0.41987	2.40746
Ru	-2.24188	-0.88629	1.27962
Cl	-0.88544	-2.56576	0.23855
C	-4.21819	-1.30833	0.09505
C	-3.4605	-0.57662	-0.87717
C	-2.96917	0.68205	-0.50314
C	-3.20872	1.20175	0.80212
C	-4.0814	0.56169	1.72001
C	-4.55934	-0.72126	1.33462
H	-4.5698	-2.30575	-0.14382

H	-2.30048	1.24317	-1.14762	C	-5.06959	-0.56699	4.07581
H	-2.70489	2.13048	1.04915	C	-4.41168	-1.02124	2.90508
H	-5.16261	-1.28745	2.03677	C	-3.41695	-0.22266	2.29277
C	-4.53286	1.19863	3.02349	C	-3.06919	1.07401	2.76706
C	-5.77936	2.07171	2.76281	C	-3.66709	1.48141	3.97627
C	-3.43435	2.0042	3.7328	H	-5.05142	1.00273	5.56778
H	-5.53712	2.90952	2.10007	H	-4.63083	-1.9971	2.48421
H	-6.58531	1.49533	2.29734	H	-2.90393	-0.63223	1.43129
H	-6.15766	2.48396	3.70367	H	-3.39524	2.43328	4.42216
H	-3.81015	2.37894	4.68982	C	-2.1232	2.00826	2.02612
H	-2.55391	1.38598	3.92965	C	-2.95261	3.07643	1.27666
H	-3.11883	2.87152	3.14405	C	-1.15595	1.29856	1.06745
C	-3.1307	-1.1968	-2.20371	H	-3.58985	2.61228	0.51777
H	-2.70165	-0.46106	-2.8865	H	-3.59445	3.64765	1.95382
H	-2.39565	-1.99644	-2.05185	H	-2.28474	3.77751	0.77078
H	-4.02267	-1.63353	-2.66415	H	-0.43446	2.01956	0.67551
H	-4.83152	0.37907	3.68988	H	-0.60644	0.49331	1.56065
O	0.61321	0.90637	1.97003	H	-1.68192	0.87301	0.20713
Cl	-0.30972	2.70157	-0.00585	C	-6.18046	-1.35845	4.71168
H	0.39923	1.575	2.64212	H	-7.13068	-1.1161	4.22216
H	0.27564	1.41198	1.10105	H	-6.01629	-2.4332	4.60411
TS3a				H	-6.28225	-1.12078	5.77311
Sum of electronic and thermal Free Energies = -1998.755597				C	-2.79101	-1.85003	6.10271
Sum of electronic and thermal Enthalpies = -1998.644477				C	-3.18837	-3.1281	6.5548
Imaginary frequency= -543.3362				C	-3.18319	-3.42197	7.94831
C	-0.42443	0.03145	8.29735	C	-3.57174	-4.13456	5.62658
C	-0.75949	-0.58884	7.081	C	-3.56741	-4.67597	8.3918
C	0.3006	-1.14718	6.31221	H	-2.88843	-2.64974	8.6517
C	1.62092	-1.09253	6.8054	C	-3.94286	-5.39051	6.08741
C	1.92085	-0.4684	8.00837	H	-3.52208	-3.92867	4.55978
C	0.88818	0.10017	8.7546	C	-3.947	-5.65814	7.46207
H	-1.22004	0.45692	8.89684	H	-3.57119	-4.90257	9.45307
H	2.42919	-1.51073	6.21729	H	-4.21794	-6.16555	5.3791
H	2.94885	-0.41755	8.35273	H	-4.24012	-6.64255	7.8158
H	1.10161	0.59211	9.69835	C	-2.21617	-0.66847	6.71702
C	0.10463	-1.76569	4.98005	C	-3.13892	0.08561	7.51546
C	1.0613	-2.82659	4.48259	C	-3.9571	0.67567	8.20008
H	1.57096	-3.30348	5.32017	C	-4.91658	1.36065	9.00324
H	0.51205	-3.59486	3.93238	C	-4.67059	2.67518	9.45081
H	1.8261	-2.39038	3.82699	C	-6.12301	0.72488	9.36234
N	-0.91585	-1.37131	4.30254	C	-5.61183	3.33242	10.23687
O	-0.77967	-1.93787	2.52749	H	-3.74241	3.16695	9.17835
Ru	-2.69199	-0.71103	4.58552	C	-7.05812	1.39255	10.14646
C	-4.63106	0.66533	4.62658	H	-6.3113	-0.29089	9.02783

C	-6.80567	2.69545	10.58541
H	-5.4144	4.3438	10.57923
H	-7.98363	0.89549	10.41961
H	-7.53642	3.21221	11.19882
H	-1.5279	-2.82111	2.39936
Cl	-2.58455	-3.99573	2.17063
H	0.10373	-2.27404	2.29246
H	-1.52904	2.52493	2.79087

IM5a

Sum of electronic and thermal Free Energies = -1922.407456

Sum of electronic and thermal Enthalpies = -1922.29798

C	-0.45382100	-2.04790500	8.48511300
C	-0.70358900	-1.45364500	7.24491500
C	0.37806500	-1.02852700	6.44624500
C	1.68404100	-1.20949700	6.92379200
C	1.92392400	-1.81593100	8.15544200
C	0.85225600	-2.23630000	8.93989900
H	-1.28473200	-2.36539000	9.10611900
H	2.52564400	-0.88478600	6.32302700
H	2.94388400	-1.95700100	8.49817800
H	1.02570200	-2.70704300	9.90236000
C	0.14132100	-0.39739400	5.11994000
C	1.24984300	0.43043100	4.48977700
H	2.09217100	-0.21299400	4.21483800
H	0.88103400	0.91284100	3.58470400
H	1.61435900	1.19116900	5.18711400
N	-0.93470200	-0.50158000	4.45064000
Ru	-2.57232000	-1.53282900	4.72585100
C	-4.91955800	-0.66915400	4.61540900
C	-5.14478900	-1.78114800	3.76895900
C	-4.46307100	-1.78636600	2.53906300
C	-3.68287700	-0.69423400	2.12603600
C	-3.53772200	0.45790300	2.91787900
C	-4.12649800	0.42734800	4.20228200
H	-5.41093800	-0.62345600	5.58231400
H	-4.54786300	-2.65086100	1.88733300
H	-3.17246400	-0.75026100	1.16956200
H	-4.01227600	1.26739700	4.87541500
C	-2.71255000	1.62717000	2.40756300
C	-3.38277700	2.25424100	1.16427900
C	-2.41901000	2.69967000	3.46352200
H	-3.55417000	1.52034200	0.37166300
H	-4.34798700	2.70116600	1.42488700
H	-2.74489000	3.04342900	0.75624600

H	-1.91409200	2.28064200	4.33850600
H	-1.76597700	3.46539000	3.03573200
H	-3.33359700	3.20531800	3.79415200
C	-6.11107300	-2.87477300	4.14295600
H	-7.12029300	-2.61286200	3.80329000
H	-5.84447500	-3.82415200	3.67192300
H	-6.15762900	-3.02437200	5.22420800
C	-2.89706800	-2.37579800	6.38394800
C	-3.49675400	-3.52835100	6.95409000
C	-3.81382100	-3.54849200	8.33957400
C	-3.78647100	-4.66577600	6.15657200
C	-4.41219900	-4.66700000	8.89848500
H	-3.61237800	-2.67063500	8.94478100
C	-4.35747800	-5.79011400	6.73683300
H	-3.50490300	-4.65432100	5.10972600
C	-4.67613900	-5.78921600	8.10032300
H	-4.66816700	-4.67768500	9.95289000
H	-4.55413100	-6.67085100	6.13436900
H	-5.13043000	-6.66886800	8.54648900
C	-2.14587100	-1.23895100	6.83398600
C	-2.80114100	-0.10071300	7.37814800
C	-3.32301400	0.87831600	7.88906400
C	-3.90949100	2.02753600	8.48522000
C	-3.09067000	3.08885400	8.92816900
C	-5.30860600	2.12021200	8.64628800
C	-3.66370200	4.21248100	9.51417900
H	-2.01473800	3.01603700	8.80824000
C	-5.86997200	3.24907800	9.23348200
H	-5.93982400	1.30185100	8.31448900
C	-5.05091700	4.29579500	9.66760100
H	-3.02919400	5.02498600	9.85385400
H	-6.94649800	3.31413500	9.35635100
H	-5.49315200	5.17450900	10.12670800
Cl	-1.32575500	-3.39968900	3.98082500
H	-1.75173900	1.19550600	2.09346900

IM1-p

Sum of electronic and thermal Free Energies = -1958.273088

Sum of electronic and thermal Enthalpies = -1958.185376

C	-1.59462600	-2.03086900	-0.17823600
C	-1.68201500	-1.41717500	1.07930700
C	-2.54581900	-0.33541800	1.28908000
C	-3.35835800	0.11859300	0.23535100
C	-3.27403400	-0.50746000	-1.00583600
C	-2.39665800	-1.57349000	-1.23123700

H	-1.05790600	-1.80441900	1.87882100
H	-4.03486400	0.95069600	0.39879000
H	-3.91059500	-0.16782000	-1.81829000
C	-2.63879500	0.24673300	2.65377000
C	-2.91808800	-0.67693800	3.81415900
H	-3.00131500	-1.70983900	3.47701400
H	-2.13736000	-0.59435100	4.57726900
H	-3.85255100	-0.37714600	4.29969000
N	-2.51247000	1.51876600	2.86894300
O	-2.68108000	1.82446600	4.20112200
H	-2.66631800	2.81821900	4.22160600
Cl	-2.40774800	4.66181000	3.57556400
C	-1.41802500	2.93276700	-0.55075300
C	-0.57992600	2.10923700	0.22633200
C	0.22050500	2.64869600	1.29264300
C	0.11489900	4.03143600	1.54266700
C	-0.72881100	4.87348100	0.74147000
C	-1.49619200	4.35385900	-0.31999200
H	-2.06500600	2.47771000	-1.29153100
H	-0.58487300	1.03926300	0.05750000
H	0.61617800	4.46132000	2.40224800
H	-0.84130000	5.91000100	1.03086100
C	1.10115500	1.75617600	2.12406200
Ru	-1.97947200	3.22436800	1.60059000
C	-2.42249700	5.19556500	-1.17815800
C	-2.86521500	6.50715900	-0.51889500
C	-1.75884400	5.44716300	-2.54912600
H	-3.32273000	6.32011800	0.45589300
H	-2.02984400	7.20631800	-0.39528900
H	-3.60748800	7.00125200	-1.15294400
H	-1.47853700	4.51248700	-3.04630700
H	-2.44953100	5.98363000	-3.20718700
H	-0.85411600	6.05622000	-2.44210800
H	1.27953300	2.18661600	3.11231000
H	0.65198000	0.76809800	2.25190500
H	2.07178300	1.61935000	1.63192300
Cl	-4.36475800	3.36343300	1.12219500
H	-2.35711000	-2.04054200	-2.20806200
O	-0.70508600	-3.06148100	-0.26775100
C	-0.58706500	-3.74209900	-1.50823100
H	0.16350900	-4.51873800	-1.35488200
H	-1.53445900	-4.20946400	-1.80533000
H	-0.25212400	-3.07016300	-2.30900100
H	-3.32206900	4.58796000	-1.33146100

IM1a-p

Sum of electronic and thermal Free Energies = -1497.828354

Sum of electronic and thermal Enthalpies = -1497.741571

C	-2.78907	-2.5745	1.93201
C	-1.64993	-1.79956	2.17329
C	-1.61969	-0.42518	1.85791
C	-2.77279	0.16263	1.29615
C	-3.8909	-0.60148	1.03079
C	-3.91482	-1.98045	1.34602
H	-2.80202	-3.61488	2.23405
H	-0.8249	-2.23579	2.73137
H	-2.77043	1.21149	1.01519
H	-4.77248	-0.16681	0.57161
C	-0.39366	0.35132	2.0714
C	-0.42019	1.72401	2.68686
H	-1.41301	2.1609	2.58289
H	-0.2094	1.67817	3.76256
H	0.29672	2.40236	2.21157
N	0.70818	-0.23727	1.71301
O	1.93272	0.3437	2.00981
H	1.78246	1.1008	2.60233
Ru	0.81055	-1.9653	0.51524
Cl	-0.35574	-0.75692	-1.15682
C	0.9938	-4.09878	-0.1993
C	1.27558	-4.10005	1.21237
C	2.29779	-3.2461	1.69284
C	2.96398	-2.35439	0.80789
C	2.68378	-2.33311	-0.59622
C	1.69701	-3.26123	-1.07895
H	0.1764	-4.70347	-0.57722
H	2.50741	-3.20147	2.75599
H	3.6438	-1.62053	1.22193
H	1.39566	-3.21226	-2.11932
C	3.39062	-1.41536	-1.57786
C	4.42518	-2.24242	-2.3753
C	4.04156	-0.1855	-0.93244
H	5.21037	-2.63356	-1.71907
H	3.96379	-3.08664	-2.89686
H	4.9007	-1.6061	-3.1274
H	4.43248	0.46919	-1.71651
H	3.32446	0.38828	-0.33876
H	4.88813	-0.45874	-0.29114
C	0.50783	-5.00437	2.1352
H	0.94967	-6.00794	2.10995

H	0.54126	-4.6526	3.16895
H	-0.5353	-5.09812	1.82295
O	-5.06796	-2.61341	1.06739
C	-5.19756	-4.00068	1.38177
H	-5.07898	-4.17452	2.45758
H	-6.20636	-4.27814	1.07873
H	-4.47062	-4.60222	0.82371
H	2.62064	-1.06595	-2.27603

TS1-p

Sum of electronic and thermal Free Energies = -1958.222914

Sum of electronic and thermal Enthalpies = -1958.136313

Imaginary frequency= -298.4286

C	-2.03375	0.33238	4.44171
C	-2.11617	0.3603	5.83303
C	-0.96433	0.23969	6.61039
C	0.32246	0.14514	5.9883
C	0.37511	0.10097	4.5865
C	-0.78637	0.18505	3.81128
H	-2.94256	0.415	3.85792
H	-3.0957	0.43395	6.29467
H	1.32688	0.05641	4.06743
C	-0.97753	0.09745	8.05534
C	-2.1065	0.48372	8.9614
H	-2.9748	0.81268	8.39425
H	-2.38464	-0.35247	9.60765
H	-1.79117	1.30632	9.6106
N	0.1142	-0.44018	8.51907
O	0.12645	-0.60722	9.90425
H	0.7649	-1.32461	10.02804
Cl	1.65668	2.6815	6.80688
C	3.20849	-2.63201	7.90423
C	3.36469	-2.43318	6.48702
C	3.55887	-1.11717	6.03396
C	3.61218	-0.02082	6.9501
C	3.53806	-0.21565	8.35157
C	3.31337	-1.55721	8.80747
H	2.97459	-3.62461	8.2718
H	3.61039	-0.92218	4.96833
H	3.66154	0.99413	6.56939
H	3.19764	-1.7508	9.86869
C	3.74799	0.96915	9.28134
Ru	1.63579	-1.09491	7.2899
C	3.27556	-3.59881	5.54417
H	3.22466	1.8122	8.81474

H	1.07052	1.06866	6.44309
Cl	0.07823	-2.90916	6.74511
O	-0.60935	0.13647	2.4634
C	-1.75248	0.22518	1.6244
H	-1.38025	0.1541	0.6016
H	-2.45439	-0.59746	1.81079
H	-2.27389	1.1822	1.75249
H	3.13672	-3.26341	4.51399
H	2.43266	-4.24221	5.81034
H	4.20107	-4.18805	5.5937
C	3.1929	0.7796	10.69845
H	3.72319	-0.00833	11.24832
H	3.32441	1.70552	11.26585
H	2.12556	0.54815	10.68745
C	5.25497	1.30421	9.33232
H	5.65607	1.51443	8.33674
H	5.41919	2.18906	9.95516
H	5.83119	0.47683	9.76366

IM2-p

Sum of electronic and thermal Free Energies = -1497.451186

Sum of electronic and thermal Enthalpies = -1497.368641

C	-3.01375	-3.64836	2.44733
C	-2.31904	-2.43851	2.5648
C	-1.46527	-2.28687	3.69354
C	-1.34668	-3.29008	4.66884
C	-2.07064	-4.46945	4.54299
C	-2.89497	-4.64301	3.42384
H	-3.64017	-3.86011	1.58604
H	-0.68096	-3.15565	5.51744
H	-1.99013	-5.26745	5.27373
C	-0.66914	-1.06998	3.69
C	0.45279	-0.7919	4.64261
H	0.06476	-0.66758	5.65996
H	1.14559	-1.63882	4.65717
H	0.99003	0.10998	4.35487
N	-1.00134	-0.27736	2.71394
O	-0.20721	0.85753	2.5028
H	0.05503	0.72671	1.57025
Ru	-2.40789	-0.8178	1.32009
Cl	-0.38264	-1.51627	0.11748
C	-4.45704	-1.29583	0.41193
C	-3.67753	-0.7956	-0.64485
C	-3.14941	0.54383	-0.52673
C	-3.33436	1.2955	0.62867

C	-4.0135	0.73615	1.7696	O	-1.34946	-1.8642	0.30963
C	-4.59737	-0.55203	1.62554	H	-2.11268	-2.43044	0.0989
H	-4.88656	-2.28838	0.33795	Ru	-3.65298	-0.54456	1.88128
H	-2.54033	0.9358	-1.33415	C	-4.36693	0.06069	-0.23842
H	-2.88677	2.2795	0.70168	C	-3.73913	1.25118	0.27579
H	-5.14352	-0.98653	2.45584	C	-4.23567	1.74601	1.49804
C	-4.2499	1.5307	3.04727	C	-5.25768	1.0575	2.20729
C	-5.66447	2.14785	3.02398	C	-5.92816	-0.0724	1.66681
C	-3.19314	2.61163	3.31891	C	-5.46553	-0.54373	0.4058
H	-5.76649	2.85599	2.19381	H	-4.01162	-0.36732	-1.16689
H	-6.43793	1.38211	2.90914	H	-3.78978	2.61965	1.95609
H	-5.85878	2.69154	3.95477	H	-5.55614	1.42684	3.18286
H	-3.3359	3.02461	4.3224	H	-5.93143	-1.41748	-0.03748
H	-2.17665	2.21744	3.24832	C	-7.07768	-0.72741	2.38392
H	-3.28484	3.44766	2.61539	C	-3.69489	-2.51317	2.4944
C	-3.4071	-1.59694	-1.88891	C	-3.78063	-3.82124	1.90444
H	-3.85242	-1.10962	-2.76442	C	-4.06041	-4.00256	0.53196
H	-2.32801	-1.68233	-2.0504	C	-3.55173	-4.96827	2.70054
H	-3.82085	-2.6049	-1.8087	C	-4.11688	-5.27973	-0.02266
O	-3.56997	-5.83841	3.26351	H	-4.26174	-3.13367	-0.08884
C	-4.88027	-5.85396	3.81796	C	-3.61194	-6.23862	2.1402
H	-5.29371	-6.8462	3.62343	H	-3.32847	-4.84278	3.75516
H	-4.86176	-5.67663	4.90218	C	-3.89251	-6.40123	0.77849
H	-5.52526	-5.09673	3.35074	H	-4.33883	-5.40097	-1.07858
H	-4.21363	0.80807	3.87295	H	-3.43603	-7.10904	2.76494

TS2-p

Sum of electronic and thermal Free Energies = -1652.458601

Sum of electronic and thermal Enthalpies = -1652.347320

Imaginary frequency= -329.0797

C	-3.06065	0.43593	4.86511	C	-5.3559	-2.49399	7.28525
C	-2.61708	-0.34443	3.79015	C	-5.09318	-1.56351	8.31361
C	-1.20298	-0.49151	3.60981	C	-6.2139	-3.58335	7.54259
C	-0.31595	0.07969	4.53161	C	-5.68068	-1.72328	9.56452
C	-0.77603	0.83256	5.60566	H	-4.43526	-0.72332	8.11404
C	-2.16149	1.02472	5.76309	C	-6.78857	-3.73682	8.80048
H	-4.1182	0.54581	5.07552	H	-6.41734	-4.29853	6.75217
H	0.75438	-0.03943	4.39377	C	-6.52578	-2.80895	9.81221
H	-0.06774	1.26252	6.30224	H	-5.47777	-1.00249	10.3507
C	-0.76002	-1.15579	2.40189	H	-7.44496	-4.57983	8.99292
C	0.62905	-1.67197	2.17708	H	-6.9786	-2.9315	10.79131
H	1.26951	-0.88046	1.77053	C	-2.65807	2.00628	-0.51425
H	1.06737	-2.01442	3.11622	C	-2.01487	1.12534	-1.60495
H	0.61843	-2.48889	1.45566	C	-3.36076	3.21089	-1.19345
N	-1.70613	-1.25148	1.51067	H	-1.58215	0.21061	-1.18927

H	-2.72862	0.85306	-2.38913
H	-1.21237	1.68591	-2.09244
H	-3.79644	3.89256	-0.45635
H	-2.63526	3.77513	-1.78764
H	-4.15993	2.88058	-1.86501
H	-7.15907	-1.78446	2.11958
H	-6.96112	-0.65442	3.46783
H	-8.02063	-0.23861	2.11231
O	-2.72763	1.73815	6.76593
C	-1.88101	2.38865	7.71428
H	-1.22246	3.11635	7.22659
H	-2.54979	2.90897	8.39972
H	-1.27816	1.66453	8.27406
H	-1.88503	2.36535	0.13257

IM1-m

Sum of electronic and thermal Free Energies = -1958.274259

Sum of electronic and thermal Enthalpies = -1958.186228

C	-1.70137	-2.08523	-0.32064
C	-1.85213	-1.50597	0.93983
C	-2.63071	-0.35578	1.13229
C	-3.31888	0.17598	0.02548
C	-3.17799	-0.39578	-1.23363
C	-2.35317	-1.51745	-1.42271
H	-1.08067	-2.96598	-0.42995
H	-1.33756	-1.95555	1.78462
H	-3.95816	1.04277	0.16603
H	-3.7108	0.00328	-2.09094
C	-2.74563	0.21379	2.49517
C	-3.11603	-0.70292	3.63643
H	-3.26644	-1.72386	3.28406
H	-2.35065	-0.68507	4.4198
H	-4.03836	-0.34198	4.10336
N	-2.54453	1.47286	2.73677
O	-2.73424	1.76108	4.07055
H	-2.65283	2.74903	4.11911
Cl	-2.24126	4.58561	3.55343
C	-1.61183	3.13508	-0.69874
C	-0.77422	2.16573	-0.11273
C	0.14059	2.51103	0.94212
C	0.17567	3.8566	1.35982
C	-0.66277	4.84514	0.74149
C	-1.56004	4.52035	-0.29743
H	-2.35317	2.82144	-1.42541
H	-0.86603	1.13173	-0.42007

H	0.78308	4.14227	2.21132
H	-0.66897	5.84211	1.16212
C	1.00702	1.45604	1.57513
Ru	-1.97818	3.20802	1.50589
C	-2.50557	5.52262	-0.93933
C	-2.65026	6.83237	-0.15402
C	-2.08187	5.78842	-2.39828
H	-2.9618	6.64774	0.87731
H	-1.7174	7.4089	-0.14379
H	-3.41209	7.45862	-0.62838
H	-2.01483	4.86338	-2.981
H	-2.81409	6.43821	-2.88837
H	-1.10741	6.28656	-2.44339
H	1.31572	1.74732	2.58207
H	0.48074	0.49971	1.63296
H	1.91041	1.30298	0.97198
Cl	-4.38543	3.39788	1.16121
O	-2.24473	-1.97648	-2.70094
C	-1.66304	-3.25725	-2.9085
H	-2.22841	-4.0348	-2.3768
H	-1.71189	-3.4398	-3.98283
H	-0.61298	-3.2945	-2.58895
H	-3.48836	5.03558	-0.94648

IM1a-m

Sum of electronic and thermal Free Energies = -1497.828497

Sum of electronic and thermal Enthalpies = -1497.744097

C	-3.17235	-2.32675	2.37148
C	-2.00607	-1.62523	2.6932
C	-1.61811	-0.5042	1.93021
C	-2.43104	-0.08036	0.86827
C	-3.58275	-0.79262	0.54734
C	-3.95308	-1.91897	1.29244
H	-3.48221	-3.17113	2.97931
H	-1.46252	-1.86656	3.60255
H	-2.14016	0.77216	0.26312
H	-4.85877	-2.46089	1.03983
C	-0.34497	0.17308	2.22548
C	-0.28365	1.41539	3.07476
H	-1.28633	1.7425	3.3468
H	0.25408	1.22174	4.01228
H	0.21321	2.24134	2.55028
N	0.71877	-0.37272	1.72071
O	1.96564	0.14118	2.03293
H	1.85048	0.93045	2.5904

Ru	0.78618	-1.97376	0.32467	C	-2.07686	0.40572	9.13444
Cl	-0.40055	-0.57843	-1.16614	H	-2.94155	0.7902	8.59696
C	0.90764	-4.06016	-0.50074	H	-2.37035	-0.47247	9.7166
C	1.22978	-4.1529	0.89885	H	-1.7447	1.17017	9.84403
C	2.27683	-3.34091	1.3909	N	0.13741	-0.49652	8.61405
C	2.93211	-2.41571	0.53345	O	0.17643	-0.72339	9.98704
C	2.63673	-2.32371	-0.86727	H	0.85675	-1.40766	10.0715
C	1.61026	-3.20021	-1.36157	Cl	1.62997	2.73151	6.81744
H	0.0657	-4.62467	-0.88737	C	3.25808	-2.65367	7.9117
H	2.5141	-3.34862	2.44909	C	3.33202	-2.46243	6.48739
H	3.6408	-1.72428	0.97091	C	3.49271	-1.15003	6.00911
H	1.27878	-3.10936	-2.38694	C	3.55603	-0.04095	6.90948
C	3.44552	-1.39797	-1.78382	C	3.53705	-0.22386	8.31572
C	4.83677	-2.0695	-1.94292	C	3.37662	-1.56694	8.79472
C	3.61517	0.00658	-1.16537	H	3.07185	-3.64868	8.29959
H	5.36347	-2.15113	-0.9867	H	3.50595	-0.97034	4.93983
H	4.75412	-3.07178	-2.3756	H	3.57789	0.97074	6.51769
H	5.45375	-1.46501	-2.61436	H	3.31795	-1.74984	9.86254
H	4.22572	0.61814	-1.83564	C	3.73279	0.97948	9.22619
H	2.64692	0.49758	-1.0398	Ru	1.61862	-1.12902	7.32909
H	4.12254	-0.01272	-0.19664	C	3.21285	-3.63934	5.56145
C	0.47337	-5.09573	1.79151	H	3.12526	1.78359	8.79386
H	0.90541	-6.10008	1.70389	H	1.01728	1.15532	6.5033
H	0.53369	-4.79898	2.84111	Cl	0.03951	-2.91946	6.77367
H	-0.57769	-5.16695	1.5004	H	-0.76633	0.38022	2.87555
O	-4.38816	-0.37253	-0.55708	O	-3.23543	0.7294	3.9891
C	-5.50873	-1.25061	-0.69195	C	-3.25999	0.78046	2.56636
H	-6.24951	-0.79082	-1.31223	H	-2.92339	-0.16514	2.12634
H	-5.19017	-2.16944	-1.13822	H	-4.301	0.95555	2.2937
H	-5.92498	-1.44858	0.27368	H	-2.64202	1.60162	2.18532
H	2.9936	-1.29404	-2.74812	C	3.28592	0.75993	10.67763
TS1-m				H	3.90511	0.01393	11.19218
Sum of electronic and thermal Free Energies =	-1958.227339			H	3.38784	1.69575	11.23514
Sum of electronic and thermal Enthalpies =	-1958.140183			H	2.23765	0.45361	10.73869
Imaginary frequency=	-350.2650			C	5.2109	1.42365	9.17459
C	-2.05629	0.51649	4.61678	H	5.52735	1.65059	8.15226
C	-2.12329	0.46712	6.01854	H	5.35004	2.32753	9.7757
C	-0.96505	0.25304	6.75131	H	5.87547	0.64751	9.57261
C	0.32306	0.13755	6.12086	H	2.39634	-4.29269	5.87737
C	0.32544	0.14879	4.70492	H	3.01281	-3.31747	4.53653
C	-0.82491	0.34389	3.95651	H	4.14892	-4.2138	5.56676
H	-3.09963	0.55975	6.48063	IM2-m			
H	1.27338	0.06612	4.18115	Sum of electronic and thermal Free Energies =	-1497.364870		
C	-0.96116	0.06097	8.1967	Sum of electronic and thermal Enthalpies =	-1497.447478		

C	-3.18063	-3.46524	2.87608	H	-2.7498	-6.74677	5.36666
C	-2.39738	-2.31084	2.77874	H	-2.43882	-6.56573	7.11277
C	-1.45394	-2.09929	3.82113	H	-3.82046	-5.71767	6.36262
C	-1.31487	-2.98407	4.89731	H	-4.64162	0.75809	3.78836
C	-2.12032	-4.12253	4.96267				
C	-3.05872	-4.35805	3.94886	TS2-m			
H	-3.90453	-3.70197	2.10069	Sum of electronic and thermal Free Energies =	-1652.457333		
H	-0.58494	-2.82009	5.68395	Sum of electronic and thermal Enthalpies =	-1652.345349		
C	-0.59329	-0.93861	3.63034	Imaginary frequency=	-317.5694		
C	0.60373	-0.62669	4.47403	C	-3.08786	0.4899	4.82129
H	0.29797	-0.43605	5.50879	C	-2.65082	-0.31058	3.75098
H	1.28012	-1.48706	4.48683	C	-1.24046	-0.48893	3.614
H	1.13369	0.24313	4.08996	C	-0.34435	0.069	4.52579
N	-0.94971	-0.23971	2.59377	C	-0.81447	0.86184	5.58103
O	-0.11329	0.8127	2.20176	C	-2.19833	1.08233	5.71227
H	0.11068	0.53678	1.29056	H	-4.1516	0.6229	4.99003
Ru	-2.45493	-0.85131	1.33937	H	0.72715	-0.06312	4.42168
Cl	-0.51647	-1.81713	0.16872	C	-0.79072	-1.20256	2.42535
C	-4.48099	-1.33703	0.36213	C	0.59071	-1.75088	2.24502
C	-3.67981	-0.81448	-0.66954	H	1.2742	-0.95619	1.92561
C	-3.14854	0.517	-0.52448	H	0.96485	-2.15304	3.18846
C	-3.35089	1.2438	0.64899	H	0.60032	-2.52727	1.48166
C	-4.09001	0.69013	1.75159	N	-1.7272	-1.30113	1.52887
C	-4.65012	-0.60404	1.57799	O	-1.36844	-1.94295	0.34695
H	-4.90809	-2.32821	0.26284	H	-2.15537	-2.46818	0.11781
H	-2.52423	0.92236	-1.31298	Ru	-3.65731	-0.543	1.8535
H	-2.89133	2.22058	0.75298	C	-4.28853	0.08827	-0.29153
H	-5.21522	-1.04903	2.39013	C	-3.66881	1.26751	0.25863
C	-4.40279	1.48998	3.00691	C	-4.20714	1.75311	1.46608
C	-5.65803	2.35598	2.7704	C	-5.26731	1.07142	2.12777
C	-3.23612	2.3495	3.51518	C	-5.92121	-0.04782	1.55324
H	-5.47033	3.11152	1.99986	C	-5.41186	-0.51464	0.30595
H	-6.51	1.75116	2.44656	H	-3.90264	-0.33481	-1.21028
H	-5.94163	2.87994	3.68911	H	-3.77016	2.61699	1.95089
H	-3.50368	2.8076	4.47288	H	-5.60627	1.43962	3.09038
H	-2.33223	1.75304	3.65588	H	-5.86928	-1.37909	-0.1635
H	-2.99935	3.16535	2.82311	C	-7.10739	-0.70172	2.20884
C	-3.37976	-1.60277	-1.91501	C	-3.79455	-2.50764	2.48976
H	-3.72169	-1.0587	-2.80252	C	-3.91772	-3.81071	1.88616
H	-2.30049	-1.76443	-1.99926	C	-4.14402	-3.97495	0.50266
H	-3.87074	-2.57823	-1.89597	C	-3.7789	-4.96965	2.68439
H	-3.69153	-5.2386	3.97639	C	-4.23252	-5.24618	-0.06236
O	-1.90705	-4.94866	6.03695	H	-4.27772	-3.09649	-0.12273
C	-2.78233	-6.04848	6.21466	C	-3.87102	-6.23405	2.11442
				H	-3.59902	-4.85928	3.74897

C	-4.09618	-6.37962	0.7407	C	-0.23031	0.0028	4.51601
H	-4.41111	-5.35237	-1.12815	C	-0.66899	0.74226	5.60492
H	-3.76387	-7.1134	2.74204	C	-2.04684	0.93254	5.7519
H	-4.16404	-7.36972	0.30148	H	-4.03004	0.53351	5.10485
C	-3.71296	-1.94988	3.67504	H	0.83438	-0.13772	4.3612
C	-4.21632	-2.16231	4.9492	H	0.01518	1.17239	6.32465
C	-4.64709	-2.3549	6.07608	C	-0.72571	-1.18661	2.36997
C	-5.12535	-2.5807	7.39549	C	0.65359	-1.71502	2.12255
C	-4.50388	-1.94409	8.49109	H	1.30768	-0.91502	1.75597
C	-6.21883	-3.44089	7.6283	H	1.08469	-2.10654	3.04613
C	-4.97004	-2.1627	9.78327	H	0.63238	-2.49849	1.36551
H	-3.65883	-1.28752	8.31092	N	-1.69047	-1.26399	1.49893
C	-6.67345	-3.65624	8.92554	O	-1.3592	-1.85808	0.28808
H	-6.69734	-3.93192	6.78704	H	-2.15861	-2.35529	0.04106
C	-6.05309	-3.01853	10.00381	Ru	-3.62942	-0.55586	1.91559
H	-4.48681	-1.67032	10.62174	C	-4.4134	0.06255	-0.18894
H	-7.51349	-4.32191	9.09803	C	-3.77421	1.24984	0.31762
H	-6.41182	-3.18926	11.01414	C	-4.23804	1.73264	1.55813
C	-2.55279	2.0203	-0.48367	C	-5.2392	1.03707	2.28869
C	-1.86214	1.13607	-1.54267	C	-5.9182	-0.09281	1.75764
C	-3.22232	3.22407	-1.19682	C	-5.49107	-0.55085	0.47987
H	-1.45897	0.21624	-1.10874	H	-4.08585	-0.35273	-1.1334
H	-2.53675	0.87086	-2.36339	H	-3.78503	2.60686	2.00812
H	-1.03096	1.69114	-1.98694	H	-5.51858	1.4015	3.27193
H	-3.69062	3.90722	-0.48137	H	-5.96746	-1.42168	0.04187
H	-2.47029	3.78704	-1.75853	C	-7.04533	-0.75564	2.5022
H	-3.99081	2.89328	-1.90338	C	-3.64884	-2.54291	2.50597
H	-7.08983	-1.78547	2.06868	C	-3.71018	-3.84188	1.89975
H	-7.13396	-0.49402	3.28071	C	-4.02324	-4.0136	0.53281
H	-8.03734	-0.32191	1.76998	C	-3.42868	-4.9912	2.67595
H	-2.58606	1.69918	6.51437	C	-4.06058	-5.28483	-0.0356
O	0.13183	1.37113	6.40108	H	-4.27009	-3.14392	-0.0706
C	-0.27104	2.19675	7.49197	C	-3.47047	-6.25579	2.10134
H	0.65131	2.49226	7.99566	H	-3.18011	-4.8721	3.72563
H	-0.79732	3.09315	7.14154	C	-3.78358	-6.40903	0.74566
H	-0.90939	1.64902	8.1925	H	-4.30952	-5.40034	-1.08602
H	-1.80834	2.38023	0.19541	H	-3.25479	-7.12859	2.70988
TS2-p-NO₂				H	-3.81101	-7.39935	0.30247
Sum of electronic and thermal Free Energies = -1742.450792				C	-3.60586	-1.95171	3.68461
Sum of electronic and thermal Enthalpies = -1742.340305				C	-4.23995	-2.13475	4.90825
Imaginary frequency= -338.5300				C	-4.79429	-2.2659	5.98898
C	-2.98079	0.39328	4.88392	C	-5.4452	-2.41505	7.24345
C	-2.55993	-0.37592	3.77907	C	-5.3467	-1.39784	8.21729
C	-1.14868	-0.52628	3.59368	C	-6.19719	-3.57532	7.52464

C	-5.99127	-1.54533	9.44141	Ru	-3.64717	-0.56024	1.96075
H	-4.77774	-0.49943	7.99984	C	-4.32078	0.12178	-0.15908
C	-6.82805	-3.71375	8.75659	C	-3.68633	1.28524	0.40592
H	-6.2735	-4.35586	6.77457	C	-4.20246	1.74629	1.63371
C	-6.72822	-2.70111	9.71528	C	-5.2492	1.05187	2.29905
H	-5.91665	-0.75806	10.185	C	-5.91947	-0.05302	1.7096
H	-7.40127	-4.61057	8.97005	C	-5.43925	-0.48772	0.44204
H	-7.22509	-2.81236	10.67416	H	-3.95314	-0.28007	-1.09457
C	-2.72337	2.01795	-0.49991	H	-3.75702	2.60151	2.1262
C	-2.0877	1.14058	-1.598	H	-5.56975	1.39882	3.27576
C	-3.46486	3.20391	-1.17154	H	-5.90957	-1.33787	-0.04066
H	-1.62691	0.23824	-1.18503	C	-7.09584	-0.7123	2.37716
H	-2.81202	0.84752	-2.36468	C	-3.72503	-2.54367	2.52932
H	-1.30738	1.71243	-2.10755	C	-3.81871	-3.8364	1.90911
H	-3.89785	3.88186	-0.42954	C	-4.09176	-3.98403	0.53106
H	-2.76279	3.778	-1.78398	C	-3.60675	-5.00145	2.68336
H	-4.27109	2.85367	-1.8242	C	-4.15622	-5.24788	-0.05129
H	-7.1504	-1.80383	2.2129	H	-4.28169	-3.10026	-0.07229
H	-6.88571	-0.71257	3.5821	C	-3.67644	-6.25866	2.09547
H	-7.99139	-0.24809	2.28065	H	-3.3905	-4.90063	3.74206
N	-2.5347	1.71974	6.90422	C	-3.94861	-6.38802	0.72845
O	-1.69408	2.23681	7.63115	H	-4.3715	-5.34517	-1.11098
O	-3.75447	1.80243	7.06043	H	-3.51479	-7.14419	2.70221
H	-1.94349	2.39698	0.12701	H	-3.99756	-7.37275	0.27479
TS2-m-NO₂				C	-3.65944	-1.99131	3.72619
Sum of electronic and thermal Free Energies = -1742.450936				C	-4.25134	-2.22245	4.96108
Sum of electronic and thermal Enthalpies = -1742.339432				C	-4.75266	-2.42358	6.0572
Imaginary frequency= -342.5097				C	-5.32171	-2.65912	7.33814
C	-3.0486	0.37512	4.94561	C	-4.74225	-2.07738	8.4863
C	-2.61457	-0.40557	3.84721	C	-6.46706	-3.47178	7.47765
C	-1.20159	-0.57598	3.68235	C	-5.30168	-2.30231	9.7401
C	-0.29463	-0.04708	4.60594	H	-3.85698	-1.45852	8.37948
C	-0.77981	0.70379	5.66705	C	-7.0154	-3.69277	8.73716
C	-2.14955	0.93901	5.83597	H	-6.91158	-3.92122	6.59542
H	-4.11072	0.50356	5.12193	C	-6.43663	-3.1089	9.86819
H	0.77584	-0.17369	4.49803	H	-4.8514	-1.8524	10.6195
C	-0.76511	-1.23977	2.46469	H	-7.8956	-4.32009	8.83942
C	0.61081	-1.78652	2.24008	H	-6.86867	-3.28383	10.84894
H	1.26881	-1.01025	1.83071	C	-2.57936	2.05304	-0.3341
H	1.04325	-2.13747	3.18032	C	-1.94867	1.21456	-1.46492
H	0.57907	-2.6045	1.52143	C	-3.24669	3.31016	-0.95293
N	-1.7136	-1.29836	1.57549	H	-1.54045	0.26884	-1.09536
O	-1.36798	-1.88912	0.36482	H	-2.66208	1.00202	-2.26822
H	-2.15227	-2.41241	0.12201	H	-1.12776	1.77929	-1.91517

H	-3.67269	3.96211	-0.18373	C	-3.66792	-2.51566	2.51493
H	-2.50077	3.88725	-1.50759	C	-3.74092	-3.82401	1.92662
H	-4.04644	3.03744	-1.64965	C	-4.03757	-4.01067	0.55838
H	-7.17666	-1.76345	2.09097	C	-3.48606	-4.96598	2.72227
H	-7.01764	-0.658	3.46557	C	-4.08545	-5.28903	0.00688
H	-8.02456	-0.21086	2.08114	H	-4.2606	-3.14581	-0.06084
H	-2.48049	1.54659	6.66982	C	-3.53795	-6.23794	2.16484
N	0.1713	1.27944	6.62695	H	-3.25024	-4.8358	3.77357
O	-0.29451	1.9485	7.54834	C	-3.83531	-6.40589	0.80739
O	1.36706	1.05365	6.44408	H	-4.32099	-5.41566	-1.04536
H	-1.80383	2.35831	0.33691	H	-3.34263	-7.105	2.7883

TS2-p-CN

Sum of electronic and thermal Free Energies = -1630.196855

Sum of electronic and thermal Enthalpies = -1630.087389

Imaginary frequency= -335.9804

C	-3.03506	0.44736	4.86688	C	-5.39465	-2.46758	7.27502
C	-2.59467	-0.3363	3.78228	C	-5.08782	-1.61253	8.35539
C	-1.18171	-0.47293	3.60857	C	-6.33452	-3.5043	7.4581
C	-0.28044	0.08771	4.52778	C	-5.71286	-1.79313	9.585
C	-0.73989	0.84084	5.59747	H	-4.36772	-0.81214	8.21909
C	-2.1282	1.03449	5.75341	C	-6.94596	-3.67982	8.695
H	-4.09557	0.55833	5.05897	H	-6.5707	-4.16136	6.62732
H	0.7876	-0.04022	4.38446	C	-6.63887	-2.82581	9.7585
H	-0.04855	1.28383	6.30499	H	-5.47579	-1.1292	10.41032
C	-0.74045	-1.14947	2.40066	H	-7.66511	-4.48149	8.83125
C	0.64509	-1.67285	2.1775	H	-7.12094	-2.96485	10.72128
H	1.29526	-0.87853	1.79207	C	-2.69656	2.00811	-0.52772
H	1.07316	-2.03528	3.11417	C	-2.04692	1.12365	-1.61178
H	0.63485	-2.47728	1.44236	C	-3.42629	3.19128	-1.21687
N	-1.69331	-1.24699	1.51873	H	-1.59181	0.22381	-1.18728
O	-1.34279	-1.86036	0.32212	H	-2.76133	0.82607	-2.386
H	-2.13889	-2.36014	0.07054	H	-1.25971	1.69206	-2.11455
Ru	-3.64193	-0.5422	1.89711	H	-3.86858	3.87454	-0.48529
C	-4.38647	0.05088	-0.22352	H	-2.71464	3.76045	-1.82279
C	-3.75992	1.24654	0.27965	H	-4.2239	2.83855	-1.87873
C	-4.24613	1.74199	1.50632	H	-7.15461	-1.79766	2.15771
C	-5.25825	1.05161	2.22711	H	-6.93069	-0.67858	3.51161
C	-5.92566	-0.08577	1.69813	H	-8.00964	-0.2483	2.17656
C	-5.47414	-0.55809	0.43372	C	-2.63189	1.80596	6.85339
H	-4.0407	-0.37541	-1.15654	N	-3.06056	2.4149	7.74679
H	-3.80298	2.62208	1.95472	H	-1.92491	2.38937	0.10796
H	-5.55512	1.42682	3.20105				
H	-5.94058	-1.43514	-0.00237				
C	-7.06473	-0.74326	2.42925				

TS2-m-CN

Sum of electronic and thermal Free Energies = -1630.196560

Sum of electronic and thermal Enthalpies = -1630.086944

Imaginary frequency= -338.8103

C	-3.05281	0.3849	4.96013
C	-2.61638	-0.39313	3.86292
C	-1.20445	-0.56111	3.70453
C	-0.30227	-0.03284	4.63318
C	-0.76962	0.727	5.71094
C	-2.15698	0.94777	5.85313
H	-4.11551	0.51283	5.13397
H	0.76543	-0.1751	4.50616
C	-0.76311	-1.22688	2.48908
C	0.6138	-1.77315	2.26948
H	1.27588	-0.99145	1.87861
H	1.03693	-2.13795	3.20734
H	0.59007	-2.58036	1.53738
N	-1.70772	-1.28757	1.59613
O	-1.35745	-1.88274	0.38917
H	-2.14596	-2.39599	0.13936
Ru	-3.64213	-0.5481	1.97047
C	-4.32304	0.12262	-0.1506
C	-3.68377	1.28886	0.40323
C	-4.19147	1.75875	1.63113
C	-5.23635	1.07055	2.30615
C	-5.91268	-0.03631	1.72753
C	-5.43919	-0.48111	0.46091
H	-3.96175	-0.28545	-1.08589
H	-3.74123	2.61568	2.11606
H	-5.55065	1.42412	3.28252
H	-5.91316	-1.3342	-0.01303
C	-7.08729	-0.68848	2.40536
C	-3.7253	-2.53229	2.53908
C	-3.81931	-3.82419	1.91598
C	-4.09556	-3.96969	0.53851
C	-3.60345	-4.99074	2.68698
C	-4.16031	-5.23269	-0.04612
H	-4.2879	-3.08509	-0.06281
C	-3.67234	-6.24699	2.0967
H	-3.3842	-4.89192	3.74526
C	-3.94842	-6.37426	0.7303
H	-4.37897	-5.32787	-1.10532
H	-3.5068	-7.13344	2.70127
H	-3.99716	-7.35818	0.2748
C	-3.66203	-1.98271	3.73638
C	-4.25274	-2.21698	4.9711
C	-4.75673	-2.42467	6.0645

C	-5.33252	-2.67141	7.34017
C	-4.7662	-2.09298	8.49624
C	-6.47226	-3.4936	7.46618
C	-5.33293	-2.3302	9.74431
H	-3.88476	-1.46738	8.39982
C	-7.02785	-3.72718	8.72004
H	-6.90656	-3.94075	6.57785
C	-6.46219	-3.14628	9.85898
H	-4.89261	-1.88289	10.62995
H	-7.9035	-4.36217	8.81163
H	-6.8998	-3.33105	10.83531
C	-2.58275	2.05	-0.35219
C	-1.93532	1.18939	-1.45643
C	-3.26365	3.27956	-1.0095
H	-1.52044	0.25796	-1.0598
H	-2.63995	0.94833	-2.25875
H	-1.11776	1.75142	-1.91591
H	-3.70042	3.94777	-0.26081
H	-2.52361	3.84968	-1.57955
H	-4.05745	2.97601	-1.69975
H	-7.16271	-1.74563	2.13906
H	-7.01101	-0.6129	3.49263
H	-8.01824	-0.19719	2.0986
H	-2.51647	1.55199	6.67965
C	0.15129	1.28504	6.6536
N	0.8981	1.73922	7.42105
H	-1.8147	2.38451	0.31347

TS2-p-COOH

Sum of electronic and thermal Free Energies = -1726.521412

Sum of electronic and thermal Enthalpies = -1726.410494

Imaginary frequency= -335.1721

C	-2.98079	0.39328	4.88392
C	-2.55993	-0.37592	3.77907
C	-1.14868	-0.52628	3.59368
C	-0.23031	0.0028	4.51601
C	-0.66899	0.74226	5.60492
C	-2.04684	0.93254	5.7519
H	-4.03004	0.53351	5.10485
H	0.83438	-0.13772	4.3612
H	0.01518	1.17239	6.32465
C	-0.72571	-1.18661	2.36997
C	0.65359	-1.71502	2.12255
H	1.30768	-0.91502	1.75597
H	1.08469	-2.10654	3.04613

H	0.63238	-2.49849	1.36551
N	-1.69047	-1.26399	1.49893
O	-1.3592	-1.85808	0.28808
H	-2.15861	-2.35529	0.04106
Ru	-3.62942	-0.55586	1.91559
C	-4.4134	0.06255	-0.18894
C	-3.77421	1.24984	0.31762
C	-4.23804	1.73264	1.55813
C	-5.2392	1.03707	2.28869
C	-5.9182	-0.09281	1.75764
C	-5.49107	-0.55085	0.47987
H	-4.08585	-0.35273	-1.1334
H	-3.78503	2.60686	2.00812
H	-5.51858	1.4015	3.27193
H	-5.96746	-1.42168	0.04187
C	-7.04533	-0.75564	2.5022
C	-3.64884	-2.54291	2.50597
C	-3.71018	-3.84188	1.89975
C	-4.02324	-4.0136	0.53281
C	-3.42868	-4.9912	2.67595
C	-4.06058	-5.28483	-0.0356
H	-4.27009	-3.14392	-0.0706
C	-3.47047	-6.25579	2.10134
H	-3.18011	-4.8721	3.72563
C	-3.78358	-6.40903	0.74566
H	-4.30952	-5.40034	-1.08602
H	-3.25479	-7.12859	2.70988
H	-3.81101	-7.39935	0.30247
C	-3.60586	-1.95171	3.68461
C	-4.23995	-2.13475	4.90825
C	-4.79429	-2.2659	5.98898
C	-5.4452	-2.41505	7.24345
C	-5.3467	-1.39784	8.21729
C	-6.19719	-3.57532	7.52464
C	-5.99127	-1.54533	9.44141
H	-4.77774	-0.49943	7.99984
C	-6.82805	-3.71375	8.75659
H	-6.2735	-4.35586	6.77457
C	-6.72822	-2.70111	9.71528
H	-5.91665	-0.75806	10.185
H	-7.40127	-4.61057	8.97005
H	-7.22509	-2.81236	10.67416
C	-2.72337	2.01795	-0.49991
C	-2.0877	1.14058	-1.598

C	-3.46486	3.20391	-1.17154
H	-1.62691	0.23824	-1.18503
H	-2.81202	0.84752	-2.36468
H	-1.30738	1.71243	-2.10755
H	-3.89785	3.88186	-0.42954
H	-2.76279	3.778	-1.78398
H	-4.27109	2.85367	-1.8242
H	-7.1504	-1.80383	2.2129
H	-6.88571	-0.71257	3.5821
H	-7.99139	-0.24809	2.28065
C	-2.55504	1.75257	6.95227
O	-3.70245	1.93961	7.3548
O	-1.54326	2.33975	7.63996
H	-1.89052	2.84953	8.39009
H	-1.94349	2.39698	0.12701

TS2-m-COOH

Sum of electronic and thermal Free Energies = -1726.521781

Sum of electronic and thermal Enthalpies = -1726.409460

Imaginary frequency= -336.8908

C	-2.99488	0.38139	4.96296
C	-2.58031	-0.39718	3.85919
C	-1.17144	-0.57313	3.67604
C	-0.2559	-0.04517	4.59054
C	-0.69836	0.71496	5.67298
C	-2.07716	0.94025	5.84054
H	-4.05429	0.51196	5.1552
H	0.81295	-0.18077	4.46212
C	-0.75136	-1.2349	2.45198
C	0.62315	-1.77723	2.20917
H	1.27803	-0.99028	1.81702
H	1.05949	-2.14555	3.13958
H	0.59152	-2.57858	1.47126
N	-1.70974	-1.29272	1.5732
O	-1.38056	-1.88134	0.35538
H	-2.16067	-2.42034	0.13348
Ru	-3.63546	-0.55223	1.98147
C	-4.34573	0.12327	-0.12766
C	-3.69342	1.28472	0.42055
C	-4.18286	1.75561	1.65546
C	-5.21981	1.06965	2.34431
C	-5.90847	-0.03376	1.77288
C	-5.45571	-0.47713	0.49857
H	-3.99888	-0.28455	-1.06831
H	-3.72143	2.60948	2.13555

H	-5.51761	1.42132	3.3265	O	-0.2089	1.99091	7.60547
H	-5.93985	-1.32735	0.02958	H	0.53433	2.30579	8.147
C	-7.07361	-0.68301	2.46962	H	-1.79603	2.32776	0.30986
C	-3.70762	-2.53776	2.54846	TS2-p-CH₃			
C	-3.79571	-3.83125	1.92912	Sum of electronic and thermal Free Energies =	-1577.259102		
C	-4.09643	-3.98312	0.55742	Sum of electronic and thermal Enthalpies =	-1577.259102		
C	-3.5475	-4.99339	2.69719	Imaginary frequency=	-326.3347		
C	-4.15329	-5.24826	-0.02392	C	-3.09501	0.53408	4.81611
H	-4.31485	-3.10221	-0.04051	C	-2.64877	-0.27827	3.75411
C	-3.6083	-6.2515	2.11001	C	-1.24123	-0.43219	3.58587
H	-3.30858	-4.88919	3.75064	C	-0.35007	0.16467	4.49222
C	-3.90865	-6.38534	0.74941	C	-0.82778	0.95472	5.52708
H	-4.39144	-5.34847	-1.07842	C	-2.21181	1.16584	5.69145
H	-3.41703	-7.13433	2.71241	H	-4.16178	0.63971	4.98866
H	-3.95067	-7.37072	0.29621	H	0.72015	0.03674	4.36169
C	-3.64137	-1.97914	3.74132	H	-0.129	1.42243	6.21459
C	-4.23999	-2.20776	4.97424	C	-0.79753	-1.1443	2.40204
C	-4.76112	-2.41409	6.05947	C	0.58897	-1.67464	2.20045
C	-5.36563	-2.66263	7.32182	H	1.23586	-0.89758	1.77694
C	-4.85566	-2.05051	8.48643	H	1.01956	-1.99114	3.15214
C	-6.48085	-3.52086	7.42461	H	0.57929	-2.51191	1.50305
C	-5.45327	-2.29038	9.71958	N	-1.7443	-1.26946	1.51729
H	-3.99339	-1.3962	8.40807	O	-1.38993	-1.92516	0.34036
C	-7.06752	-3.75691	8.66372	H	-2.16656	-2.47414	0.13289
H	-6.87193	-3.99383	6.52956	Ru	-3.68399	-0.53509	1.86479
C	-6.55772	-3.1425	9.81132	C	-4.3774	0.05375	-0.27789
H	-5.05638	-1.81648	10.61199	C	-3.74933	1.23711	0.24478
H	-7.92415	-4.41975	8.7367	C	-4.24672	1.74672	1.45907
H	-7.01937	-3.32906	10.77609	C	-5.28736	1.07661	2.15905
C	-2.59363	2.0405	-0.34299	C	-5.95523	-0.05376	1.6163
C	-2.00606	1.20017	-1.49499	C	-5.48309	-0.53995	0.36232
C	-3.25391	3.31314	-0.93571	H	-4.01158	-0.37592	-1.20301
H	-1.60168	0.24676	-1.14128	H	-3.77907	2.61662	1.90765
H	-2.74374	1.00225	-2.2793	H	-5.59874	1.45451	3.12693
H	-1.18962	1.75568	-1.964	H	-5.9531	-1.41307	-0.07764
H	-3.63346	3.97412	-0.14962	C	-7.11912	-0.6983	2.31984
H	-2.51659	3.87332	-1.51925	C	-3.7475	-2.49561	2.51597
H	-4.08698	3.06082	-1.60035	C	-3.84402	-3.81156	1.94257
H	-7.19163	-1.72418	2.15937	C	-4.12336	-4.00912	0.57266
H	-6.9484	-0.66096	3.55521	C	-3.62858	-4.94912	2.75541
H	-8.00153	-0.15167	2.22633	C	-4.19173	-5.29345	0.03565
H	-2.41943	1.54525	6.67297	H	-4.31548	-3.14705	-0.06057
C	0.32899	1.26772	6.5976	C	-3.70082	-6.22664	2.21278
O	1.52395	1.09506	6.46938	H	-3.40663	-4.81114	3.80874

C	-3.98042	-6.40568	0.85294	C	-2.14586	0.97205	5.81326
H	-4.41299	-5.42713	-1.01893	H	-4.11741	0.52463	5.11856
H	-3.5352	-7.08987	2.85024	H	0.75145	-0.12547	4.4436
H	-4.03218	-7.40604	0.43505	C	-0.7805	-1.20805	2.45964
C	-3.68143	-1.90035	3.68838	C	0.59924	-1.74952	2.24383
C	-4.24234	-2.10831	4.94198	H	1.26636	-0.95705	1.88452
C	-4.73442	-2.31171	6.04124	H	1.00799	-2.13507	3.17996
C	-5.31109	-2.56579	7.31577	H	0.58725	-2.53889	1.49281
C	-4.87716	-1.84995	8.45171	N	-1.72654	-1.28858	1.57025
C	-6.32456	-3.537	7.45953	O	-1.37854	-1.90556	0.37138
C	-5.44928	-2.09845	9.69536	H	-2.16799	-2.42384	0.13554
H	-4.09259	-1.10807	8.34339	Ru	-3.65842	-0.54347	1.93908
C	-6.88486	-3.7821	8.70924	C	-4.36248	0.11744	-0.18062
H	-6.65806	-4.08969	6.58704	C	-3.70945	1.27591	0.36577
C	-6.45182	-3.06365	9.8276	C	-4.18392	1.76187	1.59887
H	-5.11133	-1.54298	10.56497	C	-5.22782	1.09079	2.29287
H	-7.66204	-4.533	8.81283	C	-5.92191	-0.0125	1.7278
H	-6.89324	-3.25685	10.80055	C	-5.47068	-0.47441	0.45731
C	-2.65025	1.98024	-0.50121	H	-4.01584	-0.29228	-1.12202
C	-1.83129	1.10874	-1.4637	H	-3.69802	2.61331	2.06324
C	-3.27203	3.18274	-1.24763	H	-5.52258	1.44801	3.27378
H	-1.44118	0.2095	-0.98023	H	-5.95876	-1.32927	0.00131
H	-2.42294	0.80426	-2.33445	C	-7.08996	-0.65376	2.42742
H	-0.98434	1.68598	-1.84472	C	-3.76041	-2.52673	2.51474
H	-3.80058	3.85651	-0.56696	C	-3.87952	-3.81669	1.88745
H	-2.48747	3.75654	-1.74946	C	-4.14653	-3.95479	0.50794
H	-3.98209	2.84637	-2.01077	C	-3.69901	-4.98967	2.65711
H	-7.15673	-1.77178	2.12103	C	-4.23568	-5.21547	-0.07985
H	-7.06026	-0.55274	3.40067	H	-4.31254	-3.0654	-0.09416
H	-8.06074	-0.2587	1.97188	C	-3.79205	-6.24324	2.06414
C	-2.71743	2.03746	6.81499	H	-3.48734	-4.89799	3.71757
H	-3.80094	2.17227	6.76708	C	-4.05845	-6.36316	0.69525
H	-2.4758	1.59823	7.78995	H	-4.44678	-5.30287	-1.14134
H	-2.24999	3.02771	6.7886	H	-3.65332	-7.13397	2.66932
H	-1.9698	2.37765	0.26235	H	-4.12677	-7.34504	0.23779
TS2-m-CH₃				C	-3.68493	-1.98334	3.71028
Sum of electronic and thermal Free Energies = -1577.259102				C	-4.23693	-2.224	4.96105
Sum of electronic and thermal Enthalpies = -1577.259102				C	-4.71722	-2.44505	6.06212
Imaginary frequency= -326.1727				C	-5.26644	-2.70951	7.34634
C	-3.05561	0.4016	4.93224	C	-4.73376	-2.07701	8.48956
C	-2.62626	-0.3726	3.83605	C	-6.34645	-3.6051	7.49424
C	-1.21876	-0.53258	3.67059	C	-5.27415	-2.33373	9.74548
C	-0.31555	0.01428	4.5934	H	-3.8989	-1.3931	8.37574
C	-0.75851	0.77394	5.67756	C	-6.87535	-3.8585	8.75588

H	-6.75594	-4.0933	6.6159	Ru	-3.66916	-0.55313	1.88981
C	-6.34328	-3.22396	9.88194	C	-4.38387	0.05119	-0.23447
H	-4.85983	-1.8435	10.62096	C	-3.75913	1.24191	0.28245
H	-7.70461	-4.55084	8.86311	C	-4.25948	1.73492	1.50413
H	-6.75998	-3.42406	10.86429	C	-5.28157	1.04414	2.21046
C	-2.60947	2.02237	-0.37526	C	-5.94811	-0.08706	1.66732
C	-1.80337	1.1609	-1.35785	C	-5.48256	-0.55563	0.40672
C	-3.22797	3.24135	-1.09732	H	-4.02594	-0.37501	-1.16276
H	-1.41709	0.25108	-0.89171	H	-3.817	2.60979	1.96325
H	-2.40275	0.87515	-2.22986	H	-5.58424	1.41305	3.18488
H	-0.95444	1.73794	-1.73483	H	-5.94572	-1.42997	-0.03838
H	-3.74689	3.90744	-0.40185	C	-7.09811	-0.74436	2.38159
H	-2.44287	3.81754	-1.59526	C	-3.70017	-2.52842	2.48976
H	-3.94561	2.92242	-1.86072	C	-3.76007	-3.83231	1.88933
H	-7.16057	-1.71723	2.18671	C	-4.0293	-4.00725	0.51369
H	-7.00678	-0.55343	3.51211	C	-3.51697	-4.98148	2.67822
H	-8.02571	-0.17526	2.11566	C	-4.06161	-5.281	-0.05086
H	-2.51595	1.57583	6.63815	H	-4.24311	-3.13704	-0.10116
C	0.21168	1.34755	6.67935	C	-3.55343	-6.24817	2.10776
H	0.3998	0.63665	7.4932	H	-3.30218	-4.86037	3.73511
H	1.17686	1.57615	6.21898	C	-3.82338	-6.40472	0.74311
H	-0.17599	2.26432	7.13209	H	-4.276	-5.39781	-1.10882
H	-1.9209	2.40275	0.38986	H	-3.36723	-7.12048	2.72682
TS2-p-OH				H	-3.84696	-7.39675	0.30341
Sum of electronic and thermal Free Energies = -1613.180071				C	-3.66468	-1.94651	3.67333
Sum of electronic and thermal Enthalpies = -1613.072308				C	-4.27393	-2.16804	4.90351
Imaginary frequency= -329.3975				C	-4.80062	-2.3328	5.99271
C	-3.10392	0.42002	4.87289	C	-5.40048	-2.50127	7.27025
C	-2.64709	-0.35408	3.79453	C	-5.13136	-1.57594	8.30174
C	-1.23181	-0.50513	3.63223	C	-6.26924	-3.58336	7.52233
C	-0.35001	0.04681	4.57419	C	-5.72361	-1.73376	9.55067
C	-0.82595	0.78453	5.64816	H	-4.46493	-0.74122	8.10729
C	-2.2116	0.98375	5.78572	C	-6.84859	-3.73484	8.77826
H	-4.16379	0.53598	5.06706	H	-6.4772	-4.29451	6.72944
H	0.72113	-0.07844	4.45034	C	-6.57957	-2.8121	9.79307
H	-0.13602	1.20787	6.37312	H	-5.51595	-1.01698	10.33922
C	-0.77886	-1.15996	2.42371	H	-7.51336	-4.57214	8.96681
C	0.61312	-1.67118	2.2062	H	-7.03605	-2.93297	10.77069
H	1.26063	-0.86764	1.83607	C	-2.67816	2.00046	-0.50435
H	1.03534	-2.04221	3.14206	C	-2.03294	1.1234	-1.59692
H	0.61477	-2.46576	1.46051	C	-3.38178	3.20627	-1.18056
N	-1.71948	-1.25246	1.5255	H	-1.59911	0.20829	-1.18323
O	-1.35514	-1.85535	0.32198	H	-2.74569	0.85227	-2.38241
H	-2.1051	-2.44083	0.11438	H	-1.2309	1.68652	-2.08218

H	-3.81893	3.88532	-0.44192	C	-3.67767	-4.98978	2.66831
H	-2.6563	3.77309	-1.77229	C	-4.18692	-5.20784	-0.07419
H	-4.17984	2.87706	-1.85396	H	-4.29622	-3.05913	-0.07742
H	-7.18432	-1.79861	2.10796	C	-3.74576	-6.24119	2.06733
H	-6.97847	-0.68147	3.4658	H	-3.47572	-4.90143	3.73104
H	-8.0398	-0.24947	2.11684	C	-3.99829	-6.35744	0.69544
O	-2.75087	1.69617	6.80818	H	-4.38794	-5.29184	-1.13801
H	-2.05158	2.04179	7.37963	H	-3.59755	-7.13308	2.66883
H	-1.90622	2.35851	0.14434	H	-4.04708	-7.33754	0.23174
TS2-m-OH				C	-3.70635	-1.99079	3.73832
Sum of electronic and thermal Free Energies = -1613.178183				C	-4.26501	-2.2255	4.98654
Sum of electronic and thermal Enthalpies = -1613.069926				C	-4.75435	-2.44195	6.08476
Imaginary frequency= -319.0430				C	-5.31747	-2.70462	7.36359
C	-3.05779	0.39393	4.96601	C	-4.73898	-2.14589	8.52299
C	-2.62853	-0.3773	3.86735	C	-6.4581	-3.52526	7.48983
C	-1.22007	-0.56129	3.72075	C	-5.29333	-2.40073	9.7733
C	-0.31292	-0.04437	4.65025	H	-3.85698	-1.52104	8.42589
C	-0.77741	0.7136	5.72738	C	-7.00174	-3.77682	8.74567
C	-2.15748	0.94416	5.86845	H	-6.90287	-3.95734	6.59917
H	-4.11938	0.53207	5.1418	C	-6.42343	-3.21549	9.88788
H	0.75654	-0.1844	4.53734	H	-4.84264	-1.96839	10.66141
C	-0.7788	-1.23663	2.50794	H	-7.87831	-4.41086	8.83577
C	0.59677	-1.7912	2.30195	H	-6.85143	-3.41425	10.8657
H	1.27733	-1.00138	1.95973	C	-2.55952	2.04875	-0.35006
H	0.99081	-2.1892	3.23885	C	-1.90424	1.17985	-1.44354
H	0.58521	-2.57262	1.54306	C	-3.22977	3.27648	-1.02082
N	-1.71834	-1.29711	1.61043	H	-1.50105	0.24696	-1.03873
O	-1.36632	-1.90169	0.40744	H	-2.60108	0.94024	-2.25282
H	-2.15571	-2.417	0.16381	H	-1.07756	1.73472	-1.89545
Ru	-3.6432	-0.5414	1.96684	H	-3.66611	3.95312	-0.27961
C	-4.30847	0.12945	-0.15748	H	-2.4848	3.83783	-1.59298
C	-3.66867	1.29366	0.40022	H	-4.02286	2.97152	-1.71112
C	-4.18188	1.76636	1.62418	H	-7.10085	-1.75442	2.19124
C	-5.23441	1.08239	2.29426	H	-7.06769	-0.52378	3.46469
C	-5.90825	-0.02309	1.71452	H	-8.02188	-0.25562	1.99879
C	-5.42612	-0.47318	0.45135	H	-2.5233	1.54231	6.70021
H	-3.94356	-0.28095	-1.09031	O	0.14799	1.20174	6.5882
H	-3.73004	2.62062	2.11218	H	-0.27778	1.72317	7.28185
H	-5.55318	1.43795	3.26846	H	-1.79578	2.38451	0.31991
H	-5.89811	-1.32747	-0.02229				
C	-7.0861	-0.67855	2.38337				
C	-3.76889	-2.52717	2.54069				
C	-3.86895	-3.81473	1.90406				
C	-4.12171	-3.94913	0.52147				