Supporting Information

The theoretical investigation of the impact of ligands on the regiodivergent Rh-catalyzed hydrothiolation of allyl amines

Lingli Han[a,*], Yaping Li[b] and Tao Liu[a,b,*]

[a] *Department of Chemistry and Chemical Engineering, Jining University, Qufu 273155, Shandong, China*
[b] *School of Chemistry and Chemical Engineering, Qufu Normal University, Qufu 273165, Shandong, China*

Author Email Address: liutao_2005@126.com

Table of Contents:

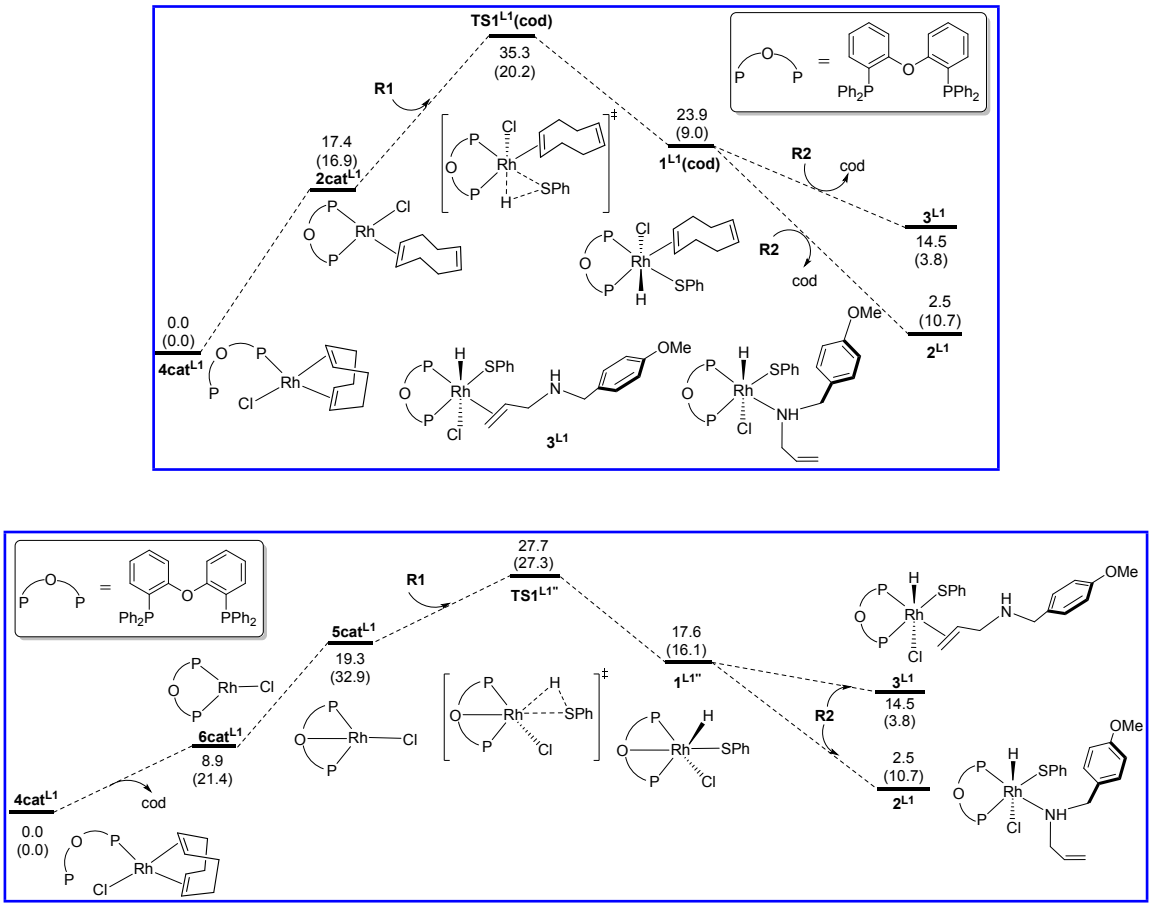

Fig. S1 The unfavorable **4cat^{L1}**-catalyzed oxidative addition pathways.

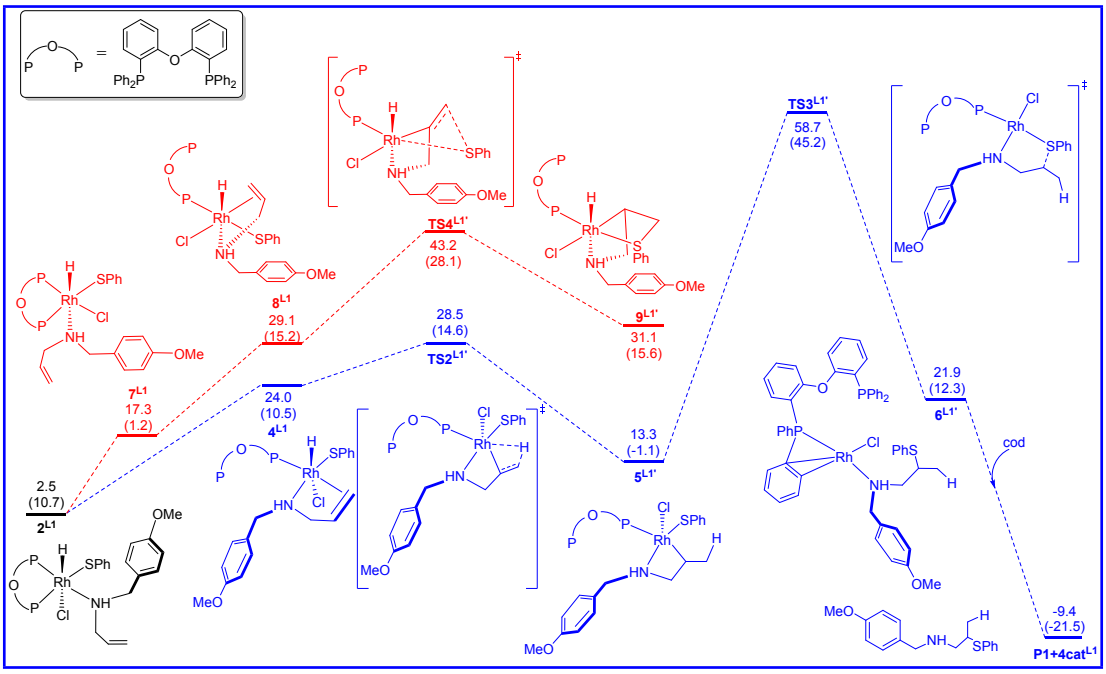

Fig. S2 Other inaccessible pathways for the 2,1-olefin insertion into the Rh-H or Rh-S bond from $\mathbf{2}^{L1}$ to **P1** and **P2**.

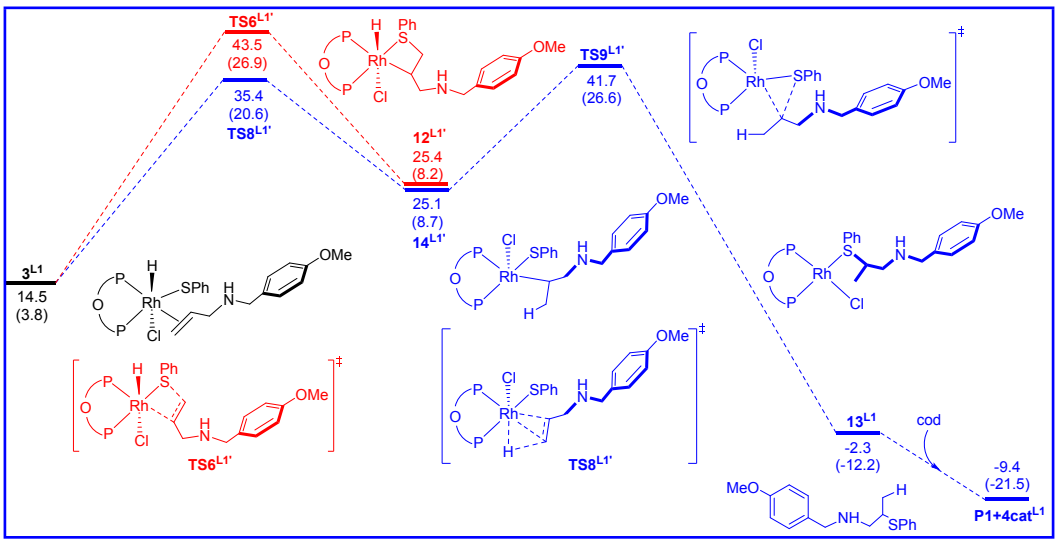

Fig. S3 Other inaccessible pathways for the 2,1-olefin insertion into the Rh-H or Rh-S bond from $\mathbf{3}^{\mathbf{L1}}$ to **P1** and **P2**.

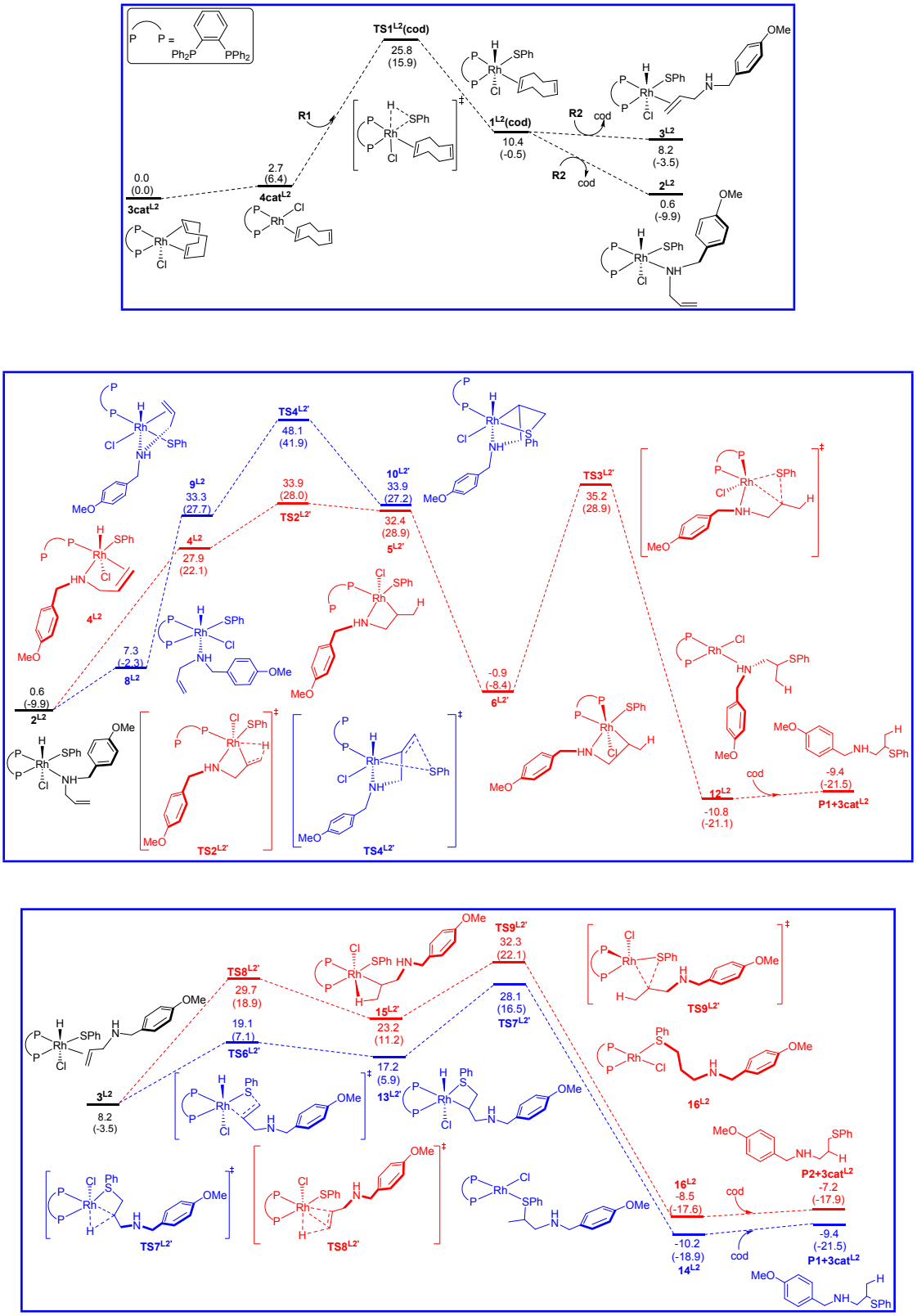

Fig. S4 Other inaccessible pathways for the **3cat^{L2}**-catalyzed hydrothiolation reaction.

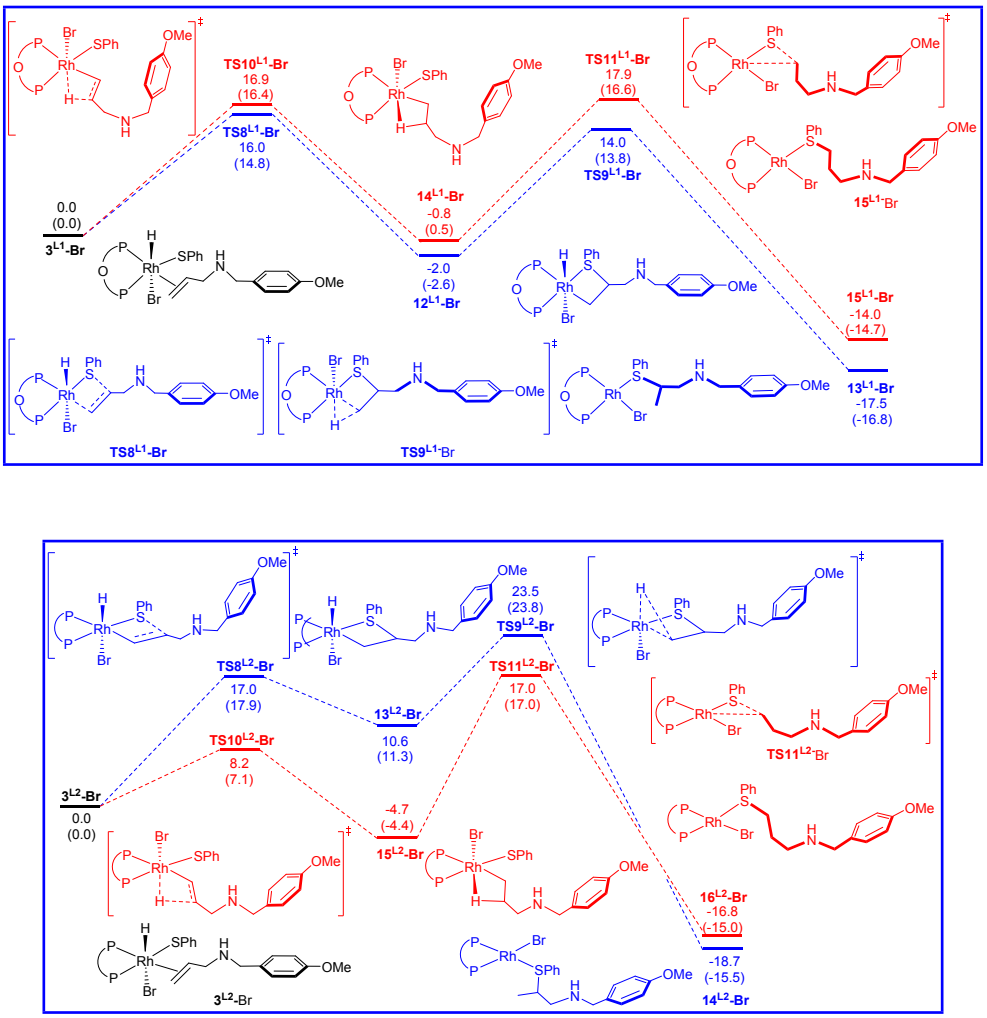

Fig. S5 The pathways in which Cl of the catalyst is replaced by Br.

.

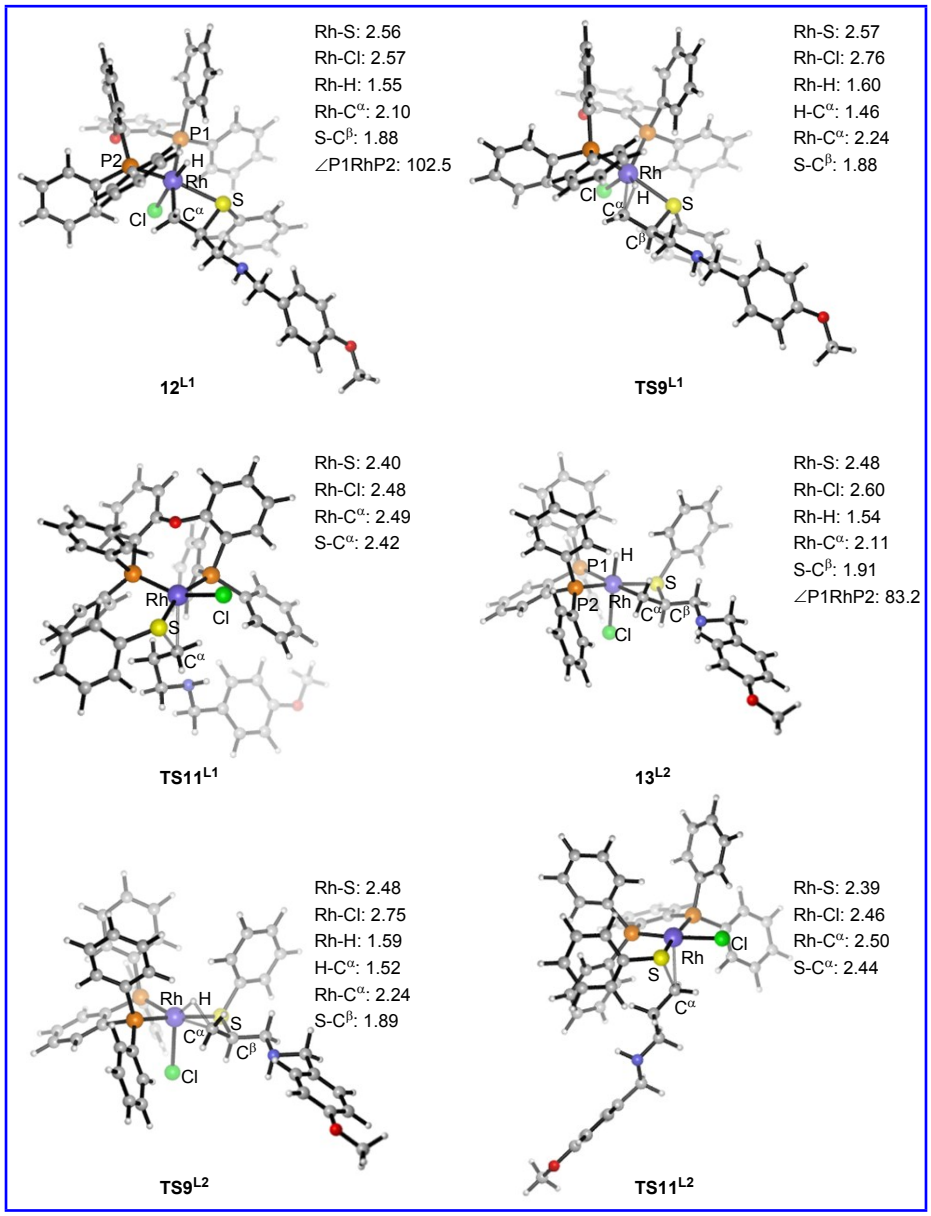

Fig. S6 Optimized geometries of the selected intermediates and transition states. Bond distances are given in Å and angles are given in degree.

.

Cartesian Coordinates and Sum of Electronic and Thermal Free Energies for All of the Calculated Structures

1cat

Sum of electronic and thermal Free Energies= -1763.421406

Cl	-0.00406800	1.68764700	-0.73462300
Cl	0.00406200	-1.68684400	-0.73596900
C	-3.02866400	1.37777000	0.83805400
C	-3.30959600	1.41754500	-0.54211300
H	-2.35929400	2.14576500	1.22040800
C	-3.91142800	0.68979700	1.87516800
H	-4.95556100	0.71628300	1.54749900
H	-3.87522900	1.25741700	2.81080700
C	-4.47793500	0.74165900	-1.23530600
H	-5.39792900	1.33229100	-1.10602900
H	-4.26321900	0.74364200	-2.30921200
H	-2.85247800	2.22547900	-1.11128400
C	-4.69672500	-0.71607800	-0.77024400
H	-5.39297000	-0.75136200	0.07393700
H	-5.17343600	-1.28302000	-1.57652700
C	-3.46315700	-0.76400200	2.14338400
H	-2.69366700	-0.76099200	2.92285100
H	-4.29808900	-1.36145800	2.54091800
C	-3.38771700	-1.39963200	-0.38636600
C	-2.86330900	-1.43378500	0.92127400
H	-3.03706500	-2.16831200	-1.07220800
H	-2.16127000	-2.23590400	1.14354200
Rh	-1.74964100	-0.00609600	-0.21436800
C	3.02847000	-1.37868300	0.83639500
C	3.30969900	-1.41668000	-0.54382800
H	2.35945900	-2.14763400	1.21749900
C	3.91077800	-0.69202800	1.87473800
H	4.95518300	-0.71898500	1.54793200
H	3.87341700	-1.26042000	2.80985300
C	4.47803600	-0.73989300	-1.23615400
H	5.39793900	-1.33092000	-1.10806300
H	4.26313800	-0.74003600	-2.31003800
H	2.85299600	-2.22417000	-1.11395900
C	4.69700600	0.71702600	-0.76877300
H	5.39265100	0.75082900	0.07593700
H	5.17441800	1.28506800	-1.57387300
C	3.46332500	0.76188200	2.14406200
H	2.69433400	0.75882700	2.92400800
H	4.29886800	1.35854100	2.54150100
C	3.38784200	1.40017500	-0.38478900
C	2.86323400	1.43290500	0.92275500
H	3.03709500	2.16921100	-1.07017600
H	2.16076200	2.23442000	1.14574500
Rh	1.74966100	0.00618400	-0.21453300

L1

Sum of electronic and thermal Free Energies= -2146.194311

P	2.51348	-0.01845	-0.90949
P	-2.51963	0.01831	-0.90633
C	4.259	-0.53588	-1.27737
C	5.40776	0.1928	-0.9334
C	4.41695	-1.72216	-2.01547
C	6.67553	-0.25681	-1.30838
H	5.3136	1.11834	-0.37558
C	5.68348	-2.18023	-2.37548
H	3.5372	-2.28774	-2.31287
C	6.81812	-1.44535	-2.02496
H	7.55345	0.32381	-1.03808
H	5.78375	-3.10272	-2.9403
H	7.80528	-1.79326	-2.31499
C	2.71588	1.72783	-0.32107
C	3.16041	2.08543	0.96247
C	2.39444	2.7487	-1.22846
C	3.28904	3.42789	1.3229
H	3.40545	1.3091	1.68192
C	2.52709	4.09134	-0.8706
H	2.02904	2.48657	-2.21827
C	2.97505	4.43373	0.40617
H	3.63668	3.68898	2.31917
H	2.2729	4.8684	-1.58598
H	3.07351	5.47818	0.68852
C	-2.71497	-1.72764	-0.31519
C	-3.14525	-2.0854	0.97285
C	-2.40085	-2.74824	-1.22532
C	-3.26774	-3.42816	1.33467
H	-3.38451	-1.30931	1.69434

C	-2.52807	-4.09108	-0.86628
H	-2.04624	-2.48591	-2.21878
C	-2.96167	-4.43364	0.41513
H	-3.60375	-3.68939	2.33463
H	-2.27985	-4.8679	-1.58391
H	-3.0559	-5.47831	0.6981
C	-4.26634	0.5316	-1.27167
C	-5.41335	-0.19962	-0.92721
C	-4.42657	1.7172	-2.01057
C	-6.68198	0.24656	-1.30388
H	-5.31724	-1.12443	-0.36813
C	-5.6939	2.17208	-2.37185
H	-3.54779	2.2847	-2.3079
C	-6.82688	1.4342	-2.02178
H	-7.55883	-0.33609	-1.03391
H	-5.79582	3.09409	-2.9374
H	-7.8147	1.77917	-2.31338
C	2.18519	-0.91674	0.68414
C	3.09612	-1.7776	1.31319
C	0.90362	-0.79969	1.25412
C	2.75156	-2.48723	2.46482
H	4.09003	-1.89065	0.8943
C	0.54239	-1.51084	2.39922
C	1.47352	-2.35243	3.0061
H	3.47966	-3.14213	2.93421
H	-0.46066	-1.40944	2.79796
H	1.1922	-2.90835	3.89566
C	-2.18759	0.92094	0.68311
C	-3.09258	1.79103	1.30786
C	-0.90568	0.79918	1.25226
C	-2.74228	2.50482	2.45534
H	-4.0866	1.90791	0.88947
C	-0.53935	1.51373	2.39376
C	-1.46475	2.36483	2.99648
H	-3.46542	3.167	2.92161
H	0.46301	1.40817	2.79314
H	-1.17924	2.9236	3.88321
O	-0.00487	-0.00518	0.57831

cod

Sum of electronic and thermal Free Energies= -311.895809

C	-0.04334	2.36464	-0.47094
C	0.04464	2.24398	0.86071
H	-1.03994	2.54875	-0.86867
C	1.02211	2.84899	-1.4408
H	0.76294	2.55344	-2.46341
H	1.98712	2.39592	-1.20977
C	1.27422	2.62343	1.68372
H	1.19267	2.19098	2.68673
H	2.18838	2.22379	1.23745
H	-0.87993	2.35203	1.42671
C	1.40305	4.13374	1.79658
H	0.41273	4.58741	1.65277
H	1.70353	4.3857	2.81802
C	1.15685	4.35127	-1.36945
H	1.30753	4.73699	-2.38211
H	0.20669	4.78075	-1.02243
C	2.40621	4.78739	0.83831
C	2.28944	4.87722	-0.50284
H	3.31679	5.1734	1.29382
H	3.12413	5.33334	-1.03277

2cat^{L1}

Sum of electronic and thermal Free Energies= -3027.823650

C	2.22984	-1.84288	-0.61936
C	1.59619	-2.17358	0.57715
H	2.95497	-1.03555	-0.56893
C	2.49106	-2.76956	-1.78482
H	2.75902	-2.1559	-2.65298
H	1.59511	-3.32857	-2.05588
C	1.04929	-3.53997	0.92891
H	0.37814	-3.44215	1.78961
H	0.46369	-3.95467	0.10709
H	1.85865	-1.57931	1.44927
C	2.22136	-4.5146	1.28576
H	3.08796	-3.92884	1.62441
H	1.92057	-5.12746	2.14265
C	3.66485	-3.75499	-1.47626
H	4.26189	-3.88692	-2.38547
H	4.33846	-3.29351	-0.73931
C	2.62143	-5.43962	0.15514
C	3.22209	-5.12192	-0.99796
H	2.35389	-6.4867	0.29576
H	3.39515	-5.93693	-1.70017
C	-4.73449	2.65622	1.46637
C	-4.14199	3.87571	1.1286
C	-2.94152	3.89854	0.42343
C	-2.86291	1.46311	0.43347
C	-4.09625	1.47181	1.11651
H	-5.6843	2.62732	1.99447

H	-4.61921	4.81408	1.39663
H	-2.50029	4.84847	0.15206
H	-4.55683	0.52638	1.38609
P	1.44844	1.135	0.11337
P	-2.09113	-0.16411	-0.04378
Rh	0.18986	-0.74318	-0.48008
Cl	-0.83522	-2.58576	-1.70766
C	-3.38233	-0.66788	-1.27606
C	-4.57005	-1.32434	-0.92773
C	-3.1818	-0.2921	-2.61205
C	-5.53201	-1.60966	-1.90014
H	-4.74504	-1.63368	0.09803
C	-4.14931	-0.56428	-3.578
H	-2.25387	0.19306	-2.89893
C	-5.32528	-1.2303	-3.22647
H	-6.44071	-2.13438	-1.61771
H	-3.97584	-0.27391	-4.60995
H	-6.07188	-1.45743	-3.98299
C	-2.41198	-1.18463	1.4721
C	-2.56309	-2.57845	1.36587
C	-2.37719	-0.60796	2.75358
C	-2.71096	-3.36329	2.50966
H	-2.5318	-3.04771	0.38848
C	-2.51656	-1.398	3.89474
H	-2.25026	0.46402	2.86626
C	-2.69269	-2.77747	3.77715
H	-2.8343	-4.43805	2.40687
H	-2.49439	-0.92933	4.8751
H	-2.8074	-3.39128	4.66492
C	2.64727	1.38918	-1.29613
C	3.9054	2.00042	-1.17234
C	2.20255	1.01871	-2.57676
C	4.7024	2.21961	-2.29765
H	4.27818	2.30266	-0.19903
C	2.99403	1.2548	-3.70211
H	1.23669	0.52925	-2.68284
C	4.24756	1.8527	-3.56589
H	5.67758	2.68273	-2.17974
H	2.62959	0.96456	-4.68384
H	4.86694	2.02819	-4.44118
C	2.46418	0.93656	1.6513
C	3.76194	0.4032	1.67544
C	1.83653	1.22113	2.87818
C	4.41574	0.1712	2.88917
H	4.27336	0.16521	0.7497
C	2.4907	0.99321	4.08672
H	0.82911	1.62785	2.888
C	3.78535	0.4666	4.09678
H	5.4208	-0.24122	2.88355
H	1.98867	1.22576	5.02175
H	4.29501	0.28623	5.03858
C	-2.31438	2.6986	0.05966
O	-1.17001	2.68614	-0.73776
C	-0.12505	3.51401	-0.35894
C	0.99897	2.95415	0.2691
C	-0.18407	4.88272	-0.64723
C	1.97114	3.8473	0.75741
C	0.8114	5.73879	-0.18481
H	-1.00895	5.25988	-1.24092
C	1.87343	5.22191	0.55965
H	2.82791	3.45503	1.29276
H	0.7539	6.80196	-0.40053
H	2.64097	5.88117	0.95365

3cat^{L1}

Sum of electronic and thermal Free Energies= -3027.819234

P	-2.3877	0.07165	-0.07479
P	2.16492	-0.49121	-0.02055
C	-3.43363	1.25973	0.89193
C	-4.53001	1.93918	0.34226
C	-3.08423	1.51642	2.23016
C	-5.25995	2.84925	1.11302
H	-4.82391	1.75354	-0.68503
C	-3.81624	2.42027	2.99784
H	-2.2361	1.00007	2.67026
C	-4.90798	3.09106	2.44018
H	-6.10987	3.36282	0.67244
H	-3.53336	2.60281	4.03059
H	-5.47854	3.79645	3.03799
C	-3.38068	-0.22815	-1.59646
C	-4.17844	-1.36277	-1.79318
C	-3.30865	0.73976	-2.6126
C	-4.90458	-1.51689	-2.97628
H	-4.2253	-2.13806	-1.03539
C	-4.05167	0.59412	-3.78178
H	-2.65412	1.59956	-2.49641
C	-4.85102	-0.5365	-3.96762
H	-5.50989	-2.40731	-3.12175
H	-3.99068	1.35501	-4.5559

H	-5.41826	-0.65761	-4.88594
C	2.98725	-0.52747	1.64357
C	4.335	-0.87312	1.83295
C	2.17425	-0.34391	2.77175
C	4.86002	-1.00398	3.11911
H	4.9791	-1.04364	0.97751
C	2.69898	-0.48339	4.05791
H	1.12727	-0.09102	2.63106
C	4.04459	-0.80768	4.23484
H	5.90621	-1.26601	3.24859
H	2.0559	-0.3344	4.92059
H	4.4552	-0.91293	5.23524
C	3.4705	-0.03542	-1.23089
C	4.49767	0.86479	-0.89836
C	3.33531	-0.45187	-2.56876
C	5.39262	1.30951	-1.87332
H	4.60291	1.22666	0.11948
C	4.23694	-0.00716	-3.53483
H	2.50456	-1.0911	-2.85252
C	5.27038	0.86849	-3.19152
H	6.18306	2.00285	-1.59824
H	4.12194	-0.34016	-4.56279
H	5.96843	1.21343	-3.94901
C	-2.55951	-1.46578	0.9556
C	-3.77884	-1.76824	1.586
C	-1.46685	-2.3192	1.20307
C	-3.91318	-2.86578	2.4335
H	-4.63076	-1.11701	1.41916
C	-1.57965	-3.39614	2.08909
C	-2.80411	-3.67173	2.69343
H	-4.869	-3.07508	2.90373
H	-0.70763	-4.00004	2.30979
H	-2.88302	-4.50982	3.37959
C	1.9068	-2.31593	-0.25004
C	2.88469	-3.16563	-0.77514
C	0.66453	-2.87495	0.09973
C	2.62799	-4.5214	-0.98836
H	3.84988	-2.75503	-1.05209
C	0.37983	-4.21633	-0.1429
C	1.37016	-5.03669	-0.68697
H	3.39899	-5.16043	-1.4075
H	-0.60408	-4.61664	0.0647
H	1.14432	-6.08146	-0.87986
O	-0.24852	-1.97703	0.64699
C	-0.03093	2.38427	-0.56727
C	0.05973	2.21085	0.85298
H	-1.01481	2.67213	-0.94486
C	1.07415	2.90594	-1.46156
H	0.84762	2.60474	-2.49023
H	2.03747	2.454	-1.21348
C	1.25656	2.66766	1.66898
H	1.17742	2.25917	2.68218
H	2.19815	2.28938	1.26226
H	-0.87083	2.37765	1.39215
C	1.34279	4.23043	1.76142
H	0.351	4.64878	1.54354
H	1.57412	4.51772	2.79364
C	1.20502	4.46414	-1.38504
H	1.37488	4.85792	-2.39294
H	0.2447	4.8837	-1.05311
C	2.38098	4.84616	0.84888
C	2.32195	4.94586	-0.48517
H	3.28185	5.21694	1.33824
H	3.17858	5.39139	-0.99121
Rh	-0.09165	0.31622	-0.24608
Cl	-0.18709	-0.96942	-2.45518

4cat^{L1}

Sum of electronic and thermal Free Energies= -3027.850933

C	-0.91791	-3.21334	-0.01599
C	-0.26108	-3.33077	-1.22863
H	-1.89552	-2.74476	-0.04762
C	-0.62088	-4.02861	1.23463
H	-0.24487	-5.0138	0.94274
H	-1.56495	-4.21452	1.75918
C	0.93994	-4.20092	-1.51697
H	0.61591	-5.22991	-1.73928
H	1.39889	-3.81333	-2.43136
H	-0.75999	-2.93406	-2.10629
C	1.98056	-4.18463	-0.3815
H	1.75737	-4.95556	0.36478
H	2.96122	-4.44585	-0.79409
C	0.3759	-3.33585	2.1891
H	-0.17433	-2.73339	2.91997
H	0.91899	-4.08984	2.7812
C	2.07662	-2.81537	0.29317
C	1.34941	-2.42694	1.46166
H	3.04477	-2.34958	0.16418
H	1.86335	-1.73475	2.12926

C	3.19883	3.001	-3.02585
C	1.99997	3.61188	-3.37723
C	0.84785	3.38923	-2.62353
C	2.07519	1.83514	-1.19977
C	3.22338	2.10911	-1.95322
H	4.10546	3.19142	-3.5915
H	1.94918	4.27288	-4.23773
H	-0.08019	3.86063	-2.91476
H	4.15296	1.60903	-1.71536
P	-2.06813	0.12371	-0.07382
P	2.00488	0.50403	0.08812
Rh	0.5573	-1.43544	-0.28169
Cl	0.42534	-0.66291	-2.74353
C	1.72466	1.45998	1.64636
C	0.8334	0.9732	2.60972
C	2.37489	2.68449	1.87697
C	0.59616	1.68927	3.78546
H	0.30919	0.04365	2.42346
C	2.14523	3.39398	3.0554
H	3.05462	3.08629	1.13065
C	1.25546	2.89683	4.01239
H	-0.11387	1.30568	4.51165
H	2.65564	4.33917	3.22358
H	1.0716	3.45643	4.92553
C	3.78477	-0.00121	0.20138
C	4.34936	-0.67396	-0.90084
C	4.57109	0.19491	1.34405
C	5.67432	-1.10531	-0.86733
H	3.73817	-0.86391	-1.77965
C	5.8961	-0.25279	1.37985
H	4.15823	0.69916	2.21093
C	6.45265	-0.89574	0.27541
H	6.09571	-1.61346	-1.73029
H	6.49016	-0.09372	2.2756
H	7.48332	-1.2382	0.304
C	-2.72018	0.28423	1.66704
C	-3.4859	1.35654	2.15164
C	-2.39414	-0.7534	2.56039
C	-3.91762	1.38317	3.47996
H	-3.75051	2.18035	1.49523
C	-2.82806	-0.73179	3.88594
H	-1.78039	-1.577	2.21308
C	-3.59457	0.34081	4.35139
H	-4.51414	2.22304	3.83032
H	-2.56177	-1.54778	4.55532
H	-3.93328	0.36354	5.3832
C	-3.40894	-0.86303	-0.89747
C	-4.58893	-1.27524	-0.25858
C	-3.1978	-1.22791	-2.24116
C	-5.54183	-2.03113	-0.94769
H	-4.77075	-1.00443	0.77651
C	-4.15698	-1.97499	-2.92551
H	-2.27416	-0.93701	-2.73847
C	-5.33024	-2.3801	-2.28185
H	-6.45081	-2.34226	-0.43864
H	-3.98276	-2.24717	-3.96314
H	-6.07269	-2.96674	-2.81621
C	0.89782	2.54178	-1.516
O	-0.15124	2.32607	-0.64677
C	-1.43833	2.75922	-0.88537
C	-2.46363	1.80982	-0.74815
C	-1.72911	4.10247	-1.14989
C	-3.7768	2.22281	-1.02902
C	-3.04476	4.48879	-1.39864
H	-0.92933	4.83334	-1.15576
C	-4.06975	3.54232	-1.36989
H	-4.58035	1.49616	-0.97052
H	-3.26421	5.52945	-1.61733
H	-5.09332	3.83283	-1.58779

5cat^{L1}

Sum of electronic and thermal Free Energies= -2715.953755

P	2.27134	0.02653	-0.195
P	-2.27218	-0.01139	-0.19671
C	3.45133	-1.04324	-1.11634
C	4.83675	-0.81812	-1.14088
C	2.91705	-2.12505	-1.83287
C	5.67645	-1.67987	-1.84785
H	5.25798	0.03698	-0.62036
C	3.7609	-2.98513	-2.53659
H	1.84055	-2.26621	-1.85355
C	5.13982	-2.76653	-2.54211
H	6.74752	-1.49806	-1.86275
H	3.33844	-3.81694	-3.09282
H	5.79443	-3.43291	-3.09697
C	3.11838	1.66058	-0.12117
C	3.91441	2.09192	0.94929
C	2.92116	2.51622	-1.21926
C	4.51341	3.35399	0.91819

H	4.06417	1.44934	1.81153
C	3.52924	3.77037	-1.24934
H	2.28098	2.19726	-2.03816
C	4.32547	4.19235	-0.18115
H	5.1255	3.68019	1.75463
H	3.37236	4.42307	-2.10339
H	4.79131	5.17356	-0.20312
C	-3.12994	-1.63936	-0.2783
C	-3.9356	-2.16233	0.74307
C	-2.93066	-2.39131	-1.4494
C	-4.5419	-3.41219	0.59203
H	-4.08729	-1.60109	1.66009
C	-3.54601	-3.63337	-1.59875
H	-2.28313	-2.00209	-2.23129
C	-4.35176	-4.14678	-0.57887
H	-5.16146	-3.81011	1.3911
H	-3.38748	-4.20553	-2.50843
H	-4.82334	-5.1187	-0.69403
C	-3.44401	1.14993	-1.01142
C	-4.83018	0.93449	-1.0628
C	-2.90252	2.29492	-1.61562
C	-5.66351	1.86524	-1.68485
H	-5.257	0.03438	-0.63016
C	-3.74001	3.22368	-2.23444
H	-1.82547	2.43349	-1.61732
C	-5.11974	3.01244	-2.26702
H	-6.73522	1.69044	-1.72145
H	-3.31199	4.10449	-2.70428
H	-5.76935	3.73289	-2.75631
C	2.31334	-0.64657	1.53855
C	3.43555	-1.2639	2.10762
C	1.11585	-0.66635	2.27785
C	3.37284	-1.88168	3.35751
H	4.36287	-1.2877	1.5441
C	1.0231	-1.31641	3.50728
C	2.16227	-1.91624	4.04731
H	4.25588	-2.35616	3.77389
H	0.07534	-1.37333	4.02787
H	2.08908	-2.42653	5.00296
C	-2.3103	0.49374	1.59307
C	-3.42854	1.06207	2.21803
C	-1.11307	0.43481	2.33084
C	-3.36276	1.55715	3.52132
H	-4.35499	1.14649	1.65885
C	-1.01716	0.96327	3.61697
C	-2.15273	1.5166	4.2116
H	-4.24282	1.99595	3.98089
H	-0.06972	0.9638	4.14121
H	-2.07682	1.93231	5.21182
O	-0.00065	-0.08893	1.65788
Rh	-0.00053	0.0186	-0.537
Cl	-0.00061	0.13248	-2.89504

6cat^{L1}

Sum of electronic and thermal Free Energies= -2715.959683

Rh	0.06482600	-1.48516100	-0.38236800
P	1.72651400	-0.06564400	-0.01921900
P	-1.72759900	-0.16921600	-0.02250400
C	2.99366600	-0.73489400	1.14933700
C	4.29598300	-0.21154700	1.19735800
C	2.64541800	-1.77986800	2.01585000
C	5.22490900	-0.71589900	2.10768400
H	4.58997400	0.58211700	0.51762400
C	3.57666600	-2.28147300	2.92665700
H	1.65355400	-2.21435400	1.94412000
C	4.86582300	-1.74985300	2.97561300
H	6.23108300	-0.30690500	2.13246700
H	3.29736200	-3.09838400	3.58573900
H	5.59277700	-2.14623100	3.67907400
C	2.71303000	0.37605700	-1.51862000
C	2.93892600	-0.60777400	-2.49387400
C	3.26930300	1.65309600	-1.69055600
C	3.71419500	-0.31387000	-3.61637400
H	2.51049300	-1.59783400	-2.36705100
C	4.04108100	1.94109900	-2.81738700
H	3.09884000	2.42787000	-0.94969300
C	4.26476700	0.95834200	-3.78276600
H	3.88331000	-1.08355700	-4.36404300
H	4.46389600	2.93452000	-2.94007700
H	4.86312400	1.18397300	-4.66118800
C	-2.13515600	0.49190500	1.65340800
C	-3.07101900	1.51384600	1.87367400
C	-1.50372200	-0.10411300	2.75573500
C	-3.37417900	1.92368500	3.17298900
H	-3.56288300	1.99171100	1.03224700
C	-1.81135700	0.30425700	4.05386900
H	-0.76933600	-0.88598600	2.58135200
C	-2.74733200	1.31855900	4.26436100
H	-4.10006600	2.71620800	3.33234100

H	-1.31634700	-0.16603700	4.89868000
H	-2.98488400	1.63965700	5.27467700
C	-3.01770700	-1.45415100	-0.33169500
C	-4.02922200	-1.78226600	0.58449000
C	-2.89485100	-2.21053900	-1.51369300
C	-4.90222000	-2.83817300	0.31929900
H	-4.13430800	-1.21526700	1.50335900
C	-3.76737600	-3.26853900	-1.77063600
H	-2.11516000	-1.96837300	-2.23245100
C	-4.77259400	-3.58343100	-0.85490700
H	-5.68327100	-3.08118700	1.03421700
H	-3.65655100	-3.84666500	-2.68309500
H	-5.45051400	-4.40859600	-1.05304500
C	1.29799100	1.56646700	0.73852700
C	1.73107100	1.96003100	2.01283400
C	0.40350100	2.41275000	0.06301000
C	1.27929000	3.14664800	2.59298900
H	2.42049000	1.32659300	2.55936700
C	-0.05747800	3.59967500	0.63031800
C	0.38195600	3.96215300	1.90363300
H	1.62513600	3.42776700	3.58289700
H	-0.74611800	4.22770900	0.07491700
H	0.02495900	4.88512500	2.35106700
C	-2.21793900	1.19944700	-1.17420000
C	-3.52134500	1.30394900	-1.68791500
C	-1.26528500	2.12843000	-1.63086100
C	-3.85959200	2.28636900	-2.61968500
H	-4.27551400	0.59289900	-1.36665600
C	-1.58821200	3.10220500	-2.57519600
C	-2.88964800	3.18242500	-3.06989800
H	-4.87494800	2.34101000	-3.00041300
H	-0.80789900	3.77496000	-2.91555200
H	-3.14115900	3.94027600	-3.80581900
O	0.05366700	2.04030800	-1.22301100
Cl	1.33915800	-3.41825500	-0.89346000

R1

Sum of electronic and thermal Free Energies= -630.376495

S	-0.94884	0.66007	0.
H	-1.38613	1.88119	-0.1837
C	0.83116	0.66007	0.
C	1.52868	0.66064	1.20828
C	1.52866	0.65938	-1.2079
C	2.92339	0.66121	1.20856
H	0.97848	0.66195	2.1604
C	2.9238	0.65896	-1.2078
H	0.97906	0.65875	-2.16031
C	3.62122	0.66001	0.00015
H	3.47325	0.66229	2.16089
H	3.47348	0.65801	-2.16033
H	4.7209	0.6604	0.00062

IM1^{L1}

Sum of electronic and thermal Free Energies= -3346.327759

Rh	0.32590200	0.67133400	-0.74912600
C	2.88886200	2.94658400	-0.44772900
C	1.99572100	4.01926000	-0.33687400
C	4.09365900	2.94818300	0.26248200
C	2.32528900	5.09655800	0.48601100
H	1.05795800	3.99695600	-0.88398500
C	4.40330100	4.02542500	1.09637000
H	4.78684700	2.11917000	0.15764700
C	3.52226500	5.10153800	1.20767900
H	1.63810700	5.93416400	0.56649500
H	5.33942600	4.02511200	1.64754700
H	3.76791900	5.94232800	1.84998500
P	1.30409000	-1.24245900	0.02477900
P	-1.87937700	0.40052400	-0.02666200
C	2.43512300	-1.84247600	-1.32207400
C	3.75427800	-2.26433400	-1.10968200
C	1.93306700	-1.83473000	-2.63630400
C	4.54967800	-2.67584600	-2.18303100
H	4.17173500	-2.26676300	-0.10897300
C	2.72498700	-2.25471900	-3.70442500
H	0.92086900	-1.48246500	-2.81654800
C	4.03833000	-2.67560400	-3.48024100
H	5.57263000	-2.99337200	-2.00057500
H	2.31914300	-2.24306000	-4.71206900
H	4.65943800	-2.99377900	-4.31277100
C	2.37354900	-1.22211800	1.53614900
C	2.70700200	0.01585300	2.10067500
C	2.84888500	-2.39640600	2.14192200
C	3.51772700	0.08270700	3.23579700
H	2.31239100	0.92397600	1.65520100
C	3.65664000	-2.32898100	3.27754800
H	2.58092400	-3.36554200	1.73078800
C	3.99578200	-1.08865300	3.82438500
H	3.76760200	1.05073000	3.66074600
H	4.01788600	-3.24462700	3.73772900
H	4.62318400	-1.03814800	4.70998100

C	-2.85970900	-0.75740100	-1.08601700
C	-3.87549800	-1.58981800	-0.59564300
C	-2.56171600	-0.78039000	-2.46004300
C	-4.57977100	-2.43108700	-1.46027300
H	-4.12040500	-1.58634100	0.46103900
C	-3.27663900	-1.61270800	-3.32099300
H	-1.78039700	-0.13082100	-2.84459000
C	-4.28389400	-2.44329500	-2.82340100
H	-5.36085400	-3.07495500	-1.06535100
H	-3.04368600	-1.61336300	-4.38215800
H	-4.83425800	-3.09650400	-3.49491700
C	-2.77387400	2.01619300	-0.18377500
C	-3.95212900	2.16710900	-0.92269100
C	-2.25099100	3.12490600	0.50021700
C	-4.59683200	3.40654200	-0.97751500
H	-4.36881700	1.32423500	-1.46331900
C	-2.90031300	4.35567400	0.45240700
H	-1.32429200	3.02539800	1.05834500
C	-4.07604500	4.50104600	-0.28944300
H	-5.50655600	3.51171600	-1.56211600
H	-2.48392300	5.20545700	0.98626900
H	-4.57834800	5.46334200	-0.33312800
C	0.26175500	-2.74325600	0.30385800
C	0.28713400	-3.90925200	-0.47179800
C	-0.67265900	-2.66543800	1.34409600
C	-0.61125800	-4.94989400	-0.22429600
H	1.00312900	-3.99985800	-1.28079000
C	-1.58004900	-3.69065600	1.60268000
C	-1.54573100	-4.83583100	0.80526700
H	-0.58208800	-5.84421800	-0.83915700
H	-2.29333300	-3.59344000	2.41391300
H	-2.24874200	-5.64131600	0.99683000
C	-2.43972600	-0.03679000	1.71483500
C	-3.59707700	0.55745000	2.25447600
C	-1.73650900	-0.91052900	2.56061400
C	-4.01179400	0.31332000	3.56350300
H	-4.17844000	1.23481600	1.64123000
C	-2.12164700	-1.13969300	3.88270800
C	-3.26466200	-0.52627200	4.38915400
H	-4.91082700	0.79357400	3.93781000
H	-1.50944100	-1.79660400	4.49199800
H	-3.56720900	-0.70483600	5.41674000
O	-0.58095800	-1.52523900	2.12009100
Cl	-0.48032900	2.34566900	-2.40064100
S	2.53327800	1.51710100	-1.49774100
H	1.92986500	2.19694500	-2.50638100

TS1^{L1}

Sum of electronic and thermal Free Energies= -3346.294383

Rh	-0.20989	0.66766	-0.93172
C	-3.62799	2.37096	-0.6127
C	-4.60172	3.20735	-1.18782
C	-3.8241	1.91221	0.69671
C	-5.73631	3.57474	-0.46671
H	-4.45455	3.58157	-2.19658
C	-4.96808	2.2753	1.40925
H	-3.083	1.27373	1.16144
C	-5.92853	3.10956	0.83641
H	-6.46868	4.23466	-0.92382
H	-5.10105	1.90247	2.42127
H	-6.81235	3.39812	1.39845
P	-0.91482	-1.31724	-0.01531
P	1.83909	0.86572	0.10678
C	-2.39915	-1.37152	1.08272
C	-3.66111	-1.71128	0.5739
C	-2.29734	-0.97814	2.42934
C	-4.78896	-1.68436	1.39646
H	-3.76727	-1.9953	-0.46612
C	-3.42368	-0.96872	3.25209
H	-1.33603	-0.68583	2.8407
C	-4.67367	-1.3237	2.7376
H	-5.75868	-1.94371	0.98248
H	-3.32514	-0.67894	4.29423
H	-5.5513	-1.31134	3.37733
C	-1.40455	-2.3592	-1.46975
C	-1.44415	-1.82414	-2.76627
C	-1.70728	-3.71933	-1.27991
C	-1.78199	-2.63775	-3.85134
H	-1.19604	-0.78215	-2.94241
C	-2.05136	-4.52405	-2.36418
H	-1.67094	-4.15273	-0.28405
C	-2.08681	-3.9841	-3.65427
H	-1.79829	-2.21096	-4.85104
H	-2.28503	-5.57286	-2.20254
H	-2.34654	-4.61381	-4.50068
C	1.92878	0.41403	1.89694
C	2.98123	-0.32051	2.45826
C	0.92554	0.91888	2.74143
C	3.02331	-0.55753	3.83512

H	3.77365	-0.70571	1.82531
C	0.9767	0.69287	4.11634
H	0.10923	1.49617	2.31596
C	2.02464	-0.05119	4.66642
H	3.84273	-1.13393	4.25535
H	0.20086	1.10089	4.75836
H	2.06323	-0.22995	5.73711
C	2.39772	2.63547	0.18073
C	3.22105	3.07808	1.23371
C	1.99829	3.55709	-0.79983
C	3.63738	4.40765	1.29793
H	3.53498	2.391	2.01064
C	2.41783	4.88666	-0.72752
H	1.37514	3.23118	-1.62506
C	3.23474	5.31681	0.31848
H	4.27072	4.73236	2.11921
H	2.0973	5.58393	-1.49577
H	3.55345	6.35385	0.37372
C	0.28263	-2.45816	0.82902
C	-0.0181	-3.20153	1.98021
C	1.55952	-2.62615	0.26189
C	0.92305	-4.05142	2.56293
H	-0.99887	-3.11428	2.4317
C	2.50965	-3.47095	0.83692
C	2.18966	-4.17873	1.9942
H	0.66284	-4.61028	3.45648
H	3.48487	-3.57234	0.37353
H	2.92849	-4.83784	2.44093
C	3.23263	-0.03925	-0.69616
C	4.45778	0.57191	-1.00084
C	3.02817	-1.35574	-1.14724
C	5.43917	-0.10491	-1.72688
H	4.63521	1.59369	-0.68378
C	3.99088	-2.0309	-1.89376
C	5.20374	-1.40288	-2.18003
H	6.37797	0.39112	-1.95351
H	3.77065	-3.03053	-2.25413
H	5.9559	-1.92542	-2.76382
O	1.80143	-1.96742	-0.92712
Cl	0.79702	1.39979	-3.07354
S	-2.17452	2.05592	-1.614
H	-1.22623	1.65911	-0.18328

1^{L1}

Sum of electronic and thermal Free Energies= -3346.315641

Rh	-0.38316	0.76466	-0.58163
H	-0.85811	1.17326	0.8387
S	-2.2503	1.76462	-1.53636
C	-3.59197	2.34225	-0.512
C	-3.77776	2.04245	0.84572
C	-4.52751	3.18108	-1.15143
C	-4.87501	2.55845	1.5379
H	-3.06758	1.40248	1.35551
C	-5.60522	3.71466	-0.44755
H	-4.39421	3.41673	-2.20408
C	-5.78854	3.40374	0.90211
H	-5.00829	2.30354	2.58613
H	-6.30182	4.37613	-0.95781
H	-6.63284	3.81399	1.44979
P	-0.94496	-1.35263	0.00441
P	1.87874	0.85961	0.10952
C	-2.34558	-1.38168	1.20757
C	-3.59807	-1.90273	0.85914
C	-2.16623	-0.84606	2.4952
C	-4.64818	-1.8929	1.7813
H	-3.76071	-2.31106	-0.13168
C	-3.2105	-0.85316	3.41748
H	-1.20627	-0.4253	2.77733
C	-4.45745	-1.37477	3.06081
H	-5.61608	-2.29153	1.49274
H	-3.05363	-0.44385	4.41142
H	-5.27454	-1.37102	3.77629
C	-1.53371	-2.37502	-1.40876
C	-2.12426	-1.77595	-2.53009
C	-1.44876	-3.77629	-1.33768
C	-2.63444	-2.5725	-3.55685
H	-2.17598	-0.69606	-2.6068
C	-1.95396	-4.56379	-2.37106
H	-0.99122	-4.25498	-0.47805
C	-2.54977	-3.96268	-3.48205
H	-3.08562	-2.09667	-4.42238
H	-1.8792	-5.64574	-2.30719
H	-2.94119	-4.5768	-4.28821
C	2.31746	0.52679	1.87225
C	3.53456	-0.06049	2.24657
C	1.42107	0.92739	2.87714
C	3.84548	-0.2481	3.59503
H	4.24378	-0.36952	1.48627
C	1.73825	0.74779	4.22352

H	0.47874	1.38972	2.59765
C	2.95058	0.15578	4.58584
H	4.79134	-0.70701	3.86848
H	1.03833	1.07012	4.98919
H	3.1959	0.01202	5.6342
C	2.33609	2.63589	-0.11908
C	2.91408	3.40022	0.9071
C	2.06747	3.2419	-1.36083
C	3.22016	4.74567	0.69519
H	3.12849	2.95272	1.87103
C	2.38126	4.58569	-1.56355
H	1.61381	2.65989	-2.15907
C	2.95473	5.34104	-0.53868
H	3.66687	5.32611	1.4976
H	2.16901	5.04182	-2.52607
H	3.1922	6.38885	-0.69967
C	0.3158	-2.42685	0.82626
C	0.08945	-3.11663	2.02735
C	1.57137	-2.57428	0.21094
C	1.08852	-3.89703	2.60973
H	-0.8748	-3.04115	2.51477
C	2.58114	-3.34512	0.78918
C	2.33594	-4.00167	1.99404
H	0.88972	-4.41842	3.54074
H	3.53938	-3.43288	0.28892
H	3.11898	-4.60574	2.44319
C	3.15906	-0.04308	-0.86776
C	4.36384	0.5678	-1.24726
C	2.91239	-1.345	-1.33323
C	5.28069	-0.09238	-2.0664
H	4.57542	1.57809	-0.9141
C	3.80788	-2.00323	-2.17201
C	4.99753	-1.37388	-2.53853
H	6.20444	0.4034	-2.34833
H	3.55092	-2.99117	-2.53905
H	5.69627	-1.88336	-3.19534
O	1.71828	-1.97307	-1.01696
Cl	0.43737	0.5241	-2.95504

2^{L1}

Sum of electronic and thermal Free Energies= -3904.245714

S	-0.80002	-2.30579	0.55877
C	-1.66741	-3.21804	-0.70924
C	-1.52195	-3.03816	-2.0929
C	-2.53493	-4.22335	-0.23755
C	-2.22433	-3.86055	-2.97809
H	-0.88333	-2.24796	-2.47002
C	-3.2219	-5.04456	-1.1308
H	-2.66632	-4.35613	0.83384
C	-3.07022	-4.86818	-2.509
H	-2.1024	-3.70807	-4.04814
H	-3.88355	-5.81732	-0.74586
H	-3.60901	-5.50448	-3.20649
P	0.97584	2.31138	-0.16496
P	1.97748	-1.55156	0.35733
C	-0.12233	3.68259	-0.78967
C	-0.46958	4.78102	0.01131
C	-0.62317	3.62481	-2.10567
C	-1.2885	5.79786	-0.48877
H	-0.10928	4.85031	1.03095
C	-1.4298	4.64658	-2.6027
H	-0.40311	2.75867	-2.72309
C	-1.7647	5.73876	-1.79754
H	-1.54743	6.63769	0.15048
H	-1.80731	4.58035	-3.61934
H	-2.3981	6.53114	-2.18626
C	1.55428	3.02559	1.44768
C	2.46915	4.09175	1.49261
C	1.02272	2.54484	2.65094
C	2.83227	4.66583	2.71036
H	2.89358	4.47899	0.57184
C	1.3829	3.12352	3.87089
H	0.33226	1.70675	2.63373
C	2.28669	4.18558	3.90339
H	3.53815	5.49213	2.72757
H	0.95753	2.73884	4.79316
H	2.56595	4.63743	4.85092
C	2.07323	-2.90662	-0.90233
C	2.27346	-4.26735	-0.61957
C	2.03292	-2.49256	-2.24241
C	2.41052	-5.19139	-1.65657
H	2.32782	-4.62142	0.40183
C	2.177	-3.42141	-3.27408
H	1.84378	-1.45203	-2.48596
C	2.36185	-4.77318	-2.98714
H	2.55318	-6.24207	-1.41867
H	2.12889	-3.07928	-4.30403
H	2.46326	-5.49628	-3.7916
C	1.95685	-2.2258	2.10024

C	1.42333	-3.4634	2.48754
C	2.54003	-1.41507	3.08929
C	1.51865	-3.89936	3.81013
H	0.91499	-4.08767	1.76122
C	2.61054	-1.83678	4.41703
H	2.95333	-0.44999	2.82386
C	2.11279	-3.08988	4.78101
H	1.1172	-4.87542	4.07521
H	3.07015	-1.1933	5.15891
H	2.187	-3.43182	5.80802
C	2.4351	2.56317	-1.28822
C	2.44447	3.38138	-2.42735
C	3.60126	1.83673	-1.00809
C	3.54466	3.42642	-3.2826
H	1.58323	3.99077	-2.66164
C	4.69756	1.8392	-1.87008
C	4.66022	2.63517	-3.01481
H	3.51874	4.0693	-4.1593
H	5.56951	1.23365	-1.65504
H	5.51463	2.64282	-3.6836
C	3.83632	-1.18055	0.4052
C	4.70895	-2.26715	0.60944
C	4.40902	0.08931	0.39404
C	6.07298	-2.08537	0.81365
H	4.31107	-3.27508	0.61668
C	5.77088	0.29601	0.64593
C	6.60765	-0.79532	0.84886
H	6.71302	-2.94954	0.96246
H	6.14924	1.31139	0.67841
H	7.66546	-0.64038	1.03573
O	3.58251	1.17947	0.20417
Rh	0.01429	-0.09016	0.00796
H	0.03198	-0.0019	1.54637
Cl	-0.09075	0.14376	-2.58034
C	-4.52721	1.94275	-2.42383
C	-4.08971	1.98191	-1.16108
H	-5.54008	2.23403	-2.68734
H	-3.88264	1.60998	-3.23428
H	-4.75608	2.32132	-0.37089
C	-2.65413	1.6904	-0.80407
H	-2.10801	1.43404	-1.71372
H	-2.221	2.59998	-0.38789
N	-2.34455	0.62013	0.19279
H	-2.32697	1.02712	1.1244
C	-3.31902	-0.50215	0.20339
H	-2.89367	-1.26467	0.85578
H	-3.33411	-0.92401	-0.80349
C	-4.73555	-0.20053	0.65758
C	-5.81244	-0.69627	-0.08375
C	-5.02618	0.47796	1.85374
C	-7.13523	-0.52808	0.32972
H	-5.61557	-1.22277	-1.01555
C	-6.3378	0.67346	2.27424
H	-4.21952	0.86816	2.47343
C	-7.40526	0.16843	1.51432
H	-7.93597	-0.93156	-0.2805
H	-6.56261	1.20558	3.19455
O	-8.65902	0.40563	2.00815
C	-9.76079	-0.1361	1.29819
H	-10.6532	0.17105	1.85062
H	-9.82066	0.25668	0.26807
H	-9.71608	-1.23148	1.26138

3^{Li}

Sum of electronic and thermal Free Energies= -3904.231923

S	0.64273700	2.97732900	0.09833000
C	1.16550600	4.00972300	1.46080000
C	2.24542900	3.72595700	2.31550000
C	0.48192900	5.23132000	1.62145100
C	2.62435300	4.64402900	3.29670100
H	2.76376300	2.77714600	2.22632800
C	0.88186200	6.15047100	2.59098300
H	-0.35944500	5.45631600	0.97211400
C	1.95432200	5.86119500	3.43766400
H	3.45729100	4.40268800	3.95235800
H	0.34473700	7.09039500	2.69119900
H	2.26015900	6.57300800	4.19936400
P	0.45390200	-1.89236800	1.04514300
P	1.51616300	0.53636700	-1.62076500
C	-0.15043900	-2.20538900	2.77333900
C	-1.41075300	-2.76039600	3.03894000
C	0.68364100	-1.86026800	3.85402000
C	-1.83063600	-2.96682700	4.35613700
H	-2.06811000	-3.03850900	2.22258800
C	0.26131000	-2.07660500	5.16522800
H	1.65702900	-1.41746200	3.65819300
C	-0.99665800	-2.62872600	5.42110200
H	-2.81036200	-3.39681900	4.54404100
H	0.91777100	-1.80851300	5.98811800

H	-1.32315500	-2.79353000	6.44397200
C	-0.78194800	-2.82960800	0.02706800
C	-0.68925100	-4.21581400	-0.17691000
C	-1.88537900	-2.14481000	-0.50394100
C	-1.67428200	-4.89497800	-0.89432500
H	0.15390500	-4.76765400	0.22446700
C	-2.87703900	-2.82671700	-1.21130200
H	-1.96825700	-1.07206500	-0.36310100
C	-2.77186500	-4.20364800	-1.41095600
H	-1.58358700	-5.96674500	-1.04746900
H	-3.72671500	-2.27587900	-1.60446200
H	-3.53818700	-4.73572600	-1.96768900
C	3.28783300	0.99334500	-1.84755700
C	4.00239600	0.52822200	-2.96439200
C	3.92378600	1.84168500	-0.93180300
C	5.32890700	0.91062100	-3.16218000
H	3.52571200	-0.12973300	-3.68392300
C	5.25198800	2.22009000	-1.13524100
H	3.38430300	2.19550200	-0.06450800
C	5.95671000	1.75763600	-2.24641800
H	5.86988500	0.54495300	-4.03053700
H	5.73447000	2.87333200	-0.41438500
H	6.99124700	2.05289000	-2.39870400
C	0.60045800	1.68586900	-2.75088400
C	1.27886500	2.58438700	-3.58621300
C	-0.80174100	1.64181700	-2.80734400
C	0.57087300	3.41421100	-4.45748200
H	2.35984500	2.64812200	-3.55079800
C	-1.50705900	2.46470200	-3.68464200
H	-1.34786100	0.96558600	-2.15754900
C	-0.82145300	3.35617400	-4.51193100
H	1.11316300	4.11160600	-5.08953900
H	-2.59182900	2.41509500	-3.71106300
H	-1.36985000	4.00496300	-5.18898100
C	1.95118100	-3.00255000	1.02965200
C	2.13832300	-4.01051500	1.99094800
C	2.96189000	-2.84656800	0.06983200
C	3.29089000	-4.79720700	2.00830800
H	1.38130400	-4.17537200	2.74757400
C	4.13133200	-3.60336800	0.09273300
C	4.29888900	-4.58341600	1.06908300
H	3.40289800	-5.56474700	2.76802100
H	4.89276700	-3.40465400	-0.65404400
H	5.20875900	-5.17558600	1.09196000
C	1.37701700	-1.05595500	-2.54779800
C	0.63498100	-1.24250700	-3.72172600
C	2.06245500	-2.15902500	-2.01964800
C	0.56527900	-2.49689100	-4.33129200
H	0.10454800	-0.40587200	-4.16053100
C	2.00305800	-3.41818100	-2.61557200
C	1.24413600	-3.58078900	-3.77480400
H	-0.01869700	-2.62297900	-5.23764300
H	2.54312300	-4.25067400	-2.17880000
H	1.19188800	-4.55840700	-4.24522100
O	2.82811600	-1.88239600	-0.90818300
Rh	0.61713500	0.55665900	0.58615000
H	-0.69040200	0.56309900	-0.23142700
Cl	2.81648000	0.27994500	1.92661600
C	-0.23578400	1.20579000	2.75096600
C	-1.37421600	0.85593100	2.08251500
H	0.30370600	0.49787000	3.36276600
H	0.06503800	2.24277400	2.83470100
H	-1.73884600	-0.16410000	2.16277800
C	-2.38089900	1.83402700	1.52292200
H	-1.92843400	2.82842600	1.40429100
H	-2.70545800	1.51230600	0.52889300
N	-3.56637100	1.81733600	2.39127000
H	-3.32816000	2.23219700	3.28832900
C	-4.71481900	2.52512500	1.81816200
H	-4.45389800	3.52553000	1.42720300
H	-5.42860300	2.69013900	2.63623200
C	-5.39250200	1.73187100	0.71441800
C	-5.62675500	0.36121200	0.85694500
C	-5.83606700	2.35589000	-0.46032300
C	-6.29087800	-0.37379000	-0.12894000
H	-5.27069100	-0.13732300	1.75350300
C	-6.50215500	1.64286500	-1.45130500
H	-5.65694500	3.41930800	-0.60149500
C	-6.73767200	0.27069800	-1.28993700
H	-6.45864700	-1.43425400	0.02089100
H	-6.84763500	2.12527600	-2.36003700
O	-7.40205200	-0.34352600	-2.31583000
C	-7.69959800	-1.72276000	-2.18981300
H	-8.24228300	-1.99994900	-3.09518200
H	-6.78851100	-2.33229400	-2.11735600
H	-8.33115400	-1.92494100	-1.31484700

IM1$^{L1'}$

Sum of electronic and thermal Free Energies= -3346.296855

Rh	-0.0753	0.28139	0.46924
C	0.54435	3.56044	-0.21259
C	0.36534	3.63563	1.17113
C	1.04026	4.655	-0.92736
C	0.67168	4.8239	1.83835
H	0.00146	2.75995	1.70309
C	1.3376	5.8403	-0.25281
H	1.2008	4.57679	-1.99848
C	1.15394	5.92579	1.12868
H	0.5321	4.88605	2.91381
H	1.72256	6.69179	-0.80657
H	1.39478	6.84696	1.65207
P	2.09093	-0.52756	0.13401
P	-2.35066	-0.14827	0.05781
C	3.40868	0.56342	-0.60443
C	4.44846	1.09608	0.17383
C	3.31659	0.95579	-1.95226
C	5.36994	1.98747	-0.37972
H	4.54954	0.80667	1.21421
C	4.23988	1.84443	-2.50363
H	2.5269	0.55738	-2.58057
C	5.27079	2.36481	-1.71926
H	6.17134	2.3807	0.23982
H	4.153	2.12713	-3.54933
H	5.99086	3.0556	-2.14904
C	2.97311	-1.29189	1.57041
C	2.95538	-0.56913	2.77506
C	3.65413	-2.51551	1.5297
C	3.64237	-1.03569	3.89485
H	2.37868	0.34806	2.83786
C	4.32613	-2.99095	2.65836
H	3.65653	-3.11249	0.62502
C	4.33089	-2.24911	3.83931
H	3.61859	-0.46244	4.81716
H	4.84406	-3.94503	2.61117
H	4.85527	-2.62037	4.71547
C	-3.01044	0.51046	-1.54124
C	-3.03114	-0.25621	-2.71539
C	-3.40963	1.85909	-1.61548
C	-3.44597	0.30366	-3.92584
H	-2.73195	-1.29818	-2.68305
C	-3.828	2.41592	-2.82567
H	-3.42105	2.46898	-0.71567
C	-3.84534	1.63944	-3.98631
H	-3.46164	-0.30995	-4.8224
H	-4.14229	3.45542	-2.85884
H	-4.16983	2.07169	-4.92841
C	-3.71656	0.27381	1.23484
C	-5.06255	0.36693	0.83995
C	-3.382	0.52547	2.575
C	-6.05082	0.70558	1.76536
H	-5.3409	0.18025	-0.19276
C	-4.37475	0.8604	3.49784
H	-2.3467	0.43292	2.88824
C	-5.70836	0.95352	3.09657
H	-7.08702	0.77532	1.44549
H	-4.10216	1.04866	4.53263
H	-6.47828	1.2181	3.81616
C	2.02894	-1.87473	-1.16394
C	3.23556	-2.31641	-1.74166
C	0.8363	-2.4453	-1.66107
C	3.27341	-3.27887	-2.74756
H	4.16729	-1.87743	-1.40067
C	0.86631	-3.38	-2.70544
C	2.07868	-3.80757	-3.23699
H	4.22684	-3.59557	-3.15905
H	-0.07231	-3.7508	-3.10234
H	2.08607	-4.53577	-4.04295
C	-2.46678	-1.99437	-0.12567
C	-3.54336	-2.71745	0.40131
C	-1.38455	-2.72683	-0.66544
C	-3.55236	-4.11285	0.41616
H	-4.3785	-2.17994	0.83551
C	-1.36599	-4.12127	-0.61844
C	-2.45291	-4.80903	-0.07767
H	-4.40082	-4.64494	0.83456
H	-0.50753	-4.66781	-0.98761
H	-2.42887	-5.89453	-0.04382
O	-0.3777	-1.96732	-1.22169
Cl	-0.3068	-1.18962	2.37269
H	-1.04727	2.35139	-1.53152
S	0.19618	2.01548	-1.10559

TS1$^{Li'}$

Sum of electronic and thermal Free Energies= -3346.285353

Rh	0.17479	0.31451	-0.55462
C	-1.70439	3.2875	-0.08026
C	-2.21468	2.93329	-1.33097
C	-2.29673	4.32024	0.65601

C	-3.32267	3.61636	-1.84083
H	-1.74787	2.12587	-1.8887
C	-3.40422	4.99253	0.14142
H	-1.88962	4.59943	1.6209
C	-3.91962	4.64372	-1.10713
H	-3.71723	3.34128	-2.81363
H	-3.85819	5.79363	0.71635
H	-4.78163	5.16958	-1.50723
P	-1.87901	-0.8123	-0.09692
P	2.46872	0.28259	-0.11622
C	-3.29027	0.07559	0.71687
C	-4.56924	0.15151	0.14765
C	-3.05736	0.72434	1.94549
C	-5.59214	0.85333	0.79196
H	-4.77306	-0.34768	-0.79348
C	-4.08024	1.41937	2.58784
H	-2.07538	0.67778	2.40165
C	-5.35341	1.48618	2.01164
H	-6.58242	0.89931	0.33333
H	-3.88323	1.90898	3.5402
H	-6.15122	2.0274	2.51269
C	-2.71686	-1.77676	-1.43303
C	-2.74848	-1.20566	-2.7152
C	-3.33846	-3.01688	-1.22914
C	-3.41451	-1.84528	-3.76102
H	-2.22482	-0.27446	-2.89736
C	-3.99402	-3.66171	-2.27974
H	-3.30929	-3.48849	-0.25268
C	-4.03869	-3.07483	-3.54573
H	-3.42608	-1.39189	-4.74836
H	-4.46804	-4.62423	-2.10718
H	-4.54832	-3.5789	-4.36267
C	2.88454	1.02958	1.52249
C	2.99053	0.24702	2.68245
C	2.98552	2.42732	1.6446
C	3.19121	0.8431	3.92809
H	2.92619	-0.83369	2.61316
C	3.19216	3.02081	2.88994
H	2.91516	3.05693	0.76288
C	3.29127	2.23108	4.03661
H	3.27336	0.2196	4.814
H	3.27096	4.10181	2.96284
H	3.44756	2.69407	5.0067
C	3.7486	0.98473	-1.25101
C	4.98148	1.48626	-0.80078
C	3.46122	1.01016	-2.62568
C	5.90706	2.00628	-1.7076
H	5.21798	1.48042	0.25823
C	4.39476	1.52281	-3.52764
H	2.51474	0.60963	-2.97733
C	5.61587	2.0242	-3.07256
H	6.85444	2.39628	-1.34576
H	4.1639	1.53126	-4.58889
H	6.33729	2.42856	-3.77738
C	-1.51029	-2.07658	1.23653
C	-2.54061	-2.55516	2.06601
C	-0.20032	-2.54203	1.49747
C	-2.29799	-3.45211	3.10671
H	-3.55491	-2.20293	1.90433
C	0.0586	-3.41674	2.55979
C	-0.99312	-3.87479	3.35623
H	-3.12377	-3.80406	3.72585
H	1.07371	-3.72636	2.76739
H	-0.78429	-4.55454	4.17998
C	2.98208	-1.49585	0.0726
C	4.27883	-1.92211	-0.23932
C	2.04378	-2.47456	0.46881
C	4.6393	-3.26878	-0.17264
H	5.01466	-1.1915	-0.55773
C	2.38244	-3.8288	0.49691
C	3.68428	-4.21936	0.18227
H	5.6527	-3.571	-0.41861
H	1.62954	-4.56946	0.73822
H	3.94186	-5.27423	0.20501
O	0.78189	-2.00758	0.72407
Cl	0.62869	-1.15176	-2.43125
S	-0.25867	2.4775	0.62924
H	0.45866	2.38875	-0.55763

1$^{Li'}$

Sum of electronic and thermal Free Energies= -3346.307953

Rh	-0.40599	0.50868	-0.98511
H	-1.76904	0.56914	-1.71671
S	-0.90107	2.50272	0.12326
C	-2.50253	3.21213	-0.22571
C	-3.21929	2.99711	-1.41417
C	-3.0257	4.10591	0.72648
C	-4.43274	3.65048	-1.6342
H	-2.81732	2.3223	-2.16378

C	-4.23003	4.77185	0.49249
H	-2.47695	4.2815	1.64758
C	-4.94127	4.54399	-0.6874
H	-4.97454	3.47045	-2.55933
H	-4.611	5.4674	1.23526
H	-5.87837	5.06273	-0.87073
P	-1.42058	-1.2323	0.02967
P	2.03184	0.60724	-0.0659
C	-3.08732	-0.88245	0.74933
C	-4.12482	-1.82489	0.64854
C	-3.32266	0.31299	1.44495
C	-5.36727	-1.57051	1.2303
H	-3.96885	-2.7561	0.11722
C	-4.56522	0.56118	2.02727
H	-2.53613	1.05544	1.51618
C	-5.59176	-0.37829	1.91939
H	-6.16039	-2.3071	1.13916
H	-4.7323	1.49994	2.54653
H	-6.56272	-0.17947	2.36356
C	-1.73808	-2.69269	-1.04083
C	-2.28049	-2.49275	-2.31873
C	-1.52357	-3.99954	-0.58168
C	-2.61641	-3.58515	-3.11634
H	-2.41902	-1.48539	-2.69406
C	-1.85159	-5.09057	-1.38913
H	-1.10464	-4.17086	0.40417
C	-2.40076	-4.88541	-2.65517
H	-3.03221	-3.41775	-4.10531
H	-1.67675	-6.09927	-1.02605
H	-2.65496	-5.73505	-3.28273
C	2.41273	0.85346	1.73134
C	3.69926	0.64212	2.25634
C	1.39023	1.26621	2.59686
C	3.95447	0.84322	3.61226
H	4.50462	0.31529	1.60642
C	1.64806	1.46553	3.95521
H	0.39392	1.44155	2.20725
C	2.92762	1.25389	4.4661
H	4.95502	0.67778	4.00184
H	0.84395	1.78497	4.61147
H	3.12644	1.4077	5.52311
C	2.89237	2.01015	-0.90379
C	3.50593	3.05761	-0.20274
C	2.85674	2.05478	-2.30998
C	4.0861	4.12421	-0.89405
H	3.53174	3.0484	0.88129
C	3.44658	3.11739	-2.99278
H	2.36295	1.26025	-2.86341
C	4.06226	4.15495	-2.28791
H	4.5561	4.93036	-0.33766
H	3.41713	3.13714	-4.07849
H	4.51561	4.98454	-2.82313
C	-0.45972	-1.85992	1.47002
C	-0.96368	-1.86516	2.77885
C	0.86346	-2.29636	1.2663
C	-0.17006	-2.27458	3.85074
H	-1.98093	-1.53852	2.96126
C	1.66655	-2.70314	2.33212
C	1.1443	-2.6846	3.62493
H	-0.57784	-2.26866	4.85668
H	2.68323	-3.02938	2.14302
H	1.76887	-2.99827	4.45622
C	3.10843	-0.84026	-0.49018
C	4.42959	-0.69526	-0.94004
C	2.60051	-2.14634	-0.39036
C	5.21141	-1.80436	-1.26746
H	4.84407	0.30103	-1.05365
C	3.36449	-3.26073	-0.72903
C	4.67802	-3.08899	-1.16538
H	6.23036	-1.66044	-1.61404
H	2.91136	-4.2445	-0.66366
H	5.27563	-3.95547	-1.43246
O	1.27359	-2.35051	-0.0412
Cl	0.47865	-0.72879	-2.87994

R2

Sum of electronic and thermal Free Energies= -557.954989

C	-2.38649	1.34074	-0.38116
C	-1.08449	1.81375	-0.29197
C	-0.03486	0.98866	0.1461
C	-0.33289	-0.33516	0.46285
C	-1.63449	-0.83783	0.35344
C	-2.6725	0.00721	-0.04973
H	-3.20025	1.98241	-0.70846
H	-0.87961	2.85073	-0.55631
H	0.46383	-0.98075	0.81718
H	-1.82363	-1.87702	0.59683
O	-3.98782	-0.36282	-0.13848
C	-4.2912	-1.75153	-0.0968

H	-5.36985	-1.82755	-0.24164
H	-3.77446	-2.29266	-0.90226
H	-4.02839	-2.2073	0.86816
C	1.36146	1.57278	0.30483
H	1.33067	2.31764	1.11037
H	1.61808	2.13437	-0.61406
N	2.38435	0.59451	0.66631
H	3.13552	1.06501	1.16175
C	2.96178	-0.15425	-0.45277
H	3.37987	0.49533	-1.24437
H	2.15103	-0.73049	-0.92113
C	4.02235	-1.09352	0.05256
C	5.24741	-1.2113	-0.45899
H	3.73237	-1.6946	0.91281
H	5.97152	-1.91142	-0.05391
H	5.56889	-0.62	-1.31155

1^{L1}(R2)

Sum of electronic and thermal Free Energies= -2967.738747

P	0.50048100	1.50295000	-0.42079100
P	-2.05651900	-0.85222000	0.18864800
C	2.11614800	2.33490800	0.01749300
C	3.31743400	2.06439000	-0.65343300
C	2.15113900	3.21947900	1.11309800
C	4.51338200	2.66637000	-0.24906100
H	3.32481200	1.38211300	-1.49551300
C	3.34282200	3.82556200	1.51139200
H	1.23326700	3.44912700	1.64669000
C	4.53159400	3.54935700	0.82994400
H	5.43095700	2.44524900	-0.78717200
H	3.34105200	4.51521500	2.35091400
H	5.46076400	4.01971100	1.13838800
C	0.86982200	0.86948800	-2.12587200
C	0.68022500	1.61538100	-3.29768500
C	1.42811200	-0.41529300	-2.22293000
C	1.03853800	1.08484800	-4.53871300
H	0.24870900	2.60949200	-3.24679100
C	1.80430000	-0.93701600	-3.46200900
H	1.57290700	-1.00127400	-1.32018300
C	1.60520500	-0.18815900	-4.62381200
H	0.87656400	1.67024700	-5.43969900
H	2.25141100	-1.92602300	-3.51226900
H	1.88723300	-0.59501800	-5.59105100
C	-3.62034300	-0.48737400	1.11580400
C	-4.87756700	-0.71204200	0.53149200
C	-3.55833600	0.04735200	2.40938000
C	-6.04810200	-0.41529000	1.23007400
H	-4.94549900	-1.11501800	-0.47456400
C	-4.73141700	0.34743000	3.10473600
H	-2.58925800	0.20877000	2.86700500
C	-5.97685900	0.11740600	2.51898200
H	-7.01367800	-0.59637400	0.76565400
H	-4.66874800	0.75990400	4.10792100
H	-6.88818300	0.35210900	3.06241400
C	-2.03219100	-2.69554400	0.01697000
C	-2.97709800	-3.53282200	0.62250900
C	-0.99817500	-3.27757600	-0.73478600
C	-2.89666300	-4.91906900	0.47053400
H	-3.77034600	-3.10838600	1.22673600
C	-0.92697700	-4.66102000	-0.89673300
H	-0.24504300	-2.64441500	-1.19317300
C	-1.87665200	-5.48756200	-0.29159100
H	-3.63344800	-5.55372400	0.95506700
H	-0.12713500	-5.09371900	-1.49194900
H	-1.81740800	-6.56591300	-0.40975400
C	-0.51121000	3.05345400	-0.76589100
C	0.09294800	4.30762700	-0.97793600
C	-1.91741600	3.03152900	-0.77241300
C	-0.65699600	5.47549200	-1.12245800
H	1.17274200	4.37989300	-1.01905800
C	-2.67942900	4.19617000	-0.87845100
C	-2.04863100	5.42634800	-1.04831600
H	-0.14860500	6.42191200	-1.28087700
H	-3.76022300	4.11072200	-0.83243500
H	-2.63987100	6.33311200	-1.13500600
C	-2.56611300	-0.34536300	-1.52291400
C	-2.78070600	-1.21258000	-2.60256000
C	-2.72879600	1.02758900	-1.74960500
C	-3.11905600	-0.71998800	-3.86507700
H	-2.67329400	-2.28128200	-2.45848800
C	-3.06363000	1.53816000	-3.00268300
C	-3.25395600	0.65346300	-4.06470600
H	-3.27468400	-1.41063400	-4.68835000
H	-3.17746000	2.60783600	-3.14024200
H	-3.51541600	1.04216400	-5.04476200
O	-2.59271200	1.83655500	-0.63156100
Rh	-0.09101300	-0.08829600	1.13719800
Cl	-0.64394300	-1.72731200	2.89510900
C	2.73781300	1.02431000	5.76284700

C	2.54544300	1.36742300	4.48852000
H	3.57143900	1.41245100	6.34137100
H	2.06023500	0.34612800	6.27636200
H	3.24656900	2.05030500	4.00532300
C	1.38215200	0.90536900	3.64787000
H	0.74666000	0.20687000	4.19617900
H	0.75748400	1.76254400	3.37322000
N	1.76386600	0.23376800	2.36749400
H	2.35717600	0.87723900	1.84673200
C	2.57436900	-0.99930700	2.62606600
H	1.92326300	-1.68644700	3.16795700
H	3.41661500	-0.73719400	3.27954300
C	3.09284200	-1.64986000	1.36680600
C	4.29646000	-1.24220400	0.78652200
C	2.39483500	-2.71216900	0.76573000
C	4.79599300	-1.84352700	-0.37418200
H	4.86792300	-0.43818100	1.24505600
C	2.88332400	-3.32966900	-0.37933400
H	1.45943100	-3.04512100	1.20505900
C	4.08080300	-2.89072200	-0.96450800
H	5.73262100	-1.49729300	-0.79507800
H	2.35341800	-4.15750200	-0.83946000
O	4.45873900	-3.54593200	-2.10556100
C	5.68563800	-3.17645100	-2.71306400
H	5.80008900	-3.82485200	-3.58338200
H	5.67702800	-2.12923100	-3.04305400
H	6.53571800	-3.32997500	-2.03566600

1^{L1}(R2)'

Sum of electronic and thermal Free Energies=-2967.731597

P	0.50048100	1.50295000	-0.42079100
P	-2.05651900	-0.85222000	0.18864800
C	2.11614800	2.33490800	0.01749300
C	3.31743400	2.06439000	-0.65343300
C	2.15113900	3.21947900	1.11309800
C	4.51338200	2.66637000	-0.24906100
H	3.32481200	1.38211300	-1.49551300
C	3.34282200	3.82556200	1.51139200
H	1.23326700	3.44912700	1.64669000
C	4.53159400	3.54935700	0.82994400
H	5.43095700	2.44524900	-0.78717200
H	3.34105200	4.51521500	2.35091400
H	5.46076400	4.01971100	1.13838800
C	0.86982200	0.86948800	-2.12587200
C	0.68022500	1.61538100	-3.29768500
C	1.42811200	-0.41529300	-2.22293000
C	1.03853800	1.08484800	-4.53871300
H	0.24870900	2.60949200	-3.24679100
C	1.80430000	-0.93701600	-3.46200900
H	1.57290700	-1.00127400	-1.32018300
C	1.60520500	-0.18815900	-4.62381200
H	0.87656400	1.67024700	-5.43969900
H	2.25141100	-1.92602300	-3.51226900
H	1.88723300	-0.59501800	-5.59105100
C	-3.62034300	-0.48737400	1.11580400
C	-4.87756700	-0.71204200	0.53149200
C	-3.55833600	0.04735200	2.40938000
C	-6.04810200	-0.41529000	1.23007400
H	-4.94549900	-1.11501800	-0.47456400
C	-4.73141700	0.34743000	3.10473600
H	-2.58925800	0.20877000	2.86700500
C	-5.97685900	0.11740600	2.51898200
H	-7.01367800	-0.59637400	0.76565400
H	-4.66874800	0.75990400	4.10792100
H	-6.88818300	0.35210900	3.06241400
C	-2.03219100	-2.69554400	0.01697000
C	-2.97709800	-3.53282200	0.62250900
C	-0.99817500	-3.27757600	-0.73478600
C	-2.89666300	-4.91906900	0.47053400
H	-3.77034600	-3.10838600	1.22673600
C	-0.92697700	-4.66102000	-0.89673300
H	-0.24504300	-2.64441500	-1.19317300
C	-1.87665200	-5.48756200	-0.29159100
H	-3.63344800	-5.55372400	0.95506700
H	-0.12713500	-5.09371900	-1.49194900
H	-1.81740800	-6.56591300	-0.40975400
C	-0.51121000	3.05345400	-0.76589100
C	0.09294800	4.30762700	-0.97793600
C	-1.91741600	3.03152900	-0.77241300
C	-0.65699600	5.47549200	-1.12245800
H	1.17274200	4.37989300	-1.01905800
C	-2.67942900	4.19617000	-0.87845100
C	-2.04863100	5.42634800	-1.04831600
H	-0.14860500	6.42191200	-1.28087700
H	-3.76022300	4.11072200	-0.83243500
H	-2.63987100	6.33311200	-1.13500600
C	-2.56611300	-0.34536300	-1.52291400
C	-2.78070600	-1.21258000	-2.60256000
C	-2.72879600	1.02758900	-1.74960500

C	-3.11905600	-0.71998800	-3.86507700	H	-6.16583600	-1.75714900	-1.82166100
H	-2.67329400	-2.28128200	-2.45848800	C	-5.11921100	-5.26309400	-0.54529400
C	-3.06363000	1.53816000	-3.00268300	H	-3.09112000	-4.60253800	-0.87454600
C	-3.25395600	0.65346300	-4.06470600	C	-6.47186100	-4.92169600	-0.60347400
H	-3.27468400	-1.41063400	-4.68835000	H	-7.89810200	-3.38238400	-1.10609400
H	-3.17746000	2.60783600	-3.14024200	H	-4.82004900	-6.24318700	-0.18418800
H	-3.51541600	1.04216400	-5.04476200	H	-7.22894000	-5.63687700	-0.29408000
O	-2.59271200	1.83655500	-0.63156100	P	4.07051100	-0.41231800	0.48915400
Rh	-0.09101300	-0.08829600	1.13719800	P	-0.92508700	0.29494700	1.48281900
Cl	-0.64394300	-1.72731200	2.89510900	C	5.92383100	-0.53225900	0.50038700
C	2.73781300	1.02431000	5.76284700	C	6.66813800	-1.53117700	-0.14586800
C	2.54544300	1.36742300	4.48852000	C	6.61157100	0.42579500	1.26582400
H	3.57143900	1.41245100	6.34137100	C	8.06099000	-1.56197600	-0.03943300
H	2.06023500	0.34612800	6.27636200	H	6.15877600	-2.28978600	-0.73151800
H	3.24656900	2.05030500	4.00532300	C	8.00242000	0.40277700	1.36194500
C	1.38215200	0.90536900	3.64787000	H	6.04959600	1.19166600	1.79516800
H	0.74666000	0.20687000	4.19617900	C	8.73165100	-0.59424100	0.70960000
H	0.75748400	1.76254400	3.37322000	H	8.62137800	-2.34443000	-0.54399000
N	1.76386600	0.23376800	2.36749400	H	8.51602500	1.15457400	1.95486100
H	2.35717600	0.87723900	1.84673200	H	9.81456700	-0.62069800	0.79156300
C	2.57436900	-0.99930700	2.62606600	C	3.57876700	-2.02783500	-0.27786500
H	1.92326300	-1.68644700	3.16795700	C	3.46285500	-2.26064300	-1.65756300
H	3.41661500	-0.73719400	3.27954300	C	3.29978000	-3.08439800	0.60546000
C	3.09284200	-1.64986000	1.36680600	C	3.07916500	-3.51469900	-2.13947800
C	4.29646000	-1.24220400	0.78652200	H	3.66678700	-1.46241900	-2.36372000
C	2.39483500	-2.71216900	0.76573000	C	2.92918500	-4.34029500	0.12375400
C	4.79599300	-1.84352700	-0.37418200	H	3.35616400	-2.91528400	1.67650300
H	4.86792300	-0.43818100	1.24505600	C	2.81395300	-4.55791700	-1.25072200
C	2.88332400	-3.32966900	-0.37933400	H	2.98456100	-3.67147000	-3.21036300
H	1.45943100	-3.04512100	1.20505900	H	2.71594700	-5.14441400	0.82224900
C	4.08080300	-2.89072200	-0.96450800	H	2.51246700	-5.53158200	-1.62606100
H	5.73262100	-1.49729300	-0.79507800	C	0.38169400	-0.41297700	2.60053100
H	2.35341800	-4.15750200	-0.83946000	C	1.22338600	0.40673200	3.37244900
O	4.45873900	-3.54593200	-2.10556100	C	0.47753200	-1.80506100	2.74625300
C	5.68563800	-3.17645100	-2.71306400	C	2.13097300	-0.15149600	4.27314300
H	5.80008900	-3.82485200	-3.58338200	H	1.17210500	1.48600200	3.27923300
H	5.67702800	-2.12923100	-3.04305400	C	1.38119200	-2.35832000	3.65615300
H	6.53571800	-3.32997500	-2.03566600	H	-0.18149100	-2.44919400	2.17496800
TS1^{L1}(R2)				C	2.21034900	-1.53700800	4.42113000
Sum of electronic and thermal Free Energies= -3598.048738				H	2.77317200	0.49900300	4.86029300
C	-4.51739400	-3.07961600	-1.39997400	H	1.42845500	-3.43812400	3.76842600
C	-5.87583900	-2.73798700	-1.45725600	H	2.91125600	-1.97147400	5.12868800
C	-4.14248400	-4.34807800	-0.93777100	C	-2.32383500	0.62774600	2.65731500
C	-6.84758200	-3.65626300	-1.05856800	C	-2.13526800	0.73186000	4.04281500

C	-3.61542700	0.79431700	2.13659100
C	-3.21473300	1.00322500	4.88577800
H	-1.14938600	0.59260600	4.47172500
C	-4.69030600	1.07735700	2.97839900
H	-3.77321800	0.67629200	1.07061800
C	-4.49326600	1.18086000	4.35664600
H	-3.05351200	1.06971000	5.95816800
H	-5.68477500	1.19842200	2.55833400
H	-5.33258300	1.38877300	5.01443000
C	3.80842900	0.77145200	-0.92358500
C	4.77461700	1.00955200	-1.91811300
C	2.60844300	1.49880200	-1.00643500
C	4.56178400	1.92106700	-2.95048000
H	5.71465700	0.47007800	-1.87022200
C	2.37713200	2.40635100	-2.04713900
C	3.35558000	2.62052800	-3.01525600
H	5.33144300	2.08248900	-3.69921900
H	1.43878200	2.94813000	-2.08081500
H	3.17125500	3.32963300	-3.81704000
C	-0.24995000	2.02557100	1.23176400
C	-0.90643200	3.11982900	1.81961500
C	0.97287500	2.29421600	0.57785500
C	-0.36517400	4.40501100	1.81988800
H	-1.85720200	2.95618000	2.31001100
C	1.55508000	3.56444400	0.63105900
C	0.88589300	4.61872900	1.24919500
H	-0.90910700	5.21863700	2.28941600
H	2.52771600	3.72888100	0.18457700
H	1.35115400	5.59982900	1.28039000
O	1.60331200	1.23871100	-0.07390000
Rh	-1.73473100	-1.02067400	-0.29257000
Cl	-2.56215200	-2.51679300	1.37540900
C	0.86484000	-0.96443300	-5.02729200
C	0.90501500	-0.51106800	-3.77288700
H	1.56081500	-0.61296500	-5.78377500
H	0.13923500	-1.71157700	-5.34086300
H	1.64682200	0.23693000	-3.49693200
C	0.00531700	-1.00993400	-2.67137100
H	-0.70669400	-1.74017800	-3.06193300
H	0.60356400	-1.51447500	-1.90476700
N	-0.78411700	0.04869500	-1.95379200
H	-0.11830800	0.68222200	-1.51307100
C	-1.62835100	0.85227200	-2.90278100
H	-2.47413900	0.22296300	-3.19009900
H	-1.04112800	1.04095700	-3.80882500
C	-2.10267700	2.16819700	-2.33914600
C	-1.39312700	3.34452200	-2.59729400
C	-3.28431700	2.26990800	-1.58514800
C	-1.80660200	4.58309100	-2.09859800
H	-0.50608200	3.30357500	-3.22554700
C	-3.71390500	3.49047700	-1.08287100
H	-3.87401200	1.37820500	-1.39941100
C	-2.97059300	4.65597900	-1.32576400
H	-1.22729900	5.47022700	-2.32440900
H	-4.62569500	3.57084100	-0.50017000
O	-3.47129000	5.80253200	-0.78246100
C	-2.74965600	7.00780000	-0.97773000
H	-3.30871100	7.78318200	-0.45157400
H	-1.73713500	6.94365600	-0.55853400
H	-2.68153400	7.27315000	-2.04082800
S	-3.29675500	-1.93730400	-2.03672200
H	-3.24845500	-0.75018100	-0.85667300

$TS1^{L1}$(R2)'

Sum of electronic and thermal Free Energies=-3598.044603

C	-4.51739400	-3.07961600	-1.39997400
C	-5.87583900	-2.73798700	-1.45725600
C	-4.14248400	-4.34807800	-0.93777100
C	-6.84758200	-3.65626300	-1.05856800
H	-6.16583600	-1.75714900	-1.82166100
C	-5.11921100	-5.26309400	-0.54529400
H	-3.09112000	-4.60253800	-0.87454600
C	-6.47186100	-4.92169600	-0.60347400
H	-7.89810200	-3.38238400	-1.10609400
H	-4.82004900	-6.24318700	-0.18418800
H	-7.22894000	-5.63687700	-0.29408000
P	4.07051100	-0.41231800	0.48915400
P	-0.92508700	0.29494700	1.48281900
C	5.92383100	-0.53225900	0.50038700
C	6.66813800	-1.53117700	-0.14586800
C	6.61157100	0.42579500	1.26582400
C	8.06099000	-1.56197600	-0.03943300
H	6.15877600	-2.28978600	-0.73151800
C	8.00242000	0.40277700	1.36194500
H	6.04959600	1.19166600	1.79516800
C	8.73165100	-0.59424100	0.70960000
H	8.62137800	-2.34443000	-0.54399000
H	8.51602500	1.15457400	1.95486100
H	9.81456700	-0.62069800	0.79156300

C	3.57876700	-2.02783500	-0.27786500
C	3.46285500	-2.26064300	-1.65756300
C	3.29978000	-3.08439800	0.60546000
C	3.07916500	-3.51469900	-2.13947800
H	3.66678700	-1.46241900	-2.36372000
C	2.92918500	-4.34029500	0.12375400
H	3.35616400	-2.91528400	1.67650300
C	2.81395300	-4.55791700	-1.25072200
H	2.98456100	-3.67147000	-3.21036300
H	2.71594700	-5.14441400	0.82224900
H	2.51246700	-5.53158200	-1.62606100
C	0.38169400	-0.41297700	2.60053100
C	1.22338600	0.40673200	3.37244900
C	0.47753200	-1.80506100	2.74625300
C	2.13097300	-0.15149600	4.27314300
H	1.17210500	1.48600200	3.27923300
C	1.38119200	-2.35832000	3.65615300
H	-0.18149100	-2.44919400	2.17496800
C	2.21034900	-1.53700800	4.42113000
H	2.77317200	0.49900300	4.86029300
H	1.42845500	-3.43812400	3.76842600
H	2.91125600	-1.97147400	5.12868800
C	-2.32383500	0.62774600	2.65731500
C	-2.13526800	0.73186000	4.04281500
C	-3.61542700	0.79431700	2.13659100
C	-3.21473300	1.00322500	4.88577800
H	-1.14938600	0.59260600	4.47172500
C	-4.69030600	1.07735700	2.97839900
H	-3.77321800	0.67629200	1.07061800
C	-4.49326600	1.18086000	4.35664600
H	-3.05351200	1.06971000	5.95816800
H	-5.68477500	1.19842200	2.55833400
H	-5.33258300	1.38877300	5.01443000
C	3.80842900	0.77145200	-0.92358500
C	4.77461700	1.00955200	-1.91811300
C	2.60844300	1.49880200	-1.00643500
C	4.56178400	1.92106700	-2.95048000
H	5.71465700	0.47007800	-1.87022200
C	2.37713200	2.40635100	-2.04713900
C	3.35558000	2.62052800	-3.01525600
H	5.33144300	2.08248900	-3.69921900
H	1.43878200	2.94813000	-2.08081500
H	3.17125500	3.32963300	-3.81704000
C	-0.24995000	2.02557100	1.23176400
C	-0.90643200	3.11982900	1.81961500
C	0.97287500	2.29421600	0.57785500
C	-0.36517400	4.40501100	1.81988800
H	-1.85720200	2.95618000	2.31001100
C	1.55508000	3.56444400	0.63105900
C	0.88589300	4.61872900	1.24919500
H	-0.90910700	5.21863700	2.28941600
H	2.52771600	3.72888100	0.18457700
H	1.35115400	5.59982900	1.28039000
O	1.60331200	1.23871100	-0.07390000
Rh	-1.73473100	-1.02067400	-0.29257000
Cl	-2.56215200	-2.51679300	1.37540900
C	0.86484000	-0.96443300	-5.02729200
C	0.90501500	-0.51106800	-3.77288700
H	1.56081500	-0.61296500	-5.78377500
H	0.13923500	-1.71157700	-5.34086300
H	1.64682200	0.23693000	-3.49693200
C	0.00531700	-1.00993400	-2.67137100
H	-0.70669400	-1.74017800	-3.06193300
H	0.60356400	-1.51447500	-1.90476700
N	-0.78411700	0.04869500	-1.95379200
H	-0.11830800	0.68222200	-1.51307100
C	-1.62835100	0.85227200	-2.90278100
H	-2.47413900	0.22296300	-3.19009900
H	-1.04112800	1.04095700	-3.80882500
C	-2.10267700	2.16819700	-2.33914600
C	-1.39312700	3.34452200	-2.59729400
C	-3.28431700	2.26990800	-1.58514800
C	-1.80660200	4.58309100	-2.09859800
H	-0.50608200	3.30357500	-3.22554700
C	-3.71390500	3.49047700	-1.08287100
H	-3.87401200	1.37820500	-1.39941100
C	-2.97059300	4.65597900	-1.32576400
H	-1.22729900	5.47022700	-2.32440900
H	-4.62569500	3.57084100	-0.50017000
O	-3.47129000	5.80253200	-0.78246100
C	-2.74965600	7.00780000	-0.97773000
H	-3.30871100	7.78318200	-0.45157400
H	-1.73713500	6.94365600	-0.55853400
H	-2.68153400	7.27315000	-2.04082800
S	-3.29675500	-1.93730400	-2.03672200
H	-3.24845500	-0.75018100	-0.85667300

3^{L1}(R2)

Sum of electronic and thermal Free Energies= -3904.230599

C	-4.01071800	-3.50077300	-1.20621700	H	1.05532500	-3.40589400	3.90344400
C	-5.34929500	-3.12486600	-1.01731700	H	2.73628900	-2.08243200	5.17959900
C	-3.63894700	-4.82974700	-0.95241600	C	-2.26307700	0.93261300	2.65515100
C	-6.29227100	-4.05634100	-0.58478800	C	-2.16804800	0.77960000	4.04405900
H	-5.64279800	-2.09778200	-1.20919300	C	-3.45032700	1.44593600	2.10904800
C	-4.58586600	-5.76133100	-0.52658200	C	-3.24011600	1.12720100	4.86926300
H	-2.60369500	-5.12450900	-1.09231100	H	-1.26311500	0.38033100	4.48739800
C	-5.91566900	-5.37893100	-0.34021800	C	-4.51350700	1.80451500	2.93556600
H	-7.32450800	-3.74829700	-0.43949500	H	-3.54865300	1.56282600	1.03446900
H	-4.28220000	-6.78743600	-0.33544600	C	-4.41355900	1.64131700	4.31929900
H	-6.65215600	-6.10455700	-0.00601200	H	-3.15474800	0.99037200	5.94360800
P	4.19112500	-0.13025800	0.46662700	H	-5.42500300	2.19905000	2.49582100
P	-0.86990400	0.49523600	1.51396600	H	-5.24744700	1.90856900	4.96220600
C	6.04448500	-0.21964800	0.41080300	C	3.84316900	0.91122600	-1.03594500
C	6.77969000	-1.27150100	-0.15708600	C	4.78203400	1.13326100	-2.05990700
C	6.74513400	0.82306000	1.04228500	C	2.60740700	1.56949100	-1.14640400
C	8.17594700	-1.27260200	-0.10503700	C	4.50991200	1.97288400	-3.13873100
H	6.26134300	-2.09490800	-0.63791700	H	5.74802900	0.64373000	-1.99625800
C	8.13886000	0.82875800	1.08269900	C	2.32042000	2.41021200	-2.22676800
H	6.19178200	1.63322800	1.51144400	C	3.27377500	2.61644700	-3.22158600
C	8.85880100	-0.22229400	0.50963300	H	5.25956000	2.12472700	-3.90944300
H	8.72934100	-2.09678500	-0.54686700	H	1.35943700	2.91147700	-2.26749600
H	8.66231200	1.64581300	1.57146600	H	3.04762700	3.27328100	-4.05623900
H	9.94436800	-0.22587400	0.54944500	C	-0.08515500	2.18349700	1.27029500
C	3.69404000	-1.81788800	-0.11316300	C	-0.61608800	3.29886400	1.94279300
C	3.56666600	-2.19671400	-1.45945300	C	1.09270200	2.39928100	0.52151200
C	3.42351600	-2.77170700	0.88191100	C	-0.01039000	4.55406800	1.91056300
C	3.18245100	-3.49570400	-1.80002800	H	-1.52165800	3.17705800	2.52190200
H	3.75656500	-1.47636500	-2.24871700	C	1.73663100	3.64152800	0.52765800
C	3.05161300	-4.07267200	0.54079000	C	1.18392000	4.71843000	1.21638400
H	3.48673900	-2.48839800	1.92823300	H	-0.46046400	5.38349400	2.44713100
C	2.92751400	-4.43740600	-0.80122400	H	2.66866200	3.76491700	-0.00888100
H	3.07700900	-3.76666700	-2.84670000	H	1.69541900	5.67655300	1.20768200
H	2.84369300	-4.79647300	1.32354900	O	1.62028200	1.32584400	-0.18744600
H	2.62474600	-5.44604400	-1.06706900	Rh	-1.79826300	-0.93352000	-0.26133900
C	0.36205600	-0.31759200	2.63915400	Cl	-2.86155800	-2.10883000	1.51194600
C	1.31439400	0.42046600	3.36120400	C	1.03853400	-1.29027400	-4.86704600
C	0.28883900	-1.70620200	2.83709100	C	1.01010200	-0.63707700	-3.70363200
C	2.16787500	-0.21336200	4.26525300	H	1.68601200	-0.97722000	-5.68127700
H	1.39105100	1.49347800	3.22644200	H	0.41779700	-2.16549500	-5.04423200
C	1.13788600	-2.33347500	3.75056100	H	1.64591000	0.23520100	-3.56370700
H	-0.46060600	-2.28604100	2.30960200	C	0.17418200	-1.07310200	-2.52802800
C	2.07893200	-1.59178200	4.46691000	H	-0.42347200	-1.94681800	-2.79491300
H	2.89930500	0.37349400	4.81346300	H	0.82420400	-1.36153900	-1.69424000

N	-0.76751600	-0.03955800	-1.97731700
H	-0.20304000	0.70609200	-1.57198700
C	-1.63860300	0.55929700	-3.04445700
H	-2.31164400	-0.23314400	-3.37892300
H	-1.00012500	0.83687700	-3.89168200
C	-2.42126600	1.76195500	-2.58058000
C	-1.82808900	3.02532300	-2.51477000
C	-3.77917800	1.65569300	-2.23154800
C	-2.53452100	4.15260700	-2.08677900
H	-0.79290600	3.14820400	-2.82548400
C	-4.50164300	2.76598300	-1.81275600
H	-4.26694400	0.68753300	-2.29292200
C	-3.88110800	4.02228100	-1.72736600
H	-2.03467400	5.11303300	-2.04810800
H	-5.55162500	2.68803000	-1.54980000
O	-4.67238600	5.04716200	-1.29886700
C	-4.09547500	6.33774000	-1.18141300
H	-4.88879800	6.99048000	-0.81399500
H	-3.26189400	6.34487800	-0.46719100
H	-3.74031100	6.71347200	-2.14988200
S	-2.82333300	-2.35524600	-1.88462400
H	-2.90869800	0.06384700	-0.37837100

TS1^{L1}(cod)

Sum of electronic and thermal Free Energies= -3658.146734

Rh	0.46847	0.23065	-0.66573
C	3.46879	-1.96527	0.90413
C	4.85135	-2.21964	0.85783
C	2.75997	-2.36767	2.04561
C	5.49457	-2.86412	1.91353
H	5.41698	-1.91259	-0.01601
C	3.4136	-2.99678	3.10781
H	1.6923	-2.20853	2.09812
C	4.78202	-3.25352	3.04926
H	6.5613	-3.05607	1.84809
H	2.84084	-3.29817	3.97968
H	5.286	-3.75408	3.86759
P	-0.86293	1.75406	0.58196
P	-0.88643	-1.69003	-0.46177
C	0.07637	2.63228	1.92962
C	0.30938	4.01631	1.9403
C	0.64862	1.86079	2.95549
C	1.07098	4.60802	2.95173
H	-0.09572	4.64347	1.1557
C	1.39312	2.45241	3.97456
H	0.5194	0.78495	2.95761
C	1.60736	3.83239	3.977
H	1.24059	5.68068	2.93279
H	1.81718	1.8319	4.75797
H	2.19498	4.29416	4.76466
C	-1.6156	3.12108	-0.42731
C	-1.55419	3.06777	-1.82594
C	-2.34526	4.15698	0.18327
C	-2.16657	4.0606	-2.5967
H	-1.07767	2.22388	-2.31582
C	-2.94968	5.14792	-0.58884
H	-2.45199	4.18595	1.2635
C	-2.85311	5.10677	-1.98291
H	-2.11438	4.00057	-3.68025
H	-3.50382	5.94574	-0.1024
H	-3.32714	5.87775	-2.58424
C	-1.49631	-2.21111	1.21242
C	-2.55303	-3.12898	1.34598
C	-0.85393	-1.75643	2.36874
C	-2.94364	-3.58135	2.60576
H	-3.06964	-3.49445	0.46474
C	-1.24136	-2.21019	3.63114
H	-0.04473	-1.04201	2.26809
C	-2.28762	-3.12552	3.75192
H	-3.76181	-4.2918	2.69127
H	-0.7283	-1.84446	4.51621
H	-2.59315	-3.48018	4.7321
C	0.00721	-3.20744	-1.03771
C	0.24731	-4.28656	-0.17546
C	0.47765	-3.27271	-2.36128
C	0.93614	-5.4138	-0.62967
H	-0.09155	-4.25962	0.85313
C	1.15138	-4.40663	-2.80977
H	0.32598	-2.42723	-3.02397
C	1.38531	-5.47982	-1.9471
H	1.12	-6.23744	0.0539
H	1.50691	-4.44335	-3.83558
H	1.91978	-6.35797	-2.29881
C	-2.38472	1.1979	1.48033
C	-2.65961	1.41131	2.83679
C	-3.34977	0.53062	0.70819
C	-3.84846	0.94888	3.40634
H	-1.94006	1.93524	3.45593
C	-4.53685	0.0568	1.26285

C	-4.77833	0.26632	2.62164
H	-4.04351	1.12066	4.46089
H	-5.25599	-0.46318	0.63915
H	-5.70165	-0.09913	3.06227
C	-2.46272	-1.73968	-1.44276
C	-2.80009	-2.83263	-2.25485
C	-3.3775	-0.67661	-1.37893
C	-3.99129	-2.85225	-2.98304
H	-2.11782	-3.6709	-2.33199
C	-4.55656	-0.6724	-2.12029
C	-4.86688	-1.76857	-2.9255
H	-4.22215	-3.711	-3.60628
H	-5.2049	0.19667	-2.0678
H	-5.78456	-1.76994	-3.50641
O	-3.05462	0.44471	-0.63613
C	5.23414	2.528	-2.55108
C	5.40062	2.87599	-1.26828
H	6.12756	2.22256	-3.09378
C	3.94785	2.4733	-3.34718
H	4.1967	2.30827	-4.40015
H	3.43945	3.44663	-3.30858
C	4.34963	3.31588	-0.26835
H	4.86263	3.65115	0.63996
H	3.80607	4.19484	-0.64704
H	6.41531	2.82291	-0.87535
C	3.32286	2.20622	0.12926
H	3.78	1.22811	0.0038
H	3.0686	2.31373	1.18367
C	2.95376	1.35407	-2.88911
H	2.45031	0.91739	-3.75447
H	3.50842	0.55481	-2.39223
C	2.05985	2.31108	-0.68563
C	1.90222	1.939	-1.98798
H	1.32413	3.00856	-0.30119
H	1.02568	2.30979	-2.49913
Cl	-0.23513	-0.00525	-3.19619
S	2.75079	-1.22031	-0.55135
H	1.59032	-0.29505	0.39621

1^{L1}(cod)

Sum of electronic and thermal Free Energies= -3658.168957

Rh	0.40162	0.45141	-0.3347
H	0.6814	0.49755	1.18743
S	2.74304	0.32246	-0.9373
C	3.90871	0.11645	0.34153
C	3.58944	0.01359	1.71487
C	5.27057	0.06874	-0.05424
C	4.59965	-0.12347	2.65733
H	2.54987	0.05932	2.01649
C	6.272	-0.07146	0.8977
H	5.51972	0.14757	-1.10762
C	5.94156	-0.16739	2.25461
H	4.34844	-0.19506	3.71117
H	7.31133	-0.10341	0.58652
H	6.72627	-0.27353	2.99729
P	-1.89842	0.95355	0.38617
P	0.26777	-1.9499	-0.24827
C	-1.81816	2.19032	1.75877
C	-2.28077	3.50601	1.60351
C	-1.21645	1.8281	2.97886
C	-2.153	4.4314	2.64376
H	-2.74692	3.81528	0.67539
C	-1.10144	2.74944	4.01795
H	-0.84286	0.81906	3.12021
C	-1.56775	4.05703	3.85194
H	-2.51651	5.44491	2.50404
H	-0.64728	2.44825	4.95734
H	-1.47405	4.77591	4.66011
C	-3.08035	1.6976	-0.825
C	-2.74008	1.90463	-2.16747
C	-4.37685	2.02404	-0.38366
C	-3.67524	2.45662	-3.04794
H	-1.76868	1.59625	-2.53814
C	-5.3018	2.57585	-1.26703
H	-4.66816	1.84697	0.64701
C	-4.95058	2.79825	-2.60171
H	-3.40172	2.60597	-4.0881
H	-6.29751	2.82705	-0.91403
H	-5.67395	3.22598	-3.28951
C	-0.14563	-2.69465	1.38973
C	-0.66778	-3.99707	1.46329
C	0.14833	-2.01713	2.58135
C	-0.88737	-4.60114	2.70131
H	-0.90194	-4.54366	0.55642
C	-0.06883	-2.62464	3.81871
H	0.54613	-1.00916	2.53773
C	-0.58858	-3.91825	3.8814
H	-1.29231	-5.60778	2.74111
H	0.1646	-2.08578	4.73226

H	-0.76087	-4.39091	4.84356
C	1.92294	-2.67168	-0.63718
C	2.66355	-3.37531	0.32038
C	2.46004	-2.49134	-1.93007
C	3.91922	-3.89573	-0.00637
H	2.26935	-3.52879	1.31821
C	3.70971	-3.02697	-2.25009
H	1.89205	-1.95081	-2.6817
C	4.4423	-3.72678	-1.29004
H	4.48276	-4.44137	0.74444
H	4.10511	-2.89419	-3.25252
H	5.41315	-4.14322	-1.54108
C	-2.92308	-0.39605	1.10438
C	-3.51125	-0.40316	2.37581
C	-3.17864	-1.4734	0.24534
C	-4.30877	-1.47624	2.77761
H	-3.35145	0.42709	3.05358
C	-3.96909	-2.55222	0.6319
C	-4.52947	-2.5471	1.91016
H	-4.75937	-1.47136	3.76477
H	-4.14744	-3.37232	-0.0544
H	-5.15149	-3.38051	2.22205
C	-0.82142	-2.84877	-1.44803
C	-0.36328	-3.97531	-2.15308
C	-2.14286	-2.43837	-1.68168
C	-1.18315	-4.63653	-3.06835
H	0.64357	-4.34083	-1.99642
C	-2.95979	-3.0715	-2.61366
C	-2.47664	-4.17715	-3.31231
H	-0.80043	-5.50267	-3.59841
H	-3.95862	-2.68348	-2.78268
H	-3.10913	-4.67532	-4.0402
O	-2.62919	-1.33221	-1.01321
C	2.16891	5.21457	-1.89292
C	2.70065	5.2401	-0.66469
H	2.76596	5.65449	-2.69022
C	0.83522	4.64603	-2.33382
H	0.68319	4.9043	-3.38577
H	0.01654	5.13428	-1.78617
C	2.11451	4.69415	0.62144
H	2.75831	4.99406	1.45347
H	1.13464	5.149	0.82107
H	3.6839	5.69694	-0.56461
C	1.97595	3.13383	0.64569
H	2.68721	2.71494	-0.06832
H	2.24528	2.75447	1.63595
C	0.69712	3.09406	-2.1935
H	0.12256	2.69242	-3.0298
H	1.68685	2.63313	-2.2488
C	0.55524	2.74314	0.33492
C	-0.00996	2.73994	-0.91177
H	-0.10919	2.73216	1.19047
H	-1.09473	2.7707	-0.96737
Cl	0.15358	0.14607	-2.84977

TS1^{L1}"

Sum of electronic and thermal Free Energies= -3346.285959

P	1.9784	-0.81029	0.01405
P	-2.32569	0.25205	-0.10821
C	3.59901	-0.47446	-0.80653
C	4.83867	-0.69995	-0.18963
C	3.56805	0.04411	-2.11196
C	6.02591	-0.40878	-0.86464
H	4.87879	-1.10006	0.81829
C	4.75705	0.32289	-2.78602
H	2.60868	0.21276	-2.5937
C	5.98753	0.10239	-2.16263
H	6.97968	-0.5833	-0.37453
H	4.72231	0.71847	-3.79692
H	6.91249	0.32927	-2.68575
C	2.44211	-1.02127	1.79167
C	2.43564	-2.27136	2.4261
C	2.79158	0.11312	2.54377
C	2.76416	-2.38459	3.7786
H	2.1794	-3.16136	1.86133
C	3.1272	-0.0023	3.89195
H	2.80498	1.09041	2.07255
C	3.10975	-1.25188	4.5153
H	2.75325	-3.36179	4.25254
H	3.3975	0.88464	4.45809
H	3.36468	-1.34083	5.56734
C	-3.37892	0.45932	-1.61024
C	-4.3381	-0.46087	-2.05156
C	-3.16683	1.62718	-2.36161
C	-5.08456	-0.20608	-3.20468
H	-4.50028	-1.38582	-1.51026
C	-3.92371	1.88815	-3.50158
H	-2.38849	2.32258	-2.06074
C	-4.88676	0.97009	-3.92681

H	-5.81887	-0.9338	-3.53869
H	-3.74717	2.79797	-4.06808
H	-5.46877	1.16534	-4.82297
C	-3.15596	1.32139	1.16093
C	-4.2177	2.19014	0.86893
C	-2.65259	1.28713	2.47391
C	-4.76499	3.00002	1.86751
H	-4.62318	2.23427	-0.13633
C	-3.20134	2.09567	3.46791
H	-1.83013	0.6204	2.72024
C	-4.26068	2.95488	3.1677
H	-5.59105	3.66272	1.62571
H	-2.7994	2.05442	4.47664
H	-4.68775	3.58598	3.94168
C	1.57601	-2.53176	-0.54174
C	2.45116	-3.29817	-1.31715
C	0.28222	-3.04402	-0.30468
C	2.05774	-4.52092	-1.8651
H	3.44661	-2.92256	-1.51548
C	-0.13218	-4.24881	-0.87002
C	0.76245	-4.982	-1.65257
H	2.75355	-5.09371	-2.46889
H	-1.14488	-4.60591	-0.72017
H	0.43272	-5.91685	-2.09704
C	-2.76238	-1.42697	0.58146
C	-4.08352	-1.64512	1.01684
C	-1.83644	-2.47143	0.78034
C	-4.48456	-2.84531	1.59709
H	-4.8084	-0.84505	0.90856
C	-2.2254	-3.66581	1.40214
C	-3.54623	-3.8587	1.7941
H	-5.51462	-2.97806	1.9131
H	-1.47623	-4.42599	1.59187
H	-3.83387	-4.78989	2.2733
O	-0.50849	-2.24961	0.49934
Rh	-0.05882	0.44972	-0.33649
Cl	-0.27408	-0.5641	-2.50184
C	1.56698	3.37945	0.37215
C	2.33925	4.3033	1.08619
C	1.7347	3.24609	-1.01403
C	3.27379	5.09296	0.41042
H	2.19845	4.41856	2.15907
C	2.65961	4.05029	-1.68027
H	1.13696	2.51625	-1.55696
C	3.43269	4.97378	-0.9726
H	3.86968	5.81104	0.96701
H	2.77442	3.94981	-2.75643
H	4.15029	5.59818	-1.4966
S	0.32197	2.4144	1.26772
H	-0.58208	2.35344	0.20585

1^{Li}”

Sum of electronic and thermal Free Energies= -3346.312274

S	-0.14659	2.17192	1.00633
C	-1.35281	3.2382	0.3323
C	-1.99456	3.05304	-0.91312
C	-1.67016	4.368	1.13265
C	-2.94626	3.97622	-1.33084
H	-1.70609	2.2206	-1.54474
C	-2.62634	5.27527	0.69971
H	-1.16703	4.50979	2.08399
C	-3.27012	5.08026	-0.53014
H	-3.4352	3.83973	-2.29004
H	-2.87319	6.13514	1.3148
H	-4.01865	5.79268	-0.86552
P	2.52004	0.15642	0.05046
P	-2.07722	-0.76695	0.10259
C	3.54787	1.60228	-0.38068
C	4.80863	1.78992	0.21122
C	3.06646	2.53572	-1.31432
C	5.58138	2.89858	-0.13581
H	5.18383	1.08097	0.94124
C	3.84814	3.64014	-1.65159
H	2.09646	2.3859	-1.77859
C	5.10217	3.8239	-1.06448
H	6.55465	3.03966	0.32384
H	3.47416	4.3588	-2.37403
H	5.70439	4.68833	-1.32818
C	3.20541	-0.50841	1.61406
C	3.97238	-1.68191	1.64953
C	2.94735	0.18439	2.80992
C	4.47447	-2.15455	2.86448
H	4.18372	-2.2246	0.73409
C	3.45595	-0.28866	4.01739
H	2.35048	1.09239	2.79976
C	4.21822	-1.46057	4.04693
H	5.06792	-3.0638	2.88253
H	3.25506	0.2544	4.9359
H	4.61013	-1.8297	4.98976

C	-3.45677	-0.58018	-1.0931
C	-4.79309	-0.79187	-0.70831
C	-3.15603	-0.31329	-2.43949
C	-5.81065	-0.73424	-1.66003
H	-5.04363	-0.99564	0.32702
C	-4.18287	-0.25777	-3.38297
H	-2.12849	-0.13787	-2.74345
C	-5.50808	-0.467	-2.99717
H	-6.83968	-0.89938	-1.3549
H	-3.94252	-0.04887	-4.42112
H	-6.30382	-0.42222	-3.73465
C	-2.81509	-0.5528	1.7675
C	-3.61991	0.57386	2.01106
C	-2.4938	-1.40641	2.83373
C	-4.11108	0.82429	3.29252
H	-3.87326	1.25127	1.20143
C	-2.98784	-1.14963	4.11338
H	-1.86244	-2.27348	2.67194
C	-3.79819	-0.03716	4.34584
H	-4.74059	1.69189	3.46561
H	-2.73963	-1.82318	4.92798
H	-4.18362	0.15786	5.34202
C	2.79036	-1.13348	-1.23065
C	3.94861	-1.1956	-2.01425
C	1.74299	-2.01987	-1.52012
C	4.05393	-2.11941	-3.05505
H	4.75895	-0.49977	-1.82237
C	1.81209	-2.91593	-2.57949
C	2.9834	-2.96542	-3.34015
H	4.95593	-2.15633	-3.65664
H	0.96827	-3.54847	-2.82592
H	3.04268	-3.65918	-4.1726
C	-1.59235	-2.54515	-0.0184
C	-2.50318	-3.56789	0.29058
C	-0.2914	-2.91395	-0.39469
C	-2.11855	-4.90628	0.27161
H	-3.52042	-3.30565	0.56342
C	0.12179	-4.24592	-0.37748
C	-0.80044	-5.2379	-0.04493
H	-2.83651	-5.68164	0.51735
H	1.14395	-4.50769	-0.61881
H	-0.47969	-6.27479	-0.03414
O	0.58294	-1.8721	-0.73336
Rh	0.12993	0.17386	-0.02846
H	0.20103	-0.35845	1.42977
Cl	0.15551	0.85263	-2.46468

TS2^{L1}

Sum of electronic and thermal Free Energies= -3904.232202

S	3.19425	-2.3733	0.21144
C	4.57368	-1.70818	-0.70095
C	4.46434	-1.22186	-2.01989
C	5.85461	-1.77375	-0.11577
C	5.60265	-0.81368	-2.71907
H	3.48512	-1.1758	-2.48787
C	6.98918	-1.39123	-0.83281
H	5.95098	-2.14265	0.9013
C	6.8706	-0.90305	-2.13706
H	5.49561	-0.44145	-3.73508
H	7.96777	-1.46426	-0.36512
H	7.75364	-0.59965	-2.69265
P	-0.21642	-2.49873	0.31642
P	-3.43001	2.1137	-0.49049
C	0.41818	-4.09389	-0.38249
C	0.27701	-5.31173	0.29608
C	1.051	-4.07869	-1.63814
C	0.75081	-6.49709	-0.27327
H	-0.19564	-5.34821	1.27063
C	1.50339	-5.26737	-2.20809
H	1.18432	-3.13552	-2.15962
C	1.35907	-6.47887	-1.52704
H	0.64147	-7.43231	0.26891
H	1.98648	-5.24116	-3.18059
H	1.72534	-7.40129	-1.96964
C	-0.71614	-2.98677	2.03438
C	-1.95623	-3.59122	2.30005
C	0.19865	-2.83826	3.08708
C	-2.27717	-4.0193	3.58995
H	-2.67135	-3.7357	1.49684
C	-0.1222	-3.26969	4.37574
H	1.16792	-2.39004	2.89421
C	-1.36195	-3.85646	4.63241
H	-3.24028	-4.4868	3.77654
H	0.60081	-3.14721	5.17726
H	-1.61161	-4.19093	5.63544
C	-4.77129	1.69226	-1.69928
C	-6.12556	1.51652	-1.36936
C	-4.37867	1.52394	-3.03666
C	-7.06	1.18313	-2.35129

H	-6.45251	1.62951	-0.33999
C	-5.31448	1.1998	-4.02075
H	-3.33117	1.63128	-3.30508
C	-6.65658	1.02587	-3.67967
H	-8.10305	1.04628	-2.07864
H	-4.99126	1.07096	-5.0497
H	-7.38428	0.76402	-4.44253
C	-3.71637	3.92036	-0.1799
C	-4.76799	4.66841	-0.73043
C	-2.75883	4.58834	0.60474
C	-4.86686	6.0418	-0.49098
H	-5.51251	4.18127	-1.35115
C	-2.86444	5.95584	0.85261
H	-1.92284	4.03085	1.02081
C	-3.92017	6.68836	0.30328
H	-5.68778	6.60455	-0.92736
H	-2.11754	6.45279	1.46547
H	-3.99895	7.75601	0.48763
C	-1.85949	-2.33947	-0.55421
C	-2.15591	-3.19252	-1.6302
C	-2.88497	-1.46478	-0.13146
C	-3.41136	-3.21721	-2.23591
H	-1.39271	-3.86782	-1.99254
C	-4.15987	-1.51977	-0.69806
C	-4.42126	-2.3909	-1.75339
H	-3.59402	-3.89208	-3.06631
H	-4.94009	-0.86859	-0.32662
H	-5.41297	-2.40669	-2.19538
C	-4.06562	1.37599	1.09979
C	-4.98626	2.04052	1.93077
C	-3.592	0.12561	1.54502
C	-5.42769	1.48678	3.13187
H	-5.3498	3.01853	1.63172
C	-4.02498	-0.43693	2.74739
C	-4.94704	0.24214	3.54105
H	-6.13829	2.03009	3.74795
H	-3.61372	-1.39396	3.05041
H	-5.27643	-0.19493	4.47915
O	-2.58266	-0.55595	0.86357
Rh	1.39656	-0.74313	0.18706
H	1.6955	-0.85876	1.6893
Cl	1.0021	-0.58944	-2.38893
C	0.14019	0.96848	1.31332
C	0.38227	1.36402	0.02623
H	0.81823	1.21493	2.12364
H	-0.8205	0.56058	1.59265
H	-0.39393	1.28263	-0.72546
C	1.718	1.97333	-0.36986
H	1.73371	2.16517	-1.44217
H	1.93824	2.90874	0.15726
N	2.74944	0.93583	-0.05109
H	3.28303	0.70532	-0.88893
C	3.69063	1.24713	1.0614
H	4.24548	0.32356	1.24475
H	3.09127	1.44899	1.95276
C	4.63378	2.39823	0.78895
C	4.5124	3.61533	1.46346
C	5.68731	2.25489	-0.13318
C	5.40533	4.67016	1.24439
H	3.71567	3.74765	2.19261
C	6.57743	3.29249	-0.36759
H	5.82233	1.31433	-0.66064
C	6.44623	4.50816	0.32384
H	5.28282	5.59552	1.79494
H	7.39683	3.18271	-1.07077
O	7.38317	5.45659	0.03396
C	7.33349	6.68732	0.73763
H	8.17272	7.27933	0.36921
H	6.39857	7.22924	0.54401
H	7.44378	6.53928	1.82008

4^{Li}

Sum of electronic and thermal Free Energies= -3904.222629

S	-4.6624	0.64229	-0.15232
C	-5.44973	1.8641	0.8874
C	-5.14796	2.01008	2.25322
C	-6.48204	2.64439	0.33512
C	-5.86176	2.91699	3.0359
H	-4.33911	1.42735	2.67872
C	-7.20542	3.53584	1.12982
H	-6.71795	2.5371	-0.71969
C	-6.8955	3.67892	2.48323
H	-5.61215	3.02352	4.08856
H	-8.00534	4.12396	0.68701
H	-7.45243	4.37761	3.10169
P	-1.97971	-1.30832	-0.70896
P	3.20966	-0.89303	0.47013
C	-3.36627	-2.21171	-1.55911
C	-3.64134	-3.56663	-1.31642

C	-4.08378	-1.54729	-2.56412	C	-0.57205	-2.52897	1.52093
C	-4.61494	-4.23646	-2.05748	C	-2.96182	-2.92535	2.89877
H	-3.10366	-4.10011	-0.53997	H	-3.91366	-2.09813	1.16945
C	-5.05318	-2.22081	-3.30843	C	-0.55595	-3.03507	2.82505
H	-3.89695	-0.49554	-2.75307	C	-1.74767	-3.24521	3.50852
C	-5.32271	-3.56595	-3.05671	H	-3.89806	-3.05778	3.4316
H	-4.8197	-5.28352	-1.85221	H	0.39927	-3.24505	3.29388
H	-5.60551	-1.6874	-4.07669	H	-1.72453	-3.63307	4.52265
H	-6.08227	-4.08804	-3.63168	C	2.93601	-2.72285	0.58971
C	-0.63009	-1.79982	-1.88877	C	3.95953	-3.66946	0.43403
C	-0.09342	-3.10222	-1.91846	C	1.62869	-3.19908	0.8147
C	-0.2319	-0.89942	-2.88007	C	3.70882	-5.04002	0.50636
C	0.85049	-3.46159	-2.87831	H	4.97127	-3.32096	0.25466
H	-0.41184	-3.83769	-1.1888	C	1.36686	-4.57196	0.8897
C	0.70725	-1.25905	-3.85092	C	2.40819	-5.48658	0.73753
H	-0.69116	0.0837	-2.91859	H	4.52238	-5.74901	0.38679
C	1.2603	-2.53903	-3.84479	H	0.35579	-4.9187	1.06927
H	1.26563	-4.4651	-2.87113	H	2.19432	-6.55009	0.79573
H	0.99756	-0.54086	-4.61285	O	0.6299	-2.24995	0.88749
H	1.99275	-2.82305	-4.59488	Rh	-2.30639	1.09844	-0.3674
C	3.60583	-0.43796	2.22232	H	-2.59741	0.76903	-1.89694
C	3.8426	-1.36705	3.24669	Cl	-1.81356	0.96415	2.04941
C	3.63808	0.93163	2.5371	C	-2.65873	3.263	-0.35727
C	4.10532	-0.93772	4.54952	C	-2.22478	2.95045	-1.61692
H	3.82222	-2.42966	3.02719	H	-1.9642	3.57993	0.4167
C	3.9116	1.35966	3.83596	H	-3.70372	3.48647	-0.16895
H	3.44943	1.66866	1.76103	H	-2.93958	2.9007	-2.4771
C	4.14215	0.42503	4.84745	C	-0.73861	2.83635	-1.90139
H	4.28253	-1.671	5.33168	H	-0.53972	2.457	-2.90456
H	3.93271	2.42251	4.05944	H	-0.24999	3.82181	-1.82405
H	4.34366	0.75695	5.86198	N	-0.20822	1.88395	-0.89056
C	4.87237	-0.82368	-0.35158	H	0.31299	1.14111	-1.34702
C	6.09131	-0.67392	0.32677	C	0.64353	2.44608	0.19583
C	4.8876	-0.86457	-1.75752	H	0.98566	1.58273	0.77112
C	7.292	-0.57445	-0.38076	H	0.00633	3.02144	0.86858
H	6.1024	-0.63137	1.41119	C	1.79987	3.29016	-0.29906
C	6.08755	-0.77655	-2.46299	C	1.83959	4.66644	-0.05903
H	3.95136	-0.96895	-2.30179	C	2.86612	2.71994	-1.02011
C	7.2945	-0.6278	-1.77519	C	2.89373	5.46501	-0.5156
H	8.22662	-0.45591	0.16076	H	1.03525	5.13298	0.50504
H	6.08047	-0.81505	-3.54895	C	3.92016	3.49558	-1.48217
H	8.2291	-0.54877	-2.3233	H	2.87718	1.64909	-1.20589
C	-1.78088	-2.21528	0.87768	C	3.94015	4.87822	-1.23505
C	-2.9702	-2.4001	1.61183	H	2.88594	6.52779	-0.30451

H	4.7471	3.0528	-2.02772
O	5.01668	5.55259	-1.73169
C	5.09773	6.95047	-1.50259
H	6.02326	7.28067	-1.97665
H	4.25148	7.4851	-1.95323
H	5.1385	7.18395	-0.43085

TS3^{L1}

Sum of electronic and thermal Free Energies= -3904.208772

S	-4.53893	0.91005	-0.07381
C	-5.11883	1.97056	1.24214
C	-4.80184	1.73034	2.59114
C	-5.99939	3.0231	0.92985
C	-5.34838	2.53079	3.594
H	-4.10889	0.93334	2.83366
C	-6.55471	3.81192	1.94017
H	-6.25236	3.20816	-0.1109
C	-6.22723	3.57139	3.27621
H	-5.08744	2.33844	4.632
H	-7.23779	4.61755	1.68124
H	-6.65331	4.18804	4.06356
P	-2.0423	-1.17847	-0.91712
P	3.04679	-1.04845	0.61878
C	-3.45551	-1.88262	-1.89404
C	-3.74677	-3.25682	-1.8876
C	-4.17737	-1.04501	-2.75494
C	-4.74115	-3.77514	-2.71596
H	-3.20267	-3.92433	-1.22734
C	-5.17003	-1.5662	-3.58749
H	-3.97571	0.02081	-2.76115
C	-5.45553	-2.93087	-3.56955
H	-4.95748	-4.83974	-2.69494
H	-5.7262	-0.89949	-4.2403
H	-6.23172	-3.33576	-4.21282
C	-0.6756	-1.70991	-2.05335
C	-0.12639	-2.99919	-2.05534
C	-0.26172	-0.80783	-3.04557
C	0.84466	-3.35917	-2.98958
H	-0.45187	-3.72961	-1.32426
C	0.70313	-1.16831	-3.98965
H	-0.72865	0.17189	-3.10247
C	1.269	-2.44332	-3.95567
H	1.26915	-4.35865	-2.96111
H	1.00581	-0.45537	-4.75191
H	2.02276	-2.72756	-4.68459
C	3.35624	-0.59715	2.38886
C	3.49433	-1.52568	3.43097
C	3.41755	0.77162	2.69834
C	3.68904	-1.0968	4.7455
H	3.44796	-2.58778	3.21649
C	3.62282	1.19881	4.00939
H	3.30258	1.50956	1.90914
C	3.75515	0.26448	5.0381
H	3.7895	-1.82956	5.54131
H	3.66563	2.26072	4.22828
H	3.90207	0.59579	6.06159
C	4.75484	-1.06222	-0.10658
C	5.93673	-0.89604	0.63024
C	4.84803	-1.19103	-1.50421
C	7.1774	-0.86575	-0.01184
H	5.88858	-0.78827	1.70889
C	6.08715	-1.17336	-2.1431
H	3.94125	-1.31147	-2.09325
C	7.25719	-1.00733	-1.39735
H	8.08274	-0.73416	0.57457
H	6.14011	-1.28135	-3.22292
H	8.22288	-0.98418	-1.89415
C	-2.01958	-2.21298	0.6112
C	-3.27442	-2.42562	1.21812
C	-0.87866	-2.5763	1.34868
C	-3.39204	-3.0023	2.47827
H	-4.17122	-2.10632	0.69949
C	-0.99114	-3.13308	2.62706
C	-2.24328	-3.35384	3.18866
H	-4.37639	-3.15362	2.91042
H	-0.0863	-3.3771	3.17301
H	-2.31833	-3.78059	4.18468
C	2.69063	-2.86596	0.71908
C	3.68901	-3.84966	0.64627
C	1.35261	-3.29604	0.82405
C	3.38564	-5.21075	0.67681
H	4.72452	-3.53823	0.56173
C	1.03799	-4.66046	0.84749
C	2.05452	-5.61144	0.77638
H	4.18142	-5.94731	0.6239
H	0.00405	-4.97356	0.92822
H	1.79748	-6.66672	0.79544
O	0.38205	-2.31448	0.83242
Rh	-2.16918	1.21285	-0.38802

H	-2.50509	1.6918	-1.92662
Cl	-1.52236	0.87531	1.9479
C	-2.38198	3.35207	-0.20277
C	-2.08025	3.10374	-1.57614
H	-1.59731	3.66544	0.47616
H	-3.38516	3.64846	0.07861
H	-2.7621	3.45421	-2.35138
C	-0.59843	2.97793	-1.92313
H	-0.46416	2.67169	-2.96496
H	-0.0635	3.92349	-1.78581
N	-0.07038	1.91071	-1.021
H	0.36865	1.1781	-1.56792
C	0.88355	2.32145	0.04955
H	1.2252	1.38764	0.49796
H	0.3231	2.84321	0.82647
C	2.04147	3.16419	-0.44073
C	2.10262	4.53157	-0.15507
C	3.08366	2.60913	-1.2076
C	3.14584	5.33873	-0.62222
H	1.32166	4.98326	0.45236
C	4.12799	3.39448	-1.68039
H	3.08448	1.54365	-1.42409
C	4.16086	4.76965	-1.39785
H	3.15196	6.39402	-0.37691
H	4.93566	2.96586	-2.26511
O	5.21409	5.4565	-1.91881
C	5.29981	6.84953	-1.66539
H	6.20038	7.19545	-2.17782
H	4.42836	7.38841	-2.06374
H	5.39283	7.06101	-0.59239

5^{L1}

Sum of electronic and thermal Free Energies= -3904.259671

P	0.54673	2.65858	0.31977
P	-1.16384	-1.83633	0.92711
C	1.78102	3.71376	-0.57846
C	1.41029	4.85754	-1.30066
C	3.11855	3.28397	-0.65429
C	2.34812	5.55222	-2.06752
H	0.38425	5.20747	-1.26952
C	4.05606	3.98363	-1.41218
H	3.43758	2.40073	-0.1083
C	3.67312	5.12147	-2.12557
H	2.03751	6.43509	-2.61942
H	5.08446	3.63509	-1.44949
H	4.40072	5.66346	-2.7226
C	-0.88441	3.80595	0.54035
C	-1.09079	4.61824	1.66703
C	-1.8294	3.83156	-0.50163
C	-2.21286	5.44488	1.74768
H	-0.37692	4.60803	2.48354
C	-2.93796	4.67643	-0.42645
H	-1.69773	3.18166	-1.36199
C	-3.13611	5.47928	0.69926
H	-2.36514	6.0629	2.62876
H	-3.65503	4.68973	-1.24062
H	-4.00751	6.1253	0.76249
C	0.29623	-2.74054	1.64006
C	0.80441	-2.49067	2.9226
C	0.91459	-3.73942	0.86514
C	1.91234	-3.19361	3.40351
H	0.32499	-1.75889	3.55993
C	2.02273	-4.44093	1.34284
H	0.50707	-4.00026	-0.1063
C	2.53152	-4.16334	2.61431
H	2.28637	-2.98567	4.40396
H	2.48096	-5.20713	0.7247
H	3.39374	-4.70684	2.9915
C	-2.39259	-3.22316	0.80118
C	-2.24697	-4.40039	1.55569
C	-3.5188	-3.09002	-0.02845
C	-3.19392	-5.42208	1.46889
H	-1.39767	-4.52601	2.21805
C	-4.46278	-4.11545	-0.11279
H	-3.66601	-2.17137	-0.58398
C	-4.30181	-5.28546	0.63054
H	-3.06345	-6.32416	2.06038
H	-5.32341	-3.99142	-0.76396
H	-5.03589	-6.08355	0.56165
C	1.29478	2.58981	2.01824
C	2.21058	3.52303	2.53655
C	0.98269	1.48193	2.82358
C	2.78426	3.35908	3.79698
H	2.47973	4.38356	1.93219
C	1.55939	1.29628	4.08264
C	2.46045	2.24163	4.57102
H	3.48595	4.09901	4.17226
H	1.29982	0.4188	4.66668
H	2.91139	2.102	5.54941

C	-1.82274	-0.82291	2.32933
C	-3.1009	-1.07043	2.852
C	-1.11561	0.29186	2.82745
C	-3.66213	-0.25043	3.82903
H	-3.67029	-1.91266	2.47846
C	-1.67593	1.12765	3.79675
C	-2.94905	0.85324	4.29255
H	-4.65443	-0.46773	4.21142
H	-1.12285	1.98935	4.15034
H	-3.38105	1.51293	5.03944
O	0.14151	0.50167	2.30207
Rh	-0.7293	-0.51514	-1.0179
Cl	-0.27652	1.03294	-2.85991
C	1.29349	-1.91802	-2.68845
H	2.20396	-2.50488	-2.86026
H	1.24619	-1.11352	-3.42575
N	1.32633	-1.27201	-1.34795
H	1.47079	-2.00457	-0.65399
C	2.42528	-0.2809	-1.16407
H	2.28573	0.13386	-0.16201
H	2.24796	0.52431	-1.87925
C	3.81561	-0.8645	-1.3022
C	4.3945	-1.58742	-0.25349
C	4.56027	-0.71233	-2.48392
C	5.66511	-2.15726	-0.36782
H	3.84898	-1.70992	0.6803
C	5.82661	-1.26899	-2.61566
H	4.14012	-0.14362	-3.30937
C	6.38697	-2.00019	-1.55791
H	6.07981	-2.70619	0.46938
H	6.40449	-1.15054	-3.52684
O	7.63251	-2.51121	-1.78404
C	8.24727	-3.26154	-0.74975
H	9.21626	-3.5763	-1.13996
H	8.40177	-2.65764	0.15451
H	7.65836	-4.15082	-0.48855
C	-1.21606	-1.97631	-2.39401
H	-2.01576	-2.60974	-2.01433
H	-1.58258	-1.38368	-3.23204
S	-2.94678	0.34837	-0.64577
C	-4.04329	0.16724	-2.04612
C	-5.36136	-0.25689	-1.7838
C	-3.69817	0.49881	-3.36869
C	-6.30479	-0.33997	-2.80852
H	-5.64258	-0.50854	-0.76489
C	-4.64293	0.39644	-4.39016
H	-2.69213	0.84327	-3.58165
C	-5.94981	-0.01931	-4.12003
H	-7.31819	-0.66185	-2.57929
H	-4.35533	0.65807	-5.40579
H	-6.68153	-0.08813	-4.92012
C	0.03417	-2.77807	-2.76671
H	-0.06679	-3.1752	-3.78711
H	0.14553	-3.65205	-2.11267

TS4^{L1}

Sum of electronic and thermal Free Energies= -3904.194812

P	2.22159	2.17666	0.25119
P	-1.91132	-1.4072	1.02144
C	3.88019	2.85506	-0.23326
C	4.22026	4.21621	-0.24784
C	4.82616	1.92591	-0.70466
C	5.47176	4.63386	-0.70804
H	3.50376	4.95566	0.09408
C	6.08121	2.34103	-1.14769
H	4.5734	0.86843	-0.73277
C	6.40721	3.69952	-1.15329
H	5.71363	5.69335	-0.71758
H	6.7983	1.60586	-1.50268
H	7.37941	4.02675	-1.51126
C	1.20696	3.70077	0.52026
C	1.32736	4.54534	1.63734
C	0.26997	4.01972	-0.47621
C	0.53668	5.69037	1.74995
H	2.04415	4.3092	2.41951
C	-0.51185	5.17267	-0.36452
H	0.13919	3.35316	-1.3254
C	-0.38195	6.00836	0.74554
H	0.64089	6.33602	2.61823
H	-1.22538	5.41015	-1.14897
H	-0.99522	6.90146	0.83221
C	-0.67082	-2.67217	1.57356
C	0.12745	-2.53929	2.71551
C	-0.55336	-3.85136	0.81373
C	1.03116	-3.54115	3.0801
H	0.02971	-1.66045	3.33674
C	0.34633	-4.85427	1.177
H	-1.19807	-4.00383	-0.04875
C	1.14716	-4.69899	2.31112

H	1.63934	-3.4147	3.97134
H	0.41787	-5.75633	0.57702
H	1.8478	-5.47818	2.59751
C	-3.47354	-2.36146	1.42739
C	-3.46903	-3.46831	2.29762
C	-4.70472	-1.96011	0.87769
C	-4.64864	-4.15594	2.59176
H	-2.54417	-3.80414	2.75296
C	-5.88565	-2.63976	1.18502
H	-4.7489	-1.10521	0.2132
C	-5.86273	-3.7448	2.03795
H	-4.61574	-5.01386	3.2594
H	-6.82395	-2.30041	0.75226
H	-6.78066	-4.27847	2.27076
C	2.53991	1.63161	2.00014
C	3.74905	1.85316	2.68069
C	1.54258	0.90353	2.67588
C	3.95618	1.39412	3.98114
H	4.53733	2.40306	2.17785
C	1.73366	0.45519	3.98635
C	2.94033	0.70094	4.63884
H	4.90128	1.58787	4.47983
H	0.93318	-0.06746	4.49822
H	3.08217	0.34673	5.65574
C	-1.93121	-0.06542	2.3232
C	-3.14715	0.22127	2.9725
C	-0.84956	0.80834	2.5865
C	-3.30406	1.31535	3.81966
H	-3.99755	-0.4273	2.80666
C	-1.01075	1.92321	3.41748
C	-2.23145	2.179	4.03192
H	-4.2617	1.49196	4.2993
H	-0.17059	2.59164	3.5642
H	-2.33944	3.05342	4.66706
O	0.3748	0.57954	1.98466
Rh	-1.47464	-0.39626	-1.00452
Cl	-0.56268	1.16446	-2.6951
C	-0.15892	-2.13615	-2.87036
H	0.44159	-3.01408	-3.14502
H	0.08788	-1.32332	-3.55695
N	0.22008	-1.67007	-1.50342
H	0.19904	-2.47429	-0.87923
C	1.60505	-1.11002	-1.42263
H	1.70331	-0.70936	-0.41323
H	1.63989	-0.25838	-2.10353
C	2.69852	-2.12012	-1.69972
C	3.13704	-2.98274	-0.68816
C	3.30249	-2.23525	-2.96377
C	4.12514	-3.94414	-0.91605
H	2.70464	-2.90319	0.30653
C	4.28889	-3.18342	-3.20967
H	2.99808	-1.56472	-3.76375
C	4.70356	-4.04975	-2.18681
H	4.43764	-4.58956	-0.10315
H	4.75791	-3.27151	-4.18461
O	5.67408	-4.94975	-2.52616
C	6.1229	-5.8567	-1.5329
H	6.87815	-6.4817	-2.01265
H	6.57664	-5.33498	-0.68004
H	5.30719	-6.49457	-1.16698
C	-2.65982	-1.32978	-3.09843
H	-3.64279	-1.73739	-3.32296
H	-2.36495	-0.55399	-3.8022
S	-3.64232	0.09428	-1.60949
C	-3.88491	1.64491	-2.4795
C	-4.61466	1.67012	-3.67665
C	-3.49632	2.84651	-1.87553
C	-4.95108	2.88928	-4.26189
H	-4.92184	0.74705	-4.14649
C	-3.86525	4.059	-2.44874
H	-2.91109	2.81699	-0.9642
C	-4.58795	4.08757	-3.64453
H	-5.50911	2.90363	-5.19382
H	-3.58822	4.98384	-1.95762
H	-4.87005	5.03659	-4.0891
C	-1.64942	-2.48096	-3.00303
H	-1.75657	-3.02669	-3.96004
H	-1.95389	-3.19632	-2.23091

6^{L1}

Sum of electronic and thermal Free Energies= -3904.221362

P	-3.02462	-1.51768	-0.53343
P	1.82058	0.22179	1.61716
C	-4.77175	-1.49116	-1.15406
C	-5.44137	-2.57201	-1.74757
C	-5.43429	-0.2519	-1.08243
C	-6.74039	-2.42185	-2.23939
H	-4.94553	-3.53291	-1.83586
C	-6.73667	-0.1063	-1.55858

H	-4.91866	0.60831	-0.6616
C	-7.39392	-1.1929	-2.14065
H	-7.24084	-3.26902	-2.70091
H	-7.23152	0.85865	-1.49026
H	-8.40395	-1.0787	-2.52412
C	-2.36347	-3.15396	-1.09278
C	-2.79195	-4.39257	-0.58227
C	-1.35525	-3.13423	-2.06887
C	-2.23874	-5.58404	-1.05288
H	-3.55691	-4.42477	0.18879
C	-0.80245	-4.32955	-2.53739
H	-0.97548	-2.18758	-2.44452
C	-1.24395	-5.55353	-2.03482
H	-2.58178	-6.53481	-0.65287
H	-0.01794	-4.29473	-3.2877
H	-0.81046	-6.48152	-2.39817
C	0.68353	1.34981	2.55949
C	-0.36535	0.95258	3.39623
C	0.9485	2.72698	2.4309
C	-1.13901	1.90055	4.07168
H	-0.5839	-0.09623	3.53186
C	0.17783	3.67413	3.10512
H	1.78751	3.05912	1.82288
C	-0.87486	3.26254	3.92643
H	-1.94902	1.56644	4.71388
H	0.40437	4.73079	2.99415
H	-1.4767	3.99685	4.45401
C	3.31993	0.49342	2.69833
C	3.22895	0.32527	4.09193
C	4.54028	0.90032	2.14697
C	4.3334	0.55303	4.90903
H	2.28899	0.01694	4.54045
C	5.64809	1.13386	2.96967
H	4.62878	1.03366	1.07554
C	5.54843	0.96065	4.34838
H	4.24694	0.41705	5.98352
H	6.58772	1.45075	2.52535
H	6.40903	1.14151	4.9864
C	-3.27533	-1.85831	1.27702
C	-4.52177	-2.10667	1.87283
C	-2.14712	-1.84653	2.1174
C	-4.64253	-2.36112	3.23983
H	-5.4095	-2.11027	1.24922
C	-2.25293	-2.12205	3.48373
C	-3.50344	-2.3804	4.04415
H	-5.62069	-2.55598	3.66952
H	-1.35877	-2.14594	4.09811
H	-3.58183	-2.59099	5.1068
C	1.45179	-1.57053	1.97699
C	2.57786	-2.39335	2.19398
C	0.20672	-2.22275	1.84031
C	2.48357	-3.77798	2.28978
H	3.55327	-1.93152	2.29216
C	0.10815	-3.61646	1.92758
C	1.23923	-4.39236	2.15325
H	3.37781	-4.36903	2.4611
H	-0.86063	-4.08276	1.79129
H	1.146	-5.47306	2.20616
O	-0.92556	-1.47888	1.55955
Rh	1.72782	0.29057	-0.63511
Cl	1.03446	-0.34325	-2.92591
C	0.93891	2.86727	-1.8815
H	0.40442	3.82645	-1.86149
H	0.70629	2.37501	-2.82789
N	0.38208	1.99565	-0.80391
H	0.44028	2.50767	0.07535
C	-1.06221	1.65747	-1.0193
H	-1.34721	1.01406	-0.18585
H	-1.10314	1.04394	-1.92062
C	-1.99555	2.84713	-1.11816
C	-2.43483	3.51522	0.03055
C	-2.45959	3.31015	-2.36126
C	-3.29449	4.61514	-0.04207
H	-2.10932	3.1703	1.00945
C	-3.31592	4.40028	-2.45405
H	-2.14917	2.79883	-3.26896
C	-3.73757	5.06348	-1.29233
H	-3.6149	5.10172	0.87182
H	-3.67771	4.75538	-3.41371
O	-4.57924	6.12247	-1.48568
C	-5.04433	6.8261	-0.34654
H	-5.69167	7.61944	-0.72429
H	-5.62365	6.17737	0.32371
H	-4.21784	7.27556	0.21985
C	3.41405	2.15499	-2.48933
H	4.3097	2.67936	-2.83693
H	2.92826	1.67065	-3.33879
S	4.02813	0.7942	-1.3711

C	5.05865	-0.11701	-2.55108
C	6.41299	0.21972	-2.67564
C	4.52617	-1.18087	-3.28993
C	7.23246	-0.50134	-3.54614
H	6.8217	1.03799	-2.08916
C	5.35399	-1.89737	-4.15665
H	3.47193	-1.42126	-3.19075
C	6.70354	-1.56102	-4.28655
H	8.28264	-0.23867	-3.64111
H	4.94014	-2.72062	-4.73273
H	7.3427	-2.12429	-4.96101
C	2.4536	3.15489	-1.80811
H	2.59665	4.10655	-2.33813
H	2.76277	3.34764	-0.77325

P2

Sum of electronic and thermal Free Energies= -1188.340780

C	-2.09234	1.16793	-0.85283
C	-0.81281	1.63407	-0.57446
C	0.01844	0.97815	0.34389
C	-0.47228	-0.17212	0.9673
C	-1.75254	-0.66001	0.69628
C	-2.57172	0.01509	-0.21684
H	-2.73621	1.67366	-1.56492
H	-0.45183	2.52592	-1.08167
H	0.16922	-0.69904	1.667
H	-2.09699	-1.55718	1.19727
O	-3.83934	-0.36787	-0.55824
C	-4.37453	-1.52998	0.05266
H	-5.37961	-1.64974	-0.35477
H	-3.78195	-2.42344	-0.18338
H	-4.43892	-1.42334	1.14336
C	1.39242	1.52627	0.68524
H	1.34237	2.05857	1.64452
H	1.66995	2.2818	-0.07367
N	2.4001	0.47466	0.83563
H	3.20766	0.85049	1.32588
C	2.84616	-0.10427	-0.43464
H	3.2717	0.64578	-1.12766
H	1.9575	-0.51782	-0.93056
C	5.21384	-1.25917	-0.80209
H	5.13642	-1.18473	-1.86669
H	5.80217	-0.44676	-0.42959
C	3.84293	-1.20285	-0.19593
H	3.28473	-2.07108	-0.47785
H	4.17685	-1.30634	0.81535
S	5.9907	-2.80132	-0.37008
C	7.63631	-2.84779	-1.04699
C	8.71449	-2.38551	-0.2918
C	7.84798	-3.34643	-2.33233
C	10.00393	-2.42129	-0.82218
H	8.54718	-1.99174	0.72121
C	9.13788	-3.38319	-2.86263
H	6.99835	-3.71098	-2.9276
C	10.21579	-2.92061	-2.10787
H	10.85373	-2.05635	-0.22723
H	9.30453	-3.77679	-3.87594
H	11.23256	-2.94877	-2.52581

7^{L1}

Sum of electronic and thermal Free Energies= -3904.229139

S	-0.56964	-2.74005	-1.72566
C	1.00127	-3.35589	-2.30433
C	2.00987	-3.78078	-1.42188
C	1.18005	-3.58421	-3.67934
C	3.1676	-4.39653	-1.89851
H	1.87517	-3.64057	-0.35218
C	2.32703	-4.22093	-4.15193
H	0.40246	-3.26761	-4.36699
C	3.33047	-4.62192	-3.26627
H	3.93438	-4.71665	-1.1967
H	2.4371	-4.40589	-5.21893
H	4.22658	-5.10925	-3.63898
P	-0.77468	2.0438	-0.64566
P	-2.0479	-1.26134	0.64962
C	0.08885	3.15085	-1.85963
C	-0.59555	4.11393	-2.61191
C	1.48175	3.04733	-2.00954
C	0.09582	4.95636	-3.48733
H	-1.66979	4.21636	-2.52202
C	2.17148	3.89933	-2.86807
H	2.03525	2.29474	-1.46203
C	1.47894	4.8557	-3.61424
H	-0.45454	5.69215	-4.06621
H	3.24798	3.80194	-2.96778
H	2.01527	5.51254	-4.29304
C	-2.5273	2.60561	-0.82388
C	-3.10086	3.59217	-0.01139
C	-3.28348	2.07377	-1.88215
C	-4.41068	4.02113	-0.23612

H	-2.52725	4.02948	0.79862
C	-4.58631	2.51414	-2.11324
H	-2.84166	1.32712	-2.53474
C	-5.15623	3.48379	-1.28546
H	-4.8447	4.77928	0.40929
H	-5.15531	2.09778	-2.93958
H	-6.17407	3.82022	-1.46034
C	-1.42972	-2.35968	2.02137
C	-1.74156	-2.11947	3.36908
C	-0.6483	-3.48473	1.70321
C	-1.27393	-2.97256	4.37165
H	-2.35729	-1.27358	3.64981
C	-0.18484	-4.33565	2.70644
H	-0.41861	-3.68628	0.66233
C	-0.4907	-4.08107	4.04526
H	-1.53062	-2.7705	5.40878
H	0.41835	-5.20094	2.43697
H	-0.12674	-4.7444	4.82522
C	-3.3674	-2.29947	-0.13999
C	-3.82199	-3.49295	0.44087
C	-3.97618	-1.85373	-1.32438
C	-4.85062	-4.2253	-0.15491
H	-3.36921	-3.86139	1.3543
C	-5.00903	-2.58163	-1.91318
H	-3.63646	-0.93727	-1.79323
C	-5.44712	-3.77298	-1.33239
H	-5.18083	-5.15335	0.30329
H	-5.46187	-2.22198	-2.83308
H	-6.24377	-4.34659	-1.79722
C	-0.19518	2.81917	0.95824
C	0.52729	4.02758	0.98366
C	-0.36683	2.16251	2.19215
C	1.07185	4.53367	2.16468
H	0.67828	4.57391	0.06061
C	0.19611	2.64355	3.37487
C	0.92073	3.8348	3.3624
H	1.62343	5.46884	2.14099
H	0.0562	2.07171	4.28668
H	1.3593	4.21231	4.28121
C	-3.08527	-0.04403	1.58798
C	-4.485	-0.0963	1.65487
C	-2.43989	0.98557	2.28646
C	-5.20764	0.84737	2.3869
H	-5.01362	-0.88142	1.12742
C	-3.14442	1.92938	3.03344
C	-4.53649	1.85676	3.07688
H	-6.29107	0.78842	2.41983
H	-2.60898	2.70494	3.57004
H	-5.09239	2.58867	3.656
O	-1.0549	0.96156	2.24661
Rh	-0.48927	-0.40221	-0.97789
H	-1.70197	-0.34461	-1.8824
Cl	0.71017	0.09489	-3.0354
C	3.54742	-1.36889	3.40021
C	2.78738	-0.53991	2.68376
H	4.22083	-1.00395	4.17098
H	3.53095	-2.44393	3.23584
H	2.83724	0.53188	2.88175
C	1.76203	-0.97266	1.66184
H	1.87563	-2.038	1.43833
H	0.77165	-0.84955	2.10857
N	1.72642	-0.23522	0.37565
H	1.64915	0.75604	0.59412
C	2.90642	-0.43773	-0.50217
H	2.66881	0.06314	-1.44581
H	2.94201	-1.49929	-0.74559
C	4.26386	-0.0005	0.01894
C	5.32091	-0.91326	0.06652
C	4.53019	1.3235	0.41434
C	6.59653	-0.54758	0.50777
H	5.14712	-1.93898	-0.24828
C	5.7877	1.70478	0.86589
H	3.74023	2.07389	0.38061
C	6.83174	0.76727	0.9208
H	7.3839	-1.29014	0.52834
H	5.99199	2.7252	1.17671
O	8.02872	1.23829	1.38718
C	9.12511	0.33958	1.44808
H	9.96639	0.91497	1.8398
H	8.92556	-0.5043	2.12247
H	9.38563	-0.05258	0.4564

TS5^{L1}

Sum of electronic and thermal Free Energies= -3904.209009

S	3.10172	2.7799	2.33259
C	2.2329	4.30506	2.00452
C	1.39917	4.8663	2.99029
C	2.43157	5.01974	0.80759
C	0.77773	6.10025	2.78247

H	1.24854	4.33024	3.92359
C	1.79203	6.24291	0.59838
H	3.08929	4.60365	0.05159
C	0.96324	6.79163	1.58282
H	0.1428	6.51871	3.55981
H	1.9559	6.77844	-0.33388
H	0.47826	7.75082	1.42064
P	2.67225	-1.12063	-0.36713
P	-2.72527	-1.43834	0.63799
C	4.38943	-1.63977	-0.86404
C	4.57301	-2.8491	-1.5585
C	5.51567	-0.87805	-0.528
C	5.84954	-3.28745	-1.90171
H	3.71722	-3.45622	-1.83391
C	6.79649	-1.32131	-0.87306
H	5.39308	0.06805	-0.01573
C	6.96762	-2.5235	-1.55666
H	5.97126	-4.2258	-2.43585
H	7.65833	-0.71636	-0.60727
H	7.96402	-2.86591	-1.82193
C	2.16231	-2.59531	0.62005
C	1.69352	-3.79694	0.07251
C	2.34953	-2.51384	2.00874
C	1.39992	-4.88466	0.89405
H	1.54584	-3.88724	-0.9971
C	2.06427	-3.60493	2.83079
H	2.71939	-1.59146	2.44775
C	1.58364	-4.79162	2.27546
H	1.02443	-5.8033	0.45345
H	2.21547	-3.52321	3.90316
H	1.35565	-5.64004	2.91383
C	-4.27434	-0.68745	-0.04342
C	-4.97021	-1.14239	-1.17296
C	-4.7339	0.47668	0.59963
C	-6.09831	-0.46019	-1.63688
H	-4.63484	-2.03093	-1.69705
C	-5.86955	1.14585	0.14756
H	-4.1947	0.86293	1.46104
C	-6.55473	0.68075	-0.97694
H	-6.62267	-0.82665	-2.51518
H	-6.20962	2.03924	0.66337
H	-7.43008	1.21005	-1.34109
C	-3.33288	-2.36473	2.12812
C	-4.65468	-2.34166	2.59412
C	-2.37325	-3.0817	2.86491
C	-5.00856	-3.02053	3.76363
H	-5.41283	-1.79145	2.0472
C	-2.73085	-3.76837	4.02325
H	-1.34019	-3.10892	2.52751
C	-4.05113	-3.7372	4.4798
H	-6.03788	-2.9901	4.11024
H	-1.97623	-4.32214	4.57444
H	-4.32853	-4.26473	5.38779
C	1.80545	-1.13792	-2.00911
C	2.54077	-0.63971	-3.10544
C	0.44442	-1.42323	-2.2309
C	1.96496	-0.45621	-4.359
H	3.58423	-0.38613	-2.96463
C	-0.14258	-1.23316	-3.48841
C	0.61591	-0.75534	-4.5521
H	2.56768	-0.07392	-5.17659
H	-1.19377	-1.46637	-3.61933
H	0.14934	-0.60788	-5.5215
C	-2.39875	-2.861	-0.5086
C	-3.25252	-3.97555	-0.58461
C	-1.24613	-2.86747	-1.3144
C	-3.0004	-5.03991	-1.44645
H	-4.13143	-3.99913	0.05238
C	-0.98005	-3.93484	-2.18303
C	-1.85979	-5.01152	-2.25128
H	-3.68347	-5.88269	-1.48809
H	-0.09107	-3.91709	-2.80314
H	-1.64333	-5.83358	-2.92748
O	-0.34277	-1.82458	-1.16245
Rh	2.56804	0.98901	0.83775
H	3.95361	0.56533	1.34342
Cl	3.65382	2.01557	-0.96512
C	0.09655	-0.07275	2.7363
C	-0.18082	1.23323	2.68563
H	0.20025	-0.58568	3.68568
H	0.19383	-0.68224	1.84635
H	-0.31418	1.7771	3.61934
C	-0.36776	2.07244	1.45344
H	-1.44426	2.20488	1.26601
H	0.03737	3.06719	1.64593
N	0.3163	1.53935	0.25813
H	-0.14216	0.66402	0.0037
C	0.23121	2.45841	-0.91429

H	0.76108	1.96197	-1.73092
H	0.80936	3.34872	-0.6591
C	-1.17009	2.84838	-1.33827
C	-1.70824	4.09161	-0.99468
C	-1.97289	1.972	-2.08804
C	-3.00456	4.46012	-1.36987
H	-1.10485	4.79486	-0.42577
C	-3.26208	2.31862	-2.469
H	-1.57529	1.00432	-2.38348
C	-3.78858	3.56784	-2.10823
H	-3.38324	5.43456	-1.08464
H	-3.88615	1.6392	-3.03945
O	-5.06628	3.81625	-2.52741
C	-5.64604	5.06646	-2.19737
H	-6.64942	5.05872	-2.62748
H	-5.72082	5.20538	-1.11092
H	-5.07898	5.90414	-2.6238

8^{L1}

Sum of electronic and thermal Free Energies= -3904.218058

S	1.94742	3.20298	2.68259
C	0.93678	4.55035	2.11928
C	-0.15216	4.98716	2.90343
C	1.26369	5.28596	0.96878
C	-0.85919	6.14765	2.55454
H	-0.41915	4.43394	3.7963
C	0.54065	6.41823	0.60839
H	2.10695	4.95504	0.37049
C	-0.51785	6.86694	1.40719
H	-1.68241	6.48515	3.18407
H	0.81965	6.97221	-0.28118
H	-1.06309	7.77127	1.14652
P	2.86718	-0.51259	-0.34962
P	-2.22055	-2.09563	0.64385
C	4.67524	-0.43566	-0.75386
C	5.23141	-1.38571	-1.62782
C	5.51909	0.50069	-0.13555
C	6.59986	-1.39462	-1.88946
H	4.59757	-2.11645	-2.10784
C	6.89245	0.48298	-0.39333
H	5.09825	1.24757	0.52425
C	7.4354	-0.45966	-1.27285
H	7.01329	-2.12514	-2.5705
H	7.53264	1.21875	0.08452
H	8.50306	-0.45931	-1.47404
C	2.81404	-2.22243	0.35738
C	2.64157	-3.37539	-0.41349
C	3.08071	-2.36903	1.72918
C	2.69709	-4.64304	0.1659
H	2.45543	-3.28971	-1.47898
C	3.1457	-3.629	2.3157
H	3.25965	-1.48618	2.34059
C	2.95094	-4.76978	1.53291
H	2.5527	-5.52359	-0.45337
H	3.3586	-3.72324	3.37033
H	2.99353	-5.75667	1.98383
C	-3.90967	-1.66555	0.01547
C	-4.44731	-2.10809	-1.20185
C	-4.66467	-0.76668	0.79161
C	-5.70721	-1.67411	-1.62418
H	-3.88631	-2.79731	-1.82364
C	-5.92661	-0.34577	0.37721
H	-4.26128	-0.39638	1.73129
C	-6.45217	-0.79717	-0.83608
H	-6.10682	-2.02878	-2.57046
H	-6.49463	0.34407	0.99467
H	-7.4298	-0.45965	-1.16702
C	-2.58654	-3.24667	2.05218
C	-3.86075	-3.74398	2.36431
C	-1.50349	-3.60581	2.87354
C	-4.04529	-4.58415	3.46539
H	-4.71372	-3.47116	1.75122
C	-1.68754	-4.45388	3.96472
H	-0.50997	-3.22924	2.65661
C	-2.96077	-4.94355	4.26599
H	-5.03926	-4.95889	3.69424
H	-0.83835	-4.72441	4.58603
H	-3.10617	-5.59629	5.12202
C	2.05577	-0.554	-2.01637
C	2.66215	0.19032	-3.04784
C	0.7832	-1.08785	-2.27274
C	2.05073	0.37085	-4.27873
H	3.62935	0.64865	-2.8613
C	0.1571	-0.90729	-3.51109
C	0.79354	-0.18499	-4.51649
H	2.55114	0.95029	-5.04789
H	-0.82477	-1.33884	-3.67468
H	0.29917	-0.04628	-5.47333
C	-1.60301	-3.29487	-0.63138

C	-2.16863	-4.5721	-0.7865
C	-0.53143	-2.94692	-1.47462
C	-1.72088	-5.46356	-1.75795
H	-2.97848	-4.86512	-0.12573
C	-0.07755	-3.83416	-2.45981
C	-0.67513	-5.08365	-2.60066
H	-2.18211	-6.44132	-1.8566
H	0.73773	-3.54535	-3.11241
H	-0.31153	-5.76306	-3.36625
O	0.09779	-1.73164	-1.24768
Rh	2.01241	1.29733	1.00506
H	3.30355	1.1239	1.82791
Cl	3.11489	2.71985	-0.62957
C	0.69839	-0.27966	2.30164
C	0.01364	0.86374	2.4026
H	1.26509	-0.64595	3.1499
H	0.6222	-0.95257	1.42456
H	0.18888	1.52461	3.35567
C	-0.85817	1.55025	1.36417
H	-1.89074	1.16233	1.34964
H	-0.89375	2.62704	1.60693
N	-0.17536	1.41465	0.0563
H	-0.40153	0.5001	-0.33268
C	-0.46475	2.47187	-0.93861
H	0.0907	2.19704	-1.84269
H	-0.03088	3.40154	-0.56869
C	-1.93166	2.67123	-1.25871
C	-2.59782	3.83485	-0.86783
C	-2.67427	1.69831	-1.95016
C	-3.95116	4.04484	-1.15467
H	-2.04589	4.60996	-0.33354
C	-4.01841	1.87769	-2.23195
H	-2.18755	0.78063	-2.27274
C	-4.66337	3.06042	-1.83791
H	-4.42245	4.97006	-0.8361
H	-4.59395	1.12338	-2.75737
O	-5.98652	3.15319	-2.17114
C	-6.67885	4.34098	-1.82637
H	-7.69968	4.21377	-2.19096
H	-6.70208	4.4984	-0.73985
H	-6.23371	5.22389	-2.30344

TS6^{L1}

Sum of electronic and thermal Free Energies= -3904.208981

S	1.76745	3.0328	2.71082
C	0.89869	4.4834	2.15208
C	-0.18814	4.95667	2.91277
C	1.3042	5.21799	1.0212
C	-0.85692	6.12697	2.55055
H	-0.49444	4.40824	3.79951
C	0.62805	6.3847	0.66383
H	2.13974	4.8556	0.43252
C	-0.45365	6.84469	1.42204
H	-1.69024	6.47871	3.15332
H	0.95415	6.94215	-0.21059
H	-0.97004	7.7583	1.14102
P	2.86733	-0.51734	-0.34002
P	-2.23202	-2.0888	0.64865
C	4.6722	-0.45253	-0.76591
C	5.21582	-1.38895	-1.66212
C	5.52661	0.46483	-0.14184
C	6.58265	-1.40286	-1.93213
H	4.5733	-2.11237	-2.15396
C	6.89822	0.44203	-0.40819
H	5.11519	1.20951	0.52752
C	7.4288	-0.48683	-1.30186
H	6.98647	-2.13042	-2.63069
H	7.54683	1.16329	0.08024
H	8.49512	-0.4983	-1.50991
C	2.80729	-2.22873	0.36368
C	2.64561	-3.37981	-0.41846
C	3.06556	-2.37872	1.73497
C	2.71142	-4.64878	0.15737
H	2.46807	-3.29149	-1.48378
C	3.14069	-3.64824	2.30989
H	3.21831	-1.49752	2.34895
C	2.9567	-4.78701	1.52408
H	2.56934	-5.52784	-0.4643
H	3.34499	-3.74505	3.37239
H	3.00908	-5.77499	1.97226
C	-3.90779	-1.63041	0.00427
C	-4.45009	-2.07717	-1.20946
C	-4.64666	-0.70609	0.76591
C	-5.69905	-1.62181	-1.64251
H	-3.90138	-2.78612	-1.82002
C	-5.89764	-0.26324	0.34075
H	-4.23916	-0.33273	1.7026
C	-6.42783	-0.71854	-0.86906
H	-6.10262	-1.97984	-2.58589

H	-6.45273	0.44709	0.94656
H	-7.39623	-0.36337	-1.20897
C	-2.63189	-3.23377	2.05259
C	-3.91715	-3.71339	2.34658
C	-1.56611	-3.60527	2.89084
C	-4.12946	-4.54864	3.4463
H	-4.7569	-3.43022	1.72009
C	-1.77792	-4.44842	3.98088
H	-0.56458	-3.23354	2.68831
C	-3.06195	-4.92052	4.26382
H	-5.13164	-4.90953	3.66097
H	-0.94215	-4.72877	4.61583
H	-3.22892	-5.56928	5.11893
C	2.04348	-0.55274	-2.00094
C	2.63842	0.20148	-3.03198
C	0.77286	-1.10168	-2.26033
C	2.01901	0.37494	-4.26685
H	3.5945	0.67509	-2.84781
C	0.13957	-0.92187	-3.49525
C	0.76545	-0.19074	-4.50084
H	2.51041	0.96215	-5.03587
H	-0.83993	-1.35987	-3.65559
H	0.26535	-0.05239	-5.45473
C	-1.62099	-3.2967	-0.62166
C	-2.1972	-4.56905	-0.77799
C	-0.54277	-2.95942	-1.46062
C	-1.75285	-5.46528	-1.74672
H	-3.01266	-4.85432	-0.12077
C	-0.09207	-3.8514	-2.4428
C	-0.69998	-5.09572	-2.58517
H	-2.22235	-6.43899	-1.84657
H	0.72854	-3.56992	-3.092
H	-0.33906	-5.77929	-3.34831
O	0.09699	-1.7499	-1.23243
Rh	2.07098	1.24906	0.98261
H	3.35851	1.03977	1.79249
Cl	3.15701	2.74933	-0.65245
C	0.82439	-0.02384	2.32055
C	0.00694	1.09843	2.514
H	1.31984	-0.43901	3.19291
H	0.52749	-0.7473	1.5683
H	-0.18735	1.47726	3.50919
C	-0.85648	1.63408	1.40123
H	-1.84158	1.14219	1.42427
H	-1.02894	2.70205	1.5542
N	-0.15693	1.44311	0.11245
H	-0.40061	0.52526	-0.25499
C	-0.4357	2.47077	-0.92345
H	0.12658	2.16342	-1.8097
H	0.01319	3.40441	-0.58112
C	-1.89973	2.68264	-1.25332
C	-2.56139	3.84948	-0.86193
C	-2.63618	1.71759	-1.96223
C	-3.91269	4.06192	-1.15658
H	-2.01406	4.61864	-0.32235
C	-3.97806	1.90776	-2.26029
H	-2.14617	0.80428	-2.2923
C	-4.62703	3.08503	-1.85666
H	-4.38706	4.98312	-0.83887
H	-4.54893	1.15969	-2.79953
O	-5.94795	3.18024	-2.19807
C	-6.64365	4.36387	-1.84592
H	-7.66171	4.23986	-2.21935
H	-6.67505	4.50987	-0.75796
H	-6.1956	5.25203	-2.3104

9^{L1}

Sum of electronic and thermal Free Energies= -3904.239900

P	-3.59957	1.16505	-0.56644
P	0.45511	-2.43126	0.39358
C	-4.52415	2.76569	-0.73607
C	-5.89752	2.88213	-0.99823
C	-3.7574	3.94255	-0.6568
C	-6.48863	4.13775	-1.1598
H	-6.51005	1.99077	-1.08183
C	-4.34973	5.19637	-0.80163
H	-2.68614	3.87327	-0.48527
C	-5.71955	5.29704	-1.0568
H	-7.55284	4.20756	-1.36844
H	-3.73995	6.09256	-0.73081
H	-6.18191	6.27174	-1.18252
C	-4.87228	-0.09023	-1.05072
C	-5.9411	-0.49301	-0.23123
C	-4.75142	-0.65448	-2.33247
C	-6.87048	-1.43118	-0.685
H	-6.0489	-0.06818	0.76532
C	-5.69001	-1.58365	-2.78954
H	-3.91482	-0.36981	-2.96477
C	-6.74884	-1.97433	-1.96779

H	-7.69183	-1.73366	-0.03923
H	-5.58905	-2.00593	-3.78512
H	-7.47523	-2.70125	-2.32177
C	1.10055	-1.9634	2.07282
C	0.48306	-2.39068	3.25915
C	2.2625	-1.1812	2.17258
C	1.00212	-2.02931	4.50438
H	-0.40115	-3.01747	3.2105
C	2.78436	-0.82188	3.41645
H	2.78137	-0.87068	1.27219
C	2.15025	-1.24003	4.58743
H	0.50948	-2.37132	5.4103
H	3.68673	-0.21928	3.46751
H	2.55176	-0.95921	5.55674
C	1.44208	-3.9449	-0.01044
C	2.3721	-4.50422	0.87733
C	1.25348	-4.55246	-1.26479
C	3.0975	-5.64303	0.51917
H	2.53378	-4.05727	1.85185
C	1.96931	-5.69634	-1.61348
H	0.54734	-4.12029	-1.9666
C	2.8973	-6.24228	-0.724
H	3.81761	-6.06046	1.21665
H	1.80929	-6.15328	-2.5857
H	3.4623	-7.12738	-1.00094
C	-3.55585	0.9745	1.2834
C	-4.18493	1.85461	2.18152
C	-2.76787	-0.05104	1.8379
C	-4.04704	1.71121	3.56263
H	-4.79799	2.65783	1.78518
C	-2.60797	-0.19426	3.21695
C	-3.25207	0.68849	4.08214
H	-4.55531	2.40137	4.2297
H	-1.97083	-0.9839	3.60007
H	-3.12535	0.57899	5.15533
C	-1.21124	-3.12909	0.80256
C	-1.44329	-4.51226	0.85342
C	-2.295	-2.27087	1.07034
C	-2.70153	-5.02925	1.15849
H	-0.62463	-5.19391	0.65457
C	-3.55864	-2.7817	1.37743
C	-3.75903	-4.15869	1.41862
H	-2.8508	-6.10355	1.18978
H	-4.37869	-2.09863	1.55982
H	-4.74756	-4.5466	1.64579
O	-2.07798	-0.9081	0.97694
Rh	0.25459	-0.88865	-1.31456
H	-0.39774	-2.09884	-2.03475
Cl	-0.45532	0.42198	-3.21478
C	2.57472	1.03041	-1.4213
H	3.3569	1.69377	-1.03402
H	2.23703	1.41571	-2.38745
N	1.39227	0.98894	-0.52463
H	1.71365	0.79075	0.42113
C	0.62639	2.26658	-0.47656
H	-0.20381	2.09999	0.21782
H	0.19463	2.40734	-1.47054
C	1.44219	3.47064	-0.04874
C	1.73906	3.70004	1.29912
C	1.95385	4.37663	-0.99342
C	2.52792	4.7794	1.70713
H	1.34353	3.02648	2.05766
C	2.73806	5.45739	-0.60868
H	1.73119	4.22997	-2.04748
C	3.0353	5.66368	0.74658
H	2.7315	4.92326	2.76205
H	3.13367	6.15681	-1.33865
O	3.81713	6.749	1.02433
C	4.17175	6.99316	2.37527
H	4.79765	7.88732	2.36623
H	3.28861	7.17858	3.00159
H	4.74327	6.15807	2.80301
C	2.04951	-1.30786	-2.22228
H	2.32185	-2.35869	-2.12442
H	1.86346	-1.06513	-3.27165
C	3.1016	-0.39404	-1.61052
H	3.44168	-0.80014	-0.65189
S	4.62784	-0.40392	-2.69455
C	5.90406	0.0135	-1.49977
C	6.47931	1.29169	-1.49997
C	6.36829	-0.94722	-0.58868
C	7.49878	1.60515	-0.59807
H	6.12532	2.03354	-2.20818
C	7.37708	-0.62589	0.31996
H	5.94293	-1.94625	-0.6051
C	7.94598	0.65017	0.31575
H	7.93955	2.59795	-0.60853
H	7.72944	-1.37691	1.02132

H	8.73796	0.89601	1.01752

10^{L1}

Sum of electronic and thermal Free Energies= -3904.236957

P	-2.73534	1.17268	-0.92305
P	-0.87845	-1.6989	0.9821
C	-2.87383	2.44001	-2.26722
C	-3.83903	2.37298	-3.28231
C	-1.97008	3.51617	-2.26508
C	-3.90247	3.36054	-4.26833
H	-4.54687	1.55311	-3.31264
C	-2.04943	4.51057	-3.23856
H	-1.1898	3.56126	-1.51462
C	-3.01265	4.43326	-4.2465
H	-4.65113	3.28651	-5.05152
H	-1.34055	5.33289	-3.22235
H	-3.06295	5.2005	-5.0141
C	-4.10177	0.00562	-1.39551
C	-5.40391	0.09666	-0.87917
C	-3.83221	-0.97861	-2.36601
C	-6.40269	-0.78223	-1.30436
H	-5.64533	0.85905	-0.14395
C	-4.8322	-1.85086	-2.79693
H	-2.83928	-1.05218	-2.80229
C	-6.12038	-1.75972	-2.26173
H	-7.404	-0.69729	-0.88834
H	-4.60305	-2.60009	-3.55222
H	-6.89838	-2.44197	-2.59264
C	-0.16824	-1.23642	2.62929
C	-0.53264	-1.92891	3.79684
C	0.68468	-0.13091	2.73288
C	-0.02743	-1.53865	5.03659
H	-1.21992	-2.76767	3.74055
C	1.185	0.26175	3.97703
H	0.96737	0.41822	1.83927
C	0.83468	-0.4429	5.129
H	-0.31371	-2.08525	5.931
H	1.84441	1.12282	4.04239
H	1.22391	-0.13698	6.09585
C	-0.34061	-3.44291	0.69022
C	0.53006	-4.13427	1.54408
C	-0.80253	-4.09033	-0.46962
C	0.918	-5.44519	1.25209
H	0.90675	-3.6564	2.44134
C	-0.42488	-5.40202	-0.75217
H	-1.46126	-3.56379	-1.15455
C	0.4392	-6.08349	0.1088
H	1.59396	-5.96574	1.92455
H	-0.79628	-5.88694	-1.65009
H	0.74033	-7.10263	-0.11514
C	-3.4576	2.10973	0.51283
C	-4.07819	3.36384	0.39116
C	-3.29119	1.60057	1.81159
C	-4.49677	4.07803	1.51463
H	-4.22112	3.7903	-0.59491
C	-3.68161	2.31288	2.94403
C	-4.29076	3.55876	2.79296
H	-4.97385	5.04506	1.38784
H	-3.49728	1.88559	3.92411
H	-4.5989	4.11963	3.67008
C	-2.65576	-1.9238	1.47874
C	-3.32761	-3.15328	1.47362
C	-3.361	-0.79438	1.93275
C	-4.65563	-3.2546	1.89329
H	-2.8099	-4.04417	1.13859
C	-4.68407	-0.8838	2.3641
C	-5.3302	-2.11917	2.33753
H	-5.15448	-4.21846	1.87516
H	-5.19867	0.00462	2.71214
H	-6.36173	-2.18896	2.67022
O	-2.6435	0.38418	1.97321
Rh	-0.34008	-0.23379	-0.75184
H	-1.18435	-1.1317	-1.61691
Cl	0.47512	1.4249	-2.30463
C	3.07541	-0.96982	0.34946
H	2.53727	-1.37777	1.21308
H	4.13855	-1.23651	0.49151
N	2.86537	0.48065	0.39338
H	3.10663	0.76124	1.34155
C	3.71146	1.29011	-0.51636
H	3.13765	1.48278	-1.42978
H	4.6133	0.736	-0.81202
C	4.13441	2.58526	0.14447
C	5.47322	2.98639	0.13957
C	3.20779	3.41314	0.80438
C	5.89764	4.16407	0.76494
H	6.21199	2.36651	-0.36183
C	3.6135	4.5785	1.44575
H	2.15592	3.13541	0.80908

C	4.96534	4.96201	1.43273
H	6.94668	4.43565	0.73352
H	2.90102	5.21499	1.96158
O	5.26556	6.12101	2.09837
C	6.6101	6.57085	2.08493
H	6.62469	7.4977	2.66142
H	7.28955	5.84648	2.55431
H	6.9594	6.77469	1.06375
C	1.20739	-1.45289	-1.52228
H	0.74456	-2.40829	-1.77475
H	1.35667	-0.89575	-2.44534
C	2.57485	-1.75796	-0.87131
H	2.56864	-2.80155	-0.54307
S	3.74125	-1.68881	-2.33613
C	5.26837	-2.48319	-1.86203
C	6.39917	-2.14448	-2.62798
C	5.40117	-3.45044	-0.85445
C	7.62306	-2.76962	-2.4021
H	6.31044	-1.38917	-3.40418
C	6.63706	-4.05895	-0.62201
H	4.54416	-3.74036	-0.25507
C	7.75176	-3.72864	-1.39389
H	8.48159	-2.49754	-3.0109
H	6.72272	-4.80424	0.16468
H	8.7085	-4.20965	-1.21284

TS7^{L1}

Sum of electronic and thermal Free Energies= -3904.205177

P	-2.37326	1.47758	-0.32362
P	-1.0019	-1.87924	0.46574
C	-2.34257	3.12046	-1.19325
C	-3.32984	3.51132	-2.10649
C	-1.29612	4.0129	-0.91106
C	-3.27159	4.76546	-2.72347
H	-4.14591	2.8415	-2.34955
C	-1.24512	5.26632	-1.51587
H	-0.51542	3.72621	-0.21347
C	-2.23419	5.64701	-2.42948
H	-4.04351	5.04781	-3.43586
H	-0.42756	5.94239	-1.28234
H	-2.19147	6.62143	-2.90928
C	-4.02145	0.81252	-0.85696
C	-5.22805	1.14804	-0.22632
C	-4.05566	-0.0029	-1.99867
C	-6.44243	0.66605	-0.71813
H	-5.22383	1.78758	0.64988
C	-5.27199	-0.4723	-2.49606
H	-3.1207	-0.2542	-2.49167
C	-6.46764	-0.14442	-1.85351
H	-7.36892	0.92806	-0.21435
H	-5.28405	-1.09568	-3.38552
H	-7.4138	-0.51642	-2.23654
C	-0.0007	-2.169	2.01807
C	-0.56849	-2.71555	3.17993
C	1.37008	-1.87927	2.03159
C	0.20706	-2.94226	4.31762
H	-1.62231	-2.96883	3.20078
C	2.15194	-2.11401	3.16424
H	1.83993	-1.4853	1.14227
C	1.5695	-2.63891	4.31658
H	-0.25737	-3.35907	5.20664
H	3.2135	-1.88576	3.14006
H	2.17125	-2.81628	5.20319
C	-0.85234	-3.53196	-0.37758
C	-0.08808	-4.58514	0.14402
C	-1.53314	-3.7373	-1.59175
C	-0.00084	-5.80564	-0.53205
H	0.44404	-4.46164	1.08046
C	-1.45625	-4.959	-2.25838
H	-2.11933	-2.92946	-2.01988
C	-0.68408	-5.99753	-1.73198
H	0.60349	-6.60585	-0.11411
H	-1.99073	-5.09518	-3.19451
H	-0.61395	-6.94575	-2.25666
C	-2.71904	2.10238	1.41555
C	-3.10816	3.4275	1.68557
C	-2.52692	1.27032	2.52989
C	-3.2566	3.89798	2.99137
H	-3.28554	4.1066	0.86135
C	-2.64186	1.73107	3.84104
C	-3.00669	3.05572	4.07451
H	-3.55724	4.92819	3.15712
H	-2.44458	1.04064	4.65472
H	-3.10066	3.42172	5.09263
C	-2.71994	-1.99838	1.15377
C	-3.63754	-3.01742	0.86652
C	-3.13041	-0.9753	2.01989
C	-4.92489	-2.99804	1.40754
H	-3.34837	-3.83207	0.21328

C	-4.40909	-0.9431	2.57389
C	-5.30919	-1.9602	2.25612
H	-5.6221	-3.79406	1.16506
H	-4.69012	-0.13586	3.24127
H	-6.30894	-1.94093	2.68024
O	-2.1552	-0.04813	2.33624
Rh	-0.54554	-0.09178	-0.99381
H	-0.62008	-1.19761	-2.11794
Cl	-0.27703	1.4574	-2.88859
C	2.57797	0.27644	-1.32452
H	3.64977	0.30828	-1.08886
H	2.41188	0.87018	-2.22741
N	1.76582	0.87103	-0.2475
H	2.00713	0.43235	0.63728
C	1.95985	2.32949	-0.09698
H	1.27478	2.65392	0.69447
H	1.62668	2.78928	-1.03198
C	3.37085	2.77081	0.24912
C	3.83306	2.7192	1.56847
C	4.26439	3.21951	-0.73817
C	5.13751	3.08515	1.90913
H	3.15915	2.39256	2.35926
C	5.56566	3.58854	-0.42133
H	3.93052	3.28386	-1.77117
C	6.01291	3.52008	0.90656
H	5.45284	3.0352	2.94521
H	6.25603	3.93589	-1.18409
O	7.30699	3.90239	1.11786
C	7.81756	3.84616	2.43817
H	8.8566	4.17602	2.3768
H	7.26859	4.51247	3.11572
H	7.78814	2.82606	2.84061
C	0.80754	-1.36544	-2.29832
H	0.64723	-2.43834	-2.41425
H	0.82062	-0.89609	-3.2816
C	2.16598	-1.17187	-1.61533
H	2.22371	-1.77952	-0.7102
S	3.44418	-1.95543	-2.76551
C	4.79545	-2.28331	-1.62873
C	5.95175	-1.49036	-1.66114
C	4.72858	-3.35926	-0.73016
C	7.02172	-1.76695	-0.80633
H	6.00502	-0.65969	-2.35738
C	5.79448	-3.62457	0.13151
H	3.84382	-3.9895	-0.71981
C	6.94422	-2.83089	0.09357
H	7.91297	-1.14631	-0.8418
H	5.7333	-4.46045	0.82305
H	7.77675	-3.04435	0.75898

11^{L1}

Sum of electronic and thermal Free Energies= -3904.260473

P	-2.83679	-0.73727	-0.77902
P	-0.62785	1.20555	1.12847
C	-3.29987	-2.10005	-1.95744
C	-3.74303	-3.35159	-1.51095
C	-3.19226	-1.8814	-3.34248
C	-4.0765	-4.35743	-2.42327
H	-3.83366	-3.55476	-0.45082
C	-3.54222	-2.8793	-4.24939
H	-2.82813	-0.93115	-3.71284
C	-3.98285	-4.12339	-3.79315
H	-4.41608	-5.32117	-2.05514
H	-3.45243	-2.68899	-5.31472
H	-4.24579	-4.9038	-4.50213
C	-3.49743	-1.4256	0.81348
C	-4.83497	-1.29797	1.21298
C	-2.62817	-2.19909	1.59894
C	-5.28972	-1.92096	2.37659
H	-5.52692	-0.71394	0.61423
C	-3.08577	-2.83343	2.75449
H	-1.59298	-2.30245	1.28534
C	-4.41846	-2.69166	3.14846
H	-6.32824	-1.80724	2.67581
H	-2.40302	-3.439	3.34507
H	-4.7762	-3.18113	4.04961
C	-0.20454	2.96159	0.67919
C	-0.04498	3.96584	1.64796
C	-0.13333	3.31256	-0.6761
C	0.21084	5.28343	1.26761
H	-0.12976	3.7212	2.70334
C	0.11277	4.63462	-1.05756
H	-0.30407	2.54138	-1.42295
C	0.2923	5.62023	-0.08686
H	0.33642	6.04881	2.02807
H	0.15341	4.89285	-2.1126
H	0.48287	6.64845	-0.38213
C	0.6584	0.75772	2.394
C	1.84284	1.4853	2.59127

C	0.49149	-0.44559	3.10642
C	2.82421	1.03005	3.4785
H	2.00882	2.41404	2.05609
C	1.4612	-0.88789	4.00482
H	-0.40523	-1.03892	2.95625
C	2.63547	-0.15228	4.19149
H	3.7357	1.60682	3.60913
H	1.3057	-1.81401	4.55109
H	3.39697	-0.50371	4.8816
C	-4.138	0.54351	-1.23156
C	-5.18779	0.2635	-2.12491
C	-4.08711	1.85387	-0.72232
C	-6.10231	1.24183	-2.52032
H	-5.28557	-0.73513	-2.53087
C	-4.97497	2.8493	-1.13123
C	-5.98888	2.54431	-2.03748
H	-6.895	0.98187	-3.21539
H	-4.85188	3.8504	-0.73068
H	-6.6832	3.31639	-2.35657
C	-2.1123	1.52723	2.19329
C	-2.18827	1.37255	3.58317
C	-3.25902	1.97333	1.51991
C	-3.37863	1.62744	4.26821
H	-1.31616	1.04459	4.13732
C	-4.45613	2.22737	2.18658
C	-4.51082	2.0459	3.56892
H	-3.41807	1.49762	5.34559
H	-5.32467	2.56443	1.63138
H	-5.43907	2.24241	4.09792
O	-3.0889	2.20849	0.16825
Rh	-0.57101	-0.19612	-0.6983
Cl	-0.19255	-1.37691	-2.79597
C	2.52028	-0.97325	-0.04689
H	2.20972	-1.01494	0.99712
H	3.56964	-0.66672	-0.05721
N	1.70481	0.10437	-0.69273
H	1.82931	0.9127	-0.08455
C	2.25982	0.53388	-2.02722
H	1.49039	1.14757	-2.49923
H	2.35451	-0.35854	-2.646
C	3.56535	1.29927	-1.94884
C	3.56058	2.69102	-1.79918
C	4.81313	0.65774	-2.06414
C	4.74434	3.43359	-1.75856
H	2.61269	3.2175	-1.72693
C	6.00091	1.37932	-2.01517
H	4.85201	-0.42138	-2.20408
C	5.97497	2.77491	-1.86662
H	4.69227	4.51158	-1.66003
H	6.96401	0.8856	-2.11334
O	7.19324	3.39414	-1.84968
C	7.22261	4.81227	-1.82917
H	8.27654	5.09376	-1.86155
H	6.70718	5.23879	-2.7002
H	6.7705	5.2198	-0.91482
S	3.96789	-3.13585	-1.23251
C	4.84241	-3.48659	0.29841
C	5.68954	-2.53219	0.8808
C	4.75489	-4.76258	0.87471
C	6.41992	-2.84427	2.02858
H	5.78641	-1.55304	0.42387
C	5.49144	-5.07368	2.01868
H	4.11768	-5.50907	0.41263
C	6.32353	-4.11494	2.59884
H	7.07485	-2.0979	2.46902
H	5.42095	-6.06806	2.45053
H	6.9023	-4.36009	3.48484
C	1.51816	-3.31469	0.17333
H	0.54061	-2.84892	0.34653
H	1.35419	-4.27097	-0.33145
H	1.99556	-3.50398	1.1432
C	2.3537	-2.36968	-0.69241
H	1.83795	-2.26296	-1.65373

P1

Sum of electronic and thermal Free Energies= -1188.342216

C	-5.01429	-0.92534	0.39067
C	-3.88113	-1.63031	-0.00111
C	-2.81711	-0.99419	-0.65531
C	-2.9189	0.37986	-0.89037
C	-4.04694	1.10609	-0.50255
C	-5.10627	0.44995	0.13717
H	-5.83873	-1.4164	0.89773
H	-3.82281	-2.69713	0.20441
H	-2.09155	0.88801	-1.37698
H	-4.08981	2.17066	-0.70326
O	-6.25923	1.05764	0.55407
C	-6.41826	2.44152	0.28477
H	-7.40136	2.71418	0.67167

H	-5.6538	3.0449	0.79099
H	-6.38343	2.65197	-0.79288
C	-1.60915	-1.77595	-1.14068
H	-1.68017	-1.91212	-2.22726
H	-1.64247	-2.78941	-0.70003
N	-0.34663	-1.08301	-0.87975
H	0.38326	-1.46136	-1.47858
C	0.08467	-1.16059	0.5114
H	0.20641	-2.20047	0.87279
H	-0.69944	-0.70973	1.13176
C	1.68825	-0.23391	2.25099
H	2.62954	0.29861	2.40773
H	0.89218	0.33365	2.74819
H	1.76703	-1.214	2.73409
C	1.37809	-0.38008	0.7628
H	1.26501	0.60357	0.29771
S	2.75127	-1.25441	-0.14712
C	4.06571	-0.03683	-0.15793
C	5.35501	-0.44882	0.2085
C	3.86053	1.28663	-0.57488
C	6.42098	0.45077	0.15747
H	5.51677	-1.47297	0.53485
C	4.92452	2.18771	-0.59716
H	2.87427	1.6111	-0.89135
C	6.20867	1.77361	-0.23487
H	7.41564	0.1172	0.44064
H	4.75114	3.21285	-0.91415
H	7.03591	2.47673	-0.26208

TS3$^{L1'}$

Sum of electronic and thermal Free Energies= -3904.220451

S	-4.81898	-0.10505	-0.03335
C	-5.84368	1.2487	0.52609
C	-5.61496	1.91069	1.74694
C	-6.96908	1.60945	-0.23766
C	-6.4884	2.90899	2.17954
H	-4.74038	1.64407	2.33133
C	-7.84998	2.59625	0.21141
H	-7.15462	1.09778	-1.17749
C	-7.61093	3.25302	1.41942
H	-6.29639	3.41367	3.12297
H	-8.72018	2.85389	-0.38723
H	-8.29298	4.02454	1.76744
P	-1.79965	-1.47286	-0.47936
P	3.65353	-0.62668	0.09062
C	-3.02389	-2.7763	-0.97299
C	-3.13701	-4.01814	-0.33176
C	-3.81407	-2.52672	-2.10596
C	-4.01956	-4.98601	-0.81465
H	-2.54478	-4.23169	0.55118
C	-4.68869	-3.49693	-2.59043
H	-3.75265	-1.56405	-2.60212
C	-4.79534	-4.72963	-1.94531
H	-4.09943	-5.94052	-0.30278
H	-5.2955	-3.28368	-3.4657
H	-5.483	-5.48278	-2.31788
C	-0.48766	-1.83859	-1.73647
C	-0.02114	-3.1455	-1.94837
C	-0.02536	-0.8187	-2.57569
C	0.9068	-3.41379	-2.95164
H	-0.38971	-3.959	-1.3319
C	0.89945	-1.08578	-3.58874
H	-0.40693	0.18588	-2.44206
C	1.37154	-2.38387	-3.77511
H	1.26422	-4.42933	-3.09447
H	1.24282	-0.28126	-4.23386
H	2.08781	-2.59745	-4.56331
C	3.81223	-0.05687	1.84555
C	4.11518	-0.89708	2.9297
C	3.58675	1.30621	2.0938
C	4.18535	-0.38712	4.22679
H	4.29501	-1.95368	2.75968
C	3.66582	1.81679	3.38866
H	3.33906	1.97053	1.26992
C	3.96084	0.97021	4.45947
H	4.41627	-1.05134	5.05614
H	3.48398	2.8732	3.56054
H	4.00917	1.36397	5.4698
C	5.39728	-0.53136	-0.53127
C	6.52229	-0.30489	0.27596
C	5.58138	-0.64166	-1.9202
C	7.79512	-0.20009	-0.28945
H	6.40418	-0.20616	1.34975
C	6.85374	-0.55189	-2.48344
H	4.71828	-0.79814	-2.5633
C	7.9656	-0.32727	-1.66803
H	8.65479	-0.02086	0.35073
H	6.97658	-0.64579	-3.55854
H	8.95656	-0.24597	-2.10535

C	-1.2297	-2.03044	1.1836
C	-2.25056	-2.12633	2.15221
C	0.0913	-2.23526	1.61149
C	-1.97668	-2.48182	3.46725
H	-3.27236	-1.89747	1.86412
C	0.37535	-2.56824	2.94133
C	-0.6559	-2.70521	3.8627
H	-2.78752	-2.55224	4.18558
H	1.41029	-2.69723	3.23898
H	-0.4247	-2.95992	4.89277
C	3.43728	-2.45831	0.3004
C	4.46343	-3.39606	0.11285
C	2.15642	-2.94869	0.62194
C	4.23644	-4.76653	0.24914
H	5.45821	-3.0434	-0.13745
C	1.9183	-4.31849	0.7641
C	2.96152	-5.22486	0.57942
H	5.05267	-5.46784	0.1043
H	0.92423	-4.66549	1.02289
H	2.77072	-6.28851	0.68993
O	1.14084	-2.01871	0.7316
Rh	-2.63319	0.81733	-0.44066
H	-3.04318	0.80937	-2.01255
Cl	-2.13258	1.20077	1.9689
C	-3.4845	2.29224	-1.94323
C	-3.11145	2.89775	-0.71029
H	-4.54161	2.13119	-2.13196
H	-2.89026	2.48355	-2.83764
H	-3.87791	3.21827	-0.01489
C	-1.68804	3.37721	-0.51868
H	-1.40482	4.25227	-1.12157
H	-1.53562	3.61358	0.52879
N	-0.84626	2.17989	-0.84423
H	-0.63754	2.1925	-1.83978
C	0.44645	2.08137	-0.11053
H	0.88923	1.11773	-0.3721
H	0.19409	2.04663	0.95426
C	1.39893	3.20847	-0.44615
C	1.44447	4.38592	0.312
C	2.24887	3.11511	-1.56265
C	2.28374	5.45099	-0.03171
H	0.81921	4.47743	1.19779
C	3.08929	4.16182	-1.9201
H	2.26695	2.19661	-2.13434
C	3.10479	5.34464	-1.16108
H	2.28591	6.34556	0.57337
H	3.75248	4.08786	-2.77209
O	3.95486	6.3193	-1.59587
C	4.01079	7.53959	-0.87145
H	4.72952	8.17061	-1.39711
H	3.03636	8.04503	-0.85077
H	4.3535	7.38326	0.16017

5$^{Li'}$

Sum of electronic and thermal Free Energies= -3904.231231

S	-4.85303	-0.33549	-0.18949
C	-6.17494	0.78252	0.26615
C	-6.25617	1.36102	1.5438
C	-7.20961	1.01888	-0.65428
C	-7.34498	2.16447	1.88156
H	-5.45739	1.18486	2.2559
C	-8.3044	1.81011	-0.30263
H	-7.1562	0.57041	-1.64214
C	-8.37571	2.38944	0.96504
H	-7.39246	2.60863	2.87257
H	-9.09934	1.97663	-1.02496
H	-9.22603	3.00756	1.23762
P	-1.63544	-1.58165	-0.42146
P	3.92431	-0.4007	-0.02069
C	-2.7013	-3.05474	-0.78733
C	-2.67336	-4.25025	-0.05514
C	-3.55452	-2.96708	-1.8999
C	-3.47755	-5.33018	-0.42733
H	-2.02987	-4.34201	0.81266
C	-4.35094	-4.04807	-2.27385
H	-3.60462	-2.04557	-2.47159
C	-4.31675	-5.23355	-1.53703
H	-3.44497	-6.24742	0.15414
H	-5.00725	-3.95887	-3.13461
H	-4.94376	-6.0732	-1.82313
C	-0.36977	-1.77418	-1.76513
C	-0.00388	-3.02741	-2.28174
C	0.18262	-0.62577	-2.34791
C	0.90343	-3.12373	-3.33691
H	-0.4364	-3.93176	-1.86674
C	1.09227	-0.71924	-3.40226
H	-0.10246	0.34802	-1.96966
C	1.4556	-1.97113	-3.89953
H	1.17721	-4.10221	-3.72106

H	1.50821	0.18464	-3.83918
H	2.15747	-2.04869	-4.72508
C	4.04938	-0.10946	1.80703
C	4.51988	-1.06503	2.72326
C	3.6298	1.13806	2.29513
C	4.57221	-0.77797	4.08889
H	4.84261	-2.03884	2.36637
C	3.68543	1.42679	3.66072
H	3.24863	1.8846	1.60337
C	4.15501	0.46925	4.56046
H	4.93834	-1.52847	4.78437
H	3.35184	2.39583	4.02168
H	4.19058	0.69005	5.62381
C	5.68036	-0.20334	-0.58946
C	6.7954	-0.13091	0.26016
C	5.88456	-0.05841	-1.97321
C	8.076	0.07068	-0.25963
H	6.66483	-0.22688	1.33305
C	7.16491	0.12958	-2.49416
H	5.03077	-0.09034	-2.64654
C	8.26552	0.19768	-1.63637
H	8.92634	0.12807	0.4149
H	7.30252	0.23502	-3.56691
H	9.26244	0.35541	-2.03839
C	-0.86873	-2.01812	1.20194
C	-1.78109	-2.14766	2.26937
C	0.49695	-2.15322	1.49924
C	-1.35988	-2.46941	3.55518
H	-2.83816	-1.9889	2.07956
C	0.929	-2.46456	2.79394
C	0.00248	-2.63458	3.8164
H	-2.09036	-2.56881	4.35178
H	1.99349	-2.54177	2.98629
H	0.34671	-2.86874	4.81966
C	3.71712	-2.24544	-0.06758
C	4.72522	-3.14797	-0.43574
C	2.45439	-2.77754	0.25805
C	4.49783	-4.5255	-0.45898
H	5.70567	-2.76544	-0.69882
C	2.21869	-4.15333	0.25178
C	3.2455	-5.02672	-0.10537
H	5.29907	-5.20113	-0.74314
H	1.23708	-4.5279	0.52031
H	3.05902	-6.09663	-0.1147
O	1.44251	-1.8747	0.52475
Rh	-2.81981	0.78336	-0.21301
H	-3.40362	1.97082	-2.57725
Cl	-2.64357	1.17615	2.09577
C	-3.9498	2.71345	-1.9678
C	-3.48296	2.72106	-0.51786
H	-5.01088	2.46186	-2.0372
H	-3.78328	3.69218	-2.45437
H	-4.2549	3.03113	0.18646
C	-2.12693	3.36642	-0.26823
H	-1.90632	4.2548	-0.87943
H	-2.0314	3.63424	0.78467
N	-1.15623	2.25105	-0.53098
H	-0.91775	2.25728	-1.52145
C	0.11182	2.28967	0.25089
H	0.62138	1.33555	0.08681
H	-0.17572	2.32815	1.30386
C	1.019	3.43752	-0.13897
C	0.94318	4.68655	0.48551
C	1.9463	3.28409	-1.18576
C	1.74093	5.761	0.079
H	0.25174	4.8305	1.31127
C	2.74818	4.33941	-1.60252
H	2.05406	2.31328	-1.66483
C	2.645	5.59136	-0.97624
H	1.65256	6.71166	0.59011
H	3.47031	4.21952	-2.40371
O	3.4696	6.56502	-1.4593
C	3.41508	7.84969	-0.85972
H	4.15221	8.45735	-1.38676
H	2.42302	8.30939	-0.96903
H	3.67481	7.80814	0.20459

TS4$^{Li'}$

Sum of electronic and thermal Free Energies= -3904.173527

S	-4.66261	1.14072	-1.86836
C	-6.27209	1.21407	-1.10048
C	-6.84176	0.07062	-0.51583
C	-7.02079	2.40385	-1.14953
C	-8.13176	0.11831	0.00822
H	-6.25819	-0.84517	-0.46462
C	-8.31043	2.44808	-0.61571
H	-6.59357	3.29017	-1.61551
C	-8.8693	1.30581	-0.0363
H	-8.55849	-0.77388	0.45708

H	-8.87806	3.37284	-0.65461
H	-9.87271	1.3375	0.37757
P	-1.64435	-1.57218	0.30005
P	4.00407	-0.57208	-0.62529
C	-2.48074	-3.17857	0.67458
C	-2.07187	-4.06211	1.68142
C	-3.58226	-3.52558	-0.12308
C	-2.74543	-5.27106	1.88033
H	-1.23953	-3.80282	2.32596
C	-4.24732	-4.73564	0.07066
H	-3.91913	-2.83232	-0.88834
C	-3.83027	-5.61203	1.07428
H	-2.42186	-5.94349	2.6689
H	-5.09689	-4.98905	-0.55557
H	-4.35382	-6.55146	1.23135
C	-0.63915	-1.95215	-1.19604
C	-0.34723	-3.2569	-1.62109
C	-0.26694	-0.86556	-2.00793
C	0.32494	-3.46861	-2.82486
H	-0.64419	-4.10617	-1.01489
C	0.40055	-1.08543	-3.21493
H	-0.48769	0.14791	-1.67546
C	0.69891	-2.38558	-3.62471
H	0.5551	-4.48219	-3.14013
H	0.68728	-0.23964	-3.83375
H	1.21448	-2.55702	-4.56583
C	4.69257	0.15802	0.93679
C	5.33624	-0.58535	1.94102
C	4.53438	1.54055	1.12384
C	5.81067	0.03946	3.09621
H	5.46457	-1.65691	1.82022
C	5.01338	2.16671	2.27629
H	4.0233	2.13164	0.36894
C	5.65096	1.41706	3.2659
H	6.30649	-0.55005	3.86301
H	4.87637	3.23701	2.40244
H	6.0175	1.90115	4.16689
C	5.50936	-0.76897	-1.69067
C	6.82645	-0.52586	-1.27339
C	5.28671	-1.12569	-3.03301
C	7.89081	-0.64487	-2.17084
H	7.02413	-0.23935	-0.24553
C	6.3502	-1.25886	-3.92453
H	4.2703	-1.29901	-3.37916
C	7.65747	-1.01521	-3.49566
H	8.90423	-0.44916	-1.83073
H	6.15854	-1.54184	-4.95603
H	8.48662	-1.1079	-4.19137
C	-0.55742	-1.32349	1.77811
C	-1.24111	-1.00895	2.97145
C	0.84289	-1.42878	1.83949
C	-0.56525	-0.85484	4.1784
H	-2.31832	-0.87802	2.93594
C	1.52738	-1.26983	3.05081
C	0.82432	-0.99387	4.21879
H	-1.12192	-0.62052	5.08069
H	2.60989	-1.34148	3.05394
H	1.3638	-0.86855	5.15323
C	3.70306	-2.32571	-0.08938
C	4.59975	-3.38471	-0.29599
C	2.49189	-2.61814	0.56419
C	4.31531	-4.67782	0.14736
H	5.53782	-3.1889	-0.80496
C	2.19773	-3.90541	1.01848
C	3.11573	-4.93429	0.81181
H	5.03041	-5.47745	-0.02144
H	1.25336	-4.09414	1.51749
H	2.88476	-5.93642	1.16163
O	1.57138	-1.59292	0.67551
Rh	-3.1071	0.01818	-0.52565
H	-2.58329	3.1659	-2.66004
Cl	-4.22435	0.22132	1.53473
C	-3.12781	3.64393	-1.84048
C	-3.22805	2.74253	-0.62664
H	-4.10569	3.92657	-2.22512
H	-2.56796	4.55314	-1.57517
H	-4.08594	2.91065	0.02235
C	-1.93624	2.684	0.17131
H	-1.79624	3.73525	0.51223
H	-2.05518	2.07008	1.0651
N	-0.78429	2.20356	-0.58434
H	-0.68223	2.75566	-1.43267
C	0.49883	2.24557	0.15113
H	1.17641	1.52566	-0.32372
H	0.30988	1.87576	1.16404
C	1.16739	3.60688	0.18777
C	0.939	4.5347	1.20751
C	2.03021	3.98617	-0.85548

C	1.53169	5.80152	1.19546
H	0.29484	4.2673	2.04005
C	2.63094	5.23721	-0.88426
H	2.24023	3.27923	-1.65428
C	2.38197	6.15758	0.14378
H	1.33037	6.49088	2.00578
H	3.30244	5.52424	-1.68582
O	3.02014	7.3585	0.02961
C	2.80361	8.33459	1.0335
H	3.40246	9.1986	0.74775
H	1.74913	8.62902	1.08979
H	3.13047	7.98478	2.01976

$6^{LI'}$

Sum of electronic and thermal Free Energies= -3904.238849

S	-3.19047	2.55258	0.62326
C	-3.87377	3.95899	1.51989
C	-4.75252	4.84049	0.87104
C	-3.49653	4.22236	2.84494
C	-5.25987	5.95344	1.54294
H	-5.02555	4.65015	-0.16297
C	-4.00461	5.33798	3.51509
H	-2.80219	3.55214	3.34348
C	-4.88845	6.20359	2.86656
H	-5.93898	6.62972	1.02941
H	-3.70838	5.53157	4.543
H	-5.28125	7.07217	3.38787
P	0.37038	0.70778	-1.59381
P	4.4993	-0.56394	1.37704
C	0.84601	2.47105	-1.59664
C	1.99052	2.98564	-0.96547
C	-0.02918	3.34276	-2.26696
C	2.25466	4.35501	-1.01102
H	2.66531	2.32239	-0.43764
C	0.2514	4.70914	-2.31942
H	-0.9296	2.94586	-2.72831
C	1.39015	5.21607	-1.69144
H	3.13736	4.7484	-0.51482
H	-0.42772	5.37677	-2.84155
H	1.60194	6.28133	-1.72621
C	0.22331	0.04069	0.08828
C	0.22729	0.79854	1.29077
C	-0.2305	-1.31548	0.11526
C	-0.18419	0.22527	2.47733
H	0.55439	1.83239	1.26668
C	-0.65341	-1.87192	1.35291
H	-0.0186	-1.98529	-0.71192
C	-0.6371	-1.11484	2.50936
H	-0.16597	0.80907	3.39272
H	-0.95615	-2.91581	1.38529
H	-0.95059	-1.55388	3.45274
C	4.42274	-2.30894	0.76161
C	5.36624	-2.88637	-0.10441
C	3.33781	-3.08967	1.19136
C	5.23282	-4.21281	-0.51984
H	6.20705	-2.29493	-0.45643
C	3.20792	-4.41822	0.78131
H	2.58508	-2.64871	1.83985
C	4.15493	-4.98237	-0.07538
H	5.97109	-4.64582	-1.18995
H	2.36249	-5.00887	1.12387
H	4.05102	-6.01401	-0.40042
C	5.78669	-0.64299	2.71024
C	6.66476	-1.71705	2.92239
C	5.83392	0.44543	3.59949
C	7.57011	-1.69681	3.98573
H	6.63855	-2.57657	2.26025
C	6.74892	0.47348	4.65205
H	5.14313	1.27481	3.46671
C	7.61902	-0.60099	4.84928
H	8.23919	-2.53957	4.13774
H	6.77388	1.32698	5.32423
H	8.32479	-0.58756	5.67509
C	1.52899	-0.24634	-2.65052
C	0.95815	-0.857	-3.78058
C	2.9021	-0.4299	-2.41001
C	1.73325	-1.61705	-4.65598
H	-0.10637	-0.72347	-3.95596
C	3.67896	-1.21248	-3.26872
C	3.09177	-1.79542	-4.39152
H	1.27716	-2.07305	-5.52913
H	4.72923	-1.36793	-3.05081
H	3.70312	-2.40195	-5.05418
C	5.4274	0.28549	0.00958
C	6.73413	0.78406	0.12588
C	4.73994	0.55024	-1.18972
C	7.33164	1.5097	-0.90672
H	7.29034	0.59879	1.03858
C	5.31815	1.28845	-2.22378

C	6.62206	1.76289	-2.08079
H	8.34739	1.87647	-0.79104
H	4.74764	1.48856	-3.12424
H	7.07404	2.33732	-2.8843
O	3.42101	0.12383	-1.25686
Rh	-1.70909	0.02393	-1.20917
H	-3.55755	0.19079	2.4833
Cl	-2.92765	0.64499	-3.17993
C	-4.50514	0.7118	2.31214
C	-4.57035	1.32583	0.90974
H	-4.58771	1.49055	3.07424
H	-5.32856	0.00186	2.46318
H	-5.48569	1.92191	0.83001
C	-4.676	0.28986	-0.21602
H	-5.62802	-0.2353	-0.05368
H	-4.71339	0.78098	-1.19012
N	-3.57614	-0.70854	-0.27859
H	-3.31559	-0.97025	0.6714
C	-3.99397	-1.95701	-0.99386
H	-3.09748	-2.57905	-1.07113
H	-4.2644	-1.65832	-2.00912
C	-5.11517	-2.72998	-0.32896
C	-6.39568	-2.78515	-0.88507
C	-4.89536	-3.4226	0.8753
C	-7.435	-3.49319	-0.27269
H	-6.5921	-2.26737	-1.82092
C	-5.91385	-4.12704	1.50214
H	-3.9051	-3.4143	1.32692
C	-7.19602	-4.16588	0.93075
H	-8.41302	-3.51081	-0.73893
H	-5.74461	-4.66411	2.43026
O	-8.12928	-4.88415	1.62062
C	-9.44282	-4.9611	1.08965
H	-10.01659	-5.56872	1.79135
H	-9.90647	-3.96915	1.00913
H	-9.4535	-5.44207	0.10285

TS6$^{L1'}$

Sum of electronic and thermal Free Energies= -3904.202969

S	3.90958	-0.29796	2.68512
C	4.62758	1.30417	2.37963
C	4.48707	2.33678	3.32334
C	5.41954	1.52796	1.23809
C	5.11072	3.57004	3.12423
H	3.90828	2.16256	4.22649
C	6.04622	2.7596	1.04987
H	5.52659	0.72761	0.51207
C	5.89097	3.7868	1.98648
H	4.99525	4.35714	3.86481
H	6.66059	2.91777	0.16734
H	6.38414	4.74297	1.83616
P	0.99069	-2.47533	-0.39274
P	-3.36638	0.34999	0.91278
C	1.79635	-4.03119	-0.99156
C	1.29555	-4.73065	-2.10207
C	2.85724	-4.58483	-0.26108
C	1.84072	-5.96074	-2.4697
H	0.48673	-4.31354	-2.69374
C	3.39444	-5.81997	-0.62734
H	3.27829	-4.03721	0.5738
C	2.88949	-6.51052	-1.72965
H	1.44607	-6.48686	-3.33499
H	4.22147	-6.23186	-0.05592
H	3.31541	-7.46804	-2.01635
C	-0.45395	-3.20849	0.50406
C	-1.4899	-3.88145	-0.16156
C	-0.44605	-3.20588	1.90511
C	-2.50962	-4.50365	0.55481
H	-1.50702	-3.92209	-1.24502
C	-1.46348	-3.83854	2.62466
H	0.37055	-2.72339	2.43119
C	-2.50112	-4.48213	1.95199
H	-3.31085	-5.00622	0.02112
H	-1.43789	-3.82962	3.71048
H	-3.29362	-4.97352	2.50934
C	-3.35888	2.03825	0.14847
C	-3.95754	2.35891	-1.07959
C	-2.64825	3.04307	0.82931
C	-3.83732	3.64364	-1.61565
H	-4.51472	1.60181	-1.62192
C	-2.5357	4.3284	0.29828
H	-2.16981	2.8117	1.77775
C	-3.12281	4.63024	-0.93222
H	-4.29939	3.87238	-2.57221
H	-1.97029	5.08761	0.83356
H	-3.003	5.62135	-1.36462
C	-4.83565	0.4077	2.0392
C	-5.7912	1.43643	2.05497
C	-4.95392	-0.63639	2.97529

C	-6.84122	1.41779	2.97867
H	-5.71315	2.25608	1.34606
C	-6.01028	-0.66162	3.88732
H	-4.21143	-1.43257	2.98808
C	-6.95556	0.36865	3.89352
H	-7.57124	2.22419	2.9807
H	-6.08944	-1.47871	4.60072
H	-7.77235	0.35601	4.61117
C	0.40594	-1.68693	-1.9663
C	1.38132	-1.58428	-2.98382
C	-0.81985	-1.02535	-2.175
C	1.13083	-0.90112	-4.16987
H	2.35708	-2.03137	-2.81924
C	-1.06981	-0.32268	-3.36265
C	-0.10325	-0.27222	-4.36235
H	1.90067	-0.85032	-4.9338
H	-2.02168	0.18408	-3.48173
H	-0.30699	0.27324	-5.27933
C	-4.00734	-0.69731	-0.47923
C	-5.36271	-1.01224	-0.6571
C	-3.0859	-1.25268	-1.38722
C	-5.7944	-1.83575	-1.69762
H	-6.09024	-0.6017	0.03464
C	-3.50494	-2.08257	-2.43114
C	-4.86095	-2.36847	-2.5851
H	-6.85093	-2.05687	-1.81262
H	-2.77646	-2.4991	-3.11696
H	-5.1804	-3.01481	-3.39752
O	-1.74707	-0.98992	-1.14974
Rh	2.37162	-1.04277	0.84819
H	2.56848	-2.31488	1.70787
Cl	4.24593	-1.56273	-0.65271
C	1.48119	0.22975	3.03
C	0.75164	0.13702	1.84111
H	1.89855	1.17908	3.34408
H	1.3528	-0.50804	3.81493
H	-0.10606	-0.52751	1.81081
C	0.80315	1.30261	0.86277
H	-0.19093	1.59216	0.50728
H	1.24562	2.18092	1.34554
N	1.69622	0.90255	-0.26049
H	1.12994	0.54293	-1.02194
C	2.58499	1.95541	-0.80285
H	3.1395	1.48924	-1.62572
H	3.3179	2.20167	-0.03166
C	1.86963	3.21495	-1.25539
C	2.11949	4.44024	-0.63423
C	0.92048	3.18836	-2.29043
C	1.44873	5.60922	-1.01155
H	2.85828	4.49152	0.16144
C	0.23797	4.33442	-2.67217
H	0.70823	2.25488	-2.80467
C	0.49408	5.55457	-2.02975
H	1.67347	6.54004	-0.50297
H	-0.50156	4.31493	-3.4634
O	-0.24189	6.62152	-2.46865
C	0.04434	7.89956	-1.92402
H	-0.61395	8.60118	-2.44138
H	-0.16228	7.94207	-0.84447
H	1.09006	8.18777	-2.09738

9$^{Li'}$

Sum of electronic and thermal Free Energies= -3904.223636

S	3.72247	-0.31401	2.67703
C	4.76778	1.1071	2.32849
C	4.77186	2.24406	3.14606
C	5.67894	0.99283	1.26903
C	5.66984	3.28074	2.88367
H	4.09205	2.32022	3.98947
C	6.5835	2.02857	1.03032
H	5.64926	0.11488	0.62752
C	6.57879	3.17472	1.82855
H	5.66729	4.16431	3.51601
H	7.28587	1.94079	0.20644
H	7.28079	3.9799	1.63239
P	0.82252	-2.50967	-0.31647
P	-3.57457	0.51618	1.00205
C	1.50364	-4.07978	-1.02534
C	0.92848	-4.68719	-2.15262
C	2.55872	-4.72713	-0.36852
C	1.39297	-5.92156	-2.60712
H	0.12692	-4.19318	-2.69232
C	3.01557	-5.96537	-0.82144
H	3.03812	-4.24561	0.4751
C	2.43561	-6.56578	-1.93913
H	0.94209	-6.3758	-3.48509
H	3.84008	-6.45013	-0.307
H	2.7997	-7.52571	-2.29457
C	-0.59951	-3.18321	0.65472

C	-1.65176	-3.87738	0.03752
C	-0.56745	-3.11175	2.05301
C	-2.66533	-4.45378	0.79914
H	-1.68364	-3.97485	-1.04201
C	-1.58004	-3.69738	2.81732
H	0.26252	-2.6104	2.53663
C	-2.63419	-4.36225	2.19324
H	-3.47885	-4.97541	0.30347
H	-1.53881	-3.63377	3.90106
H	-3.42311	-4.81614	2.78641
C	-3.26963	2.0698	0.03534
C	-3.85552	2.36204	-1.20708
C	-2.3582	2.99027	0.5777
C	-3.52905	3.53612	-1.88994
H	-4.56549	1.66621	-1.64397
C	-2.03299	4.16376	-0.10311
H	-1.88834	2.77622	1.53425
C	-2.61237	4.43672	-1.34349
H	-3.98805	3.74435	-2.85286
H	-1.30676	4.8506	0.3208
H	-2.33552	5.33624	-1.88551
C	-5.12666	0.91085	1.93709
C	-5.96882	2.00004	1.66554
C	-5.4393	0.07525	3.02355
C	-7.09672	2.2408	2.45328
H	-5.74083	2.66494	0.83857
C	-6.57342	0.30753	3.80186
H	-4.78556	-0.76065	3.2609
C	-7.40427	1.39413	3.5196
H	-7.73623	3.09099	2.23172
H	-6.80186	-0.35202	4.63453
H	-8.28208	1.58305	4.13117
C	0.19539	-1.63042	-1.82524
C	1.15155	-1.49068	-2.85613
C	-1.03493	-0.96738	-1.98711
C	0.87678	-0.76844	-4.01342
H	2.1324	-1.93927	-2.72297
C	-1.30864	-0.22524	-3.14488
C	-0.36249	-0.13678	-4.15952
H	1.63084	-0.69107	-4.7904
H	-2.26026	0.28886	-3.2235
H	-0.58502	0.44075	-5.0521
C	-4.21597	-0.61223	-0.32627
C	-5.57085	-0.92958	-0.50214
C	-3.28828	-1.22523	-1.19022
C	-5.99402	-1.80648	-1.50262
H	-6.30627	-0.47503	0.15278
C	-3.69913	-2.10005	-2.19877
C	-5.05519	-2.3865	-2.35448
H	-7.05086	-2.02764	-1.61731
H	-2.96252	-2.54873	-2.85596
H	-5.37026	-3.06878	-3.1387
O	-1.9486	-0.96806	-0.94974
Rh	2.35624	-1.22536	0.79487
H	2.45799	-2.49524	1.6879
Cl	4.2512	-1.82378	-0.77177
C	2.01945	0.35264	3.13036
C	1.10074	-0.01656	1.97794
H	2.10513	1.42638	3.33427
H	1.75789	-0.15778	4.06025
H	0.15937	-0.43157	2.33817
C	0.88893	1.08045	0.92764
H	-0.14098	1.06708	0.56087
H	1.07651	2.09368	1.31092
N	1.81947	0.79148	-0.20942
H	1.28287	0.55658	-1.03837
C	2.79884	1.83779	-0.57287
H	3.4625	1.38722	-1.31853
H	3.411	2.04649	0.30507
C	2.1848	3.12584	-1.08769
C	2.28767	4.31599	-0.36444
C	1.48559	3.15969	-2.30722
C	1.70949	5.50816	-0.81756
H	2.84014	4.32297	0.57229
C	0.90152	4.32936	-2.77174
H	1.3971	2.25412	-2.9034
C	1.00385	5.51318	-2.0243
H	1.81712	6.41068	-0.22708
H	0.36039	4.35635	-3.71198
O	0.37653	6.60653	-2.55719
C	0.50815	7.84706	-1.88157
H	-0.03524	8.57818	-2.48231
H	0.06984	7.81163	-0.87547
H	1.55871	8.15465	-1.80144

TS8^{L1}

Sum of electronic and thermal Free Energies=-3904.213966

C	-2.09943800	-0.70049000	2.91949900
C	-3.31615500	-1.39093500	3.08589700

C	-1.30060300	-0.44459500	4.04575600	C	3.34764300	-3.92222600	-1.34259200
C	-3.73168800	-1.79643400	4.35472800	C	3.19649200	-3.57970000	1.04696700
H	-3.92818000	-1.60345000	2.21386800	C	3.60986300	-5.27806400	-1.12854500
C	-1.71910300	-0.86679500	5.30749700	H	3.30627700	-3.54838100	-2.35899200
H	-0.34993600	0.05602800	3.92267500	C	3.46994700	-4.93180300	1.25351300
C	-2.93417600	-1.53712200	5.47072800	H	3.00528000	-2.92536200	1.89383300
H	-4.67663400	-2.32164000	4.46768600	C	3.67753200	-5.78594700	0.16805600
H	-1.08818400	-0.66838800	6.16985100	H	3.76399500	-5.93345400	-1.98123200
H	-3.25404700	-1.85800300	6.45835000	H	3.51137300	-5.31787300	2.26812400
Rh	0.60935800	-0.57598400	0.44576500	H	3.88506800	-6.83954100	0.33265100
H	-0.04540900	-0.57728800	-0.95198100	C	2.98173400	-1.05135200	-2.32934600
Cl	1.85331900	-0.76974900	2.70113000	C	4.26161700	-1.02268000	-2.90752100
C	0.10146300	-2.85477800	0.51717700	C	1.86142600	-0.95628100	-3.16440300
C	-1.27133600	-2.73138300	0.52023800	C	4.41315800	-0.90011800	-4.28823700
H	0.61195800	-3.06220300	1.45004300	H	5.14173700	-1.09264200	-2.27561700
H	0.57938900	-3.18547000	-0.39846200	C	2.01413900	-0.83853600	-4.54831900
H	-1.81023800	-2.74459400	1.46084900	H	0.86828600	-0.96011400	-2.72624600
C	-2.10011900	-2.89119200	-0.72033800	C	3.28915700	-0.80863100	-5.11314000
H	-2.26042300	-3.97873600	-0.82908200	H	5.40986700	-0.87561300	-4.71990400
H	-1.50436100	-2.58493700	-1.59992700	H	1.13406100	-0.76427600	-5.18091100
N	-3.40347700	-2.25315300	-0.63595900	H	3.40855000	-0.71246300	-6.18863200
H	-3.26850800	-1.27593800	-0.38153500	C	-0.01468300	2.80463300	1.63575100
C	-4.17242500	-2.35809400	-1.87522100	C	-0.98590300	3.81786200	1.64351500
H	-3.60866400	-2.00329500	-2.75890600	C	0.70083700	2.53619900	2.81327200
H	-4.37196300	-3.42586000	-2.05483700	C	-1.24163500	4.54220600	2.80914300
C	-5.47625800	-1.59453600	-1.78698100	H	-1.55113700	4.04745500	0.74759200
C	-6.36504800	-1.81002300	-0.72918400	C	0.44523900	3.26997400	3.97233100
C	-5.83164200	-0.65221200	-2.76224100	H	1.43044000	1.73124300	2.83448500
C	-7.57460700	-1.11796200	-0.63794600	C	-0.52607400	4.27213300	3.97595600
H	-6.09940300	-2.52568100	0.04322100	H	-2.00324800	5.31702100	2.80138900
C	-7.03372200	0.04410500	-2.69137900	H	1.00384200	3.04659200	4.87674700
H	-5.15371900	-0.45907900	-3.59019300	H	-0.72728100	4.83649600	4.88217300
C	-7.91467200	-0.18482100	-1.62589000	C	-0.76307100	2.16758100	-1.20475000
H	-8.23637400	-1.31128200	0.19829100	C	-2.14540400	2.22268900	-0.96368900
H	-7.31150800	0.77282900	-3.44621900	C	-0.31495700	2.21363100	-2.53761100
O	-9.06810100	0.54868300	-1.64046500	C	-3.04936600	2.32571800	-2.02532400
C	-9.98894000	0.36950400	-0.57757600	H	-2.52413100	2.16450800	0.04768600
H	-10.82208000	1.04402800	-0.78231100	C	-1.21879200	2.31706100	-3.59312900
H	-10.36386700	-0.66147600	-0.53329000	H	0.74651100	2.16469500	-2.75752600
H	-9.54549100	0.62929000	0.39254500	C	-2.59162400	2.37473600	-3.34080800
S	-1.71488000	-0.10270400	1.28216900	H	-4.11456900	2.35893200	-1.81590000
P	2.76342800	-1.25281800	-0.50042800	H	-0.84796600	2.35512500	-4.61369200
P	0.51082600	1.88550300	0.11948000	H	-3.29632600	2.45894700	-4.16332000
C	3.14431900	-3.05443300	-0.25845400	C	4.26897400	-0.44379500	0.19910300

C	5.25100600	-1.07862800	0.96642800
C	4.37352300	0.94255400	0.01213400
C	6.27949200	-0.34476300	1.56055800
H	5.20829400	-2.14969400	1.11769200
C	5.37397000	1.69600200	0.62171100
C	6.32578600	1.03876100	1.40408900
H	7.02867200	-0.85487300	2.15765500
H	5.41177200	2.77075800	0.49541700
H	7.10847000	1.61827100	1.88496700
C	1.78474800	3.12526700	-0.50070100
C	1.41794400	4.47672700	-0.63768200
C	3.07839300	2.77465900	-0.89436900
C	2.30101500	5.42458800	-1.14665200
H	0.42571000	4.79293100	-0.33841600
C	3.96771600	3.70791700	-1.44006500
C	3.57952500	5.03828700	-1.55684300
H	1.98714300	6.46024500	-1.23358400
H	4.94185300	3.37356600	-1.77999700
H	4.26694700	5.76710900	-1.97584100
O	3.41659000	1.44367100	-0.84194800

12^{L1}

Sum of electronic and thermal Free Energies=-3904.240421

P	1.79990100	-1.82583000	0.26650300
P	2.38523800	1.90601400	-0.08239500
C	0.59832500	-3.23439700	0.27766300
C	0.41517300	-4.07153500	1.38805200
C	-0.16188400	-3.46358700	-0.88285500
C	-0.49884300	-5.12701200	1.33486100
H	0.98824000	-3.91102700	2.29434100
C	-1.05729300	-4.53090200	-0.93581900
H	-0.05259200	-2.79846900	-1.73532900
C	-1.22948700	-5.36502500	0.17121300
H	-0.63028900	-5.76583800	2.20400500
H	-1.63856600	-4.69491100	-1.83772400
H	-1.93480900	-6.19026200	0.12807300
C	2.70865700	-2.08905500	1.86442300
C	3.74752400	-3.02376300	2.00108900
C	2.30141200	-1.36807200	2.99710100
C	4.36262800	-3.22843200	3.23658800
H	4.07798400	-3.59569400	1.14016100
C	2.91222400	-1.57850900	4.23484300
H	1.50071500	-0.64068700	2.90346400
C	3.94620000	-2.50746100	4.35737800
H	5.16683000	-3.95403100	3.32301700
H	2.58084300	-1.01325300	5.10153400
H	4.42517600	-2.66850900	5.31915000
C	2.92092100	2.67254900	-1.67675700
C	4.16815800	3.31601200	-1.76421700
C	2.08272300	2.64919700	-2.79828100
C	4.56150800	3.93493000	-2.94975400
H	4.83410800	3.33404900	-0.90684200
C	2.48327900	3.27125100	-3.98403300
H	1.14830700	2.10016100	-2.76368600
C	3.71689800	3.91607000	-4.06298100
H	5.52815300	4.42804800	-3.00441500
H	1.82883000	3.23482400	-4.85012700
H	4.02562200	4.39501700	-4.98818800
C	2.03667100	3.38305400	0.98964500
C	2.09350500	4.69289200	0.49330800
C	1.67249300	3.19351100	2.33452900
C	1.80489600	5.78245300	1.32025700
H	2.35970100	4.87145800	-0.54173400
C	1.39945100	4.28121400	3.16212600
H	1.59105700	2.18681700	2.73229400
C	1.46304100	5.58229900	2.65607800
H	1.84821200	6.78833200	0.91227800
H	1.12611000	4.11137600	4.19974900
H	1.24057100	6.42989600	3.29799200
C	3.02709600	-2.42554300	-0.99954300
C	3.06297000	-3.75557800	-1.45037600
C	3.93857000	-1.53122500	-1.58492900
C	3.95064400	-4.16583400	-2.44626800
H	2.37427600	-4.47763400	-1.02743300
C	4.81475100	-1.92111900	-2.59596600
C	4.82145900	-3.24593200	-3.02946300
H	3.94894400	-5.20151000	-2.77263000
H	5.47002600	-1.17486900	-3.03302900
H	5.50137000	-3.55369800	-3.81829600
C	3.98580500	1.28849500	0.60281200
C	4.63684500	1.80587100	1.72941100
C	4.57665900	0.20120900	-0.06111200
C	5.82496000	1.23746000	2.19384400
H	4.21174000	2.65499800	2.25159300
C	5.76036200	-0.37894500	0.39293200
C	6.37828300	0.14320100	1.52953700
H	6.31223800	1.64903200	3.07229900
H	6.18628200	-1.22259600	-0.13861100
H	7.29942900	-0.30590900	1.88934000

O	3.93449000	-0.19757500	-1.21147600
Rh	0.61951100	0.40607700	-0.05164300
H	0.70841100	0.68215300	1.46951400
Cl	0.25741300	-0.18919400	-2.53145600
C	-3.18915600	2.22839800	0.31767400
H	-3.14973200	3.23007200	-0.15759900
H	-2.99617100	2.38777800	1.38639000
N	-4.48508900	1.57979000	0.17929500
H	-4.68433900	1.40539800	-0.80350300
C	-5.58537500	2.33914900	0.76898300
H	-5.37536600	2.42713700	1.84578800
H	-5.64621700	3.37773500	0.39007200
C	-6.92356400	1.66033200	0.55959800
C	-8.07397900	2.40874600	0.30605200
C	-7.04921200	0.26328000	0.63944800
C	-9.32542700	1.80427700	0.14664500
H	-8.00177700	3.49134900	0.22819800
C	-8.28235800	-0.35408600	0.47610100
H	-6.16161800	-0.33645700	0.81408100
C	-9.43186300	0.41246100	0.23213600
H	-10.19362500	2.42214900	-0.05055000
H	-8.38280900	-1.43352400	0.53006300
O	-10.59629600	-0.29051000	0.08677800
C	-11.78646700	0.43512900	-0.16655900
H	-12.58283500	-0.30683800	-0.24705000
H	-11.72617800	1.00109300	-1.10569300
H	-12.02279600	1.12862600	0.65145500
C	-0.67438000	2.06064500	-0.20177900
H	-0.45720700	2.63403100	-1.10591200
H	-0.58591300	2.70637600	0.67437100
C	-2.04703500	1.40925300	-0.28046700
H	-2.26368700	1.13401100	-1.31575600
S	-1.77685400	-0.22651600	0.60105400
C	-2.85390200	-1.37742700	-0.26974300
C	-3.68088300	-2.18642800	0.51975100
C	-2.90079000	-1.47364800	-1.66594400
C	-4.56474600	-3.08028800	-0.08640600
H	-3.63917700	-2.10473500	1.60143800
C	-3.80166900	-2.35867500	-2.26155000
H	-2.21271800	-0.89339500	-2.27252400
C	-4.63503200	-3.16098400	-1.47873700
H	-5.20557700	-3.70359100	0.53107000
H	-3.84142200	-2.42674200	-3.34533600
H	-5.33359300	-3.84650100	-1.95029900

TS9^{L1}

Sum of electronic and thermal Free Energies=-3904.205346

P	1.52722300	-1.67311000	0.59684300
P	2.51352100	1.70276200	-0.21884800
C	0.23977400	-3.00541200	0.58269600
C	-0.31846800	-3.53680500	1.75466600
C	-0.18622400	-3.49804000	-0.66412900
C	-1.27701300	-4.55101100	1.68294500
H	-0.00637900	-3.16916200	2.72565900
C	-1.13581600	-4.51755200	-0.72635200
H	0.22375200	-3.07133000	-1.57705400
C	-1.68314400	-5.04745800	0.44434100
H	-1.70067600	-4.95310700	2.59924600
H	-1.46024600	-4.88393500	-1.69577000
H	-2.42637300	-5.83822700	0.39056900
C	1.86299700	-1.47644900	2.40960400
C	2.80430900	-2.24265500	3.11139100
C	1.08432200	-0.54788200	3.11859600
C	2.96677000	-2.07874100	4.48877800
H	3.41341300	-2.96985400	2.58431800
C	1.23683900	-0.39519400	4.49709400
H	0.35649500	0.04965100	2.57524700
C	2.18299800	-1.15792300	5.18535100
H	3.70532300	-2.67535700	5.01716000
H	0.61978100	0.32130900	5.03246600
H	2.30905800	-1.03454100	6.25734900
C	3.47339300	2.22373900	-1.71019800
C	4.62817200	3.01401700	-1.56803400
C	3.05319300	1.84188300	-2.98971200
C	5.33682200	3.43326100	-2.69231000
H	4.97541200	3.30125400	-0.57986100
C	3.77162400	2.26349100	-4.11294400
H	2.20747700	1.16872200	-3.10463200
C	4.90595400	3.06087100	-3.96929500
H	6.22684200	4.04478100	-2.57168500
H	3.44424400	1.94948500	-5.09983500
H	5.46181100	3.38412600	-4.84535000
C	1.91770500	3.31712200	0.48621400
C	2.01177800	4.52676200	-0.21467800
C	1.27916000	3.31619200	1.74038300
C	1.49012000	5.70669400	0.32654900
H	2.48993600	4.55563500	-1.18689700
C	0.77348300	4.49525200	2.28481500
H	1.17633200	2.38584800	2.29044100

C	0.87527100	5.69668800	1.57672100
H	1.56803600	6.63256500	-0.23637400
H	0.29408300	4.47551300	3.25962400
H	0.47391200	6.61431400	1.99725100
C	3.00371400	-2.62492200	-0.02393700
C	3.01554100	-4.02846700	-0.08467300
C	4.13287500	-1.95811600	-0.52558800
C	4.08877200	-4.72600100	-0.64073600
H	2.16402600	-4.58375400	0.29020400
C	5.19817900	-2.63911900	-1.11033000
C	5.17616000	-4.03160500	-1.16944200
H	4.06271600	-5.81101400	-0.67442500
H	6.02318500	-2.06400200	-1.51759000
H	6.00334100	-4.56711500	-1.62581000
C	3.86866500	1.24649000	0.95244900
C	4.26414400	1.98820200	2.07299000
C	4.55698200	0.05718200	0.67134300
C	5.29562200	1.53899900	2.90008500
H	3.76154500	2.91945200	2.30634500
C	5.58509900	-0.40721700	1.49091800
C	5.94749400	0.34006700	2.61154500
H	5.58494300	2.12495700	3.76702400
H	6.09149700	-1.33471700	1.24786600
H	6.74805900	-0.01503000	3.25406200
O	4.18281600	-0.57397900	-0.49477700
Rh	0.69224600	0.30537800	-0.53964900
H	-0.07107700	1.58473700	0.03573200
Cl	1.18434200	-1.01917400	-2.91059600
C	-2.99147500	2.25800400	-0.36644300
H	-3.00687800	3.25805500	-0.84577000
H	-2.58240000	2.40851400	0.64215200
N	-4.31285100	1.66367400	-0.23761700
H	-4.70030500	1.46397100	-1.15737500
C	-5.25696300	2.49021900	0.51619000
H	-4.81857600	2.65128300	1.51161200
H	-5.39639100	3.49679000	0.07854600
C	-6.60368200	1.81444600	0.65126300
C	-7.77581900	2.43042200	0.21431500
C	-6.70503300	0.53766200	1.23068300
C	-9.02549500	1.81351100	0.34872100
H	-7.72393700	3.41632700	-0.24212000
C	-7.93355800	-0.09088000	1.37104500
H	-5.80060800	0.03896700	1.56670700
C	-9.10610100	0.54529900	0.93088500
H	-9.91301700	2.32561900	-0.00382200
H	-8.01790200	-1.07518000	1.82058200
O	-10.26429500	-0.15558900	1.11567500
C	-11.48044500	0.43935200	0.69547700
H	-12.26708100	-0.27788800	0.93548500
H	-11.48671700	0.63201100	-0.38541000
H	-11.67706000	1.38028600	1.22609000
C	-0.61679400	1.97196800	-1.26851000
H	-0.19060000	1.88460300	-2.27017800
H	-0.56643400	3.02142700	-0.96315800
C	-2.02664400	1.39301800	-1.17719100
H	-2.44111400	1.19785300	-2.17058000
S	-1.80136100	-0.30921800	-0.40488700
C	-2.70231400	-1.34770000	-1.57301900
C	-3.92572400	-1.87866000	-1.14568300
C	-2.22010100	-1.61057400	-2.86063100
C	-4.67401000	-2.67475100	-2.01409300
H	-4.29060500	-1.65461300	-0.14916400
C	-2.98115800	-2.40637300	-3.72052300
H	-1.24521600	-1.23376700	-3.16193500
C	-4.20325200	-2.93828100	-3.30244600
H	-5.62571800	-3.08216100	-1.68466700
H	-2.60689700	-2.61678400	-4.71855800
H	-4.78765600	-3.55721400	-3.97793700

13^{L1}

Sum of electronic and thermal Free Energies= -3904.257310

P	-1.61535	1.20757	0.99577
P	-1.83082	-1.94878	-0.62058
C	-0.88458	2.89006	1.35146
C	-1.49119	4.08397	0.93807
C	0.29141	2.97103	2.11809
C	-0.9473	5.32298	1.29249
H	-2.39995	4.05675	0.34722
C	0.82812	4.20603	2.48207
H	0.77141	2.06109	2.46337
C	0.20659	5.39032	2.07149
H	-1.43786	6.23477	0.96275
H	1.72578	4.2435	3.09418
H	0.61905	6.35337	2.35951
C	-3.28345	1.68585	0.34085
C	-4.40498	1.91669	1.14887
C	-3.39387	1.88281	-1.04514
C	-5.61312	2.32741	0.58137
H	-4.34111	1.77242	2.22228

C	-4.59741	2.30755	-1.60939
H	-2.52403	1.69991	-1.67122
C	-5.71193	2.52629	-0.79638
H	-6.47727	2.49281	1.21887
H	-4.66533	2.4619	-2.68262
H	-6.65257	2.84782	-1.23463
C	-1.18475	-3.52383	0.11415
C	-2.03132	-4.62792	0.30525
C	0.15299	-3.61736	0.5202
C	-1.54606	-5.80338	0.87983
H	-3.0745	-4.57252	0.00926
C	0.63396	-4.7928	1.09965
H	0.81315	-2.77373	0.36246
C	-0.21118	-5.88754	1.27995
H	-2.21244	-6.65015	1.01734
H	1.67411	-4.85056	1.40752
H	0.16663	-6.80127	1.73066
C	-2.23291	-2.35687	-2.37981
C	-1.99293	-3.61788	-2.94003
C	-2.7815	-1.35037	-3.19065
C	-2.30113	-3.86802	-4.27886
H	-1.54714	-4.40327	-2.34041
C	-3.09878	-1.60487	-4.52432
H	-2.95766	-0.3627	-2.77649
C	-2.85656	-2.86579	-5.0742
H	-2.09687	-4.84871	-4.70002
H	-3.52557	-0.81484	-5.13675
H	-3.09336	-3.06216	-6.11613
C	-1.98586	0.71135	2.77866
C	-1.9445	1.64013	3.83643
C	-2.2506	-0.62304	3.13735
C	-2.08866	1.25289	5.1693
H	-1.78385	2.68817	3.6196
C	-2.35598	-1.03121	4.46778
C	-2.26795	-0.09154	5.49205
H	-2.04618	2.00473	5.95174
H	-2.51503	-2.08511	4.67152
H	-2.35296	-0.40622	6.52791
C	-3.52682	-1.91159	0.12752
C	-4.72829	-2.0864	-0.57241
C	-3.60259	-1.68178	1.50667
C	-5.95862	-2.01684	0.0849
H	-4.70204	-2.2719	-1.63989
C	-4.82094	-1.60863	2.18
C	-6.00319	-1.77498	1.45774
H	-6.87774	-2.15159	-0.47721
H	-4.84052	-1.42908	3.24929
H	-6.95741	-1.72123	1.97408
O	-2.3846	-1.59091	2.16241
Rh	-0.40349	-0.13185	-0.45568
Cl	0.86253	-1.51592	-2.04113
C	4.18772	2.05331	-0.48044
H	4.12201	3.02915	-0.99467
H	4.94386	2.16562	0.30762
N	4.60639	0.97224	-1.35424
H	4.03082	0.93691	-2.18576
C	6.03151	0.90644	-1.67086
H	6.51618	1.89983	-1.68182
H	6.11964	0.51909	-2.6949
C	6.79487	-0.02051	-0.73425
C	8.03932	0.31769	-0.20252
C	6.26734	-1.28858	-0.42924
C	8.76115	-0.57386	0.60588
H	8.46901	1.29482	-0.41944
C	6.96607	-2.18457	0.36805
H	5.2922	-1.5585	-0.82618
C	8.22302	-1.83356	0.88955
H	9.72474	-0.27401	1.00386
H	6.56458	-3.16681	0.60145
O	8.83023	-2.7908	1.65907
C	10.11166	-2.50812	2.19178
H	10.41476	-3.40125	2.74316
H	10.84497	-2.30719	1.40031
H	10.08905	-1.65236	2.87987
C	2.84949	1.75608	0.22508
H	2.54185	2.63811	0.79175
S	1.52877	1.37982	-1.03174
C	1.15635	2.93601	-1.84886
C	0.66099	2.81061	-3.1583
C	1.3482	4.20796	-1.29983
C	0.35214	3.94822	-3.90058
H	0.53103	1.82048	-3.58641
C	1.04837	5.343	-2.05897
H	1.71723	4.32609	-0.28715
C	0.54998	5.22039	-3.35601
H	-0.02632	3.83909	-4.91409
H	1.20027	6.3265	-1.62497
H	0.32081	6.10651	-3.94113

C	2.94748	0.54048	1.15182
H	3.36745	-0.30914	0.61001
H	3.61419	0.77694	1.98903
H	1.97103	0.24843	1.54815

TS10^{L1}

Sum of electronic and thermal Free Energies=-3904.206691

S	0.10041700	2.98902000	-0.33145300
C	-0.03633500	4.24166000	0.92855300
C	1.00163600	4.51376900	1.84014400
C	-1.18613300	5.05343100	0.95282800
C	0.87933600	5.56334500	2.74999200
H	1.88735600	3.88717700	1.82712900
C	-1.28979100	6.11687700	1.85130200
H	-1.99049300	4.85183900	0.25116600
C	-0.26057900	6.37333200	2.75868600
H	1.68819100	5.75768800	3.44991100
H	-2.18142600	6.73893700	1.84670900
H	-0.34403900	7.19572200	3.46388300
P	1.23371300	-1.45829400	1.59386000
P	1.32817400	0.35510000	-1.91742900
C	0.84448400	-1.47366600	3.40340300
C	-0.11909600	-2.32435900	3.96367900
C	1.50030200	-0.54653800	4.23903900
C	-0.40782500	-2.26665600	5.33029400
H	-0.64411200	-3.03952600	3.34049200
C	1.21587100	-0.50204400	5.60332800
H	2.21628600	0.14933300	3.80814200
C	0.26183000	-1.36277300	6.15350800
H	-1.15756200	-2.93308200	5.74725600
H	1.73395700	0.21436900	6.23433300
H	0.03852900	-1.32238300	7.21579200
C	0.36502200	-2.96565000	0.95937900
C	0.77235100	-4.25140200	1.35435800
C	-0.70494900	-2.84107700	0.06444500
C	0.11465600	-5.38201300	0.87196200
H	1.60936700	-4.36702700	2.03637700
C	-1.36317600	-3.97457300	-0.41932600
H	-1.01268500	-1.85821400	-0.27535600
C	-0.95663700	-5.24571300	-0.01531500
H	0.44105500	-6.36965100	1.18557100
H	-2.18458900	-3.85629800	-1.11976300
H	-1.46563500	-6.12792300	-0.39332900
C	1.88362800	1.90710100	-2.75117000
C	1.31196400	2.40948300	-3.92699900
C	2.98274900	2.56804200	-2.17885700
C	1.84106700	3.55374400	-4.53102700
H	0.45175200	1.91964500	-4.37189400
C	3.51184600	3.70100800	-2.79258500
H	3.39334800	2.21710900	-1.23580600
C	2.94344000	4.19672600	-3.96921900
H	1.38696800	3.93985500	-5.43947800
H	4.35843100	4.20887600	-2.33969000
H	3.35269900	5.08642700	-4.43976300
C	-0.23216600	-0.14289800	-2.80112900
C	-1.36549100	0.68671000	-2.70017700
C	-0.35502100	-1.36285300	-3.48190700
C	-2.57781400	0.30595100	-3.27425400
H	-1.30279500	1.62861000	-2.16224700
C	-1.57574600	-1.74536100	-4.04704600
H	0.49591600	-2.02772400	-3.57374000
C	-2.68957400	-0.91398900	-3.94737100
H	-3.44097500	0.95932200	-3.18454900
H	-1.64791800	-2.69681500	-4.56685400
H	-3.63804900	-1.21143500	-4.38530300
C	3.00812800	-1.96981000	1.57905900
C	3.81494100	-2.11618800	2.71258100
C	3.60372300	-2.14102700	0.31867300
C	5.18168000	-2.37439300	2.59380800
H	3.38198000	-2.01214200	3.69917000
C	4.97360600	-2.35730000	0.18175600
C	5.75922300	-2.46800800	1.33046700
H	5.78980600	-2.48021100	3.48654900
H	5.42799800	-2.43092600	-0.79740700
H	6.82736300	-2.63508600	1.22683100
C	2.54644300	-0.82173200	-2.71234100
C	2.89253800	-0.67210800	-4.06731200
C	3.06801300	-1.93066100	-2.03579000
C	3.69690200	-1.60256100	-4.72128700
H	2.52420800	0.18709300	-4.61594400
C	3.83774300	-2.89860000	-2.69122500
C	4.15786300	-2.72769300	-4.03516100
H	3.94988700	-1.45551300	-5.76676000
H	4.16490100	-3.77720600	-2.14691900
H	4.76027600	-3.47444300	-4.54396300
O	2.70057600	-2.09058300	-0.72009800
Rh	0.63193300	0.75180300	0.57392100
H	-0.75983200	0.22724600	0.04746600
Cl	2.88113700	1.48875500	1.39577600

C	-0.51148000	1.32762400	2.33685300
C	-1.44294600	0.59614400	1.56133500
H	-0.04988100	0.86485200	3.19642100
H	-0.57933000	2.40804400	2.36981500
H	-1.60011800	-0.44672400	1.83199600
C	-2.67248400	1.24432000	0.94652400
H	-2.41597300	2.24168100	0.56472000
H	-3.03326000	0.65008500	0.10125200
N	-3.72648300	1.25133500	1.96765400
H	-3.43307800	1.85222000	2.73421800
C	-5.01883100	1.72418200	1.46031500
H	-4.93671300	2.67375700	0.90044500
H	-5.64495400	1.93541800	2.33730200
C	-5.71266300	0.69961700	0.58127500
C	-5.76118800	-0.64785500	0.94965300
C	-6.35499900	1.08079400	-0.60515900
C	-6.43234000	-1.59416300	0.17164400
H	-5.25215600	-0.95933600	1.85699000
C	-7.03204000	0.15434000	-1.39112900
H	-6.32661000	2.12212200	-0.91817600
C	-7.07568200	-1.19248000	-1.00596700
H	-6.44756100	-2.63012500	0.49016100
H	-7.53069000	0.44829000	-2.30919400
O	-7.76031500	-2.02919700	-1.84358300
C	-7.85084700	-3.39915800	-1.49247400
H	-8.43943400	-3.87511500	-2.27867000
H	-6.86177500	-3.87415500	-1.44631600
H	-8.35756700	-3.53954800	-0.52866600

14^{L1}

Sum of electronic and thermal Free Energies=-3904.239326

S	0.48695900	-1.45550400	2.17571300
C	1.69998300	-0.72674500	3.26210000
C	3.06739300	-0.88831000	2.98570600
C	1.32240200	-0.11442500	4.46923100
C	4.03373700	-0.44530800	3.89003100
H	3.36869300	-1.37117000	2.06198600
C	2.28997100	0.32448500	5.37090900
H	0.26886100	0.01579700	4.68658600
C	3.64852100	0.16326400	5.08533600
H	5.08729800	-0.57850700	3.65881400
H	1.98188400	0.79725700	6.29981700
H	4.40002800	0.50734900	5.79077900
Rh	-0.76631200	0.10387100	0.83467400
H	2.27736500	-0.60448500	-0.13564600
Cl	-0.16201000	1.88458700	2.31928400
C	0.66529300	0.76546100	-0.53664800
C	2.10945600	0.47723200	-0.16719600
H	0.49077400	1.84397700	-0.58349100
H	0.41036000	0.30270900	-1.49270300
H	2.34135900	0.87334700	0.82373800
C	3.07517700	1.10050700	-1.19049000
H	2.96113700	2.19312900	-1.18887000
H	2.80805100	0.75998400	-2.21161400
N	4.46155500	0.79323600	-0.84581000
H	4.57518600	-0.21570100	-0.77296100
C	5.43710300	1.31242100	-1.80022300
H	5.26145900	0.96751800	-2.83842800
H	5.31415400	2.40562700	-1.82522800
C	6.85528600	0.96571300	-1.39590500
C	7.78735400	0.51396600	-2.33024800
C	7.27455600	1.10972900	-0.06202500
C	9.10790700	0.21995900	-1.97057500
H	7.48525300	0.38496800	-3.36734500
C	8.57859300	0.81892600	0.31428700
H	6.55359800	1.44046700	0.67918400
C	9.50724700	0.37392600	-0.63967800
H	9.80077800	-0.13032100	-2.72681200
H	8.90695800	0.92756000	1.34318700
O	10.76525500	0.11515700	-0.16822300
C	11.74342900	-0.33310600	-1.08929100
H	12.66113500	-0.47040500	-0.51463700
H	11.46160000	-1.28946900	-1.54985900
H	11.92316300	0.40379600	-1.88347700
P	-2.44227400	1.72246200	-0.15269000
P	-1.40013300	-1.88859300	-0.36282000
C	-2.02128400	3.53040300	-0.11195000
C	-1.72983800	4.23211700	-1.29311500
C	-1.92540900	4.21560300	1.11370300
C	-1.35930100	5.57783400	-1.25220400
H	-1.79615500	3.73987000	-2.25574100
C	-1.57102200	5.56365700	1.14751000
H	-2.11250400	3.69455600	2.04269800
C	-1.28240500	6.24941900	-0.03324400
H	-1.13745900	6.09825900	-2.17959400
H	-1.50587500	6.07178000	2.10511200
H	-0.99746600	7.29723300	-0.00213900
C	-3.03298700	1.55502400	-1.90700600
C	-4.36552000	1.78623400	-2.27906200

C	-2.09453500	1.27641600	-2.91337000
C	-4.75025400	1.72900400	-3.61940500
H	-5.10799400	2.01388500	-1.52184300
C	-2.47774900	1.23155400	-4.25536400
H	-1.05579800	1.11193700	-2.65097400
C	-3.80886200	1.45277000	-4.61169700
H	-5.78796700	1.90667800	-3.88728400
H	-1.73412300	1.02542300	-5.02021700
H	-4.10939900	1.41408000	-5.65475300
C	-1.62743100	-3.43060300	0.64874600
C	-1.42974200	-4.70374300	0.09184300
C	-2.15041100	-3.33138800	1.94685500
C	-1.72746500	-5.85195700	0.82587000
H	-1.03864600	-4.80614900	-0.91461700
C	-2.45347600	-4.48248800	2.67482700
H	-2.30602400	-2.35769700	2.39359300
C	-2.23902900	-5.74423900	2.12003400
H	-1.55965300	-6.82994100	0.38360500
H	-2.84711200	-4.38844400	3.68271200
H	-2.46900900	-6.63878100	2.69191800
C	-0.16770500	-2.35621700	-1.65106900
C	0.99161900	-3.04532800	-1.25116200
C	-0.25842500	-1.90626900	-2.97855400
C	2.01021700	-3.30866300	-2.16707400
H	1.10170500	-3.36280800	-0.21969300
C	0.76526600	-2.17157800	-3.89120900
H	-1.12582200	-1.34486700	-3.30751400
C	1.89923400	-2.87805400	-3.49069700
H	2.89409000	-3.84962500	-1.84144800
H	0.67324900	-1.82249500	-4.91588200
H	2.69347800	-3.08581000	-4.20182800
C	-4.02505900	1.61305300	0.81369800
C	-4.74447600	2.72926900	1.27007000
C	-4.52443400	0.34412900	1.15813000
C	-5.88303500	2.58382500	2.06474800
H	-4.40331100	3.72469600	1.01213200
C	-5.64311900	0.18585700	1.97350800
C	-6.32532100	1.31313600	2.43116600
H	-6.41435500	3.46717000	2.40552300
H	-5.96043000	-0.81730400	2.23891800
H	-7.19780300	1.19575700	3.06668600
C	-3.06001500	-1.93097100	-1.18978900
C	-3.34145700	-2.61952600	-2.37834300
C	-4.13728500	-1.34399500	-0.50542700
C	-4.63552200	-2.67005100	-2.89607600
H	-2.54138900	-3.12367500	-2.90764600
C	-5.43646500	-1.38598000	-1.01110400
C	-5.67947000	-2.04378100	-2.21566100
H	-4.82513600	-3.20180000	-3.82329700
H	-6.24456900	-0.91599900	-0.46230200
H	-6.69042200	-2.07861600	-2.61092300
O	-3.84632100	-0.78997600	0.73258000

TS11^{L1}

Sum of electronic and thermal Free Energies=-3904.195749

S	-1.78889800	1.87342800	-2.42372600
C	-2.65131600	3.27803400	-1.71112800
C	-4.02933500	3.19444200	-1.44536000
C	-2.02327000	4.53107700	-1.60103000
C	-4.74659900	4.32558000	-1.05213500
H	-4.53968400	2.24565200	-1.56256800
C	-2.74077900	5.65528000	-1.19035200
H	-0.97425000	4.63400600	-1.85781300
C	-4.10476400	5.55782700	-0.90939300
H	-5.81290400	4.24040900	-0.86030700
H	-2.23377400	6.61283300	-1.10690700
H	-4.66518100	6.43624000	-0.60227300
P	0.51417700	-1.74721900	-0.54984400
P	-2.30458800	0.02423600	0.70056600
C	2.25262200	-1.71088500	-1.23087900
C	3.25696600	-2.48589700	-0.61987500
C	2.60617500	-0.90136000	-2.32046100
C	4.56954700	-2.45526400	-1.08931500
H	3.01879700	-3.11400800	0.23169100
C	3.92654900	-0.86084200	-2.77707600
H	1.83863900	-0.34147500	-2.84130200
C	4.91149900	-1.63453500	-2.16605900
H	5.32502100	-3.06954100	-0.60680700
H	4.17702100	-0.22552900	-3.62182000
H	5.93629700	-1.60017600	-2.52464100
C	0.96856000	-1.93975300	1.24179400
C	0.82762600	-3.13561300	1.95615700
C	1.57346600	-0.84058800	1.87718000
C	1.25877100	-3.22791900	3.28261100
H	0.38496400	-4.00224800	1.47823200
C	2.01314200	-0.93805100	3.19754000
H	1.72821200	0.09018300	1.33718700
C	1.85138100	-2.13139300	3.90709400
H	1.13387500	-4.16220300	3.82262500

H	2.48687600	-0.08135400	3.66896600
H	2.19153700	-2.20587200	4.93606900
C	-4.08857200	0.01101500	0.17125300
C	-5.12670400	0.26491400	1.08280000
C	-4.41494400	-0.39113200	-1.13222700
C	-6.45985000	0.16011400	0.68688800
H	-4.89807400	0.54774900	2.10541800
C	-5.75164800	-0.50851600	-1.52210600
H	-3.62280700	-0.60282900	-1.84189300
C	-6.77593400	-0.22473000	-0.61837100
H	-7.25098800	0.37368800	1.40031500
H	-5.98640200	-0.81815600	-2.53642300
H	-7.81477500	-0.30950700	-0.92498800
C	-2.17347600	1.39437400	1.93907900
C	-2.96794600	2.54794500	1.85412900
C	-1.14470900	1.36238600	2.89873800
C	-2.75129500	3.62906500	2.71187100
H	-3.75250600	2.61765900	1.11161500
C	-0.93686300	2.43897100	3.76051900
H	-0.49887600	0.49417900	2.97496800
C	-1.73999800	3.57815100	3.67071600
H	-3.37678000	4.51223900	2.62029500
H	-0.14209800	2.38737200	4.49955200
H	-1.57496200	4.41844600	4.33906400
C	-0.13714600	-3.40615000	-1.05581300
C	0.62879800	-4.34077200	-1.76832000
C	-1.49738300	-3.70483500	-0.85170400
C	0.06507700	-5.52176800	-2.25307900
H	1.67376900	-4.13200200	-1.96564400
C	-2.07555500	-4.86937000	-1.35252900
C	-1.28905500	-5.78509800	-2.05152100
H	0.68264100	-6.22376100	-2.80500200
H	-3.13746900	-5.03327300	-1.20076300
H	-1.73756400	-6.69292400	-2.44382500
C	-2.40670500	-1.49632800	1.77921700
C	-2.60390500	-1.46176200	3.16764200
C	-2.40408200	-2.75823000	1.15899400
C	-2.75271400	-2.63199700	3.91280300
H	-2.63811800	-0.50737300	3.67922500
C	-2.55644800	-3.93624600	1.89198800
C	-2.72312400	-3.87086500	3.27379800
H	-2.89618000	-2.57092800	4.98730300
H	-2.54715700	-4.89034100	1.37656000
H	-2.84311100	-4.78744100	3.84419400
O	-2.31706300	-2.77809700	-0.22144600
Rh	-0.93685600	-0.00933600	-1.19358500
H	-0.45456200	3.36074400	0.14262700
Cl	-0.43909100	-0.74246600	-3.50852900
C	0.38135800	2.09117900	-1.38291000
C	0.42115700	2.72382900	-0.01547300
H	1.05629800	1.25097400	-1.52987500
H	0.50993500	2.79591200	-2.19877100
H	0.40507900	1.96029300	0.76173600
C	1.68000200	3.59112200	0.18194000
H	1.70662700	4.39468400	-0.58029500
H	1.59776100	4.09156200	1.15552300
N	2.90275700	2.78974700	0.19880300
H	3.02521700	2.32538300	-0.69877100
C	4.09910900	3.58305200	0.48206800
H	3.97341600	4.00790700	1.48991600
H	4.20534500	4.45155400	-0.19542900
C	5.37069400	2.76089700	0.42437500
C	5.40399000	1.43289500	0.85729600
C	6.56458600	3.32948200	-0.04504800
C	6.58473200	0.68530000	0.83025300
H	4.48822500	0.97009300	1.21067000
C	7.74982000	2.60490700	-0.07057100
H	6.56501300	4.35813800	-0.39854500
C	7.76739300	1.27336700	0.36815700
H	6.56515200	-0.34537400	1.16418400
H	8.67310800	3.04379600	-0.43489300
O	8.97788900	0.64065000	0.29825900
C	9.05231600	-0.70768500	0.72688400
H	10.09138300	-1.01231000	0.59032100
H	8.78219700	-0.81399200	1.78588300
H	8.40416900	-1.36149100	0.12810400

15^{L1}

Sum of electronic and thermal Free Energies= -3904.245056

S	1.90471	-2.00025	-2.08303
C	3.30182	-3.03543	-1.61013
C	4.49164	-2.41284	-1.20591
C	3.28526	-4.42988	-1.76921
C	5.63207	-3.17322	-0.94319
H	4.52993	-1.33512	-1.10003
C	4.42889	-5.18307	-1.49758
H	2.3911	-4.93549	-2.11701
C	5.60643	-4.56267	-1.07793
H	6.54204	-2.67155	-0.62713

H	4.39446	-6.26215	-1.62289
H	6.49471	-5.15236	-0.86904
P	-0.74861	1.75383	-0.81223
P	1.88701	0.30823	0.94532
C	-2.30936	1.57646	-1.81971
C	-3.41507	2.40015	-1.53558
C	-2.44541	0.59088	-2.80561
C	-4.60948	2.26386	-2.24098
H	-3.35085	3.14887	-0.75293
C	-3.64909	0.44703	-3.50241
H	-1.59896	-0.03715	-3.05135
C	-4.73015	1.2847	-3.23015
H	-5.44694	2.91659	-2.0109
H	-3.73135	-0.31973	-4.26736
H	-5.66091	1.17631	-3.78028
C	-1.57295	1.80482	0.85223
C	-1.82239	2.97962	1.57143
C	-2.08155	0.59159	1.34355
C	-2.54632	2.93991	2.76645
H	-1.45482	3.93096	1.20199
C	-2.81965	0.55413	2.52599
H	-1.91151	-0.32373	0.78401
C	-3.04773	1.73018	3.24555
H	-2.72166	3.8597	3.31738
H	-3.22841	-0.39053	2.87371
H	-3.62043	1.70341	4.16831
C	3.6989	0.64757	0.68914
C	4.63301	0.54304	1.732
C	4.12596	1.12716	-0.55879
C	5.97081	0.87838	1.52218
H	4.31631	0.20074	2.71255
C	5.46495	1.46991	-0.7649
H	3.40282	1.23477	-1.36393
C	6.39021	1.34057	0.2719
H	6.68365	0.78562	2.33698
H	5.77981	1.83873	-1.73693
H	7.43138	1.60653	0.11109
C	1.8275	-1.20505	2.01402
C	2.85642	-2.15893	2.02424
C	0.64789	-1.48875	2.7284
C	2.71902	-3.35046	2.74135
H	3.76828	-1.98534	1.4655
C	0.51801	-2.67327	3.4533
H	-0.17346	-0.77901	2.72172
C	1.55447	-3.61033	3.46285
H	3.52915	-4.07417	2.73109
H	-0.39616	-2.86469	4.00874
H	1.45184	-4.53444	4.02466
C	-0.2086	3.50389	-1.11587
C	-0.84589	4.3585	-2.02848
C	0.96962	3.97814	-0.50677
C	-0.34613	5.63259	-2.30358
H	-1.73527	4.01826	-2.5449
C	1.48442	5.2432	-0.78438
C	0.81789	6.07916	-1.68013
H	-0.86217	6.26702	-3.01776
H	2.41447	5.5438	-0.31278
H	1.21795	7.06455	-1.89991
C	1.56152	1.68736	2.1576
C	1.45293	1.53088	3.54594
C	1.49581	2.99499	1.64472
C	1.25476	2.62912	4.38528
H	1.51905	0.54022	3.98045
C	1.30159	4.10151	2.47033
C	1.17288	3.91247	3.8457
H	1.16846	2.47841	5.45711
H	1.25521	5.09383	2.03474
H	1.02178	4.77125	4.49352
O	1.71694	3.12358	0.28839
Rh	0.91136	0.22754	-1.14306
H	1.15034	-4.25521	-0.16475
Cl	0.71309	0.63903	-3.5352
C	0.46116	-3.12835	-1.88298
C	0.2527	-3.718	-0.4873
H	-0.38425	-2.49896	-2.16964
H	0.54919	-3.91433	-2.64127
H	0.10705	-2.90437	0.22891
C	-0.93472	-4.6939	-0.44144
H	-0.85362	-5.39519	-1.28159
H	-0.85563	-5.30096	0.47961
N	-2.23362	-4.02142	-0.54104
H	-2.91928	-4.6554	-0.94152
C	-2.7418	-3.54751	0.74833
H	-2.02691	-2.80682	1.13261
H	-2.77322	-4.35168	1.50914
C	-4.11723	-2.92592	0.62969
C	-5.12179	-3.22295	1.55259
C	-4.41548	-2.01526	-0.39885

C	-6.38871	-2.63251	1.4782
H	-4.92194	-3.93431	2.35095
C	-5.66765	-1.42347	-0.49101
H	-3.65559	-1.77719	-1.13605
C	-6.66407	-1.72634	0.44943
H	-7.14147	-2.89217	2.21344
H	-5.8921	-0.71365	-1.27983
O	-7.8616	-1.09056	0.27163
C	-8.89988	-1.34652	1.20088
H	-9.75043	-0.74221	0.87991
H	-9.1936	-2.40461	1.20487
H	-8.61495	-1.05375	2.21996

TS8$^{L1'}$

Sum of electronic and thermal Free Energies= -3904.194809

S	-0.74076	2.40283	-0.53854
C	-0.20041	3.27606	-1.99584
C	-0.35714	4.67826	-1.97055
C	0.32563	2.69187	-3.16169
C	-0.00196	5.45815	-3.06872
H	-0.75734	5.14959	-1.07779
C	0.67643	3.48135	-4.26133
H	0.47108	1.61664	-3.20248
C	0.51696	4.86688	-4.22463
H	-0.1305	6.537	-3.01955
H	1.07781	3.00163	-5.15096
H	0.79328	5.47786	-5.07995
P	1.05377	-2.19319	-0.57804
P	2.06935	1.17905	0.85494
C	0.31675	-3.16881	-1.98874
C	1.03658	-3.3692	-3.1791
C	-0.99658	-3.66804	-1.927
C	0.46629	-4.0448	-4.25951
H	2.05248	-3.00595	-3.2708
C	-1.56128	-4.35672	-3.00166
H	-1.59206	-3.5203	-1.03476
C	-0.83239	-4.54596	-4.17595
H	1.04768	-4.18247	-5.16696
H	-2.5758	-4.73612	-2.91854
H	-1.27203	-5.07536	-5.01642
C	2.85301	-2.40018	-0.95991
C	3.57597	-3.49665	-0.46588
C	3.48797	-1.50904	-1.83479
C	4.90547	-3.6926	-0.8378
H	3.09899	-4.20131	0.20733
C	4.81558	-1.71429	-2.21695
H	2.9445	-0.65305	-2.2182
C	5.52773	-2.80428	-1.71721
H	5.45279	-4.54409	-0.44366
H	5.29222	-1.01019	-2.89133
H	6.5623	-2.96074	-2.0089
C	1.68405	2.91366	1.39454
C	2.38547	4.02834	0.91526
C	0.68276	3.10256	2.36525
C	2.09771	5.30767	1.40074
H	3.16317	3.91222	0.16982
C	0.40514	4.37932	2.84775
H	0.11333	2.24879	2.71994
C	1.11051	5.48689	2.3684
H	2.65335	6.16021	1.01944
H	-0.3733	4.50876	3.59458
H	0.89005	6.4816	2.74636
C	3.60701	1.41177	-0.1574
C	3.47517	1.95005	-1.44934
C	4.89082	1.10677	0.31628
C	4.60075	2.19672	-2.23549
H	2.49149	2.18937	-1.84011
C	6.01575	1.3415	-0.47854
H	5.02189	0.68562	1.30598
C	5.8765	1.89212	-1.75233
H	4.47694	2.62904	-3.22451
H	7.00203	1.09507	-0.0951
H	6.75371	2.08331	-2.36467
C	0.80604	-3.25854	0.90807
C	0.07283	-4.44828	0.97797
C	1.32507	-2.7263	2.1048
C	-0.20326	-5.04767	2.20869
H	-0.28825	-4.91456	0.07007
C	1.01005	-3.2821	3.34363
C	0.23645	-4.44301	3.38466
H	-0.77311	-5.97082	2.24453
H	1.336	-2.81255	4.26123
H	-0.01278	-4.87718	4.34855
C	2.75422	0.52982	2.46315
C	3.39834	1.40452	3.3543
C	2.72703	-0.83161	2.80259
C	4.00312	0.94372	4.52294
H	3.42983	2.46287	3.12777
C	3.3702	-1.31209	3.94805

C	3.99775	-0.4189	4.81277
H	4.48561	1.64755	5.19334
H	3.40155	-2.37606	4.14213
H	4.49097	-0.79447	5.70439
O	2.15999	-1.6635	1.87664
Rh	0.19877	0.12008	-0.32123
H	0.85573	0.27179	-1.71733
Cl	-0.75107	-0.07107	2.04586
C	-2.16724	0.69418	-1.75776
C	-1.96519	-0.58407	-1.27741
H	-3.00129	1.27503	-1.38937
H	-1.70187	1.0188	-2.68078
H	-1.42039	-1.26122	-1.9238
C	-2.92614	-1.18226	-0.26263
H	-2.96697	-2.27623	-0.41194
H	-2.5485	-1.02381	0.75299
N	-4.26149	-0.57798	-0.33132
H	-4.67706	-0.75703	-1.24517
C	-5.15623	-1.0983	0.70857
H	-4.69455	-0.86055	1.67795
H	-5.25246	-2.20448	0.67852
C	-6.53603	-0.48219	0.63172
C	-7.67847	-1.2744	0.51858
C	-6.70432	0.91234	0.69327
C	-8.96245	-0.71663	0.4803
H	-7.57448	-2.3562	0.46339
C	-7.96842	1.48435	0.65609
H	-5.82507	1.54577	0.76764
C	-9.10956	0.67173	0.5531
H	-9.82422	-1.36818	0.39299
H	-8.10417	2.56003	0.7102
O	-10.30927	1.33143	0.53096
C	-11.4923	0.5572	0.44217
H	-12.32164	1.26644	0.46086
H	-11.53257	-0.01938	-0.49188
H	-11.59123	-0.13413	1.28978

12$^{L1'}$

Sum of electronic and thermal Free Energies= -3904.223144

S	0.23523	2.71973	-0.22244
C	-0.56818	3.80221	0.97569
C	-1.10327	4.99748	0.48174
C	-0.67131	3.50546	2.34088
C	-1.7301	5.8931	1.35016
H	-1.03316	5.22043	-0.57783
C	-1.28306	4.41436	3.20501
H	-0.29104	2.56355	2.72263
C	-1.81493	5.60895	2.71315
H	-2.14529	6.81634	0.95719
H	-1.35062	4.18278	4.26438
H	-2.29462	6.31087	3.38875
P	-0.1111	-1.97461	0.64605
P	-2.74807	0.51821	-0.60326
C	1.36993	-2.41386	1.68681
C	1.23075	-2.69787	3.05485
C	2.66827	-2.40585	1.14485
C	2.34701	-2.96983	3.84903
H	0.24826	-2.71245	3.51068
C	3.78179	-2.69096	1.93626
H	2.81594	-2.17904	0.09644
C	3.62592	-2.9718	3.29433
H	2.20932	-3.18729	4.90443
H	4.77148	-2.68816	1.48806
H	4.49244	-3.18856	3.91221
C	-1.4811	-2.61184	1.71365
C	-1.85974	-3.9627	1.66213
C	-2.10031	-1.77007	2.64623
C	-2.83772	-4.45698	2.52447
H	-1.38845	-4.62942	0.94742
C	-3.07457	-2.26829	3.51429
H	-1.82364	-0.72262	2.68725
C	-3.44629	-3.61138	3.45451
H	-3.12262	-5.50404	2.47003
H	-3.55228	-1.5978	4.22159
H	-4.20864	-3.99763	4.12528
C	-3.08091	2.18597	-1.36045
C	-4.09148	3.05022	-0.91116
C	-2.29498	2.57523	-2.46065
C	-4.31349	4.27537	-1.54526
H	-4.71338	2.77155	-0.06811
C	-2.52501	3.79874	-3.09215
H	-1.50716	1.91554	-2.81669
C	-3.53287	4.65291	-2.63833
H	-5.102	4.92996	-1.18377
H	-1.91156	4.08146	-3.94318
H	-3.71002	5.60356	-3.1343
C	-3.96189	0.48759	0.80345
C	-3.69007	1.30002	1.91869
C	-5.11178	-0.31367	0.82611

C	-4.55637	1.32868	3.01085
H	-2.80046	1.92229	1.92894
C	-5.96976	-0.29862	1.92912
H	-5.34511	-0.95399	-0.01684
C	-5.70073	0.52591	3.02101
H	-4.33547	1.97788	3.8538
H	-6.85353	-0.93076	1.92778
H	-6.37498	0.54408	3.87281
C	-0.06174	-3.17646	-0.75515
C	0.99654	-4.05126	-1.02761
C	-1.11782	-3.10161	-1.68658
C	1.04873	-4.77227	-2.22148
H	1.79517	-4.16968	-0.3065
C	-1.04769	-3.77271	-2.90706
C	0.04379	-4.60067	-3.17001
H	1.87949	-5.44436	-2.41194
H	-1.81506	-3.63866	-3.65635
H	0.0955	-5.11867	-4.1233
C	-3.60433	-0.56666	-1.84893
C	-4.70376	-0.101	-2.58775
C	-3.23555	-1.91312	-2.01005
C	-5.43064	-0.94446	-3.4271
H	-4.99864	0.93886	-2.49859
C	-3.99473	-2.78299	-2.80088
C	-5.08541	-2.29259	-3.51666
H	-6.2725	-0.55292	-3.99015
H	-3.7466	-3.83669	-2.83393
H	-5.66682	-2.97002	-4.13538
O	-2.18267	-2.35381	-1.24406
Rh	-0.23868	0.28866	0.00394
H	-0.43835	0.52343	1.53409
Cl	0.0467	-0.03897	-2.52555
C	1.7892	2.16382	0.66016
C	1.82475	0.67014	0.36968
H	2.64798	2.71874	0.2727
H	1.65412	2.39013	1.71751
H	2.13306	0.12197	1.26205
C	2.7554	0.36797	-0.80223
H	2.60927	-0.6569	-1.177
H	2.50475	1.00894	-1.65384
N	4.14825	0.64269	-0.41475
H	4.39705	0.05425	0.3787
C	5.10558	0.40746	-1.49622
H	4.84811	1.09828	-2.31198
H	5.0269	-0.60787	-1.93022
C	6.53338	0.64412	-1.04985
C	7.54914	-0.26052	-1.3613
C	6.87972	1.79538	-0.32092
C	8.87781	-0.03887	-0.97924
H	7.30747	-1.16313	-1.91859
C	8.19074	2.03099	0.07055
H	6.09873	2.50112	-0.05459
C	9.20213	1.11477	-0.25917
H	9.63611	-0.76754	-1.24211
H	8.462	2.91922	0.63295
O	10.46065	1.43818	0.17065
C	11.51863	0.54764	-0.13815
H	12.42145	0.98945	0.28779
H	11.35893	-0.44404	0.30671
H	11.6513	0.43332	-1.22237

TS10$^{L1'}$

Sum of electronic and thermal Free Energies= -3904.206265

S	-0.18677	-2.63399	0.34746
C	-1.55057	-3.20368	-0.65049
C	-1.52599	-3.20193	-2.05597
C	-2.6674	-3.75654	0.00505
C	-2.59833	-3.72496	-2.77812
H	-0.67842	-2.76697	-2.56751
C	-3.72693	-4.29918	-0.72473
H	-2.68951	-3.76565	1.09189
C	-3.6995	-4.27793	-2.12059
H	-2.57198	-3.70236	-3.86353
H	-4.57608	-4.72928	-0.20047
H	-4.52839	-4.68895	-2.69068
P	0.83592	2.21891	-0.22632
P	2.82822	-1.37587	0.29595
C	-0.58834	3.3208	-0.66827
C	-1.00309	4.37725	0.158
C	-1.31063	3.06328	-1.84907
C	-2.10269	5.16548	-0.19231
H	-0.47325	4.592	1.07866
C	-2.39535	3.86567	-2.20305
H	-1.03463	2.21609	-2.4708
C	-2.79672	4.91816	-1.37663
H	-2.40995	5.97661	0.46244
H	-2.93576	3.65642	-3.12191
H	-3.64625	5.53723	-1.65167
C	1.60948	3.11055	1.20663

C	2.17142	4.38755	1.03652
C	1.66042	2.51859	2.47477
C	2.75544	5.05615	2.11156
H	2.15459	4.85847	0.05812
C	2.24372	3.18923	3.5532
H	1.26485	1.51942	2.61928
C	2.79042	4.45956	3.37488
H	3.18541	6.04271	1.96217
H	2.27421	2.71229	4.5289
H	3.24607	4.98075	4.21199
C	3.09127	-2.83867	-0.80202
C	3.74218	-4.0171	-0.40447
C	2.66706	-2.70838	-2.13396
C	3.96836	-5.04391	-1.32303
H	4.06	-4.14969	0.62453
C	2.90437	-3.73443	-3.0498
H	2.12324	-1.82	-2.44385
C	3.55402	-4.90333	-2.64834
H	4.46592	-5.95426	-0.99918
H	2.56752	-3.62233	-4.07654
H	3.7294	-5.7043	-3.3615
C	2.88193	-2.00319	2.04403
C	2.31354	-3.22267	2.43936
C	3.40732	-1.16082	3.03891
C	2.28051	-3.58747	3.78826
H	1.88567	-3.88608	1.69839
C	3.37264	-1.52866	4.38299
H	3.8557	-0.21441	2.76324
C	2.80769	-2.74458	4.76428
H	1.83681	-4.53637	4.07129
H	3.79422	-0.86572	5.13142
H	2.78236	-3.03291	5.81135
C	2.03184	2.58795	-1.59511
C	1.71694	3.28479	-2.7678
C	3.33505	2.07632	-1.4712
C	2.64818	3.42872	-3.7977
H	0.73226	3.71604	-2.88989
C	4.26665	2.18188	-2.50397
C	3.91236	2.85869	-3.67176
H	2.3752	3.97133	-4.69743
H	5.25198	1.74488	-2.40061
H	4.6357	2.94198	-4.47787
C	4.54535	-0.62207	0.24005
C	5.69653	-1.37824	0.52417
C	4.72384	0.7386	-0.0244
C	6.96107	-0.79589	0.55283
H	5.60077	-2.43904	0.72496
C	5.98177	1.34884	0.03708
C	7.10345	0.57485	0.31906
H	7.83226	-1.40729	0.76923
H	6.06159	2.41761	-0.13096
H	8.08362	1.04059	0.36265
O	3.59406	1.49589	-0.25117
Rh	0.24498	-0.22704	0.09533
H	0.55489	-0.17717	1.63368
Cl	0.03356	-0.19428	-2.38615
C	-1.12226	0.00187	1.84558
C	-1.88309	-0.07859	0.65093
H	-1.05871	-0.87274	2.4871
H	-1.04717	0.96202	2.35138
H	-2.25032	-1.06308	0.38813
C	-2.77742	1.0325	0.15709
H	-2.44547	1.99562	0.54768
H	-2.73039	1.08026	-0.94011
N	-4.15404	0.80726	0.63806
H	-4.63327	1.70404	0.6578
C	-4.93739	-0.10541	-0.20683
H	-4.5142	-1.11334	-0.11071
H	-4.86511	0.1532	-1.2794
C	-6.39324	-0.11832	0.20375
C	-7.40661	0.15009	-0.71704
C	-6.767	-0.39767	1.52989
C	-8.75777	0.13783	-0.35161
H	-7.14445	0.37389	-1.74838
C	-8.10126	-0.41144	1.91242
H	-5.99247	-0.59528	2.26494
C	-9.10865	-0.14338	0.97174
H	-9.51302	0.35129	-1.09884
H	-8.3942	-0.62744	2.93497
O	-10.3904	-0.17829	1.44768
C	-11.4459	0.09427	0.54186
H	-12.3688	0.01975	1.11979
H	-11.36752	1.10464	0.11803
H	-11.47657	-0.6342	-0.27943

$14^{Li'}$

Sum of electronic and thermal Free Energies= -3904.220013 S

S	0.56104	2.71208	0.97454
C	0.72953	4.06627	-0.17089

C	1.05013	3.96686	-1.53548
C	0.57983	5.36211	0.37619
C	1.19745	5.11144	-2.32396
H	1.22411	2.9924	-1.98041
C	0.75746	6.49876	-0.40779
H	0.33077	5.46621	1.42892
C	1.05941	6.38544	-1.76872
H	1.4424	4.99877	-3.37778
H	0.6556	7.48179	0.04917
H	1.18746	7.27336	-2.38114
P	-0.02257	-1.92837	-0.53802
P	2.78659	0.44516	0.45334
C	-1.72293	-2.33523	-1.15001
C	-1.96943	-2.74899	-2.4672
C	-2.81421	-2.16574	-0.27543
C	-3.27575	-2.99585	-2.8998
H	-1.14632	-2.89057	-3.15866
C	-4.11447	-2.41938	-0.71086
H	-2.63601	-1.82611	0.74148
C	-4.349	-2.83396	-2.02504
H	-3.4484	-3.31912	-3.92253
H	-4.94731	-2.27485	-0.0294
H	-5.36345	-3.02479	-2.3629
C	1.04089	-2.59819	-1.90097
C	1.33764	-3.96619	-2.00485
C	1.51242	-1.73189	-2.89777
C	2.08776	-4.45092	-3.07615
H	0.98439	-4.65556	-1.24571
C	2.25541	-2.21857	-3.97485
H	1.3007	-0.67041	-2.832
C	2.54733	-3.57962	-4.06466
H	2.31306	-5.51157	-3.13723
H	2.60961	-1.53286	-4.73872
H	3.13128	-3.95901	-4.89801
C	3.36256	0.78166	2.18235
C	4.73507	0.89338	2.46238
C	2.44368	0.84448	3.23708
C	5.17765	1.08581	3.77059
H	5.46276	0.82796	1.65914
C	2.89241	1.02913	4.5473
H	1.38388	0.73301	3.04098
C	4.25479	1.15475	4.81729
H	6.24165	1.17541	3.97181
H	2.16797	1.07334	5.35551
H	4.59896	1.30023	5.83778
C	3.65303	1.71172	-0.57884
C	4.13291	2.9126	-0.0377
C	3.7564	1.51427	-1.96711
C	4.71839	3.87862	-0.85877
H	4.03935	3.10101	1.02501
C	4.35286	2.47514	-2.78436
H	3.38182	0.59696	-2.413
C	4.83683	3.66231	-2.2308
H	5.07391	4.80646	-0.42063
H	4.43491	2.29809	-3.85328
H	5.29382	4.41576	-2.86613
C	0.19511	-3.18715	0.81234
C	-0.72102	-4.22844	1.0325
C	1.30336	-3.11468	1.67252
C	-0.55109	-5.13597	2.07927
H	-1.58547	-4.3287	0.38776
C	1.46926	-3.99857	2.73731
C	0.5375	-5.01494	2.94201
H	-1.27967	-5.92787	2.22393
H	2.32294	-3.86767	3.39414
H	0.6631	-5.70489	3.77099
C	3.80063	-1.07992	0.11544
C	4.97913	-1.1535	-0.63771
C	3.33375	-2.26255	0.71042
C	5.64792	-2.36773	-0.81206
H	5.377	-0.2567	-1.0987
C	3.98328	-3.48413	0.54414
C	5.1456	-3.52964	-0.22743
H	6.55847	-2.40148	-1.40276
H	3.58967	-4.37922	1.01246
H	5.65992	-4.47695	-0.36216
O	2.21457	-2.09497	1.50458
Rh	0.24547	0.47964	0.01541
Cl	-0.80087	-0.10735	2.12927
C	-1.67496	1.02545	-0.77056
H	-2.28444	0.12859	-0.733
C	-2.42333	2.23151	-0.20527
H	-2.17773	2.36868	0.84965
H	-2.09751	3.14359	-0.71875
N	-3.88348	2.10821	-0.31453
H	-4.14105	1.67269	-1.19803
C	-4.49082	1.36981	0.79252
H	-4.30293	1.95566	1.70378

H	-4.02026	0.38811	0.97733
C	-5.98189	1.17118	0.6143
C	-6.62452	0.08921	1.22215
C	-6.76832	2.07127	-0.12257
C	-8.00523	-0.10392	1.11641
H	-6.03927	-0.61767	1.80744
C	-8.14102	1.88909	-0.24869
H	-6.2863	2.9208	-0.59659
C	-8.77104	0.80147	0.37316
H	-8.46332	-0.95376	1.6092
H	-8.75099	2.58189	-0.82053
O	-10.12531	0.71216	0.19449
C	-10.81169	-0.35214	0.82966
H	-11.86659	-0.22591	0.57904
H	-10.47088	-1.33197	0.46679
H	-10.69518	-0.31837	1.92145
C	-0.86244	1.16563	-2.00263
H	-1.03718	0.40468	-2.76637
H	-0.85055	2.17212	-2.4253
H	0.2981	1.03002	-1.76855

TS11$^{LI'}$

Sum of electronic and thermal Free Energies= -3904.189922

S	0.2229	2.66163	0.9717
C	1.04789	3.93387	0.04566
C	1.48645	3.81034	-1.28434
C	1.174	5.18795	0.67779
C	2.02393	4.9077	-1.95961
H	1.41679	2.8522	-1.78211
C	1.72036	6.27545	0.00094
H	0.83555	5.29843	1.70396
C	2.14354	6.14411	-1.32556
H	2.35753	4.78712	-2.98796
H	1.81077	7.23118	0.50952
H	2.56155	6.99558	-1.85428
P	-0.01158	-1.81807	-0.42747
P	2.80091	0.32473	0.2817
C	-1.72806	-2.06666	-1.11226
C	-1.95153	-2.35921	-2.46877
C	-2.84329	-1.91943	-0.26488
C	-3.25025	-2.49773	-2.96537
H	-1.11705	-2.48537	-3.14815
C	-4.1382	-2.06773	-0.76527
H	-2.68952	-1.67104	0.78133
C	-4.34754	-2.35397	-2.1169
H	-3.39783	-2.72371	-4.01861
H	-4.98768	-1.94569	-0.09965
H	-5.35744	-2.46184	-2.50295
C	1.00185	-2.39456	-1.86752
C	1.35885	-3.73618	-2.06199
C	1.33901	-1.45592	-2.85488
C	2.0463	-4.12722	-3.21298
H	1.10055	-4.47828	-1.31369
C	2.0108	-1.8493	-4.01337
H	1.06916	-0.41347	-2.70693
C	2.37009	-3.18745	-4.19248
H	2.32485	-5.16939	-3.34442
H	2.2552	-1.112	-4.77329
H	2.89916	-3.49525	-5.08997
C	3.40032	0.63644	2.0177
C	4.77392	0.54128	2.30621
C	2.50633	0.88909	3.06533
C	5.24292	0.72871	3.60474
H	5.48205	0.31849	1.51437
C	2.97971	1.06634	4.3687
H	1.44146	0.92978	2.87182
C	4.34442	0.99404	4.64123
H	6.30823	0.6611	3.80718
H	2.27069	1.25578	5.1689
H	4.70878	1.13439	5.65514
C	3.81342	1.49562	-0.74164
C	4.51325	2.5768	-0.18709
C	3.8394	1.32848	-2.13851
C	5.24171	3.44673	-1.00154
H	4.49094	2.74598	0.88287
C	4.57688	2.19029	-2.94903
H	3.29617	0.50666	-2.59514
C	5.28508	3.25273	-2.38121
H	5.77343	4.27993	-0.55104
H	4.59825	2.03192	-4.02394
H	5.85832	3.92665	-3.01145
C	0.13836	-3.1966	0.80459
C	-0.82926	-4.19925	0.96966
C	1.22701	-3.19619	1.69444
C	-0.72915	-5.14103	1.99533
H	-1.68167	-4.23256	0.3011
C	1.32104	-4.11055	2.74144
C	0.33755	-5.08818	2.89205
H	-1.49532	-5.90318	2.10067

H	2.16045	-4.03825	3.42535
H	0.40729	-5.80308	3.70653
C	3.69778	-1.2862	-0.01023
C	4.81685	-1.44374	-0.84037
C	3.25043	-2.41959	0.69177
C	5.44748	-2.681	-0.98607
H	5.20405	-0.59041	-1.3839
C	3.87129	-3.6619	0.557
C	4.97074	-3.79094	-0.29024
H	6.3103	-2.77091	-1.63917
H	3.49666	-4.51283	1.11534
H	5.45666	-4.75715	-0.39493
O	2.20173	-2.22034	1.57186
Rh	0.3929	0.37111	0.3544
Cl	-1.29707	-0.03305	2.14366
C	-1.71422	1.61678	-0.60582
H	-1.97876	0.57116	-0.49214
C	-2.65439	2.53849	0.14422
H	-2.50791	2.44766	1.21884
H	-2.44571	3.57823	-0.13487
N	-4.05722	2.20814	-0.14574
H	-4.18406	1.81793	-1.0756
C	-4.73245	1.3907	0.86186
H	-4.63199	1.92695	1.81605
H	-4.25474	0.41194	1.02612
C	-6.20355	1.18731	0.55559
C	-6.87812	0.08043	1.07525
C	-6.94509	2.11122	-0.19608
C	-8.24757	-0.11382	0.86844
H	-6.3296	-0.64522	1.67145
C	-8.30532	1.92846	-0.42221
H	-6.44047	2.98178	-0.60084
C	-8.9688	0.81528	0.11174
H	-8.73119	-0.98339	1.29528
H	-8.8808	2.64167	-1.0033
O	-10.30765	0.72627	-0.16272
C	-11.03496	-0.33948	0.41554
H	-12.07299	-0.20056	0.10963
H	-10.68053	-1.31439	0.05808
H	-10.97754	-0.32065	1.50889
C	-1.32816	2.02299	-1.99473
H	-2.23988	2.04594	-2.61599
H	-0.89512	3.02564	-2.02712
H	-0.6402	1.31347	-2.45827

3^{Li}-Br

Sum of electronic and thermal Free Energies= -6015.45

S	-0.49553200	2.97656400	0.07019700
C	-0.94131900	4.07408000	-1.26859700
C	-2.06339200	3.90762600	-2.10004300
C	-0.15092900	5.22942500	-1.42847100
C	-2.37764300	4.87235400	-3.05844600
H	-2.66531000	3.00943600	-2.01253200
C	-0.48564100	6.19837100	-2.37441400
H	0.72146300	5.36507800	-0.79563100
C	-1.59955300	6.02399400	-3.19823700
H	-3.24474100	4.72103800	-3.69644100
H	0.13374400	7.08629000	-2.47387700
H	-1.85546800	6.77377900	-3.94169700
P	-0.42014400	-1.87931900	-1.00957100
P	-1.38454600	0.49826700	1.74633800
C	0.15008400	-2.17131400	-2.75426100
C	1.39770700	-2.74046500	-3.04969400
C	-0.69597100	-1.79935700	-3.81657200
C	1.79292500	-2.93324600	-4.37648600
H	2.06512100	-3.04064800	-2.24958300
C	-0.29835500	-2.00187600	-5.13765600
H	-1.65915000	-1.34380100	-3.59946800
C	0.94686600	-2.56793500	-5.42272200
H	2.76324100	-3.37420900	-4.58648700
H	-0.96465300	-1.71197700	-5.94510500
H	1.25423600	-2.72218400	-6.45313300
C	0.82905900	-2.84770000	-0.03500600
C	0.72712000	-4.23731100	0.14013800
C	1.95164500	-2.18666900	0.48569800
C	1.72080800	-4.94239000	0.81956900
H	-0.12982500	-4.77207100	-0.25485000
C	2.95187700	-2.89420000	1.15482200
H	2.04380300	-1.11215900	0.36661100
C	2.83700000	-4.27407700	1.32637800
H	1.62226900	-6.01642100	0.95038200
H	3.81616100	-2.36077000	1.54012600
H	3.61019600	-4.82609100	1.85339600
C	-3.14274500	0.97712900	2.03390800
C	-3.86309800	0.43369900	3.11038000
C	-3.75849700	1.92810000	1.20871400
C	-5.17554500	0.83687400	3.35664700
H	-3.40246500	-0.30131200	3.76221200
C	-5.07132900	2.32864400	1.46168000

H	-3.21093900	2.35077400	0.37753900
C	-5.78283100	1.78514600	2.53129600
H	-5.72108700	0.40852700	4.19289800
H	-5.53735600	3.06317700	0.81169700
H	-6.80607700	2.09723300	2.72152800
C	-0.42847600	1.60785900	2.88369900
C	-1.07804900	2.46365000	3.78460400
C	0.97500800	1.57113500	2.88372400
C	-0.34077700	3.26037500	4.66251900
H	-2.16001100	2.51925900	3.79731100
C	1.70988100	2.36018800	3.76777500
H	1.49836700	0.92802900	2.18360600
C	1.05290400	3.21046700	4.65912800
H	-0.86155800	3.92498000	5.34591400
H	2.79509900	2.31729900	3.74940300
H	1.62425300	3.83346000	5.34141500
C	-1.92374200	-2.98139200	-0.97822700
C	-2.14576600	-3.96594300	-1.95600100
C	-2.90334300	-2.84278100	0.01607400
C	-3.30270100	-4.74658700	-1.95511600
H	-1.41384000	-4.11727800	-2.73963000
C	-4.07657500	-3.59363600	0.01289000
C	-4.27947300	-4.55044800	-0.97985000
H	-3.44253700	-5.49577900	-2.72841300
H	-4.81373900	-3.40823300	0.78694700
H	-5.19253400	-5.13806000	-0.98755600
C	-1.23765500	-1.11776700	2.63026100
C	-0.46670500	-1.33526000	3.78008700
C	-1.94155400	-2.20515200	2.09396800
C	-0.38828500	-2.60354600	4.35879400
H	0.07974300	-0.51164300	4.22375100
C	-1.87424400	-3.47785700	2.65962800
C	-1.08738200	-3.67082800	3.79530200
H	0.21814400	-2.75340500	5.24657500
H	-2.42972700	-4.29740200	2.21788100
H	-1.02880700	-4.65927800	4.24172600
O	-2.73377900	-1.89932600	1.00896400
Rh	-0.53596700	0.56621700	-0.48969600
H	0.79209000	0.51778500	0.29453700
C	0.25799400	1.23438000	-2.65213800
C	1.40643000	0.85897100	-2.01051300
H	-0.29675600	0.54527100	-3.27146800
H	-0.02822400	2.27679000	-2.71745000
H	1.75822600	-0.16253600	-2.12184600
C	2.44382900	1.81510200	-1.46829100
H	2.00752100	2.81059800	-1.30881700
H	2.80579000	1.46720900	-0.49626100
N	3.59199100	1.80706900	-2.38548500
H	3.32092500	2.24415900	-3.26241800
C	4.77098500	2.49017300	-1.84579800
H	4.53767200	3.48451500	-1.42305300
H	5.45196700	2.66566800	-2.68927000
C	5.48502500	1.66622900	-0.78835800
C	5.68368600	0.29356900	-0.96177100
C	5.99812100	2.26331600	0.37201700
C	6.37879700	-0.46957200	-0.01960300
H	5.27487400	-0.18368800	-1.84730900
C	6.69675800	1.52217400	1.31892400
H	5.84827600	3.32787700	0.53690800
C	6.89505400	0.14801800	1.12705300
H	6.51594700	-1.53099700	-0.19221000
H	7.09589100	1.98376300	2.21642000
O	7.59526500	-0.49531900	2.11037200
C	7.85254400	-1.87930200	1.95202500
H	8.43260400	-2.18192600	2.82551000
H	6.92426300	-2.46577000	1.91724800
H	8.43470300	-2.08419300	1.04402800
Br	-2.90524000	0.37205400	-1.81869300

TS8^{L1}-Br

Sum of electronic and thermal Free Energies= -6015.428284

S	0.61015100	2.28980500	0.80488700
C	1.06522800	3.58026200	-0.34608400
C	1.67758600	4.71270500	0.22539700
C	0.86737500	3.54041600	-1.73297300
C	2.07317800	5.78262300	-0.57522700
H	1.83610600	4.75058300	1.29971600
C	1.27759600	4.61501300	-2.52555600
H	0.40683400	2.67063800	-2.18675400
C	1.87770400	5.73955200	-1.95790400
H	2.54131200	6.64926100	-0.11527600
H	1.12137700	4.56525600	-3.60011000
H	2.19220800	6.57084400	-2.58264800
P	-1.17019200	-2.18745700	-0.20005500
P	-2.44681500	1.25105400	0.50851300
C	0.17773500	-3.29498100	-0.82195300
C	0.23975900	-3.59237100	-2.19237300
C	1.21069400	-3.75629800	0.01273100
C	1.29158400	-4.35237500	-2.70654200

H	-0.52622500	-3.22082000	-2.86248400	H	-0.67128800	-4.88487100	1.10815900
C	2.25345300	-4.52672800	-0.50218700	C	-3.13104700	-2.96580200	3.38611200
H	1.20553500	-3.51811100	1.07155000	C	-2.70015700	-4.24121300	3.74612900
C	2.29599900	-4.82901700	-1.86434500	H	-1.48630500	-5.92812500	3.16959700
H	1.32231700	-4.56875000	-3.77029900	H	-3.81679700	-2.39949800	4.00771400
H	3.03581500	-4.88310800	0.16189000	H	-3.05569300	-4.69447700	4.66653100
H	3.11085600	-5.42409200	-2.26626400	C	-4.03213700	0.32105500	0.30220200
C	-2.57054500	-2.65771100	-1.33608900	C	-5.10223800	0.68574400	-0.52295200
C	-3.11667200	-3.95166900	-1.25781500	C	-4.14709900	-0.86423700	1.04584700
C	-3.06368300	-1.77330300	-2.30144000	C	-6.23677300	-0.12348600	-0.61818300
C	-4.13180600	-4.34712000	-2.12612200	H	-5.04561000	1.60214400	-1.09972200
H	-2.75283500	-4.65672800	-0.51832000	C	-5.26727700	-1.68609000	0.95810200
C	-4.08396900	-2.17317700	-3.16900800	C	-6.31243700	-1.30876900	0.11317900
H	-2.61414100	-0.79401700	-2.40397100	H	-7.05639900	0.17206400	-1.26588900
C	-4.62089500	-3.45611600	-3.08473900	H	-5.31951500	-2.60046800	1.53883300
H	-4.53940500	-5.35161700	-2.05361900	H	-7.18977700	-1.94401200	0.03466500
H	-4.45115300	-1.47460500	-3.91525600	O	-3.09277400	-1.10505800	1.90810500
H	-5.41237700	-3.76429700	-3.76232900	Rh	-0.39308800	0.12080300	0.03394800
C	-2.67155600	1.83258700	2.25958300	C	1.78811200	-0.62820900	-0.10721100
C	-3.88959400	2.43497200	2.61893600	C	2.40077800	0.61615400	-0.06390600
C	-1.69787000	1.64718300	3.24783000	H	1.59296300	-1.05707600	-1.08332300
C	-4.12055300	2.85130800	3.92981700	H	1.96329100	-1.31077500	0.71891600
H	-4.66622900	2.57609000	1.87367200	H	2.43349100	1.20291100	-0.97800300
C	-1.93092700	2.06129700	4.56074900	C	3.38842100	0.99373500	1.01230400
H	-0.75784700	1.17389800	2.99356200	H	3.04394900	0.62173900	1.99351900
C	-3.13935200	2.66639800	4.90564000	H	3.46762200	2.08151300	1.08344000
H	-5.06858000	3.31523100	4.18719400	N	4.69471800	0.46763900	0.60532500
H	-1.16222600	1.90883600	5.31299800	H	4.67474700	-0.54919400	0.60933500
H	-3.31795800	2.98880300	5.92766200	C	5.80282300	0.93955400	1.43723700
C	-2.69013400	2.77071500	-0.50540500	H	5.82689400	2.03535000	1.34864800
C	-2.69223500	4.05389100	0.06305500	H	5.65761900	0.72485300	2.51304400
C	-2.82122800	2.64775000	-1.89958700	C	7.12551500	0.35493300	0.98942700
C	-2.85273700	5.18376700	-0.74061600	C	8.04554000	-0.14091900	1.91348000
H	-2.56319400	4.17791100	1.13125400	C	7.47133800	0.31761500	-0.37240700
C	-2.99563700	3.77894200	-2.69601300	C	9.28579900	-0.65233200	1.51509900
H	-2.74535700	1.67472500	-2.37029500	H	7.79828100	-0.13103800	2.97270000
C	-3.01474800	5.04997400	-2.11902500	C	8.69417700	-0.19144600	-0.78673100
H	-2.84387000	6.16939200	-0.28435300	H	6.75886100	0.68410300	-1.10497200
H	-3.09578400	3.66422200	-3.77142000	C	9.61366100	-0.67786100	0.15612400
H	-3.13995300	5.93086200	-2.74228900	H	9.97250000	-1.02799900	2.26457500
C	-1.74807300	-3.03375100	1.36269200	H	8.96552900	-0.22334000	-1.83717500
C	-1.35326300	-4.32915300	1.73940000	O	10.78892700	-1.15589000	-0.35304400
C	-2.67436000	-2.38678000	2.20230500	C	11.75927300	-1.64793100	0.55478500
C	-1.81876900	-4.92707400	2.91197500	H	12.60890800	-1.96517600	-0.05226800

H	11.38411600	-2.50804300	1.12525900
H	12.08902600	-0.87156700	1.25777600
H	-0.32076700	-0.17853800	1.54709500
Br	-0.28499500	0.25236800	-2.69797800

12^{L1}-Br

Sum of electronic and thermal Free Energies= -6015.459

P	-2.15963100	0.76269100	1.15547300
P	-0.60478300	-2.18380500	-0.66809300
C	-2.16953300	2.58666400	1.48596100
C	-1.93531800	3.12920000	2.75845100
C	-2.40741700	3.45764100	0.40789400
C	-1.94960400	4.51276900	2.95214600
H	-1.74750400	2.47809300	3.60448900
C	-2.43532900	4.83680500	0.61136200
H	-2.55974900	3.04964200	-0.58780100
C	-2.20613700	5.36919100	1.88200000
H	-1.76511300	4.91637500	3.94403800
H	-2.61595000	5.49622800	-0.23187400
H	-2.22146000	6.44481100	2.03435800
C	-2.02107900	0.07319600	2.87359200
C	-3.12871000	-0.07941700	3.72233400
C	-0.74741300	-0.24680300	3.36768200
C	-2.96534900	-0.54195300	5.02868100
H	-4.12292000	0.16491800	3.36269000
C	-0.58320900	-0.70113700	4.67750400
H	0.11678400	-0.13450500	2.71978900
C	-1.69239000	-0.85216400	5.51085600
H	-3.83429200	-0.65674700	5.67091800
H	0.41143400	-0.93978500	5.04379500
H	-1.56651200	-1.21022800	6.52883000
C	-1.33060500	-2.94752200	-2.18814100
C	-1.79393600	-4.27472300	-2.15088400
C	-1.38772300	-2.23789800	-3.39364100
C	-2.29473100	-4.88046500	-3.30217700
H	-1.76390300	-4.83694300	-1.22279700
C	-1.89115000	-2.85018900	-4.54448500
H	-1.09257400	-1.19573200	-3.42196800
C	-2.34182700	-4.16891100	-4.50381500
H	-2.65034100	-5.90621400	-3.25922700
H	-1.94056800	-2.28337600	-5.46963600
H	-2.73562000	-4.64017100	-5.40018400
C	1.02899100	-3.05472700	-0.51384300
C	1.49475000	-3.93887400	-1.49718100
C	1.84733100	-2.80279700	0.60087100
C	2.74055900	-4.55909700	-1.36617600
H	0.89077100	-4.14500000	-2.37275300
C	3.08232500	-3.43412700	0.73846200
H	1.52131500	-2.09940300	1.36036700
C	3.53527500	-4.31430200	-0.24818900
H	3.08562800	-5.23364500	-2.14455300
H	3.69464400	-3.22949200	1.61222000
H	4.50224300	-4.79879700	-0.14715200
C	-3.94732300	0.46081800	0.73916700
C	-4.95533700	1.40791600	0.98138700
C	-4.33155700	-0.73241500	0.10452100
C	-6.27704600	1.18112600	0.59415900
H	-4.69871700	2.34447800	1.46305900
C	-5.64238800	-0.96275000	-0.30738900
C	-6.62114400	-0.00085900	-0.06089200
H	-7.03150900	1.93621800	0.79357100
H	-5.87097300	-1.88839000	-0.82530900
H	-7.64368500	-0.17523400	-0.38219600
C	-1.60938400	-2.97405000	0.66606800
C	-1.13475700	-3.93100300	1.57200800
C	-2.95094800	-2.57117400	0.77203200
C	-1.96663000	-4.45127300	2.56573400
H	-0.10720600	-4.26934400	1.50475300
C	-3.79263400	-3.08234400	1.75907200
C	-3.29008600	-4.02167600	2.65952400
H	-1.57882100	-5.18806400	3.26233200
H	-4.82251800	-2.74780300	1.81537900
H	-3.94089800	-4.42160600	3.43167000
O	-3.37789700	-1.69136600	-0.19661000
Rh	-0.35795100	0.10586600	-0.51552500
H	0.57830200	-0.30998700	0.64527200
C	3.19877400	1.62140100	-2.32409400
H	3.34306400	2.70703900	-2.48873500
H	3.42197000	1.12865200	-3.28142700
N	4.09458400	1.07426700	-1.31311400
H	3.87012800	1.48825800	-0.41021100
C	5.50806000	1.29893100	-1.60638700
H	5.72216600	0.80974400	-2.56862700
H	5.75535800	2.36799900	-1.75364700
C	6.40913700	0.72818500	-0.52995600
C	6.15573800	-0.52590700	0.03396400
C	7.53903600	1.43192700	-0.08896800
C	6.99954200	-1.07195800	1.00491900
H	5.27729300	-1.07788800	-0.28611600

C	8.39238600	0.90208000	0.87227600
H	7.75383400	2.41357500	-0.50504000
C	8.12721100	-0.35726000	1.42673400
H	6.77020600	-2.04678000	1.42014300
H	9.26596600	1.44687500	1.21560700
O	9.01985100	-0.79283300	2.36770600
C	8.79933000	-2.05953100	2.96201300
H	9.61606800	-2.20846000	3.67051400
H	8.81725400	-2.86730700	2.21830500
H	7.84402600	-2.09528900	3.50256100
C	1.29828100	-0.08587400	-1.81255500
H	0.99385900	-0.53247200	-2.76227100
H	2.09451700	-0.67261100	-1.35670300
C	1.72320200	1.35920500	-2.01480500
H	1.10005600	1.81902900	-2.78379400
S	1.16900700	2.18167700	-0.41302000
C	0.82682700	3.87709400	-0.92084400
C	1.42562400	4.89663200	-0.16975300
C	0.01423500	4.19537800	-2.01689600
C	1.22044200	6.23233800	-0.51893100
H	2.05388000	4.64268600	0.67862700
C	-0.17150000	5.53390400	-2.36593000
H	-0.49433500	3.40575300	-2.56153900
C	0.42832000	6.55349000	-1.62245600
H	1.68967000	7.01857300	0.06575800
H	-0.79802200	5.77825400	-3.21939500
H	0.27826700	7.59280500	-1.90113300
Br	-1.90664100	1.10756000	-2.49953200

TS9^{L1}-Br

Sum of electronic and thermal Free Energies= -6015.42714

P	-2.07291200	0.74184100	1.15158900
P	-0.91726600	-2.11490100	-0.68932500
C	-1.88100300	2.52263000	1.62810000
C	-1.59295800	2.92710000	2.94059400
C	-2.05496600	3.50102900	0.63358500
C	-1.48819200	4.28426700	3.25495800
H	-1.45569900	2.19023400	3.72349800
C	-1.96068800	4.85404400	0.95842300
H	-2.24968800	3.19710000	-0.39241400
C	-1.67723300	5.25052100	2.26708200
H	-1.26281900	4.58142100	4.27556900
H	-2.09056900	5.59831300	0.17879600
H	-1.59827000	6.30585000	2.51304900
C	-1.83491600	-0.11333800	2.77839400
C	-2.87662600	-0.35810200	3.68389300
C	-0.52522700	-0.46520500	3.14215300
C	-2.61474300	-0.94859600	4.92227500
H	-3.89498900	-0.08661000	3.42524900
C	-0.26272200	-1.04155000	4.38529500
H	0.28321900	-0.27879900	2.43952800
C	-1.30883800	-1.28899200	5.27722100
H	-3.43353800	-1.13828300	5.61081600
H	0.75748300	-1.29945000	4.65615600
H	-1.10711600	-1.74442400	6.24270000
C	-1.64734800	-2.73618400	-2.27235600
C	-2.02744000	-4.08572300	-2.38601000
C	-1.82200800	-1.87897000	-3.36481300
C	-2.55602400	-4.57039300	-3.58083800
H	-1.91287600	-4.75845800	-1.54122900
C	-2.35634700	-2.37128800	-4.55949300
H	-1.59178500	-0.82086600	-3.27149200
C	-2.71883300	-3.71247500	-4.67272600
H	-2.84541000	-5.61485800	-3.65761200
H	-2.49761100	-1.69262200	-5.39562300
H	-3.13543300	-4.08995400	-5.60263800
C	0.66487200	-3.07746300	-0.54441500
C	1.18239000	-3.83879200	-1.60092300
C	1.41426300	-2.97722600	0.64211600
C	2.41367600	-4.48946000	-1.47265300
H	0.63131300	-3.92462800	-2.53027200
C	2.63382300	-3.63870800	0.77351500
H	1.04235700	-2.37429300	1.46487000
C	3.13986900	-4.39633300	-0.28717600
H	2.80170700	-5.06755800	-2.30642700
H	3.19263400	-3.55605800	1.70148600
H	4.09443800	-4.90534200	-0.18913900
C	-3.91039800	0.65224300	0.86658200
C	-4.78327100	1.68279000	1.25275000
C	-4.47174200	-0.43203400	0.17233700
C	-6.14256500	1.64148700	0.93901800
H	-4.39077600	2.53802300	1.79008900
C	-5.82080100	-0.47336000	-0.17258400
C	-6.66139100	0.57007300	0.21277600
H	-6.78917900	2.45665500	1.24941700
H	-6.18732300	-1.31894200	-0.74524800
H	-7.71346400	0.54391300	-0.05491000
C	-2.00551500	-2.94375400	0.55384600
C	-1.62864700	-4.01209900	1.37813000

C	-3.32073700	-2.46548400	0.65299100	H	2.54935600	4.39148200	0.95190000
C	-2.53178700	-4.56672300	2.28722000	C	0.40803900	5.75082900	-1.97816100
H	-0.62343000	-4.41201100	1.31390100	H	-0.17406500	3.69462100	-2.30927200
C	-4.23262000	-3.00767300	1.55724500	C	1.13438100	6.63759200	-1.17919800
C	-3.82819100	-4.06010300	2.37846000	H	2.46346000	6.83104700	0.51018900
H	-2.22027300	-5.39148700	2.92069100	H	-0.19598200	6.12669700	-2.79941100
H	-5.24057600	-2.61127300	1.61010400	H	1.10527200	7.70446600	-1.38254900
H	-4.53361800	-4.48789500	3.08495100	Br	-1.85925600	1.62787700	-2.55651700
O	-3.65742400	-1.47341400	-0.24384200	**13^{L1}-Br**			
Rh	-0.48135400	0.12912100	-0.56964100	Sum of electronic and thermal Free Energies= -6015.476			
H	0.99162700	-0.42263200	-0.40483500	P	1.60161000	1.61606800	-0.59513100
C	3.28240100	1.58059400	-2.26025000	P	2.51657600	-1.74365500	0.14229300
H	3.48018600	2.66420200	-2.36010700	C	0.32223800	2.90881600	-0.99359800
H	3.46003400	1.13868200	-3.25117300	C	0.29230200	4.17689500	-0.39835100
N	4.16490600	0.92053300	-1.30524400	C	-0.61033700	2.61791600	-2.00347800
H	3.99508700	1.30530100	-0.37769900	C	-0.64089200	5.13405600	-0.81033800
C	5.58367100	1.05434500	-1.62907000	H	1.00168900	4.42836700	0.38180200
H	5.73651900	0.59636500	-2.61794500	C	-1.54099900	3.57180000	-2.41437200
H	5.90497600	2.10799300	-1.73477600	H	-0.59406900	1.64295700	-2.48133600
C	6.46711900	0.37062800	-0.60476800	C	-1.55794300	4.83705600	-1.81798000
C	6.12371500	-0.87372600	-0.06760900	H	-0.64601500	6.11327500	-0.33954600
C	7.67038400	0.95800100	-0.18753000	H	-2.24674200	3.33023900	-3.20426600
C	6.94950300	-1.52240300	0.85458100	H	-2.27853500	5.58329000	-2.14045300
H	5.18902000	-1.33665000	-0.36891100	C	2.57441900	2.44438900	0.75011300
C	8.50702500	0.32478700	0.72432000	C	3.57703300	3.39710200	0.51250300
H	7.95652300	1.92986500	-0.58310200	C	2.23730300	2.13398900	2.07571400
C	8.15072800	-0.92347900	1.25259700	C	4.22369900	4.02512700	1.57822500
H	6.64905900	-2.48536000	1.25125400	H	3.85665700	3.65066500	-0.50500400
H	9.43741100	0.77947300	1.04898900	C	2.87744700	2.76931900	3.14039100
O	9.03422100	-1.46529200	2.14538600	H	1.46641100	1.39271400	2.26258300
C	8.72546600	-2.72747800	2.70956000	C	3.87407700	3.71481100	2.89385700
H	9.55141300	-2.96985200	3.38053800	H	5.00148900	4.75728400	1.37915800
H	8.64540700	-3.50833000	1.94159800	H	2.59921100	2.52175800	4.16082000
H	7.79114600	-2.69863400	3.28602500	H	4.37826300	4.20535700	3.72183100
C	1.35706100	-0.08480300	-1.82160500	C	3.01548600	-2.95276900	-1.17147500
H	0.85840300	-0.42649700	-2.73004500	C	4.30332900	-3.51373600	-1.18346700
H	2.20678100	-0.74331600	-1.62103700	C	2.11910500	-3.28992500	-2.19451800
C	1.80392700	1.37006400	-1.92443900	C	4.68045500	-4.40472000	-2.18910700
H	1.17103100	1.88189400	-2.65158900	H	5.01988200	-3.25001700	-0.41136200
S	1.32671800	2.13780300	-0.27599100	C	2.50162500	-4.17780200	-3.20164700
C	1.21887200	3.89043600	-0.66992700	H	1.11964200	-2.87095000	-2.18422600
C	1.94580600	4.77676100	0.13560700	C	3.77944600	-4.73842800	-3.20191700
C	0.43522300	4.37852700	-1.72453100	H	5.67942200	-4.83228600	-2.18247500
C	1.89655900	6.14855600	-0.11683200	H	1.79476800	-4.43089800	-3.98688200

H	4.07366900	-5.42929200	-3.98734700
C	2.36138800	-2.74526900	1.69368200
C	2.79800900	-4.07222700	1.79621400
C	1.80197300	-2.12912000	2.82428600
C	2.68160100	-4.76437100	3.00416300
H	3.21669700	-4.57683400	0.93295700
C	1.69773800	-2.81663400	4.03232200
H	1.42845800	-1.11292000	2.74075200
C	2.13646500	-4.13953500	4.12528000
H	3.01440700	-5.79693700	3.06336200
H	1.26139600	-2.32474100	4.89744000
H	2.04579400	-4.68084700	5.06287500
C	2.69244200	1.88624400	-2.11026200
C	2.52928500	3.01488800	-2.93686700
C	3.68275100	0.96794300	-2.50526600
C	3.28032400	3.19976400	-4.09836000
H	1.79303700	3.76432100	-2.67728400
C	4.42213700	1.12713100	-3.67824700
C	4.22122700	2.24596200	-4.48244700
H	3.11642700	4.08556600	-4.70467500
H	5.14361400	0.35928400	-3.93764000
H	4.79702700	2.37080700	-5.39463800
C	4.12571400	-0.88186900	0.45585500
C	4.84774800	-0.91133800	1.65562400
C	4.62701200	-0.09798600	-0.59016600
C	6.02144700	-0.16730000	1.80088700
H	4.48732300	-1.51287400	2.48244300
C	5.79474500	0.65057400	-0.46551400
C	6.48968100	0.61445500	0.74450500
H	6.56591700	-0.19893400	2.73975300
H	6.14998500	1.24518100	-1.30044500
H	7.40095000	1.19496500	0.85571800
O	3.91213400	-0.17655500	-1.77219300
Rh	0.63584500	-0.44639300	-0.12796900
C	-4.43545900	0.40867200	0.24177700
H	-4.47641600	1.08727200	1.11402100
H	-5.23244700	0.73523200	-0.44017800
N	-4.67984400	-0.98320500	0.59264600
H	-3.88006600	-1.35428700	1.09952500
C	-5.90640000	-1.19760500	1.35467200
H	-6.00654000	-0.50763200	2.21462800
H	-5.84762000	-2.20993200	1.77562100
C	-7.15486100	-1.08423700	0.49650500
C	-8.29137400	-0.41699200	0.95271500
C	-7.20672500	-1.68256700	-0.77365000
C	-9.46097100	-0.34573200	0.18657800
H	-8.27360400	0.06306200	1.92888500
C	-8.35542100	-1.61878300	-1.55020100
H	-6.32218600	-2.18935800	-1.14741400
C	-9.49423200	-0.95049200	-1.07333500
H	-10.32226300	0.18401200	0.57662700
H	-8.40005000	-2.07903800	-2.53232600
O	-10.57377600	-0.94275800	-1.91405700
C	-11.74949000	-0.28052700	-1.48345400
H	-12.47493900	-0.39404100	-2.29099800
H	-12.15789900	-0.72872300	-0.56782600
H	-11.57279900	0.78888900	-1.30653400
C	-3.09978700	0.59925900	-0.49079300
H	-3.01894800	1.64062900	-0.81171800
S	-1.67360100	0.27911500	0.68303700
C	-1.78320600	1.63640700	1.85909200
C	-1.43843000	1.32161400	3.18330500
C	-2.18831500	2.93904100	1.54702400
C	-1.48256000	2.30061800	4.17488000
H	-1.15159200	0.30338800	3.42962500
C	-2.24972400	3.90931200	2.55002300
H	-2.45017900	3.20897500	0.53097000
C	-1.89342200	3.59865200	3.86251300
H	-1.21474400	2.04302000	5.19582800
H	-2.57020900	4.91589000	2.29621400
H	-1.94089100	4.35891900	4.63664700
C	-2.94997100	-0.31964200	-1.70453900
H	-2.95413900	-1.36978300	-1.41339500
H	-3.79246600	-0.14297400	-2.38275200
H	-2.01914400	-0.12423300	-2.24192900
Br	-0.59195900	-2.71995600	-0.05027200

TS10^{L1}-Br

Sum of electronic and thermal Free Energies= -6015.42331

S	-0.10437800	2.92113000	0.55076900
C	0.03389300	4.25316000	-0.62546000
C	-1.00387400	4.58695100	-1.51657000
C	1.18193000	5.06745900	-0.59289700
C	-0.88328900	5.69648800	-2.35226900
H	-1.89006000	3.96149200	-1.54610300
C	1.28443900	6.19002400	-1.41646700
H	1.98495000	4.82187300	0.09611700
C	0.25565200	6.50648700	-2.30511900
H	-1.69256200	5.93729400	-3.03704900

H	2.17464100	6.81221400	-1.36775000
H	0.33833900	7.37531400	-2.95229600
P	-1.11825500	-1.47109900	-1.59458700
P	-1.17797500	0.16622300	2.00931900
C	-0.75027900	-1.39243800	-3.40718700
C	0.25925400	-2.15723700	-4.00911500
C	-1.47367000	-0.47875900	-4.20059100
C	0.52875100	-2.02775500	-5.37472100
H	0.83552200	-2.86160400	-3.41966200
C	-1.20795000	-0.36297400	-5.56441200
H	-2.22851400	0.15191300	-3.73672800
C	-0.20639400	-1.13767700	-6.15615000
H	1.31486300	-2.62805200	-5.82388400
H	-1.77851300	0.34213400	-6.16199900
H	0.00230200	-1.04176100	-7.21783300
C	-0.16891300	-2.96063200	-1.03606400
C	-0.52457100	-4.24709100	-1.47664200
C	0.91534800	-2.82253100	-0.16057700
C	0.19666600	-5.36403100	-1.05742000
H	-1.37061400	-4.37459700	-2.14518200
C	1.63791600	-3.94239100	0.25919400
H	1.18548500	-1.84129100	0.21393700
C	1.28158300	-5.21362200	-0.18915600
H	-0.09053300	-6.35220000	-1.40579100
H	2.46951300	-3.81367400	0.94552000
H	1.84039900	-6.08544500	0.13943700
C	-1.71485700	1.64817200	2.97672700
C	-1.08570800	2.07432700	4.15340700
C	-2.85670800	2.32648500	2.51949300
C	-1.59828100	3.15883000	4.87114200
H	-0.19480700	1.56978700	4.51260000
C	-3.36759700	3.40021600	3.24504900
H	-3.31785800	2.03793700	1.57878900
C	-2.74140900	3.81891600	4.42220000
H	-1.09961000	3.48484800	5.77975700
H	-4.24736100	3.92199800	2.87966900
H	-3.13820800	4.66212200	4.98077700
C	0.41829400	-0.36491000	2.80503900
C	1.54150100	0.47730000	2.69460300
C	0.57371700	-1.60925600	3.43192600
C	2.77724500	0.08373800	3.20653700
H	1.44871900	1.44124300	2.20144800
C	1.81729300	-2.00384300	3.93604800
H	-0.26943600	-2.28318500	3.52891800
C	2.92141600	-1.16086000	3.82673100
H	3.63260700	0.74640000	3.11051700
H	1.91501200	-2.97413500	4.41527200
H	3.88746400	-1.46766800	4.21728500
C	-2.86392400	-2.07622500	-1.58803700
C	-3.66388800	-2.25169700	-2.72206700
C	-3.44515100	-2.29864600	-0.32885300
C	-5.01470600	-2.58431200	-2.60349100
H	-3.23968700	-2.11120100	-3.70807400
C	-4.80188600	-2.58537200	-0.19119500
C	-5.58328100	-2.72225500	-1.34016000
H	-5.61880400	-2.71230900	-3.49607800
H	-5.25049600	-2.69108100	0.78756400
H	-6.64123900	-2.94487600	-1.23661200
C	-2.35763400	-1.07468300	2.76297200
C	-2.66925000	-1.01537100	4.13299700
C	-2.88250900	-2.14612600	2.03040300
C	-3.44447400	-1.99641600	4.74725600
H	-2.29657600	-0.18765100	4.72533300
C	-3.62140300	-3.16494900	2.64313200
C	-3.90825600	-3.08248700	4.00287400
H	-3.67214500	-1.91898300	5.80589900
H	-3.94880800	-4.01518100	2.05617800
H	-4.48670600	-3.86906000	4.47843200
O	-2.53860700	-2.21009600	0.70228200
Rh	-0.58929800	0.72057000	-0.47320900
H	0.84035700	0.22611800	-0.02814900
C	0.46352200	1.43664300	-2.24584500
C	1.45170900	0.70068400	-1.55089900
H	-0.01750800	1.00410100	-3.11032300
H	0.48915900	2.51863600	-2.21840600
H	1.63539300	-0.31931800	-1.88422600
C	2.67944700	1.35749300	-0.94181800
H	2.40791200	2.32910100	-0.50822300
H	3.08041500	0.73688200	-0.13458000
N	3.70519500	1.44120900	-1.98799200
H	3.37867200	2.07351000	-2.71488400
C	4.99898200	1.91797700	-1.48726500
H	4.90952300	2.83636600	-0.87863400
H	5.59969600	2.18658300	-2.36629600
C	5.73329500	0.86609200	-0.67601400
C	5.80525000	-0.45853200	-1.11638400
C	6.38650700	1.19831000	0.51920400
C	6.50969300	-1.42916900	-0.40038600

H	5.28697500	-0.73333200	-2.03029100
C	7.09658400	0.24707400	1.24428900
H	6.34029300	2.22059300	0.88793700
C	7.16358400	-1.07603000	0.78700000
H	6.54180000	-2.44626700	-0.77374800
H	7.60382300	0.50333300	2.16892600
O	7.88016600	-1.94033700	1.56784000
C	7.99252200	-3.28781100	1.14345200
H	8.60453800	-3.79164800	1.89354300
H	7.01260100	-3.78051100	1.08868000
H	8.48478000	-3.36655800	0.16525700
Br	-3.00541300	1.46096600	-1.23170200

14^{L1}-Br

Sum of electronic and thermal Free Energies= -6015.457

S	-0.46098500	1.37873500	2.21473900
C	-1.67820000	0.61917500	3.27672100
C	-3.04559400	0.75993200	2.99077900
C	-1.30058000	0.00398700	4.48257700
C	-4.01141000	0.29233800	3.88344100
H	-3.34902200	1.24555800	2.06947200
C	-2.26741000	-0.45693900	5.37403000
H	-0.24661700	-0.10768700	4.70916500
C	-3.62608600	-0.31792700	5.07776600
H	-5.06514800	0.40930700	3.64434700
H	-1.95867100	-0.92991200	6.30262800
H	-4.37746000	-0.67984200	5.77433800
Rh	0.76722000	-0.10249900	0.75617000
H	-2.29045500	0.70051600	-0.12813300
C	-0.67985400	-0.62741700	-0.65857500
C	-2.12362800	-0.37346500	-0.26160000
H	-0.51294000	-1.69684100	-0.81558200
H	-0.42638900	-0.07318800	-1.56556300
H	-2.35614900	-0.86102100	0.68760300
C	-3.08802800	-0.89983200	-1.33903100
H	-2.97515100	-1.98846100	-1.43357600
H	-2.81716400	-0.47100600	-2.32518800
N	-4.47582700	-0.62395100	-0.97378000
H	-4.59503400	0.37703800	-0.83213100
C	-5.44753500	-1.08172100	-1.96307900
H	-5.27173600	-0.66637400	-2.97515400
H	-5.31818200	-2.17001300	-2.06205400
C	-6.86897600	-0.77194800	-1.54046700
C	-7.80822500	-0.29016000	-2.45245600
C	-7.28514800	-0.98513100	-0.21498900
C	-9.13270500	-0.03324300	-2.07957400
H	-7.50876400	-0.10771800	-3.48226100
C	-8.59310000	-0.73120000	0.17452600
H	-6.55913800	-1.34142800	0.50921900
C	-9.52895700	-0.25597600	-0.75741700
H	-9.83109200	0.34205100	-2.81854800
H	-8.91929200	-0.89335800	1.19706300
O	-10.79052300	-0.03936000	-0.27457800
C	-11.77758900	0.43125700	-1.17482900
H	-12.69767000	0.52396100	-0.59508200
H	-11.51508300	1.41312500	-1.59100500
H	-11.94281500	-0.27205600	-2.00191500
P	2.40874200	-1.65089500	-0.39521400
P	1.42651100	1.98333800	-0.28274300
C	1.96018500	-3.44690300	-0.55860500
C	1.60942100	-3.98832000	-1.80627400
C	1.89515500	-4.28183700	0.57257000
C	1.21153700	-5.32167100	-1.92216800
H	1.65123200	-3.37951600	-2.70104800
C	1.51465400	-5.61774500	0.44884200
H	2.12640100	-3.88640700	1.55182200
C	1.16683500	-6.14249200	-0.79646400
H	0.94365200	-5.71513400	-2.89861000
H	1.47616000	-6.24317800	1.33591500
H	0.86165800	-7.18109400	-0.88709600
C	2.99859400	-1.30869600	-2.12614500
C	4.32309400	-1.54032000	-2.52633100
C	2.06917400	-0.89497200	-3.09333300
C	4.70890200	-1.35266500	-3.85426200
H	5.05850600	-1.87163100	-1.80109400
C	2.45322100	-0.71948900	-4.42456200
H	1.03573400	-0.72570300	-2.81277200
C	3.77618900	-0.94286600	-4.80787200
H	5.74039300	-1.53312600	-4.14348000
H	1.71578700	-0.41001300	-5.16002000
H	4.07720200	-0.80290500	-5.84207400
C	1.63849300	3.44297600	0.84689300
C	1.39534500	4.75383200	0.40976600
C	2.19752100	3.24363800	2.11874500
C	1.68522500	5.84043300	1.23584200
H	0.97580800	4.93485600	-0.57388200
C	2.49297700	4.33332700	2.93781800
H	2.38973700	2.23854500	2.47303300
C	2.23321800	5.63315400	2.50234000

H	1.48215300	6.84874900	0.88611900
H	2.91557300	4.16144600	3.92347200
H	2.45652000	6.47975600	3.14538300
C	0.20976800	2.54980900	-1.54662800
C	-0.97927700	3.15306800	-1.09666900
C	0.33935100	2.25732200	-2.91393100
C	-1.98975100	3.48562400	-1.99875000
H	-1.11902200	3.34626700	-0.03792100
C	-0.67668000	2.59133300	-3.81271700
H	1.23062400	1.76513500	-3.28537800
C	-1.84107300	3.21106600	-3.35991300
H	-2.89706100	3.95802800	-1.63329300
H	-0.55413800	2.36419500	-4.86806600
H	-2.62932900	3.47238200	-4.05995800
C	3.99773300	-1.66459000	0.56692000
C	4.70594500	-2.82988700	0.90127200
C	4.51357700	-0.44403500	1.03844400
C	5.84721300	-2.78111400	1.70392800
H	4.35457700	-3.78883000	0.54008000
C	5.63386000	-0.38457500	1.86459400
C	6.30348600	-1.56098700	2.20130800
H	6.36937800	-3.70110300	1.94824100
H	5.96310200	0.58178100	2.23233200
H	7.17724600	-1.52031900	2.84453800
C	3.10038200	2.08312200	-1.07353600
C	3.40720000	2.89446000	-2.17589800
C	4.16115100	1.41265900	-0.44229900
C	4.70788900	2.98231600	-2.67076600
H	2.62110700	3.46656600	-2.65498100
C	5.46678700	1.48919600	-0.92798400
C	5.73408100	2.26914400	-2.05142000
H	4.91670800	3.60984400	-3.53160000
H	6.26221800	0.95194200	-0.42449600
H	6.75042500	2.33105800	-2.42916300
O	3.85163600	0.73716500	0.72962600
Br	0.14558400	-2.06466300	2.21128000

TS11^{L1}-Br

Sum of electronic and thermal Free Energies= -6015.415

S	-1.81569800	1.79484200	-2.37215700
C	-2.67408200	3.22424900	-1.70324400
C	-4.04749200	3.14255400	-1.41458500
C	-2.05278300	4.48422500	-1.65311800
C	-4.76722300	4.28425000	-1.05837800
H	-4.55186300	2.18581300	-1.48453200
C	-2.77237200	5.61971300	-1.27850000
H	-1.00793100	4.58291300	-1.92823400
C	-4.13181100	5.52532600	-0.97530400
H	-5.83018000	4.20040600	-0.84821600
H	-2.27081300	6.58301700	-1.24087800
H	-4.69398800	6.41215800	-0.69693800
P	0.54717000	-1.71183700	-0.36632200
P	-2.27623600	0.07853400	0.85107600
C	2.26871200	-1.68354100	-1.08991400
C	3.30175100	-2.40299600	-0.45931900
C	2.58198900	-0.93222300	-2.23202600
C	4.60223000	-2.37650500	-0.96145500
H	3.09473000	-2.98497600	0.43229300
C	3.89028100	-0.89457800	-2.72253100
H	1.79397600	-0.41593700	-2.76699900
C	4.90349800	-1.61392200	-2.09182000
H	5.38045100	-2.94814400	-0.46302300
H	4.10888200	-0.30450900	-3.60795000
H	5.91897900	-1.58228900	-2.47614800
C	1.04706200	-1.77507300	1.42333700
C	0.92354800	-2.91542000	2.22655200
C	1.66442700	-0.63262500	1.96384500
C	1.38068000	-2.90988500	3.54764800
H	0.47414900	-3.81626600	1.82432800
C	2.13004500	-0.63301800	3.27897100
H	1.81024400	0.25651100	1.35559400
C	1.98325500	-1.77033500	4.07822700
H	1.26773100	-3.80224000	4.15674600
H	2.61229100	0.25611900	3.67579700
H	2.34332200	-1.76851400	5.10312700
C	-4.06767800	0.01958000	0.35171500
C	-5.09234900	0.29721900	1.27158200
C	-4.41233900	-0.43623100	-0.92917600
C	-6.43098500	0.16291000	0.90462300
H	-4.84827600	0.62158800	2.27812000
C	-5.75455000	-0.58288200	-1.28951100
H	-3.63152700	-0.66878200	-1.64500400
C	-6.76580400	-0.27546400	-0.37894300
H	-7.21158900	0.39513900	1.62380000
H	-6.00353300	-0.93420400	-2.28670400
H	-7.80888300	-0.38327100	-0.66311800
C	-2.14297300	1.51339600	2.01453500
C	-2.95742200	2.64883200	1.88850700
C	-1.09565300	1.54415400	2.95404700

C	-2.74155900	3.77449100	2.68715400
H	-3.75767600	2.66807600	1.16009500
C	-0.88893500	2.66489400	3.75778800
H	-0.43426700	0.69070300	3.05853200
C	-1.71169900	3.78617100	3.62734700
H	-3.38240100	4.64274700	2.56431200
H	-0.07964100	2.66187400	4.48270200
H	-1.54761300	4.66090800	4.25021500
C	-0.07622200	-3.41501300	-0.74495700
C	0.69670700	-4.38233300	-1.40436900
C	-1.42697200	-3.72337800	-0.49924400
C	0.14713100	-5.60197600	-1.80151900
H	1.73506200	-4.17053300	-1.63134400
C	-1.99215600	-4.92712700	-0.91481400
C	-1.19969300	-5.87342600	-1.56441400
H	0.76945900	-6.32874500	-2.31467700
H	-3.04893800	-5.09780900	-0.73709300
H	-1.63771400	-6.81201600	-1.89057600
C	-2.34041800	-1.38205400	2.01266600
C	-2.52003600	-1.27256100	3.39967600
C	-2.32425800	-2.67658100	1.46383500
C	-2.64066800	-2.40120700	4.21105500
H	-2.56102000	-0.29141500	3.85731700
C	-2.44833100	-3.81382100	2.26379700
C	-2.59907000	-3.67336900	3.64180200
H	-2.77132400	-2.28222300	5.28233500
H	-2.42969000	-4.79533200	1.80319500
H	-2.69727400	-4.55824100	4.26409500
O	-2.25115300	-2.77163200	0.08593600
Rh	-0.93913900	-0.02977200	-1.07173400
H	-0.45807400	3.39200500	0.10918300
C	0.36617900	2.05795500	-1.36499200
C	0.41649800	2.74841300	-0.02652000
H	1.04446900	1.21545600	-1.48567400
H	0.48336700	2.72827800	-2.21128800
H	0.40238600	2.01870800	0.78209600
C	1.67762300	3.62110900	0.12727400
H	1.70007400	4.39382600	-0.66613100
H	1.60251100	4.15930200	1.08102600
N	2.89992000	2.81915500	0.16764600
H	3.01950700	2.32486000	-0.71421100
C	4.09795800	3.62014900	0.42131400
H	3.97355400	4.08082800	1.41343100
H	4.20450400	4.46390700	-0.28663900
C	5.36932600	2.79593800	0.39249600
C	5.40316300	1.48318900	0.86968300
C	6.56388500	3.34970500	-0.09293400
C	6.58516800	0.73700400	0.87137500
H	4.48781800	1.02968700	1.23586400
C	7.75017400	2.62642000	-0.09075400
H	6.56409500	4.36590600	-0.48078200
C	7.76842500	1.31064800	0.39321400
H	6.56602300	-0.28163100	1.24033700
H	8.67384500	3.05410900	-0.46721700
O	8.97996100	0.67767800	0.34869600
C	9.05485000	-0.65518300	0.82315500
H	10.09472300	-0.96282000	0.70023300
H	8.78154700	-0.72586000	1.88431300
H	8.40947200	-1.32988000	0.24489500
Br	-0.58653300	-1.00338400	-3.46740600

15^{L1}-Br

Sum of electronic and thermal Free Energies= -6015.468

S	-0.25329900	2.59767200	-1.32331100
C	-1.32399800	3.97636500	-0.86474700
C	-2.48255800	4.14013000	-1.64178000
C	-1.03146700	4.92377800	0.12497900
C	-3.33884300	5.21602500	-1.41588100
H	-2.70946800	3.42909900	-2.42834800
C	-1.88547600	6.00987500	0.33292900
H	-0.14539400	4.83036600	0.73949500
C	-3.04405400	6.15972400	-0.42822500
H	-4.23029300	5.32333200	-2.02723700
H	-1.63906900	6.73794300	1.10093400
H	-3.70427200	7.00602000	-0.26258500
P	0.01866300	-2.02808700	-0.06049200
P	-2.56675700	0.27884400	0.35119900
C	1.81154200	-2.52535200	0.11740000
C	2.12621100	-3.78421800	0.66500000
C	2.86341100	-1.66049800	-0.20959500
C	3.45134800	-4.17321000	0.85208100
H	1.33422800	-4.46613900	0.95611500
C	4.19265900	-2.04843100	-0.01210200
H	2.64449500	-0.69747300	-0.65221900
C	4.49089700	-3.30374900	0.51402600
H	3.66895200	-5.15262000	1.26934500
H	4.99098600	-1.36192700	-0.27704400
H	5.52458800	-3.60297400	0.66393400
C	-0.50927200	-2.61612100	1.62433800

C	-1.15976800	-3.83031600	1.87312500
C	-0.10724500	-1.83101000	2.71721400
C	-1.42380700	-4.23985200	3.18335000
H	-1.46231400	-4.46390600	1.04640900
C	-0.35843500	-2.24573200	4.02454000
H	0.41341900	-0.89423200	2.53594600
C	-1.02460300	-3.45113900	4.26138000
H	-1.93924800	-5.18028900	3.35696200
H	-0.03190300	-1.62975700	4.85810500
H	-1.22505200	-3.77404900	5.27900400
C	-3.78105700	0.82258700	-0.95202500
C	-5.10914300	1.15610900	-0.64007500
C	-3.39279600	0.78429600	-2.29950100
C	-6.01406500	1.48717200	-1.64879400
H	-5.44304800	1.15298100	0.39296300
C	-4.30316200	1.10525100	-3.30984300
H	-2.37780200	0.48893100	-2.55224500
C	-5.61171700	1.46637600	-2.98667400
H	-7.03560900	1.75203100	-1.39014800
H	-3.98588800	1.06735300	-4.34817800
H	-6.31918700	1.71786700	-3.77209600
C	-2.80391600	1.45787900	1.76402100
C	-3.41262700	2.71410500	1.63030600
C	-2.25100500	1.11491700	3.01258400
C	-3.48710000	3.59002000	2.71726100
H	-3.82290700	3.02557400	0.67777800
C	-2.33380300	1.98640300	4.09697800
H	-1.76418500	0.15412800	3.14190200
C	-2.95550000	3.22972800	3.95384000
H	-3.95855200	4.55929800	2.58498300
H	-1.91099900	1.69389300	5.05432900
H	-3.01841500	3.91089500	4.79784600
C	-0.67743000	-3.28836300	-1.23551200
C	0.11892500	-4.24543000	-1.88390000
C	-2.03338500	-3.22080200	-1.61346200
C	-0.41197600	-5.10694200	-2.84525100
H	1.17427300	-4.30680900	-1.64789600
C	-2.57006300	-4.06804100	-2.58143100
C	-1.75847800	-5.02215100	-3.19469700
H	0.23486300	-5.83248700	-3.32908400
H	-3.61292700	-3.94915800	-2.85707800
H	-2.17504300	-5.68087900	-3.95090300
C	-3.50659200	-1.22275400	0.92927900
C	-4.26152400	-1.29347600	2.10740400
C	-3.51581400	-2.34523800	0.08329100
C	-4.98010300	-2.44412100	2.43878200
H	-4.28631200	-0.44277100	2.77859500
C	-4.23325200	-3.49861100	0.39758400
C	-4.96309700	-3.54642600	1.58488300
H	-5.55334500	-2.47358200	3.36048600
H	-4.21621900	-4.34282900	-0.28338400
H	-5.52435400	-4.44247900	1.83409000
O	-2.83864100	-2.20978100	-1.11268300
Rh	-0.49243600	0.12962600	-0.64731900
H	0.60538300	2.97720300	1.52472700
C	1.34503300	3.03809800	-0.52631800
C	1.48754100	2.66698000	0.95463100
H	2.07900300	2.50298500	-1.12974200
H	1.49100000	4.10973000	-0.69592900
H	1.52269000	1.57490200	1.03896100
C	2.72381300	3.31721800	1.59672600
H	2.63772000	4.40703500	1.49694800
H	2.71170400	3.10035500	2.68203600
N	3.98289500	2.91754600	0.96563800
H	4.68329100	3.63787700	1.11746100
C	4.51989500	1.64378400	1.45174500
H	3.80771800	0.85163200	1.18692900
H	4.60904000	1.61671100	2.55481600
C	5.86953700	1.34173800	0.83742200
C	6.96509300	0.99664600	1.62932900
C	6.05274800	1.39305700	-0.55638000
C	8.21290800	0.69659000	1.07053600
H	6.85152600	0.95643300	2.71024000
C	7.28338200	1.10041300	-1.12835100
H	5.21668800	1.67444500	-1.18944800
C	8.37443800	0.74859400	-0.31716400
H	9.03839300	0.43347700	1.72149600
H	7.42841300	1.13675300	-2.20328500
O	9.54133400	0.48118800	-0.97631400
C	10.67535000	0.11822500	-0.20790500
H	11.48354900	-0.05012400	-0.92161600
H	10.96911600	0.91672400	0.48629700
H	10.50207100	-0.80356300	0.36317100
Br	1.15300200	-0.03685400	-2.62239100

L2

Sum of electronic and thermal Free Energies= -1839.997568

C	0.69277	0.05526	1.10378
C	-0.7168	-0.09863	1.09303

C	-1.40139	-0.19935	2.31279
C	-0.72492	-0.11961	3.53065
C	0.65509	0.06205	3.54174
C	1.35414	0.14834	2.33539
H	-2.47819	-0.33724	2.31201
H	-1.27915	-0.19295	4.46295
H	1.19202	0.13278	4.48302
H	2.42977	0.28965	2.35462
P	1.59018	0.18065	-0.52932
P	-1.59082	-0.19383	-0.55166
C	-3.2527	-0.87489	-0.07292
C	-4.36695	-0.09946	0.28307
C	-3.39995	-2.27185	-0.12646
C	-5.58837	-0.70544	0.58728
H	-4.28207	0.98164	0.31866
C	-4.61644	-2.87802	0.18831
H	-2.55466	-2.88675	-0.42485
C	-5.71579	-2.09457	0.54455
H	-6.44121	-0.08936	0.85851
H	-4.70953	-3.96006	0.14417
H	-6.66726	-2.56408	0.77965
C	-1.96641	1.59263	-0.88402
C	-2.22674	1.9489	-2.21713
C	-1.99992	2.59601	0.09767
C	-2.53571	3.26614	-2.55779
H	-2.17802	1.18878	-2.99289
C	-2.30293	3.91588	-0.24392
H	-1.78437	2.34789	1.13259
C	-2.57689	4.25276	-1.57033
H	-2.73586	3.52312	-3.59403
H	-2.32567	4.68032	0.52915
H	-2.81238	5.28021	-1.83393
C	3.23597	0.8778	-0.03206
C	3.40078	2.26498	-0.18643
C	4.32231	0.12246	0.4379
C	4.60756	2.88501	0.13952
H	2.5772	2.85879	-0.57435
C	5.53238	0.74123	0.75969
H	4.22454	-0.95408	0.54757
C	5.67712	2.12339	0.61443
H	4.71615	3.95844	0.01202
H	6.36374	0.14235	1.12436
H	6.62076	2.60229	0.86172
C	2.00286	-1.59003	-0.88795
C	2.37191	-1.89806	-2.20873
C	1.94564	-2.62959	0.05209
C	2.69555	-3.20379	-2.57487
H	2.39728	-1.10812	-2.95574
C	2.26079	-3.9392	-0.31692
H	1.64909	-2.41692	1.07446
C	2.63942	-4.2294	-1.62818
H	2.98027	-3.42277	-3.60021
H	2.20999	-4.73298	0.42351
H	2.88284	-5.24893	-1.91326

2cat^{L2}

Sum of electronic and thermal Free Energies= -2721.673649

C	2.6058	-1.3734	-0.47131
C	2.36744	-1.47958	0.88206
H	2.9744	-0.41585	-0.83339
C	2.82987	-2.52351	-1.42634
H	2.71229	-2.14868	-2.4495
H	2.07497	-3.29922	-1.28354
C	2.3105	-2.76652	1.6718
H	1.8505	-2.55706	2.64363
H	1.68	-3.504	1.17298
H	2.54629	-0.59447	1.48823
C	3.74615	-3.35071	1.88955
H	4.48299	-2.53657	1.83116
H	3.81484	-3.74416	2.90929
C	4.26217	-3.13248	-1.2699
H	4.63952	-3.39848	-2.26342
H	4.94344	-2.3583	-0.88831
C	4.11425	-4.45823	0.92375
C	4.32656	-4.36698	-0.39495
H	4.18299	-5.4528	1.36261
H	4.5517	-5.29486	-0.92018
C	-3.26363	3.60895	-0.96318
C	-2.08235	4.354	-0.90595
C	-0.87279	3.72209	-0.62353
C	-0.83307	2.34077	-0.38417
C	-2.02378	1.59518	-0.42071
C	-3.23447	2.23603	-0.72388
H	-4.20447	4.09644	-1.20106
H	-2.10216	5.42298	-1.09671
H	0.04491	4.30186	-0.60497
H	-4.15033	1.65569	-0.78353
P	0.75097	1.41019	-0.09857
P	-1.88384	-0.22014	-0.08619

Rh	0.33191	-0.81654	-0.09675
Cl	-0.43431	-3.13659	-0.34621
C	-3.0906	-0.95786	-1.26294
C	-4.4206	-1.23058	-0.90841
C	-2.66098	-1.22151	-2.57383
C	-5.30837	-1.74765	-1.85506
H	-4.76244	-1.05168	0.10759
C	-3.55366	-1.72454	-3.51848
H	-1.62088	-1.05142	-2.83894
C	-4.87904	-1.99072	-3.16064
H	-6.33368	-1.96577	-1.56815
H	-3.2106	-1.92668	-4.529
H	-5.57073	-2.39516	-3.89452
C	-2.64852	-0.45533	1.57733
C	-2.59217	-1.74061	2.14734
C	-3.23982	0.5896	2.30296
C	-3.13298	-1.96908	3.41212
H	-2.11154	-2.54729	1.60022
C	-3.77055	0.35449	3.57434
H	-3.28941	1.58912	1.88368
C	-3.72091	-0.92397	4.13005
H	-3.08546	-2.96634	3.84114
H	-4.22223	1.174	4.12706
H	-4.13316	-1.10525	5.11915
C	1.81369	2.04391	-1.48061
C	2.59634	3.20605	-1.39658
C	1.78655	1.33205	-2.69127
C	3.33387	3.64419	-2.49868
H	2.64193	3.76694	-0.46889
C	2.51694	1.7756	-3.79385
H	1.19653	0.42187	-2.75213
C	3.29496	2.93185	-3.69864
H	3.94006	4.54276	-2.41773
H	2.48381	1.21435	-4.72409
H	3.87152	3.27348	-4.55354
C	1.4697	2.21814	1.40234
C	2.8294	2.02146	1.70699
C	0.67787	2.9385	2.31134
C	3.37896	2.53223	2.88258
H	3.46812	1.47263	1.01813
C	1.23089	3.4554	3.48514
H	-0.3742	3.10344	2.10462
C	2.58093	3.2543	3.77543
H	4.43207	2.36898	3.09837
H	0.60335	4.02134	4.17036
H	3.00817	3.65454	4.6907

3cat^{L2}

Sum of electronic and thermal Free Energies= -2721.664327

C	-1.73355	0.62326	2.69851
C	-1.35879	-0.68279	2.97333
H	-2.583	0.77303	2.03754
C	-1.35364	1.83529	3.53697
H	-1.22251	1.5247	4.57822
H	-2.19315	2.54032	3.53567
C	-0.43743	-1.13608	4.08507
H	-1.00404	-1.22472	5.02626
H	-0.10549	-2.14126	3.81322
H	-1.91661	-1.48323	2.49512
C	0.80327	-0.23705	4.27764
H	0.59158	0.57409	4.98519
H	1.5938	-0.83546	4.7437
C	-0.08623	2.54305	3.02337
H	-0.3722	3.27104	2.25408
H	0.37922	3.13077	3.83248
C	1.3318	0.34487	2.96531
C	0.92535	1.5915	2.41033
H	2.33673	0.01614	2.71422
H	1.66739	2.10679	1.80375
C	0.85833	0.05708	-4.51262
C	-0.53799	0.02832	-4.56473
C	-1.27453	-0.02261	-3.38456
C	-0.62902	-0.05709	-2.13854
C	0.7742	-0.03345	-2.0858
C	1.50868	0.03367	-3.2814
H	1.43806	0.10813	-5.42951
H	-1.05029	0.05671	-5.52205
H	-2.35915	-0.02784	-3.42736
H	2.59272	0.07636	-3.24624
P	-1.56971	-0.04771	-0.54343
P	1.61953	0.01661	-0.43274
Rh	0.00522	-0.03103	1.27991
Cl	0.13996	-2.66576	0.95087
C	2.68044	1.52743	-0.66905
C	4.06776	1.48022	-0.8717
C	2.04105	2.77951	-0.68659
C	4.7952	2.65585	-1.07902
H	4.58673	0.52815	-0.8704
C	2.76626	3.94986	-0.90279

H	0.96716	2.83268	-0.53066
C	4.14942	3.89137	-1.09613
H	5.86918	2.59922	-1.22893
H	2.25248	4.90755	-0.91577
H	4.717	4.80336	-1.25717
C	2.84007	-1.36512	-0.45625
C	2.85058	-2.35265	-1.44922
C	3.76203	-1.46098	0.59836
C	3.77226	-3.39989	-1.39711
H	2.13159	-2.32262	-2.25935
C	4.68011	-2.50805	0.64995
H	3.76725	-0.71662	1.3871
C	4.68811	-3.4823	-0.34947
H	3.76164	-4.15916	-2.17377
H	5.38079	-2.56734	1.47704
H	5.39872	-4.3028	-0.30682
C	-2.69918	1.41045	-0.77578
C	-3.98422	1.32721	-1.335
C	-2.22171	2.669	-0.37359
C	-4.76738	2.47352	-1.4885
H	-4.38332	0.36533	-1.6367
C	-2.99653	3.81642	-0.54333
H	-1.23933	2.73535	0.09304
C	-4.27618	3.71952	-1.0971
H	-5.76579	2.3882	-1.91389
H	-2.60746	4.78212	-0.23047
H	-4.88862	4.60792	-1.21807
C	-2.71193	-1.48976	-0.678
C	-3.82237	-1.57126	0.17958
C	-2.43629	-2.57275	-1.52352
C	-4.64813	-2.69492	0.17162
H	-4.05238	-0.75256	0.85497
C	-3.26682	-3.69341	-1.53434
H	-1.56511	-2.55113	-2.16741
C	-4.37449	-3.75845	-0.6897
H	-5.50308	-2.73913	0.84041
H	-3.03684	-4.52175	-2.19758
H	-5.01599	-4.63455	-0.69549

4cat[1,2]

Sum of electronic and thermal Free Energies=-2721.660733

C	-0.36616200	-3.58006800	-1.05349100
C	-1.70862400	-3.63224700	-0.68738200
H	0.35830100	-3.84658600	-0.28791800
C	0.14348200	-3.54338600	-2.48624600
H	-0.54535300	-4.08891600	-3.13918300
H	1.09599800	-4.08138300	-2.53835800
C	-2.89831100	-3.60791500	-1.62357300
H	-3.07248300	-4.60932700	-2.04784600
H	-3.78259400	-3.37471500	-1.02086900
H	-1.92325000	-3.95522500	0.32768700
C	-2.76904600	-2.55956700	-2.74806600
H	-2.26952300	-2.99188100	-3.62141200
H	-3.77115800	-2.27656200	-3.08852300
C	0.35231000	-2.10178100	-3.00582800
H	1.35298400	-1.76877600	-2.71153900
H	0.33334600	-2.08577900	-4.10730900
C	-2.02462100	-1.30342200	-2.30100300
C	-0.63920900	-1.09868000	-2.44694800
H	-2.63930700	-0.41040000	-2.25219500
H	-0.30181800	-0.06525300	-2.50250400
C	0.30627700	2.40931300	3.78183900
C	1.64990100	2.04875000	3.72082100
C	2.11529100	1.32386500	2.62551000
C	-0.10884200	1.29162300	1.65163200
C	-0.56004000	2.02707300	2.75929100
H	-0.07696100	2.97052100	4.62921900
H	2.33246800	2.32202600	4.52057500
H	3.15943700	1.02961100	2.58926700
H	-1.60834100	2.28750400	2.84120000
P	-1.35770000	0.72010600	0.38787700
Rh	-1.02176600	-1.54616200	-0.37433500
Cl	-0.71353100	-2.15814000	1.97924200
C	-1.37996100	2.06792600	-0.88242300
C	-2.47751200	2.18032600	-1.75659400
C	-0.30162100	2.94743000	-1.05333500
C	-2.48745400	3.13466400	-2.77296200
H	-3.34419800	1.54040600	-1.62383300
C	-0.30936300	3.89863300	-2.07631200
H	0.54938400	2.90229600	-0.38538700
C	-1.39893400	3.99393000	-2.94089500
H	-3.34817900	3.20794800	-3.43170600
H	0.54156000	4.56391400	-2.18982100
H	-1.40542500	4.73512900	-3.73488000
C	-2.99746400	0.95213300	1.22131900
C	-3.61377700	-0.15386500	1.82790500
C	-3.64612800	2.19898700	1.26577400
C	-4.84958300	-0.01239400	2.46236400
H	-3.11132700	-1.11513400	1.81796400

C	-4.88256000	2.33416700	1.89836200
H	-3.18939500	3.06721500	0.80236000
C	-5.48831900	1.22769000	2.49694400
H	-5.31134000	-0.87732400	2.92998800
H	-5.37097300	3.30438300	1.92158600
H	-6.45206600	1.33301100	2.98735000
C	1.26427500	0.94734700	1.57324800
P	1.93934600	-0.00235800	0.12322000
C	2.87313500	1.29948000	-0.82410500
C	3.30909300	2.52939300	-0.30414700
C	3.13953700	1.01965100	-2.17555600
C	3.98593100	3.44736800	-1.11052000
H	3.11634200	2.77768600	0.73430000
C	3.82896300	1.92895900	-2.97874900
H	2.80142900	0.07946600	-2.60294900
C	4.25056900	3.14957900	-2.44868200
H	4.31165200	4.39456500	-0.68889000
H	4.02651400	1.68812600	-4.01956800
H	4.77908000	3.86394800	-3.07357900
C	3.31369200	-0.97703700	0.89617300
C	2.95832200	-2.04408000	1.74308400
C	4.67164400	-0.75961600	0.61589100
C	3.94303000	-2.85539000	2.30546900
H	1.91087800	-2.23222700	1.96444900
C	5.65263900	-1.58295800	1.17506500
H	4.97012900	0.05332900	-0.03754500
C	5.29288500	-2.63025800	2.02285500
H	3.65166000	-3.66919800	2.96383500
H	6.69952300	-1.39888400	0.94845700
H	6.05715900	-3.26781400	2.45868500

5cat[1,2]

Sum of electronic and thermal Free Energies=-2409.783974

C	0.41124500	-0.39356000	4.14516400
C	-0.98425600	-0.37551300	4.08259500
C	-1.62649200	-0.25862400	2.84948900
C	-0.87535400	-0.14680700	1.67230800
C	0.52917100	-0.15515800	1.73579100
C	1.16675500	-0.28839000	2.97660000
H	0.91150600	-0.50389900	5.10292500
H	-1.57119400	-0.46997500	4.99159100
H	-2.71129700	-0.27551000	2.80244500
H	2.25014900	-0.33186400	3.02942500
P	-1.59666800	-0.08182200	-0.03160600
P	1.42131300	-0.04367000	0.11215200
Rh	0.03546200	-0.34322700	-1.55106100
Cl	1.49832700	-0.66744000	-3.37551000
C	2.80324600	-1.25040900	0.26476500
C	4.01077400	-0.91459400	0.89711500
C	2.63152300	-2.54396600	-0.24832200
C	5.01960500	-1.86906600	1.03516400
H	4.17226600	0.09424100	1.26478700
C	3.64290200	-3.49421400	-0.10843500
H	1.71569300	-2.78508900	-0.77893600
C	4.83556300	-3.15992400	0.53605800
H	5.95265900	-1.59995900	1.52210900
H	3.50411300	-4.49118000	-0.51626200
H	5.62523000	-3.89908400	0.63723000
C	2.25320600	1.60066200	0.10124800
C	2.84569600	2.01247000	-1.10592500
C	2.30907400	2.44694800	1.21814300
C	3.49762600	3.24205300	-1.18002700
H	2.77667600	1.37509900	-1.98391400
C	2.95827600	3.68129900	1.13352800
H	1.84565200	2.15259400	2.15378900
C	3.55550200	4.07912800	-0.06245800
H	3.95216600	3.55033600	-2.11702400
H	2.99342600	4.33035000	2.00413000
H	4.05787500	5.04023100	-0.12654200
C	-2.91479700	-1.37484800	-0.01624400
C	-4.23049300	-1.12468600	0.40456100
C	-2.56530500	-2.66823500	-0.43599200
C	-5.17327600	-2.15385600	0.41682800
H	-4.52310700	-0.12449300	0.70909900
C	-3.50976300	-3.69494500	-0.42115200
H	-1.55110900	-2.85506600	-0.78011900
C	-4.81434000	-3.43940500	0.00616200
H	-6.18951300	-1.94961900	0.74206800
H	-3.22867800	-4.69093000	-0.75090300
H	-5.55144800	-4.23732100	0.01197400
C	-2.54392000	1.49992700	-0.10966900
C	-3.27502500	1.76602800	-1.28111700
C	-2.49995700	2.47556000	0.89579400
C	-3.95610400	2.97169900	-1.43405300
H	-3.31163300	1.02716500	-2.07739800
C	-3.17999500	3.68586400	0.73786000
H	-1.93287200	2.29704000	1.80321900
C	-3.90997400	3.93609500	-0.42359400
H	-4.51769500	3.16100400	-2.34424800

H	-3.13584600	4.43264300	1.52561500
H	-4.43671500	4.87815900	-0.54498000

IM1^{L2}

Sum of electronic and thermal Free Energies= -3040.158490

C	2.54823	1.34459	3.87055
C	1.21558	1.50583	4.26151
C	0.18815	1.22088	3.36514
C	0.48113	0.77754	2.06692
C	1.81945	0.62744	1.66927
C	2.848	0.90665	2.58247
H	3.3513	1.5567	4.57052
H	0.97947	1.84572	5.26586
H	-0.84424	1.3379	3.67898
H	3.88416	0.77779	2.28699
P	-0.82728	0.31533	0.82964
P	2.11531	0.02255	-0.05975
S	-1.74614	-1.37076	-2.37157
C	-3.44957	-0.86147	-2.09378
C	-4.04305	0.19033	-2.8014
C	-4.20345	-1.58863	-1.16299
C	-5.38441	0.50651	-2.58026
H	-3.46437	0.76196	-3.52111
C	-5.5396	-1.25606	-0.9381
H	-3.74924	-2.40972	-0.61669
C	-6.13623	-0.21063	-1.64731
H	-5.83961	1.31899	-3.13957
H	-6.11597	-1.82405	-0.21359
H	-7.17969	0.03858	-1.47861
Rh	0.14964	-0.45226	-1.03981
H	-1.52345	-0.61466	-3.46314
Cl	1.30415	-1.26194	-3.04845
C	3.19687	1.30643	-0.82764
C	3.37814	2.58159	-0.27112
C	3.82497	1.00121	-2.04945
C	4.18649	3.52527	-0.90996
H	2.89939	2.8435	0.66634
C	4.63379	1.94564	-2.67903
H	3.65912	0.03393	-2.51295
C	4.82027	3.20855	-2.11083
H	4.32064	4.50684	-0.46345
H	5.11475	1.69402	-3.62041
H	5.45299	3.94106	-2.60389
C	3.25029	-1.41292	0.17901
C	4.62311	-1.25659	0.42593
C	2.70447	-2.70395	0.15367
C	5.42657	-2.37121	0.66995
H	5.07138	-0.26798	0.40779
C	3.50959	-3.81673	0.3983
H	1.65234	-2.82344	-0.08547
C	4.87045	-3.652	0.6614
H	6.48842	-2.23871	0.85784
H	3.07538	-4.812	0.36905
H	5.49843	-4.51894	0.84708
C	-1.85704	1.84834	0.72659
C	-1.25068	3.11103	0.83513
C	-3.22703	1.7846	0.42301
C	-1.9969	4.27684	0.66341
H	-0.19136	3.18727	1.05835
C	-3.97227	2.95326	0.25518
H	-3.72116	0.82428	0.3212
C	-3.36153	4.20218	0.37635
H	-1.51035	5.244	0.75563
H	-5.0316	2.88054	0.02537
H	-3.94284	5.11072	0.24594
C	-1.87133	-0.88082	1.78726
C	-2.84854	-0.50376	2.72219
C	-1.61844	-2.2474	1.58844
C	-3.5546	-1.47216	3.43796
H	-3.07555	0.54566	2.8808
C	-2.32059	-3.21487	2.30877
H	-0.86743	-2.53873	0.85865
C	-3.29211	-2.82859	3.23426
H	-4.31227	-1.16583	4.15393
H	-2.11058	-4.26798	2.14353
H	-3.84356	-3.58005	3.79213

TS1^{L2}

Sum of electronic and thermal Free Energies= -3040.133179

C	2.42889	-1.14771	3.96074
C	1.08525	-1.26604	4.32524
C	0.08379	-1.01568	3.38894
C	0.41306	-0.64443	2.07796
C	1.76528	-0.50638	1.71615
C	2.76756	-0.76991	2.66253
H	3.21098	-1.35834	4.68427
H	0.81799	-1.56702	5.33397
H	-0.95611	-1.13162	3.67606
H	3.81234	-0.69672	2.37614
P	-0.8817	-0.34794	0.77228

P	2.12148	-0.02066	-0.03125
S	-1.63858	0.12199	-2.83466
C	-3.26912	0.39555	-2.1385
C	-3.79429	1.69573	-2.05793
C	-4.10048	-0.69194	-1.814
C	-5.11394	1.9022	-1.65398
H	-3.16266	2.54008	-2.31394
C	-5.42045	-0.48209	-1.4087
H	-3.70927	-1.70055	-1.89013
C	-5.93258	0.81526	-1.32667
H	-5.50453	2.91472	-1.59808
H	-6.05082	-1.33041	-1.17851
H	-6.96411	0.97535	-1.01495
Rh	0.18097	-0.27197	-1.25623
H	-0.53555	1.08974	-1.65102
Cl	1.53998	-0.41603	-3.25612
C	2.64205	1.74436	0.03092
C	2.95692	2.41364	1.22254
C	2.68695	2.44525	-1.18693
C	3.31096	3.76523	1.19764
H	2.92411	1.88824	2.17154
C	3.04861	3.79167	-1.20384
H	2.42778	1.93284	-2.10959
C	3.3572	4.45532	-0.01372
H	3.54816	4.27576	2.12673
H	3.07864	4.32465	-2.14952
H	3.62834	5.50714	-0.03065
C	3.6519	-0.95338	-0.43497
C	4.92793	-0.40115	-0.24967
C	3.53296	-2.26989	-0.90466
C	6.06844	-1.16296	-0.51171
H	5.03294	0.62447	0.08899
C	4.67423	-3.02933	-1.15727
H	2.54827	-2.68734	-1.09245
C	5.9432	-2.47793	-0.9603
H	7.05259	-0.72459	-0.37041
H	4.57365	-4.04657	-1.52349
H	6.8314	-3.06831	-1.16695
C	-1.75617	1.13876	1.42327
C	-0.99899	2.16141	2.0198
C	-3.13527	1.32798	1.25361
C	-1.61062	3.33629	2.45157
H	0.07256	2.04822	2.1448
C	-3.74469	2.50376	1.69722
H	-3.73919	0.56994	0.76944
C	-2.98788	3.50831	2.29735
H	-1.00924	4.1166	2.90783
H	-4.81331	2.63234	1.55647
H	-3.46493	4.42334	2.636
C	-2.02471	-1.7771	0.9799
C	-3.00563	-1.85827	1.98212
C	-1.85425	-2.86105	0.10374
C	-3.79745	-3.00204	2.10425
H	-3.16921	-1.02304	2.65529
C	-2.64329	-4.00565	0.23257
H	-1.11585	-2.79352	-0.69173
C	-3.61685	-4.07734	1.23223
H	-4.559	-3.04969	2.87847
H	-2.50343	-4.83515	-0.4542
H	-4.23664	-4.96517	1.3281

1^{L2}

Sum of electronic and thermal Free Energies= -3040.141192

C	3.03337	-2.1818	3.05244
C	1.77084	-2.54732	3.52133
C	0.62442	-2.10384	2.86113
C	0.73437	-1.28511	1.7304
C	2.00745	-0.9031	1.26445
C	3.15165	-1.36407	1.92751
H	3.92651	-2.54232	3.55396
H	1.67679	-3.19292	4.3895
H	-0.35358	-2.41867	3.21022
H	4.13469	-1.10185	1.54932
P	-0.753	-0.7147	0.78475
P	2.05367	0.18512	-0.2264
S	-1.97128	-0.35036	-2.58202
C	-3.19741	0.90259	-2.25128
C	-2.90119	2.25817	-2.01974
C	-4.55086	0.51064	-2.28317
C	-3.9231	3.18319	-1.80338
H	-1.86289	2.57819	-2.00745
C	-5.57036	1.44072	-2.07762
H	-4.79143	-0.53149	-2.46888
C	-5.26329	2.78066	-1.83125
H	-3.67151	4.22534	-1.62143
H	-6.60557	1.11332	-2.10898
H	-6.05692	3.5061	-1.66907
Rh	-0.05275	-0.16585	-1.26078
H	-0.46158	1.28284	-0.9099

Cl	0.6853	-2.40532	-2.1454
C	2.31869	1.88292	0.45128
C	3.00879	2.11928	1.65039
C	1.84233	2.97885	-0.28419
C	3.20974	3.42359	2.10603
H	3.38582	1.28717	2.23685
C	2.05434	4.2827	0.16718
H	1.29511	2.80813	-1.20615
C	2.73479	4.50789	1.36494
H	3.73876	3.59089	3.04003
H	1.67996	5.12054	-0.41405
H	2.89154	5.52274	1.72078
C	3.6458	-0.20236	-1.06275
C	4.59486	0.79794	-1.3319
C	3.90239	-1.52401	-1.47113
C	5.78545	0.47979	-1.98761
H	4.4119	1.82363	-1.02946
C	5.09859	-1.83343	-2.11638
H	3.15489	-2.29385	-1.31328
C	6.04206	-0.83591	-2.37583
H	6.51148	1.26248	-2.19083
H	5.28558	-2.85751	-2.42706
H	6.97032	-1.0819	-2.8836
C	-1.46652	0.66521	1.76035
C	-0.76223	1.28353	2.80327
C	-2.73479	1.15283	1.39992
C	-1.32178	2.36941	3.47956
H	0.22214	0.92711	3.0878
C	-3.28804	2.23462	2.08091
H	-3.28622	0.69595	0.58449
C	-2.58346	2.84545	3.12168
H	-0.76761	2.84219	4.28526
H	-4.26584	2.60462	1.78725
H	-3.01593	3.69203	3.64801
C	-1.97646	-2.07673	0.93129
C	-2.84473	-2.13374	2.03668
C	-2.01167	-3.09522	-0.0336
C	-3.7322	-3.20108	2.17455
H	-2.84178	-1.34491	2.78137
C	-2.90408	-4.15714	0.11477
H	-1.34523	-3.05375	-0.89075
C	-3.76354	-4.21318	1.21341
H	-4.40246	-3.23497	3.02889
H	-2.928	-4.938	-0.63945
H	-4.46022	-5.03986	1.31846

2[L2]

Sum of electronic and thermal Free Energies= -3598.086126

S	1.36381	1.92444	-1.54746
C	2.10875	3.36576	-0.79541
C	2.94331	3.31224	0.33555
C	1.89642	4.61161	-1.41763
C	3.54001	4.47661	0.82319
H	3.09963	2.36501	0.84069
C	2.51271	5.76683	-0.9339
H	1.25205	4.66494	-2.291
C	3.3363	5.70728	0.19215
H	4.17636	4.41533	1.70274
H	2.34082	6.71608	-1.43652
H	3.81214	6.60717	0.57301
P	1.7078	-1.2169	-0.81166
C	3.51862	-1.09762	-0.50938
C	4.15726	-1.86772	0.47153
C	4.27126	-0.17415	-1.25328
C	5.52877	-1.73382	0.68921
H	3.58881	-2.56233	1.07849
C	5.64081	-0.04156	-1.02753
H	3.77962	0.45354	-1.98851
C	6.27396	-0.82279	-0.05957
H	6.01009	-2.33593	1.45422
H	6.21032	0.67977	-1.60642
H	7.34086	-0.71611	0.11561
C	1.59668	-1.52678	-2.63243
C	2.6415	-2.16247	-3.32571
C	0.43481	-1.18115	-3.33724
C	2.51556	-2.45968	-4.68259
H	3.5654	-2.40758	-2.81262
C	0.31023	-1.48217	-4.69418
H	-0.36244	-0.65237	-2.82593
C	1.34761	-2.12481	-5.36973
H	3.33559	-2.94744	-5.20304
H	-0.59548	-1.20269	-5.22453
H	1.25182	-2.35483	-6.42694
C	1.21072	-2.85563	-0.08909
C	1.84314	-4.04995	-0.47052
C	0.14891	-2.90696	0.83076
C	1.43731	-5.2717	0.05966
H	2.65729	-4.02345	-1.1869
C	-0.26035	-4.14435	1.35285

C	0.38332	-5.31975	0.97609
H	1.93831	-6.18588	-0.24519
H	-1.0902	-4.18588	2.05171
H	0.05922	-6.27113	1.38766
Rh	0.34297	0.39699	0.0964
H	-0.67432	0.26311	-1.05058
Cl	2.00461	0.40119	2.1008
C	-1.28509	4.85753	3.13012
C	-1.31696	3.54218	2.91287
H	-1.98915	5.34545	3.79862
H	-0.53771	5.48998	2.6585
H	-2.07665	2.94006	3.41629
C	-0.34363	2.78363	2.0514
H	0.40038	3.44913	1.6077
H	0.20846	2.04682	2.64207
N	-0.99833	2.03459	0.92784
H	-1.77883	1.51393	1.32585
C	-1.58864	2.97937	-0.08025
H	-0.76952	3.30588	-0.72187
H	-1.97581	3.85093	0.46118
C	-2.69982	2.37141	-0.89928
C	-3.99057	2.25088	-0.37479
C	-2.48344	1.94873	-2.22173
C	-5.04067	1.70624	-1.11945
H	-4.19464	2.60276	0.63481
C	-3.51701	1.41248	-2.97974
H	-1.49001	2.05191	-2.64913
C	-4.801	1.27898	-2.42991
H	-6.02671	1.63007	-0.67658
H	-3.35826	1.09478	-4.00552
O	-5.74477	0.72729	-3.25156
C	-7.07251	0.61545	-2.76497
H	-7.65466	0.16738	-3.57298
H	-7.1274	-0.03108	-1.87847
H	-7.49738	1.59723	-2.51772
P	-0.75337	-1.34655	1.24705
C	-0.80977	-1.26997	3.08247
C	-1.74878	-0.4334	3.70982
C	0.1427	-1.92649	3.87463
C	-1.74673	-0.27323	5.09549
H	-2.50205	0.08322	3.12031
C	0.14015	-1.76831	5.26065
H	0.89661	-2.55112	3.41076
C	-0.80168	-0.94293	5.87506
H	-2.48262	0.3739	5.56421
H	0.88663	-2.28311	5.85857
H	-0.79667	-0.81702	6.95391
C	-2.48861	-1.78658	0.75608
C	-2.8266	-1.71565	-0.60515
C	-3.45144	-2.25951	1.66426
C	-4.08579	-2.11575	-1.05036
H	-2.10267	-1.33639	-1.31762
C	-4.71904	-2.64092	1.21955
H	-3.21954	-2.32668	2.72135
C	-5.0375	-2.57718	-0.13822
H	-4.32568	-2.05126	-2.10867
H	-5.45495	-2.99284	1.93776
H	-6.02142	-2.88307	-0.48307

3^{L2}

Sum of electronic and thermal Free Energies= -3598.070922

C	-4.78592200	-1.40071700	2.83074700
C	-4.79159100	-0.02652500	3.06856100
C	-3.85357200	0.79423000	2.43989700
C	-2.90391800	0.24566200	1.57031300
C	-2.89790400	-1.14243700	1.32967600
C	-3.84141100	-1.95624900	1.96605300
H	-5.52280000	-2.04071200	3.30729600
H	-5.53235100	0.41052200	3.73164200
H	-3.87251700	1.86594500	2.60995800
H	-3.86200000	-3.02226700	1.76395700
P	-1.64684100	1.29047800	0.70563000
P	-1.60241300	-1.79060200	0.18030700
S	-0.75567000	2.12421300	-2.52534400
C	0.71217900	3.01390200	-2.02761900
C	0.58733800	4.38006400	-1.71132600
C	1.99880300	2.44208800	-1.99765800
C	1.70680900	5.14624200	-1.38159300
H	-0.39925800	4.83256900	-1.72434300
C	3.11221600	3.20667500	-1.64762800
H	2.13157500	1.39364600	-2.24314900
C	2.97488500	4.56366200	-1.34030400
H	1.58293800	6.19973300	-1.14373400
H	4.09269500	2.73761200	-1.62137300
H	3.84499000	5.15767100	-1.07489900
Rh	-1.07369400	0.10018100	-1.20084900
H	0.40205100	0.18179700	-0.74743200
Cl	-3.56028900	0.09790800	-1.88843500
C	-1.00639900	-1.20300600	-3.22043100

C	0.32441100	-0.97289400	-3.03804300
H	-1.61490800	-0.50976700	-3.78690000
H	-1.46355000	-2.15384400	-2.96668900
H	0.74578800	-0.05446600	-3.43518400
C	1.32460500	-1.99778300	-2.57603900
H	1.66122200	-2.54210400	-3.47269400
H	0.84006900	-2.75135000	-1.92914300
N	2.50557800	-1.38100200	-1.98427500
H	2.22789400	-0.82990500	-1.17552000
C	3.53551000	-2.34485200	-1.59637900
H	3.15792800	-3.12363600	-0.90791100
H	3.84444900	-2.87320700	-2.51084700
C	4.73159900	-1.66406000	-0.96642100
C	5.28592100	-2.13377400	0.22465500
C	5.33194900	-0.55035700	-1.57937900
C	6.40854100	-1.52975900	0.80348000
H	4.83968900	-2.99417800	0.71801800
C	6.44314200	0.06397900	-1.01857100
H	4.90985000	-0.16632800	-2.50309900
C	6.99159100	-0.42300500	0.17922200
H	6.80930400	-1.92667000	1.72876200
H	6.91259500	0.92143800	-1.49035800
O	8.08408800	0.25000200	0.64806100
C	8.68898000	-0.20790400	1.84544400
H	9.53467500	0.45636900	2.03057400
H	7.99713600	-0.15517900	2.69658500
H	9.05507300	-1.23836200	1.74745400
C	-2.32310500	-3.29691600	-0.59363100
C	-1.54848200	-4.45661700	-0.76938500
C	-3.62522600	-3.25899900	-1.12374600
C	-2.07229700	-5.56231500	-1.44110500
H	-0.53932100	-4.50473400	-0.37411100
C	-4.14345200	-4.37127100	-1.78757800
H	-4.21269200	-2.35122700	-1.04426900
C	-3.37237100	-5.52443500	-1.94693800
H	-1.46252900	-6.45269000	-1.56516400
H	-5.15163100	-4.32910300	-2.18919600
H	-3.78006600	-6.38633300	-2.46738800
C	-0.33364800	-2.46995600	1.34799900
C	0.94445400	-1.90136800	1.40116000
C	-0.64036700	-3.52351200	2.22817100
C	1.90144300	-2.37463100	2.30296400
H	1.18207600	-1.07206500	0.74533900
C	0.31301300	-3.99622400	3.12766400
H	-1.62320200	-3.98309600	2.20725000
C	1.58776400	-3.42343700	3.16585900
H	2.88635300	-1.91815800	2.32437900
H	0.06104200	-4.81182200	3.79950600
H	2.32905700	-3.79356000	3.86847700
C	-2.40119100	2.96435000	0.60807700
C	-2.06355200	3.96289000	1.53564500
C	-3.35356200	3.23653300	-0.38841500
C	-2.67958900	5.21469800	1.47455000
H	-1.32014200	3.77248200	2.30159100
C	-3.96412200	4.48904500	-0.43863200
H	-3.60622200	2.47013000	-1.11351800
C	-3.63017000	5.47916600	0.48837700
H	-2.40998900	5.98072400	2.19602400
H	-4.69758700	4.69177200	-1.21348500
H	-4.10617400	6.45472600	0.43954300
C	-0.28723700	1.48164200	1.93970600
C	0.91818000	2.06794600	1.51936400
C	-0.42142400	1.07996500	3.27641600
C	1.96489500	2.24968400	2.42214300
H	1.04257400	2.38122100	0.48880100
C	0.63263500	1.25922900	4.17580600
H	-1.34226800	0.62201100	3.62048200
C	1.82590700	1.84400200	3.75204100
H	2.88814700	2.70692900	2.07911100
H	0.51729000	0.93762300	5.20697100
H	2.64410300	1.98282200	4.45315300

IM1$^{L2'}$

Sum of electronic and thermal Free Energies= -3040.101071

Rh	0.07785	0.43964	-1.16176
C	1.89678	3.19621	-0.88748
C	1.90909	2.99397	-2.27171
C	2.82174	4.05076	-0.28172
C	2.85242	3.66366	-3.05278
H	1.19246	2.31629	-2.72908
C	3.75684	4.72208	-1.07271
H	2.81201	4.18517	0.79543
C	3.77342	4.52729	-2.45535
H	2.86661	3.50705	-4.12762
H	4.4751	5.38985	-0.60635
H	4.50671	5.04564	-3.0677
P	-1.96947	0.10801	-0.11385
P	1.23208	-1.16045	0.09169
C	-2.2837	1.24275	1.31201

C	-1.96027	0.9283	2.64021
C	-2.78213	2.53087	1.03198
C	-2.13378	1.86963	3.65863
H	-1.57544	-0.05595	2.88371
C	-2.96574	3.46451	2.05129
H	-3.04225	2.79546	0.00962
C	-2.6382	3.13755	3.37039
H	-1.8766	1.60552	4.68067
H	-3.36213	4.44828	1.81512
H	-2.77407	3.86647	4.16414
C	-3.67835	-0.13952	-0.79192
C	-4.84686	0.11752	-0.0529
C	-3.80025	-0.58169	-2.1204
C	-6.10525	-0.07093	-0.62679
H	-4.77864	0.47042	0.97116
C	-5.06124	-0.77485	-2.68604
H	-2.90477	-0.76965	-2.70481
C	-6.21604	-0.52004	-1.94395
H	-6.9984	0.13337	-0.04227
H	-5.13811	-1.11926	-3.7136
H	-7.19617	-0.66627	-2.38938
C	2.07601	-0.54183	1.61941
C	1.62093	-0.77406	2.92536
C	3.22865	0.24539	1.44175
C	2.29948	-0.2362	4.0227
H	0.74013	-1.385	3.09139
C	3.91202	0.77056	2.53704
H	3.59013	0.44765	0.43598
C	3.44663	0.53381	3.83383
H	1.93134	-0.42766	5.02729
H	4.80496	1.36915	2.378
H	3.97387	0.94868	4.68817
C	2.3584	-2.54297	-0.42472
C	3.36956	-3.05984	0.40338
C	2.20926	-3.06824	-1.72044
C	4.20439	-4.08324	-0.05004
H	3.51036	-2.66444	1.40378
C	3.04236	-4.09526	-2.16479
H	1.44587	-2.66307	-2.37715
C	4.04153	-4.60596	-1.33368
H	4.98096	-4.47161	0.60346
H	2.91259	-4.49147	-3.16806
H	4.69172	-5.40244	-1.68519
C	-0.26631	-2.07494	0.75696
C	-0.08105	-3.34299	1.33218
C	-1.58501	-1.54344	0.69045
C	-1.14626	-4.07679	1.85107
H	0.91704	-3.76692	1.36708
C	-2.64451	-2.30244	1.2136
C	-2.43535	-3.55174	1.7945
H	-0.96686	-5.05497	2.28813
H	-3.65569	-1.91474	1.15233
H	-3.27814	-4.11287	2.18774
Cl	-0.39593	-1.02775	-2.98259
S	0.729	2.29457	0.16437
H	-0.31519	3.15118	0.05765

TS1$^{L2'}$

Sum of electronic and thermal Free Energies= -3040.094212

Rh	-0.07338	0.62274	-1.09638
C	1.53553	3.41929	-0.7502
C	1.71129	3.06962	-2.0968
C	2.41197	4.3276	-0.13182
C	2.75934	3.63534	-2.82762
H	1.01787	2.3849	-2.5838
C	3.457	4.88291	-0.86957
H	2.26848	4.59822	0.91417
C	3.63059	4.53911	-2.22135
H	2.88701	3.36907	-3.87618
H	4.12979	5.59041	-0.39404
H	4.44141	4.97826	-2.79575
P	-1.90169	-0.09523	-0.03946
P	1.32164	-1.07784	0.05093
C	-2.23988	0.81609	1.52926
C	-1.75308	0.37811	2.76502
C	-2.92614	2.04089	1.4701
C	-1.9555	1.14404	3.91383
H	-1.23022	-0.55501	2.82882
C	-3.12761	2.80063	2.62111
H	-3.325	2.39632	0.51573
C	-2.63643	2.35385	3.84677
H	-1.55361	0.79117	4.87136
H	-3.65758	3.74035	2.5599
H	-2.78333	2.94602	4.74407
C	-3.58461	-0.22121	-0.7955
C	-4.74278	-0.33135	-0.00303
C	-3.71927	-0.15404	-2.19037
C	-6.00401	-0.39127	-0.59723
H	-4.66485	-0.3528	1.07954

C	-4.98471	-0.21171	-2.77832
H	-2.83125	-0.06431	-2.80712
C	-6.12754	-0.33158	-1.98699
H	-6.88932	-0.47631	0.0267
H	-5.07229	-0.15624	-3.85957
H	-7.11067	-0.37091	-2.44848
C	2.08578	-0.55443	1.65352
C	1.85608	-1.16056	2.89902
C	2.95516	0.54999	1.59557
C	2.48537	-0.68135	4.05107
H	1.19162	-2.01643	2.97138
C	3.59388	1.01963	2.74379
H	3.13122	1.04172	0.64187
C	3.35845	0.40607	3.9767
H	2.2983	-1.16533	5.00662
H	4.26971	1.86843	2.67568
H	3.84995	0.77423	4.87325
C	2.55605	-2.29781	-0.60108
C	3.70093	-2.70701	0.10089
C	2.34201	-2.79349	-1.90076
C	4.60472	-3.60215	-0.47736
H	3.88907	-2.32963	1.10069
C	3.2425	-3.69444	-2.46764
H	1.47563	-2.46138	-2.46603
C	4.37605	-4.10211	-1.75925
H	5.48588	-3.91017	0.07949
H	3.06015	-4.07329	-3.46976
H	5.07843	-4.80061	-2.20622
C	-0.07327	-2.21715	0.56783
C	0.21532	-3.53041	0.97667
C	-1.4331	-1.81398	0.5073
C	-0.79271	-4.42577	1.33192
H	1.24868	-3.86094	1.00135
C	-2.4376	-2.73083	0.85516
C	-2.12599	-4.02503	1.2692
H	-0.5348	-5.43456	1.64277
H	-3.47936	-2.43845	0.78386
H	-2.92261	-4.71702	1.52764
Cl	-0.46563	-0.69328	-3.06464
S	0.2328	2.68656	0.23516
H	-0.75721	2.64508	-0.75568

$1^{L2'}$

Sum of electronic and thermal Free Energies= -3040.129037

C	1.61746	3.68146	2.40577
C	2.83817	3.00753	2.32031
C	2.92438	1.81232	1.60991
C	1.79518	1.25723	0.98474
C	0.56617	1.93929	1.07444
C	0.49154	3.15449	1.77779
H	1.54522	4.62019	2.94746
H	3.72409	3.41808	2.79696
H	3.88177	1.30798	1.52703
H	-0.45048	3.69285	1.8241
P	1.90294	-0.32438	0.01063
P	-0.95863	1.29008	0.24534
S	-1.0773	-2.17833	0.3202
C	-2.29184	-3.00689	-0.6971
C	-1.86693	-3.91157	-1.68703
C	-3.67135	-2.85782	-0.46672
C	-2.79544	-4.64313	-2.42936
H	-0.80373	-4.04413	-1.85798
C	-4.5969	-3.57233	-1.22456
H	-4.00814	-2.18013	0.31331
C	-4.16248	-4.47385	-2.2051
H	-2.44744	-5.35245	-3.17542
H	-5.66023	-3.43973	-1.04165
H	-4.88556	-5.0398	-2.78656
Rh	-0.39253	-0.39124	-1.08376
H	-1.86063	-0.31093	-1.58858
Cl	0.20723	0.69275	-3.17516
C	-2.14695	0.90963	1.59694
C	-1.81465	1.04018	2.95152
C	-3.42631	0.44308	1.24965
C	-2.74796	0.71885	3.94162
H	-0.8301	1.38686	3.24415
C	-4.35887	0.13984	2.23956
H	-3.68407	0.30158	0.204
C	-4.02055	0.2735	3.58986
H	-2.47371	0.81788	4.9883
H	-5.34618	-0.21476	1.95752
H	-4.74446	0.02364	4.36059
C	-1.63481	2.79557	-0.57594
C	-2.88552	3.34043	-0.24521
C	-0.83906	3.43843	-1.53889
C	-3.33507	4.50166	-0.87873
H	-3.513	2.8699	0.50456
C	-1.2886	4.60281	-2.15612
H	0.11367	3.01082	-1.82905

C	-2.53904	5.13505	-1.83285
H	-4.30869	4.90814	-0.62076
H	-0.66387	5.08638	-2.90216
H	-2.891	6.0369	-2.32603
C	2.2397	-1.60907	1.28925
C	2.10338	-1.38439	2.66626
C	2.57341	-2.90036	0.844
C	2.3145	-2.42244	3.57769
H	1.8347	-0.39987	3.03632
C	2.79622	-3.92988	1.75522
H	2.66291	-3.09996	-0.21998
C	2.66677	-3.69392	3.12638
H	2.20451	-2.23158	4.64177
H	3.06103	-4.91949	1.39408
H	2.83334	-4.4989	3.83624
C	3.53056	-0.16297	-0.85187
C	4.74201	-0.57191	-0.26858
C	3.54949	0.43376	-2.12442
C	5.94966	-0.36919	-0.93791
H	4.74257	-1.0612	0.70177
C	4.76298	0.63673	-2.78512
H	2.61667	0.71776	-2.60176
C	5.96317	0.24365	-2.19375
H	6.87968	-0.68801	-0.47514
H	4.76469	1.10039	-3.76745
H	6.90513	0.40399	-2.71122

1^{L2}(R2)

Sum of electronic and thermal Free Energies= -2967.738747

C	3.73130400	0.73112700	3.71546400
C	3.81543400	-0.66237400	3.66407300
C	3.18090500	-1.36088800	2.63770200
C	2.45103600	-0.67440100	1.65614300
C	2.37106100	0.72928000	1.70523000
C	3.01366700	1.42260600	2.74055300
H	4.23367500	1.27912900	4.50746500
H	4.38355800	-1.20283700	4.41570200
H	3.26999400	-2.44158900	2.58684000
H	2.97459300	2.50666400	2.77450500
P	1.60695100	-1.51070900	0.23358000
P	1.38281800	1.56355700	0.37027000
Rh	0.99867900	0.09932300	-1.30269500
Cl	0.71555300	-1.66651800	-2.99064800
C	1.08586100	1.55165600	-3.03993900
C	-0.18917800	1.68671100	-2.53439200
H	1.86253000	2.26377000	-2.78083100
H	1.28288500	0.89209500	-3.87884800
H	-0.38783600	2.51508400	-1.85420900
C	-1.42098700	1.05532700	-3.13616400
H	-1.15242000	0.09499600	-3.58336700
H	-1.77592300	1.71337900	-3.95809900
N	-2.46261600	0.82872100	-2.13231800
H	-2.74838100	1.71957900	-1.72917200
C	-3.64770200	0.16066600	-2.67515400
H	-4.09362300	0.70124400	-3.53186700
H	-3.31779900	-0.81189700	-3.06355800
C	-4.70125200	-0.03719500	-1.60775500
C	-5.97221100	0.52523600	-1.72137800
C	-4.41524100	-0.79415100	-0.45729700
C	-6.94861000	0.34739300	-0.73319600
H	-6.21796200	1.11652400	-2.60062700
C	-5.36852600	-0.97884200	0.53493700
H	-3.43163600	-1.24158500	-0.34742300
C	-6.64563500	-0.40835200	0.40276600
H	-7.92495100	0.79980000	-0.86180200
H	-5.15247900	-1.56890400	1.42003800
O	-7.51297400	-0.65083900	1.43205300
C	-8.82240900	-0.11708300	1.34023800
H	-9.34327600	-0.43391100	2.24546200
H	-8.81288100	0.98016600	1.29644600
H	-9.35811600	-0.50292300	0.46288000
C	0.18085300	-2.41856300	0.96811300
C	-0.11003000	-2.41976200	2.33962100
C	-0.67244200	-3.10213900	0.08239600
C	-1.22934700	-3.10331700	2.82210900
H	0.52923700	-1.88698300	3.03562500
C	-1.78262000	-3.78869700	0.57266700
H	-0.46831800	-3.07616400	-0.98504200
C	-2.06453100	-3.79141000	1.94229100
H	-1.44513200	-3.09521700	3.88688200
H	-2.43274000	-4.31737000	-0.11860700
H	-2.93293600	-4.32455900	2.31915600
C	2.79167400	-2.83006900	-0.25333900
C	2.81136800	-4.08517600	0.37318300
C	3.72608800	-2.55038400	-1.26125700
C	3.76681700	-5.03663200	0.01136300
H	2.07300300	-4.32709500	1.13170500
C	4.68167600	-3.50192800	-1.61628300
H	3.67840800	-1.59901100	-1.78121700

C	4.70536200	-4.74466000	-0.97968300
H	3.77150800	-6.00759100	0.49873700
H	5.39645200	-3.27827900	-2.40290700
H	5.44486900	-5.48808100	-1.26386100
C	-0.08831600	2.21273100	1.28836400
C	-0.00754900	3.22994600	2.25484400
C	-1.32840800	1.60440500	1.04125400
C	-1.14301700	3.62387200	2.96178000
H	0.93818100	3.72592500	2.45054700
C	-2.46421000	1.99931500	1.75372100
H	-1.40668200	0.83583800	0.27657000
C	-2.37251200	3.00605200	2.71499000
H	-1.06842200	4.41265700	3.70531400
H	-3.41509600	1.51496800	1.55065400
H	-3.25512200	3.31348900	3.26909100
C	2.37512000	3.06686200	-0.03340100
C	1.76137000	4.29441900	-0.32844800
C	3.76658500	2.95260200	-0.19802900
C	2.52168900	5.38379500	-0.76087400
H	0.68866200	4.40863300	-0.20873400
C	4.52374700	4.04282700	-0.62378700
H	4.25963200	2.00776500	0.01060000
C	3.90343400	5.26252900	-0.90678600
H	2.03019500	6.32726300	-0.98087700
H	5.59904100	3.93872400	-0.73758600
H	4.49401600	6.11054900	-1.24107900

1^{L2}(R2)`

Sum of electronic and thermal Free Energies=-2967.731597

C	3.73130400	0.73112700	3.71546400
C	3.81543400	-0.66237400	3.66407300
C	3.18090500	-1.36088800	2.63770200
C	2.45103600	-0.67440100	1.65614300
C	2.37106100	0.72928000	1.70523000
C	3.01366700	1.42260600	2.74055300
H	4.23367500	1.27912900	4.50746500
H	4.38355800	-1.20283700	4.41570200
H	3.26999400	-2.44158900	2.58684000
H	2.97459300	2.50666400	2.77450500
P	1.60695100	-1.51070900	0.23358000
P	1.38281800	1.56355700	0.37027000
Rh	0.99867900	0.09932300	-1.30269500
Cl	0.71555300	-1.66651800	-2.99064800
C	1.08586100	1.55165600	-3.03993900
C	-0.18917800	1.68671100	-2.53439200
H	1.86253000	2.26377000	-2.78083100
H	1.28288500	0.89209500	-3.87884800
H	-0.38783600	2.51508400	-1.85420900
C	-1.42098700	1.05532700	-3.13616400
H	-1.15242000	0.09499600	-3.58336700
H	-1.77592300	1.71337900	-3.95809900
N	-2.46261600	0.82872100	-2.13231800
H	-2.74838100	1.71957900	-1.72917200
C	-3.64770200	0.16066600	-2.67515400
H	-4.09362300	0.70124400	-3.53186700
H	-3.31779900	-0.81189700	-3.06355800
C	-4.70125200	-0.03719500	-1.60775500
C	-5.97221100	0.52523600	-1.72137800
C	-4.41524100	-0.79415100	-0.45729700
C	-6.94861000	0.34739300	-0.73319600
H	-6.21796200	1.11652400	-2.60062700
C	-5.36852600	-0.97884200	0.53493700
H	-3.43163600	-1.24158500	-0.34742300
C	-6.64563500	-0.40835200	0.40276600
H	-7.92495100	0.79980000	-0.86180200
H	-5.15247900	-1.56890400	1.42003800
O	-7.51297400	-0.65083900	1.43205300
C	-8.82240900	-0.11708300	1.34023800
H	-9.34327600	-0.43391100	2.24546200
H	-8.81288100	0.98016600	1.29644600
H	-9.35811600	-0.50292300	0.46288000
C	0.18085300	-2.41856300	0.96811300
C	-0.11003000	-2.41976200	2.33962100
C	-0.67244200	-3.10213900	0.08239600
C	-1.22934700	-3.10331700	2.82210900
H	0.52923700	-1.88698300	3.03562500
C	-1.78262000	-3.78869700	0.57266700
H	-0.46831800	-3.07616400	-0.98504200
C	-2.06453100	-3.79141000	1.94229100
H	-1.44513200	-3.09521700	3.88688200
H	-2.43274000	-4.31737000	-0.11860700
H	-2.93293600	-4.32455900	2.31915600
C	2.79167400	-2.83006900	-0.25333900
C	2.81136800	-4.08517600	0.37318300
C	3.72608800	-2.55038400	-1.26125700
C	3.76681700	-5.03663200	0.01136300
H	2.07300300	-4.32709500	1.13170500
C	4.68167600	-3.50192800	-1.61628300
H	3.67840800	-1.59901100	-1.78121700

C	4.70536200	-4.74466000	-0.97968300
H	3.77150800	-6.00759100	0.49873700
H	5.39645200	-3.27827900	-2.40290700
H	5.44486900	-5.48808100	-1.26386100
C	-0.08831600	2.21273100	1.28836400
C	-0.00754900	3.22994600	2.25484400
C	-1.32840800	1.60440500	1.04125400
C	-1.14301700	3.62387200	2.96178000
H	0.93818100	3.72592500	2.45054700
C	-2.46421000	1.99931500	1.75372100
H	-1.40668200	0.83583800	0.27657000
C	-2.37251200	3.00605200	2.71499000
H	-1.06842200	4.41265700	3.70531400
H	-3.41509600	1.51496800	1.55065400
H	-3.25512200	3.31348900	3.26909100
C	2.37512000	3.06686200	-0.03340100
C	1.76137000	4.29441900	-0.32844800
C	3.76658500	2.95260200	-0.19802900
C	2.52168900	5.38379500	-0.76087400
H	0.68866200	4.40863300	-0.20873400
C	4.52374700	4.04282700	-0.62378700
H	4.25963200	2.00776500	0.01060000
C	3.90343400	5.26252900	-0.90678600
H	2.03019500	6.32726300	-0.98087700
H	5.59904100	3.93872400	-0.73758600
H	4.49401600	6.11054900	-1.24107900

TS1^{L2}(R2)

Sum of electronic and thermal Free Energies=-3598.048738

C	-2.75419200	3.22656500	3.44526300
C	-2.96623400	2.04839000	4.16227900
C	-2.73055300	0.81181800	3.55933400
C	-2.28062000	0.75144200	2.23671000
C	-2.06471300	1.93727400	1.51309100
C	-2.30562400	3.17299700	2.12437800
H	-2.92298200	4.18993700	3.91759500
H	-3.30162700	2.09067700	5.19435800
H	-2.87604700	-0.10426800	4.12308400
H	-2.11221900	4.09453000	1.58500800
P	-1.93139700	-0.82017000	1.34644400
P	-1.48514600	1.75204000	-0.23486100
S	0.01154600	-2.88325500	-0.73864800
C	0.56740200	-3.25864900	-2.40021000
C	-0.33615000	-3.37438300	-3.46815300
C	1.92758500	-3.52050400	-2.61996300
C	0.12016400	-3.72992400	-4.73738900
H	-1.39382200	-3.19402100	-3.29954600
C	2.37490600	-3.89130600	-3.88948500
H	2.62884600	-3.43266600	-1.79582100
C	1.47561100	-3.99198600	-4.95187100
H	-0.58707800	-3.81186200	-5.55806800
H	3.43048500	-4.09331400	-4.04721500
H	1.82679600	-4.27435100	-5.93991800
Rh	-0.37382800	-0.24900900	-0.39772400
H	-0.96083900	-1.77960800	-1.10644700
Cl	1.29935700	0.50912400	1.61119700
C	1.23774500	0.12401400	-1.97823400
H	1.71809000	-0.85055100	-1.97824000
C	2.19093500	1.30337600	-1.84889700
H	1.63290300	2.20860700	-1.59930600
H	2.60751700	1.47028200	-2.85674100
N	3.31077200	1.17779600	-0.93056200
H	2.94830900	1.02824300	0.01304500
C	4.27840500	0.14012800	-1.26669100
H	3.89202300	-0.89105200	-1.16237500
H	4.52852000	0.25968800	-2.33321200
C	5.54812800	0.25739800	-0.44404400
C	6.19973200	-0.87435600	0.04532300
C	6.12451100	1.51159700	-0.18545100
C	7.39894600	-0.78330700	0.76148700
H	5.76571100	-1.85691400	-0.12703200
C	7.31184600	1.62320800	0.52519400
H	5.61002800	2.40000900	-0.53768600
C	7.96032000	0.47381300	1.00193300
H	7.86998500	-1.68755200	1.12915800
H	7.75945400	2.59084000	0.73018600
O	9.12502800	0.68999100	1.69063800
C	9.81039700	-0.43581000	2.20677100
H	10.69653500	-0.04723100	2.71233800
H	9.19796100	-0.98990800	2.93080700
H	10.12471900	-1.12362900	1.40996600
C	-3.59845500	-1.40143000	0.78805500
C	-4.76272000	-0.63946000	0.95980900
C	-3.69277200	-2.64154500	0.13002200
C	-5.99196100	-1.10383700	0.48424600
H	-4.71773900	0.31899000	1.46518100
C	-4.92116000	-3.10262100	-0.33950300
H	-2.80550400	-3.25141100	-0.01122200
C	-6.07585100	-2.33443500	-0.16519500

H	-6.88311800	-0.49908800	0.62621300
H	-4.97670100	-4.06575400	-0.83915200
H	-7.03262100	-2.69562900	-0.53143500
C	-1.48654000	-2.06484700	2.63165900
C	-2.48095100	-2.80219100	3.29911900
C	-0.13777700	-2.26937600	2.96334600
C	-2.13059800	-3.72246600	4.28708500
H	-3.52668100	-2.66678900	3.04422800
C	0.20271300	-3.19600800	3.95033200
H	0.63085900	-1.68410800	2.46758700
C	-0.78748700	-3.92273200	4.61242100
H	-2.90732800	-4.28592900	4.79646500
H	1.24915500	-3.34570400	4.19943400
H	-0.51570000	-4.64407600	5.37818600
C	-3.04101600	1.93404400	-1.22371500
C	-3.86795700	3.06397000	-1.09603500
C	-3.42939800	0.90544000	-2.09112400
C	-5.04976000	3.16178800	-1.82856100
H	-3.59059100	3.87215400	-0.42676200
C	-4.61266400	1.00589400	-2.82657000
H	-2.80271600	0.02252900	-2.16754700
C	-5.42322600	2.13311400	-2.69809200
H	-5.67897800	4.04072800	-1.72067100
H	-4.90104800	0.19907600	-3.49399300
H	-6.34433600	2.21140200	-3.26867000
C	-0.55605300	3.30250900	-0.56980300
C	-0.79002800	4.07178500	-1.72078800
C	0.47366900	3.67859500	0.31259300
C	-0.02085800	5.20880100	-1.97624900
H	-1.57393200	3.79252300	-2.41640400
C	1.23131200	4.82004100	0.05308900
H	0.70329300	3.05388300	1.17091600
C	0.98648900	5.58748500	-1.08831400
H	-0.21170700	5.79604800	-2.86994100
H	2.02633600	5.09834600	0.73828900
H	1.58465100	6.47181900	-1.28878200
C	-0.01594100	0.21296500	-2.57759300
H	-0.40476300	1.18704900	-2.86572900
H	-0.44046800	-0.62578900	-3.11910700

TS^{L2}(R2)`

Sum of electronic and thermal Free Energies=-3598.044603

C	-2.75419200	3.22656500	3.44526300
C	-2.96623400	2.04839000	4.16227900
C	-2.73055300	0.81181800	3.55933400
C	-2.28062000	0.75144200	2.23671000
C	-2.06471300	1.93727400	1.51309100
C	-2.30562400	3.17299700	2.12437800
H	-2.92298200	4.18993700	3.91759500
H	-3.30162700	2.09067700	5.19435800
H	-2.87604700	-0.10426800	4.12308400
H	-2.11221900	4.09453000	1.58500800
P	-1.93139700	-0.82017000	1.34644400
P	-1.48514600	1.75204000	-0.23486100
S	0.01154600	-2.88325500	-0.73864800
C	0.56740200	-3.25864900	-2.40021000
C	-0.33615000	-3.37438300	-3.46815300
C	1.92758500	-3.52050400	-2.61996300
C	0.12016400	-3.72992400	-4.73738900
H	-1.39382200	-3.19402100	-3.29954600
C	2.37490600	-3.89130600	-3.88948500
H	2.62884600	-3.43266600	-1.79582100
C	1.47561100	-3.99198600	-4.95187100
H	-0.58707800	-3.81186200	-5.55806800
H	3.43048500	-4.09331400	-4.04721500
H	1.82679600	-4.27435100	-5.93991800
Rh	-0.37382800	-0.24900900	-0.39772400
H	-0.96083900	-1.77960800	-1.10644700
Cl	1.29935700	0.50912400	1.61119700
C	1.23774500	0.12401400	-1.97823400
H	1.71809000	-0.85055100	-1.97824000
C	2.19093500	1.30337600	-1.84889700
H	1.63290300	2.20860700	-1.59930600
H	2.60751700	1.47028200	-2.85674100
N	3.31077200	1.17779600	-0.93056200
H	2.94830900	1.02824300	0.01304500
C	4.27840500	0.14012800	-1.26669100
H	3.89202300	-0.89105200	-1.16237500
H	4.52852000	0.25968800	-2.33321200
C	5.54812800	0.25739800	-0.44404400
C	6.19973200	-0.87435600	0.04532300
C	6.12451100	1.51159700	-0.18545100
C	7.39894600	-0.78330700	0.76148700
H	5.76571100	-1.85691400	-0.12703200
C	7.31184600	1.62320800	0.52519400
H	5.61002800	2.40000900	-0.53768600
C	7.96032000	0.47381300	1.00193300
H	7.86998500	-1.68755200	1.12915800
H	7.75945400	2.59084000	0.73018600

O	9.12502800	0.68999100	1.69063800
C	9.81039700	-0.43581000	2.20677100
H	10.69653500	-0.04723100	2.71233800
H	9.19796100	-0.98990800	2.93080700
H	10.12471900	-1.12362900	1.40996600
C	-3.59845500	-1.40143000	0.78805500
C	-4.76272000	-0.63946000	0.95980900
C	-3.69277200	-2.64154500	0.13002200
C	-5.99196100	-1.10383700	0.48424600
H	-4.71773900	0.31899000	1.46518100
C	-4.92116000	-3.10262100	-0.33950300
H	-2.80550400	-3.25141100	-0.01122200
C	-6.07585100	-2.33443500	-0.16519500
H	-6.88311800	-0.49908800	0.62621300
H	-4.97670100	-4.06575400	-0.83915200
H	-7.03262100	-2.69562900	-0.53143500
C	-1.48654000	-2.06484700	2.63165900
C	-2.48095100	-2.80219100	3.29911900
C	-0.13777700	-2.26937600	2.96334600
C	-2.13059800	-3.72246600	4.28708500
H	-3.52668100	-2.66678900	3.04422800
C	0.20271300	-3.19600800	3.95033200
H	0.63085900	-1.68410800	2.46758700
C	-0.78748700	-3.92273200	4.61242100
H	-2.90732800	-4.28592900	4.79646500
H	1.24915500	-3.34570400	4.19943400
H	-0.51570000	-4.64407600	5.37818600
C	-3.04101600	1.93404400	-1.22371500
C	-3.86795700	3.06397000	-1.09603500
C	-3.42939800	0.90544000	-2.09112400
C	-5.04976000	3.16178800	-1.82856100
H	-3.59059100	3.87215400	-0.42676200
C	-4.61266400	1.00589400	-2.82657000
H	-2.80271600	0.02252900	-2.16754700
C	-5.42322600	2.13311400	-2.69809200
H	-5.67897800	4.04072800	-1.72067100
H	-4.90104800	0.19907600	-3.49399300
H	-6.34433600	2.21140200	-3.26867000
C	-0.55605300	3.30250900	-0.56980300
C	-0.79002800	4.07178500	-1.72078800
C	0.47366900	3.67859500	0.31259300
C	-0.02085800	5.20880100	-1.97624900
H	-1.57393200	3.79252300	-2.41640400
C	1.23131200	4.82004100	0.05308900
H	0.70329300	3.05388300	1.17091600
C	0.98648900	5.58748500	-1.08831400
H	-0.21170700	5.79604800	-2.86994100
H	2.02633600	5.09834600	0.73828900
H	1.58465100	6.47181900	-1.28878200
C	-0.01594100	0.21296500	-2.57759300
H	-0.40476300	1.18704900	-2.86572900
H	-0.44046800	-0.62578900	-3.11910700

TS1^{L2}(cod)

Sum of electronic and thermal Free Energies= -3351.988712

C	-1.12714	-2.41649	-0.76822
C	-1.1794	-2.23063	0.61042
H	-0.21857	-2.855	-1.17665
C	-2.32999	-2.57737	-1.66622
H	-2.01048	-2.37803	-2.69145
H	-3.10508	-1.84481	-1.43104
C	-2.44992	-2.17818	1.42854
H	-2.22188	-1.73769	2.40538
H	-3.21081	-1.5521	0.96279
H	-0.31805	-2.53681	1.1955
C	-3.03838	-3.61484	1.63122
H	-2.22725	-4.35103	1.53733
H	-3.40225	-3.70112	2.66077
C	-2.92255	-4.02052	-1.54716
H	-3.21291	-4.36508	-2.54529
H	-2.13051	-4.70696	-1.21324
C	-4.17565	-3.96489	0.69341
C	-4.12555	-4.13501	-0.63391
H	-5.15243	-4.06547	1.16589
H	-5.06765	-4.36246	-1.13225
C	4.68561	2.6393	-0.14612
C	5.22759	1.35286	-0.07163
C	4.38801	0.24515	0.00905
C	2.99357	0.40903	0.02481
C	2.45179	1.69925	-0.04118
C	3.30454	2.81101	-0.13523
H	5.33797	3.50419	-0.22298
H	6.30438	1.21233	-0.0916
H	4.81781	-0.74975	0.03736
H	2.87974	3.80697	-0.20891
P	1.83895	-1.04194	0.09788
P	0.61861	1.88583	-0.01617
Rh	-0.36173	-0.29674	-0.40458
Cl	-0.21682	-0.2152	-3.09513

C	0.38766	3.26716	-1.21585
C	0.06587	4.57771	-0.83263
C	0.66597	2.98877	-2.56566
C	0.04262	5.59904	-1.7864
H	-0.15893	4.80908	0.20314
C	0.64994	4.01622	-3.50754
H	0.85864	1.96736	-2.88036
C	0.34474	5.32293	-3.12139
H	-0.20589	6.61179	-1.48125
H	0.87225	3.78708	-4.54632
H	0.33887	6.12158	-3.85869
C	0.28484	2.64597	1.64443
C	-1.02868	3.01376	1.99118
C	1.3026	2.84164	2.59147
C	-1.30764	3.55634	3.24541
H	-1.83387	2.86831	1.27956
C	1.01752	3.38142	3.84815
H	2.3286	2.58742	2.35196
C	-0.28745	3.7404	4.18075
H	-2.32836	3.83695	3.48935
H	1.82253	3.52536	4.56333
H	-0.50815	4.1628	5.15687
C	2.69129	-2.23617	-1.04189
C	3.76981	-3.04064	-0.62532
C	2.35005	-2.21084	-2.40277
C	4.49561	-3.78548	-1.55649
H	4.05455	-3.08559	0.42017
C	3.08326	-2.95918	-3.32756
H	1.52199	-1.59185	-2.74583
C	4.15877	-3.74208	-2.91188
H	5.33013	-4.39506	-1.2213
H	2.80746	-2.91481	-4.37756
H	4.73458	-4.31229	-3.63661
C	2.18358	-1.74171	1.77711
C	2.02526	-3.11457	2.03819
C	2.57921	-0.90249	2.83069
C	2.28754	-3.63361	3.30792
H	1.7305	-3.79046	1.24155
C	2.84009	-1.42344	4.09835
H	2.69644	0.16204	2.66254
C	2.70279	-2.79132	4.33994
H	2.1781	-4.69982	3.48431
H	3.16052	-0.75826	4.89498
H	2.92118	-3.19765	5.3235
S	-2.48819	1.09577	-0.60592
H	-1.5229	0.3544	0.61044
C	-4.14805	0.63187	-0.11984
C	-4.62438	0.75487	1.19666
C	-5.0633	0.37326	-1.15504
C	-5.99011	0.64315	1.46297
H	-3.92706	0.96209	2.00333
C	-6.43025	0.28277	-0.88379
H	-4.69636	0.28072	-2.17252
C	-6.89897	0.42215	0.42342
H	-6.34906	0.75316	2.48298
H	-7.12828	0.11217	-1.69944
H	-7.96472	0.36761	0.63064

1^{L2}(cod)

Sum of electronic and thermal Free Energies= -3352.015436

C	1.29287	2.67741	0.32981
C	1.52899	2.50991	-1.00594
H	1.97007	2.18231	1.02296
C	0.43498	3.7594	0.94147
H	0.21694	3.48909	1.97996
H	-0.52329	3.83338	0.42188
C	0.96293	3.35536	-2.11585
H	1.08202	2.8048	-3.05183
H	-0.10814	3.51687	-1.97258
H	2.34339	1.85276	-1.29608
C	1.69503	4.73472	-2.2048
H	2.7087	4.63832	-1.79023
H	1.82838	4.98647	-3.26172
C	1.15628	5.14616	0.9164
H	0.9505	5.66351	1.85942
H	2.24355	4.98552	0.89285
C	0.96164	5.87598	-1.5314
C	0.73468	6.04929	-0.22404
H	0.55223	6.62846	-2.20458
H	0.15894	6.92736	0.06632
C	1.86055	-4.92141	0.37139
C	0.51305	-5.19201	0.1221
C	-0.37884	-4.14264	-0.0831
C	0.05972	-2.80957	-0.04266
C	1.41107	-2.53631	0.23247
C	2.30331	-3.60269	0.42931
H	2.56334	-5.73549	0.52483
H	0.15917	-6.21805	0.08403
H	-1.42266	-4.35963	-0.28421

H	3.3518	-3.40243	0.62106
P	-1.13624	-1.41238	-0.30997
P	1.93953	-0.77036	0.40144
S	-1.90677	1.70646	-1.06162
C	-3.10097	2.04228	0.21907
C	-2.81439	2.19409	1.58702
C	-4.43576	2.23533	-0.19489
C	-3.81709	2.52196	2.50005
H	-1.79595	2.05563	1.93132
C	-5.43188	2.57465	0.71895
H	-4.68165	2.12549	-1.24743
C	-5.13225	2.71772	2.07587
H	-3.56358	2.63176	3.55206
H	-6.45012	2.72153	0.36749
H	-5.90959	2.97681	2.78881
Rh	0.09111	0.53577	-0.3074
H	-0.33346	0.82827	1.14854
Cl	0.77637	-0.099	-2.69223
C	2.48672	-0.65218	2.17284
C	3.67625	-1.25522	2.62144
C	1.69287	0.0315	3.1045
C	4.04698	-1.18766	3.96337
H	4.33047	-1.76096	1.91923
C	2.06458	0.09947	4.44941
H	0.78547	0.52169	2.76698
C	3.24013	-0.51253	4.88276
H	4.97046	-1.65798	4.28975
H	1.43565	0.63642	5.15386
H	3.53208	-0.45841	5.92756
C	3.52822	-0.64692	-0.51761
C	4.495	0.29337	-0.12152
C	3.74695	-1.3935	-1.68597
C	5.66345	0.46495	-0.8645
H	4.34657	0.88638	0.77543
C	4.92152	-1.22591	-2.419
H	2.99509	-2.09169	-2.03202
C	5.88169	-0.29854	-2.01209
H	6.40196	1.19348	-0.54305
H	5.07799	-1.81443	-3.31791
H	6.79245	-0.16743	-2.58914
C	-2.36657	-1.71151	1.03842
C	-3.4719	-2.55932	0.85273
C	-2.14589	-1.16311	2.30936
C	-4.33164	-2.84506	1.9142
H	-3.67311	-2.98713	-0.12287
C	-3.00241	-1.45563	3.37044
H	-1.30406	-0.49863	2.46349
C	-4.09935	-2.29573	3.17568
H	-5.18665	-3.49523	1.7508
H	-2.81778	-1.01597	4.34633
H	-4.77265	-2.51562	3.99945
C	-2.02831	-1.85236	-1.8544
C	-3.29227	-1.29293	-2.10974
C	-1.44249	-2.6859	-2.8185
C	-3.9647	-1.58943	-3.29557
H	-3.74687	-0.62205	-1.39043
C	-2.12066	-2.98003	-4.0018
H	-0.45278	-3.09487	-2.65803
C	-3.3816	-2.4332	-4.24338
H	-4.94015	-1.14988	-3.48213
H	-1.65336	-3.62586	-4.73979
H	-3.90329	-2.65712	-5.16949

TS2^{L2}

Sum of electronic and thermal Free Energies= -3598.036476

S	-1.79636	2.33798	0.85932
C	-3.30014	2.5159	-0.07795
C	-3.43726	2.18015	-1.43833
C	-4.39994	3.09835	0.58625
C	-4.64291	2.41983	-2.10381
H	-2.60331	1.72939	-1.96899
C	-5.58773	3.36	-0.0958
H	-4.31119	3.34916	1.6389
C	-5.72065	3.01571	-1.44419
H	-4.73003	2.14801	-3.15304
H	-6.41827	3.81919	0.43424
H	-6.65105	3.20861	-1.9715
P	1.40473	1.48822	0.07649
P	2.96869	-1.58117	-0.07106
C	1.14932	3.28507	-0.29398
C	1.78671	4.30016	0.4298
C	0.28944	3.6341	-1.35081
C	1.56967	5.64292	0.10419
H	2.45386	4.05593	1.25019
C	0.08549	4.97171	-1.67916
H	-0.2047	2.85412	-1.91735
C	0.72086	5.98094	-0.94924
H	2.07168	6.42202	0.67662
H	-0.57866	5.22649	-2.49873

H	0.55364	7.02443	-1.20112
C	2.41075	1.52728	1.62569
C	3.80696	1.67222	1.59998
C	1.75832	1.49188	2.86844
C	4.53275	1.76746	2.78929
H	4.3322	1.70677	0.65098
C	2.48507	1.59558	4.05523
H	0.67937	1.38251	2.9035
C	3.87406	1.73051	4.01938
H	5.61348	1.86505	2.75078
H	1.96363	1.56875	5.00817
H	4.43974	1.8044	4.94455
C	2.94644	-3.08691	-1.15605
C	2.0496	-3.11089	-2.24216
C	3.69564	-4.23883	-0.87707
C	1.91958	-4.25579	-3.02785
H	1.46056	-2.22842	-2.48387
C	3.55797	-5.3848	-1.66523
H	4.39576	-4.24439	-0.04772
C	2.67199	-5.39817	-2.74206
H	1.22947	-4.25194	-3.86691
H	4.15186	-6.26577	-1.43706
H	2.56857	-6.28917	-3.35503
C	4.58253	-1.74499	0.83259
C	5.82697	-1.28433	0.37641
C	4.52379	-2.36479	2.09195
C	6.9762	-1.44806	1.15148
H	5.90329	-0.78723	-0.58399
C	5.6743	-2.54259	2.86129
H	3.56585	-2.70384	2.47698
C	6.90505	-2.08156	2.39296
H	7.92984	-1.08146	0.78193
H	5.60611	-3.0288	3.82985
H	7.80121	-2.20936	2.99324
C	2.64213	1.00506	-1.25789
C	2.94316	1.95397	-2.24975
C	3.27548	-0.26079	-1.334
C	3.81787	1.67253	-3.29754
H	2.48486	2.93131	-2.21711
C	4.14103	-0.53022	-2.40857
C	4.41713	0.42023	-3.38688
H	4.01534	2.4345	-4.04501
H	4.5933	-1.51448	-2.48309
H	5.08982	0.1804	-4.20551
Rh	-0.69623	0.33898	0.20829
H	-0.62101	0.27896	1.7424
Cl	-0.66096	0.10864	-2.36255
C	-0.33499	-2.29035	1.27973
C	-0.81223	-2.37322	0.02665
H	-0.96663	-2.06109	2.13087
H	0.71215	-2.4737	1.48623
H	-0.145	-2.66631	-0.77624
C	-2.24409	-2.06943	-0.35903
H	-2.31883	-2.04628	-1.44756
H	-2.94637	-2.82298	0.02016
N	-2.61577	-0.71148	0.14753
H	-3.1024	-0.21241	-0.59771
C	-3.49988	-0.70425	1.35422
H	-3.5899	0.34163	1.65226
H	-2.97394	-1.22484	2.15629
C	-4.858	-1.32757	1.11806
C	-5.20336	-2.55808	1.68095
C	-5.815	-0.67516	0.31622
C	-6.45389	-3.14383	1.45786
H	-4.48915	-3.07501	2.31849
C	-7.05687	-1.24531	0.07829
H	-5.5883	0.29562	-0.11869
C	-7.38541	-2.48761	0.64544
H	-6.68436	-4.09492	1.91834
H	-7.79831	-0.74357	-0.53794
O	-8.62948	-2.96124	0.34814
C	-9.02018	-4.20846	0.89555
H	-10.02732	-4.40101	0.52838
H	-8.35699	-5.01624	0.56904
H	-9.03903	-4.1815	1.99051

4^{L2}

Sum of electronic and thermal Free Energies= -3598.032157

S	-3.95711	0.8121	-0.34647
C	-4.68043	1.73959	0.99896
C	-4.45218	1.41433	2.34752
C	-5.59629	2.76398	0.69557
C	-5.11953	2.10431	3.35934
H	-3.73377	0.64068	2.5892
C	-6.27088	3.44224	1.71285
H	-5.78196	3.01299	-0.34541
C	-6.03176	3.11714	3.04942
H	-4.92691	1.84621	4.39758
H	-6.98	4.22628	1.4592

H	-6.5518	3.64718	3.84291
P	-1.25405	-0.96422	-1.00286
P	1.64324	-1.65801	1.04016
C	-2.53007	-1.76303	-2.09703
C	-2.63258	-3.1626	-2.17809
C	-3.29259	-0.9819	-2.97548
C	-3.48668	-3.76022	-3.10297
H	-2.05207	-3.79259	-1.51305
C	-4.1454	-1.58371	-3.90341
H	-3.23264	0.09909	-2.92716
C	-4.24707	-2.97201	-3.96961
H	-3.55597	-4.84345	-3.14631
H	-4.73623	-0.95936	-4.56724
H	-4.91385	-3.4387	-4.68901
C	0.18697	-1.28978	-2.12219
C	0.84299	-2.52723	-2.14474
C	0.50953	-0.34343	-3.10903
C	1.83528	-2.79148	-3.08949
H	0.58674	-3.29263	-1.42295
C	1.49903	-0.609	-4.05767
H	-0.05328	0.58361	-3.16682
C	2.17365	-1.83066	-4.0428
H	2.34473	-3.7499	-3.07107
H	1.73222	0.13507	-4.81416
H	2.94631	-2.03737	-4.77749
C	2.26396	-1.47449	2.78549
C	1.80487	-0.37185	3.52839
C	3.21583	-2.32822	3.36697
C	2.27591	-0.14468	4.82134
H	1.05988	0.29353	3.10026
C	3.69205	-2.08964	4.65877
H	3.59129	-3.18358	2.81607
C	3.22319	-0.999	5.39074
H	1.90063	0.70631	5.38312
H	4.42896	-2.7619	5.09096
H	3.59312	-0.81538	6.39586
C	2.65002	-3.11572	0.47508
C	2.23242	-4.4549	0.51042
C	3.92425	-2.83036	-0.04559
C	3.06109	-5.47572	0.03611
H	1.25405	-4.7063	0.90757
C	4.75961	-3.84916	-0.50307
H	4.2635	-1.79852	-0.09457
C	4.32752	-5.17746	-0.46889
H	2.71666	-6.50593	0.06872
H	5.74349	-3.60562	-0.89451
H	4.97257	-5.97224	-0.83278
C	-1.18546	-2.07398	0.48726
C	-2.45869	-2.51981	0.89126
C	-0.06444	-2.37427	1.30665
C	-2.63666	-3.29356	2.03448
H	-3.33184	-2.2366	0.31545
C	-0.2737	-3.16684	2.44936
C	-1.53389	-3.63603	2.81084
H	-3.63575	-3.61341	2.31505
H	0.57333	-3.39351	3.08836
H	-1.65117	-4.24094	3.7055
Rh	-1.58923	1.3046	-0.50735
H	-1.86178	1.39548	-2.03997
Cl	-1.07267	1.01898	1.97248
C	-1.9293	3.56371	0.22282
C	-1.49369	3.578	-1.07165
H	-1.25309	3.54453	1.06906
H	-2.98165	3.68062	0.45116
H	-2.20037	3.76251	-1.87481
C	-0.02174	3.4603	-1.4376
H	0.09513	3.47095	-2.52462
H	0.57573	4.28744	-1.0382
N	0.46381	2.15147	-0.90329
H	0.87753	1.61123	-1.65745
C	1.47884	2.23746	0.1888
H	1.65642	1.20928	0.51179
H	1.02259	2.75571	1.03283
C	2.76369	2.90548	-0.24818
C	3.11752	4.17989	0.20195
C	3.64417	2.25456	-1.13223
C	4.29924	4.80556	-0.20981
H	2.46615	4.69875	0.90144
C	4.81863	2.85959	-1.55532
H	3.40737	1.25315	-1.48622
C	5.15476	4.14445	-1.09706
H	4.5382	5.79293	0.16712
H	5.50213	2.35803	-2.23292
O	6.32942	4.65111	-1.57007
C	6.726	5.94339	-1.13771
H	7.67805	6.14705	-1.63009
H	5.99693	6.70993	-1.43111
H	6.86712	5.9811	-0.04979

TS3^{L2}

Sum of electronic and thermal Free Energies= -3598.018479

S	1.58638	-3.45411	0.07545
C	1.21423	-4.33404	1.58099
C	1.45741	-3.77168	2.84636
C	0.79539	-5.67468	1.5074
C	1.28021	-4.53308	4.00254
H	1.7671	-2.73621	2.90833
C	0.63156	-6.43774	2.6686
H	0.6189	-6.1196	0.53227
C	0.87113	-5.8688	3.92
H	1.46789	-4.08274	4.97354
H	0.31789	-7.47718	2.59364
H	0.74433	-6.46126	4.82489
P	1.76603	-0.27605	-1.00759
P	0.50293	2.59395	0.6824
C	3.15365	-1.12017	-1.93087
C	4.43657	-0.56068	-2.06085
C	2.8589	-2.28182	-2.6587
C	5.39892	-1.16243	-2.87091
H	4.69584	0.34532	-1.52359
C	3.8198	-2.87924	-3.47716
H	1.87633	-2.73261	-2.57711
C	5.09451	-2.32566	-3.58213
H	6.38764	-0.71825	-2.94822
H	3.56858	-3.78499	-4.02206
H	5.84551	-2.79415	-4.21209
C	1.47462	1.01516	-2.31452
C	2.31153	2.13162	-2.4607
C	0.52023	0.76321	-3.31008
C	2.18113	2.98066	-3.55983
H	3.07312	2.33663	-1.71542
C	0.38154	1.61839	-4.40649
H	-0.08839	-0.1353	-3.25214
C	1.20995	2.73282	-4.53268
H	2.84481	3.83546	-3.65907
H	-0.36441	1.40466	-5.16705
H	1.11057	3.39604	-5.3869
C	-0.41567	2.44116	2.2872
C	0.10122	1.93533	3.48754
C	-1.75241	2.8711	2.266
C	-0.69075	1.88194	4.6361
H	1.11684	1.55929	3.5276
C	-2.54357	2.81917	3.4137
H	-2.17903	3.2621	1.34484
C	-2.01327	2.32528	4.6062
H	-0.27178	1.48159	5.55478
H	-3.57356	3.15652	3.37294
H	-2.62724	2.27881	5.50236
C	0.93136	4.40943	0.72814
C	0.63663	5.252	1.81681
C	1.51399	4.99045	-0.41186
C	0.91335	6.62055	1.76275
H	0.17892	4.84367	2.71063
C	1.8048	6.35224	-0.46037
H	1.73389	4.3752	-1.27236
C	1.50006	7.17597	0.62632
H	0.6699	7.25421	2.61767
H	2.26106	6.77475	-1.352
H	1.71495	8.24115	0.58601
C	2.60197	0.59975	0.40913
C	3.73843	-0.04633	0.9286
C	2.15985	1.79839	1.03289
C	4.49473	0.51256	1.95636
H	4.03867	-1.00356	0.51966
C	2.97139	2.36809	2.02974
C	4.13239	1.74855	2.48482
H	5.36903	-0.01396	2.32594
H	2.66841	3.31184	2.47263
H	4.73012	2.2177	3.2608
Rh	-0.07341	-1.77156	-0.39409
H	-0.23417	-2.41929	-1.89765
Cl	-0.1834	-0.98386	1.89586
C	-1.66206	-3.20203	-0.12575
C	-1.61913	-2.92165	-1.52345
H	-2.39096	-2.70411	0.50179
H	-1.29871	-4.15956	0.24423
H	-1.47434	-3.73491	-2.23494
C	-2.4103	-1.69934	-1.98081
H	-2.22284	-1.48541	-3.03742
H	-3.4883	-1.84117	-1.85759
N	-1.90578	-0.56137	-1.15404
H	-1.58508	0.18551	-1.75994
C	-2.81608	0.02655	-0.12091
H	-2.39539	1.00973	0.10578
H	-2.71164	-0.55548	0.79676
C	-4.26998	0.12105	-0.5305
C	-5.23027	-0.67183	0.10439

C	-4.70542	0.97459	-1.56113
C	-6.57681	-0.6457	-0.2705
H	-4.92406	-1.32817	0.91573
C	-6.0373	1.01173	-1.95238
H	-3.99006	1.61997	-2.06722
C	-6.98401	0.19235	-1.31406
H	-7.28547	-1.27861	0.25032
H	-6.37544	1.66553	-2.75031
O	-8.26182	0.2852	-1.78121
C	-9.24995	-0.55158	-1.19765
H	-10.17711	-0.34516	-1.73468
H	-8.99678	-1.61403	-1.30958
H	-9.39269	-0.32855	-0.13258

5^{L2}

Sum of electronic and thermal Free Energies= -3598.051935

S	-4.03681	-0.00838	-0.90996
C	-4.39184	1.65858	-1.44626
C	-4.42359	1.96737	-2.82141
C	-4.69683	2.67395	-0.51569
C	-4.77524	3.2455	-3.25413
H	-4.18873	1.18855	-3.5416
C	-5.03877	3.95436	-0.95751
H	-4.65151	2.44529	0.54355
C	-5.08474	4.24348	-2.32307
H	-4.80936	3.46423	-4.31816
H	-5.28079	4.72447	-0.22907
H	-5.36375	5.23798	-2.66208
P	-1.26882	-1.34192	0.59221
P	1.92085	-2.24633	-0.92348
C	-2.26853	-1.97373	2.02698
C	-1.70068	-2.85884	2.96076
C	-3.63058	-1.66345	2.12813
C	-2.48318	-3.42816	3.96476
H	-0.64296	-3.09611	2.92776
C	-4.40932	-2.24158	3.13237
H	-4.07734	-0.95464	1.44167
C	-3.84252	-3.12372	4.05103
H	-2.02562	-4.10441	4.68141
H	-5.46193	-1.98343	3.19987
H	-4.45151	-3.56499	4.83512
C	-1.35657	-2.82109	-0.51449
C	-0.91663	-4.07488	-0.05363
C	-1.9785	-2.73865	-1.76451
C	-1.06672	-5.21094	-0.84387
H	-0.46058	-4.17137	0.92547
C	-2.12889	-3.88265	-2.55428
H	-2.37221	-1.79124	-2.10833
C	-1.66878	-5.11699	-2.10265
H	-0.72348	-6.17306	-0.47348
H	-2.61696	-3.80145	-3.52126
H	-1.78905	-6.00505	-2.71651
C	2.83906	-0.81563	-1.67559
C	3.56938	0.16635	-0.98667
C	2.76997	-0.73172	-3.07803
C	4.21385	1.19563	-1.67791
H	3.63417	0.13945	0.09556
C	3.42521	0.28719	-3.77057
H	2.19206	-1.46959	-3.62845
C	4.1477	1.25601	-3.07104
H	4.75897	1.95336	-1.12248
H	3.3614	0.3302	-4.85414
H	4.64833	2.0572	-3.60705
C	3.27374	-3.50327	-0.71993
C	4.62637	-3.26602	-1.00991
C	2.89387	-4.79549	-0.31452
C	5.57244	-4.2866	-0.88222
H	4.94556	-2.28277	-1.33966
C	3.84015	-5.80955	-0.17596
H	1.84758	-5.0104	-0.11781
C	5.18467	-5.55824	-0.46028
H	6.61464	-4.08339	-1.11306
H	3.52659	-6.79955	0.1438
H	5.92159	-6.35008	-0.36092
C	0.43451	-1.21531	1.34959
C	0.40122	-0.57633	2.60929
C	1.68115	-1.66996	0.84306
C	1.5397	-0.47373	3.40405
H	-0.53584	-0.15806	2.96719
C	2.80244	-1.60258	1.69372
C	2.74155	-1.02541	2.95967
H	1.47584	0.01391	4.37232
H	3.74644	-2.00613	1.34229
H	3.6305	-0.99071	3.58332
Rh	-1.87412	0.68364	-0.18565
Cl	-2.62527	1.50156	2.11998
C	-1.12351	0.47181	-2.11133
H	-1.91948	0.17099	-2.79641
H	-0.30314	-0.25019	-2.18003

C	0.4822	2.25201	-1.41354
H	1.39042	1.69953	-1.67262
H	0.73275	3.31774	-1.45464
N	0.07635	1.88638	-0.01286
H	0.76246	1.23332	0.35913
C	0.0274	3.05476	0.91934
H	-0.35408	2.6767	1.87008
H	-0.73471	3.74213	0.5399
C	1.35078	3.77312	1.08212
C	1.53004	5.07792	0.61777
C	2.44031	3.15129	1.7186
C	2.74483	5.75567	0.76659
H	0.70084	5.5899	0.13502
C	3.65706	3.80299	1.86841
H	2.32971	2.14435	2.11483
C	3.81843	5.11406	1.39165
H	2.83666	6.76973	0.39641
H	4.49636	3.32802	2.36658
O	5.04954	5.6697	1.59089
C	5.2545	7.00876	1.17155
H	6.28368	7.25448	1.43739
H	5.12635	7.11911	0.08691
H	4.57477	7.70156	1.68331
C	-0.64001	1.89284	-2.38278
H	-1.47228	2.6052	-2.27406
H	-0.28257	2.01006	-3.4176

$6^{L,2}$

Sum of electronic and thermal Free Energies= -3598.078448

C	1.27638	1.44715	4.74303
C	1.34764	2.72809	4.1887
C	1.18921	2.89625	2.81656
C	0.97606	1.78956	1.97497
C	0.95991	0.49284	2.5211
C	1.0829	0.34419	3.91566
H	1.37396	1.30865	5.81595
H	1.5107	3.59303	4.825
H	1.22007	3.89433	2.39137
H	1.01668	-0.64646	4.35327
P	0.60638	2.07565	0.17604
P	0.77489	-0.96173	1.38634
Cl	0.39384	-2.23439	-1.95508
C	-2.15358	0.62791	-2.45249
H	-3.11151	0.2208	-2.79368
H	-2.29642	1.70171	-2.31511
N	-1.80472	0.0504	-1.1122
H	-2.12664	0.70775	-0.40483
C	-2.49137	-1.25187	-0.83962
H	-2.15579	-1.95659	-1.59935
H	-2.10657	-1.61531	0.11397
C	-4.00306	-1.16271	-0.79812
C	-4.7921	-1.76535	-1.78164
C	-4.6639	-0.4844	0.24203
C	-6.1892	-1.70077	-1.75076
H	-4.30997	-2.30878	-2.59055
C	-6.04859	-0.40305	0.28851
H	-4.08253	-0.02228	1.03742
C	-6.82371	-1.01267	-0.71172
H	-6.76135	-2.18582	-2.53312
H	-6.55942	0.11774	1.09249
O	-8.17576	-0.8806	-0.57548
C	-9.0092	-1.48388	-1.55305
H	-10.03473	-1.25971	-1.25511
H	-8.82579	-1.07017	-2.55365
H	-8.87296	-2.57317	-1.58642
C	0.30567	0.84224	-2.88984
H	1.1482	0.48269	-3.47973
H	0.37823	1.93525	-2.84343
C	-1.0169	2.97731	0.25837
C	-1.52944	3.60524	-0.89322
C	-1.8017	2.99641	1.42349
C	-2.75855	4.26561	-0.86621
H	-0.97018	3.57819	-1.82191
C	-3.0415	3.64064	1.44242
H	-1.44223	2.52179	2.32878
C	-3.51996	4.28564	0.30252
H	-3.12307	4.75535	-1.76444
H	-3.62826	3.64224	2.35582
H	-4.47935	4.7939	0.32162
C	1.85229	3.39158	-0.22245
C	3.20017	3.11321	0.07379
C	1.53466	4.63813	-0.78293
C	4.19651	4.05095	-0.19688
H	3.47563	2.1621	0.51361
C	2.53656	5.57414	-1.05254
H	0.50634	4.90764	-0.99076
C	3.87005	5.28297	-0.76483
H	5.23031	3.81144	0.03594
H	2.26601	6.5351	-1.48162

H	4.64768	6.01225	-0.9738
C	2.27193	-2.00962	1.67906
C	3.18887	-1.82178	2.72498
C	2.47456	-3.07347	0.78223
C	4.25969	-2.70167	2.89385
H	3.08839	-0.98575	3.40704
C	3.53884	-3.958	0.96543
H	1.82152	-3.18453	-0.07916
C	4.42996	-3.78065	2.02434
H	4.96123	-2.53948	3.70827
H	3.68238	-4.76988	0.25834
H	5.26217	-4.46587	2.16098
C	-0.56716	-1.91887	2.2469
C	-0.60025	-3.32149	2.19772
C	-1.64108	-1.24822	2.86056
C	-1.66637	-4.02925	2.7558
H	0.21203	-3.86712	1.73006
C	-2.70392	-1.95802	3.42093
H	-1.64605	-0.16347	2.91438
C	-2.72076	-3.35296	3.37096
H	-1.6679	-5.11458	2.70961
H	-3.51822	-1.41947	3.89863
H	-3.54834	-3.90617	3.80552
Rh	0.48977	0.01791	-0.96657
S	2.91225	0.17232	-1.19615
C	3.7086	-1.18754	-2.03526
C	3.35154	-1.62515	-3.32255
C	4.85509	-1.73849	-1.43584
C	4.11904	-2.58131	-3.98442
H	2.46469	-1.22396	-3.79633
C	5.63336	-2.68008	-2.11202
H	5.13394	-1.41892	-0.43665
C	5.26765	-3.11027	-3.38802
H	3.82084	-2.91007	-4.97702
H	6.52208	-3.08363	-1.63234
H	5.86797	-3.84859	-3.91287
C	-1.03421	0.37885	-3.45469
H	-1.27808	0.90607	-4.39164
H	-0.97961	-0.68741	-3.68936

TS4^{L2}

Sum of electronic and thermal Free Energies= -3598.020723

C	2.98483	3.94015	2.40403
C	2.46075	4.69941	1.35529
C	1.62712	4.10188	0.41194
C	1.31253	2.73772	0.50531
C	1.84757	1.96866	1.55382
C	2.67762	2.58465	2.50227
H	3.63825	4.40186	3.13879
H	2.70553	5.75418	1.26918
H	1.23173	4.69506	-0.40566
H	3.09985	1.99645	3.31016
P	0.1784	1.88651	-0.69468
P	1.3906	0.16851	1.6193
Cl	0.43627	-2.69624	0.4807
C	-1.95817	-1.22301	-2.35037
H	-2.87768	-1.78594	-2.56444
H	-1.98901	-0.31508	-2.96511
N	-1.91669	-0.81194	-0.92998
H	-2.38283	0.0859	-0.83299
C	-2.59601	-1.77187	-0.01405
H	-2.19257	-2.76473	-0.21546
H	-2.27316	-1.52701	1.00036
C	-4.1096	-1.77062	-0.09437
C	-4.82147	-2.87303	-0.57349
C	-4.85038	-0.67135	0.37777
C	-6.22116	-2.90119	-0.58349
H	-4.27711	-3.74431	-0.93
C	-6.23786	-0.67602	0.37004
H	-4.33122	0.19941	0.77229
C	-6.93548	-1.79849	-0.10475
H	-6.73374	-3.78167	-0.95335
H	-6.80923	0.16696	0.74579
O	-8.29776	-1.71512	-0.04732
C	-9.05554	-2.85189	-0.42978
H	-10.1016	-2.5874	-0.26522
H	-8.91011	-3.10146	-1.48924
H	-8.80482	-3.72869	0.18129
C	0.56114	-1.25236	-2.88697
H	1.27526	-1.84964	-3.44798
H	0.41204	-0.28877	-3.37345
C	-1.49708	2.52223	-0.20688
C	-2.56649	2.45292	-1.11902
C	-1.75368	3.00447	1.08591
C	-3.85073	2.85726	-0.74909
H	-2.39163	2.11036	-2.13559
C	-3.03838	3.40886	1.45428
H	-0.94863	3.07321	1.80876
C	-4.09056	3.33755	0.5401

H	-4.66072	2.79851	-1.46981
H	-3.21272	3.78534	2.45822
H	-5.08786	3.6569	0.82764
C	0.47793	2.81868	-2.27639
C	1.42553	2.33525	-3.19328
C	-0.17711	4.03028	-2.56433
C	1.70276	3.04066	-4.36641
H	1.95649	1.41011	-2.99268
C	0.10452	4.73259	-3.73676
H	-0.91288	4.42929	-1.87523
C	1.04364	4.2382	-4.64336
H	2.43684	2.64699	-5.06337
H	-0.41314	5.66571	-3.94009
H	1.25941	4.78371	-5.55769
C	2.98065	-0.67179	1.98933
C	4.18802	-0.18847	1.46019
C	2.98592	-1.89797	2.67555
C	5.37677	-0.89742	1.64532
H	4.20515	0.7423	0.90462
C	4.17648	-2.59892	2.86191
H	2.05733	-2.31084	3.05016
C	5.37542	-2.10061	2.34957
H	6.3025	-0.50938	1.23114
H	4.16315	-3.5431	3.39816
H	6.30061	-2.6528	2.49083
C	0.44567	0.06852	3.21228
C	1.05769	0.02181	4.47566
C	-0.95514	0.09872	3.1433
C	0.28357	0.01249	5.63695
H	2.1399	-0.02707	4.55499
C	-1.73019	0.09782	4.30423
H	-1.42958	0.11849	2.16719
C	-1.11156	0.05395	5.55477
H	0.77137	-0.03116	6.6073
H	-2.81505	0.11985	4.22994
H	-1.71167	0.04473	6.46048
Rh	0.36741	-0.39076	-0.39629
S	2.48537	-0.63936	-1.73386
C	3.39269	-2.15114	-1.98331
C	2.84784	-3.44809	-1.93785
C	4.77461	-1.99714	-2.21905
C	3.67752	-4.5564	-2.13681
H	1.80722	-3.58775	-1.71365
C	5.58978	-3.10907	-2.40447
H	5.20493	-0.99748	-2.25396
C	5.0435	-4.4006	-2.36473
H	3.24573	-5.5513	-2.0964
H	6.65946	-2.96853	-2.58279
H	5.68491	-5.26289	-2.5097
C	-0.73372	-2.04966	-2.73266
H	-0.92947	-2.51197	-3.71511
H	-0.60368	-2.87302	-2.02563

7^{L2}

Sum of electronic and thermal Free Energies= -3598.110124

C	5.28683	-3.02731	0.46995
C	4.5825	-3.55486	1.55607
C	3.29643	-3.0971	1.84177
C	2.70428	-2.11037	1.04212
C	3.42253	-1.55704	-0.0327
C	4.71043	-2.0328	-0.31961
H	6.28313	-3.39292	0.23692
H	5.03171	-4.32747	2.17335
H	2.74879	-3.51679	2.68088
H	5.25511	-1.63624	-1.17124
P	1.00026	-1.43097	1.32583
P	2.56248	-0.23283	-1.01066
Cl	-0.07691	1.07694	-2.50303
C	-2.62572	0.62686	0.61945
H	-3.69753	0.46141	0.45438
H	-2.44886	0.4773	1.69181
N	-1.85957	-0.43675	-0.09953
H	-1.89131	-1.26328	0.49417
C	-2.49683	-0.83894	-1.39683
H	-2.54376	0.04808	-2.02896
H	-1.79304	-1.51972	-1.88067
C	-3.85316	-1.49521	-1.25712
C	-5.02387	-0.85878	-1.68311
C	-3.97234	-2.78753	-0.71638
C	-6.28137	-1.46888	-1.57551
H	-4.95943	0.13455	-2.11953
C	-5.21164	-3.40705	-0.59388
H	-3.07938	-3.32303	-0.3942
C	-6.37766	-2.75121	-1.02725
H	-7.16391	-0.94094	-1.92243
H	-5.30499	-4.40589	-0.18095
O	-7.54222	-3.44943	-0.8793
C	-8.74231	-2.85607	-1.3476
H	-9.53342	-3.5803	-1.14986

H	-8.96861	-1.9218	-0.81806
H	-8.70003	-2.65362	-2.42575
C	-1.28124	2.67493	1.25107
H	-1.76342	2.76685	2.233
H	-0.40393	2.01917	1.36397
C	-0.04475	-2.9125	1.68689
C	-1.1901	-2.79527	2.49516
C	0.18076	-4.12976	1.02107
C	-2.07184	-3.86849	2.64803
H	-1.38718	-1.86764	3.02551
C	-0.69796	-5.20172	1.179
H	1.04871	-4.24135	0.37893
C	-1.82688	-5.07607	1.99324
H	-2.94737	-3.75814	3.28147
H	-0.50039	-6.13745	0.66352
H	-2.5092	-5.91225	2.1148
C	1.21585	-0.61814	2.98192
C	1.55694	0.74357	2.98395
C	1.14284	-1.29745	4.20894
C	1.81264	1.41308	4.18108
H	1.62778	1.27305	2.03845
C	1.39135	-0.62497	5.40628
H	0.88381	-2.35116	4.23676
C	1.72558	0.73102	5.3954
H	2.07432	2.46694	4.16094
H	1.3246	-1.1618	6.34843
H	1.91707	1.25197	6.32886
C	3.50069	1.31998	-0.66295
C	4.68799	1.37054	0.08074
C	2.95058	2.5164	-1.1563
C	5.32492	2.59274	0.31273
H	5.11758	0.46339	0.48707
C	3.59544	3.73169	-0.92643
H	2.01408	2.48672	-1.7063
C	4.78384	3.77356	-0.19389
H	6.24297	2.6187	0.89249
H	3.15959	4.64824	-1.31227
H	5.2806	4.72304	-0.01271
C	3.01584	-0.6526	-2.74692
C	4.18166	-0.17066	-3.35741
C	2.17592	-1.51696	-3.46333
C	4.50922	-0.5616	-4.658
H	4.82753	0.52129	-2.82575
C	2.50802	-1.90907	-4.75929
H	1.25134	-1.85238	-3.00618
C	3.6757	-1.43346	-5.35868
H	5.4115	-0.17766	-5.12443
H	1.84547	-2.57255	-5.30773
H	3.9284	-1.73235	-6.37234
Rh	0.3845	-0.22343	-0.46142
S	-0.51982	4.29486	0.80083
C	-1.94611	5.35717	0.5179
C	-2.38855	5.57811	-0.79419
C	-2.56256	6.04068	1.57739
C	-3.42794	6.47168	-1.04187
H	-1.90338	5.05344	-1.61274
C	-3.60154	6.93193	1.32568
H	-2.21012	5.88422	2.59243
C	-4.03449	7.15068	0.01584
H	-3.75815	6.64018	-2.06315
H	-4.06466	7.46414	2.15033
H	-4.83508	7.85428	-0.18011
C	-2.24018	2.06744	0.22649
H	-3.14489	2.68289	0.16019
H	-1.76461	2.06412	-0.76072

8^{L2}

Sum of electronic and thermal Free Energies= -3598.077285

S	-0.71188	-2.32184	-1.99512
C	0.92218	-2.98005	-2.27437
C	1.4072	-4.04172	-1.48884
C	1.71773	-2.51573	-3.33793
C	2.64974	-4.61985	-1.75439
H	0.80138	-4.41301	-0.66778
C	2.96276	-3.09065	-3.59503
H	1.35358	-1.69223	-3.94211
C	3.43566	-4.14391	-2.80677
H	3.00354	-5.44376	-1.13872
H	3.5661	-2.71425	-4.41725
H	4.4034	-4.59242	-3.01461
P	-2.23585	-0.94815	0.54885
C	-1.71414	-2.19479	1.80799
C	-1.56559	-1.89994	3.17101
C	-1.39205	-3.48598	1.35246
C	-1.11026	-2.87503	4.0616
H	-1.79654	-0.91075	3.54896
C	-0.94587	-4.45712	2.24729
H	-1.47093	-3.71041	0.29316
C	-0.80167	-4.15541	3.60373

H	-0.99671	-2.62876	5.11311
H	-0.70697	-5.45111	1.88059
H	-0.44979	-4.91339	4.29721
C	-3.75379	-1.70229	-0.18512
C	-4.51362	-2.64527	0.52793
C	-4.19455	-1.29757	-1.45394
C	-5.69068	-3.16202	-0.01366
H	-4.17931	-2.99459	1.49898
C	-5.37238	-1.81654	-1.99203
H	-3.6057	-0.5919	-2.03006
C	-6.12375	-2.74789	-1.27414
H	-6.26296	-3.89539	0.54766
H	-5.69296	-1.49948	-2.97999
H	-7.03612	-3.15666	-1.6987
C	-2.89648	0.46217	1.56888
C	-3.90364	0.27074	2.52771
C	-2.3371	1.74471	1.40468
C	-4.30835	1.31645	3.35473
H	-4.3647	-0.70544	2.63609
C	-2.72621	2.78249	2.26882
C	-3.70081	2.56925	3.24181
H	-5.08623	1.15082	4.09422
H	-2.26787	3.76187	2.17261
H	-3.9946	3.38055	3.90116
Rh	-0.63788	-0.10946	-0.87538
H	-1.7809	0.12959	-1.85872
Cl	0.87642	0.92993	-2.54316
C	3.12715	-1.3568	3.51198
C	2.58605	-0.41953	2.72922
H	3.97259	-1.14522	4.16178
H	2.74304	-2.37459	3.52577
H	2.998	0.5892	2.73044
C	1.37783	-0.65447	1.85357
H	1.11309	-1.71581	1.86778
H	0.52567	-0.11007	2.27765
N	1.47153	-0.23176	0.43609
H	1.59529	0.77833	0.40991
C	2.60814	-0.844	-0.30369
H	2.37205	-0.74264	-1.36344
H	2.61753	-1.91226	-0.07466
C	3.98079	-0.24464	-0.05101
C	5.10081	-1.07162	0.07966
C	4.19026	1.14592	-0.03156
C	6.3879	-0.55067	0.2428
H	4.97232	-2.1524	0.04397
C	5.45824	1.68271	0.15238
H	3.35543	1.82914	-0.17803
C	6.56862	0.83692	0.29642
H	7.22823	-1.23032	0.33513
H	5.61544	2.75784	0.17573
O	7.77234	1.46179	0.48379
C	8.939	0.65702	0.52854
H	9.77379	1.34269	0.68242
H	8.91096	-0.06454	1.35805
H	9.08931	0.1095	-0.4131
P	-1.19844	2.01178	-0.02472
C	-2.16541	3.08015	-1.19292
C	-1.71291	3.17342	-2.52204
C	-3.32643	3.77918	-0.82283
C	-2.38639	3.97916	-3.44166
H	-0.84583	2.59811	-2.83583
C	-4.00113	4.57295	-1.75287
H	-3.73416	3.70347	0.17838
C	-3.52948	4.68371	-3.06162
H	-2.01797	4.04174	-4.46213
H	-4.901	5.1016	-1.44931
H	-4.056	5.30465	-3.78129
C	0.14793	3.09044	0.6269
C	0.85707	3.93502	-0.2452
C	0.58232	2.97483	1.95962
C	1.95992	4.65792	0.21223
H	0.55454	4.02307	-1.28252
C	1.68431	3.70403	2.41293
H	0.0572	2.32189	2.65259
C	2.37465	4.54957	1.54048
H	2.49826	5.30429	-0.47475
H	2.00165	3.60713	3.448
H	3.23415	5.11396	1.89181

TS5^{L2}

Sum of electronic and thermal Free Energies= -3598.012786

S	0.42716	-2.93396	-1.38133
C	2.11753	-3.4486	-1.62098
C	2.72885	-4.33398	-0.71366
C	2.8439	-3.05018	-2.7594
C	4.02952	-4.79623	-0.92977
H	2.16869	-4.67295	0.1533
C	4.14696	-3.50227	-2.96331
H	2.37574	-2.37562	-3.46823

C	4.74743	-4.37591	-2.05109
H	4.47956	-5.48748	-0.22135
H	4.6949	-3.17741	-3.84408
H	5.76017	-4.73205	-2.21857
P	-0.85278	1.51498	-0.14192
P	-3.14578	-0.85395	0.8609
C	0.47424	2.77156	0.14913
C	1.03036	3.46163	-0.9412
C	1.07135	2.92724	1.41439
C	2.12925	4.30468	-0.76252
H	0.60931	3.33463	-1.9316
C	2.16798	3.77285	1.59011
H	0.66666	2.40208	2.27448
C	2.69828	4.46859	0.50155
H	2.5394	4.83365	-1.61789
H	2.60614	3.8863	2.57746
H	3.54995	5.12845	0.63804
C	-1.82682	2.24345	-1.54209
C	-2.2543	3.58179	-1.48478
C	-2.18456	1.46588	-2.65062
C	-3.01394	4.12974	-2.51612
H	-1.99395	4.20398	-0.63468
C	-2.95423	2.01566	-3.67886
H	-1.85174	0.43861	-2.71786
C	-3.36698	3.34513	-3.61723
H	-3.33078	5.16732	-2.45868
H	-3.22365	1.39705	-4.52938
H	-3.96058	3.77122	-4.42133
C	-4.20977	-1.78446	2.06394
C	-3.66377	-2.10782	3.32082
C	-5.48144	-2.2845	1.74369
C	-4.37425	-2.88496	4.23344
H	-2.67789	-1.74086	3.59239
C	-6.18718	-3.07543	2.65428
H	-5.92504	-2.05699	0.78044
C	-5.63982	-3.3757	3.90128
H	-3.93627	-3.11507	5.20086
H	-7.16985	-3.45333	2.3854
H	-6.19069	-3.98972	4.60792
C	-4.28251	-0.62803	-0.57812
C	-5.25552	0.37879	-0.67415
C	-4.15339	-1.54969	-1.6309
C	-6.08331	0.45771	-1.79486
H	-5.36248	1.10711	0.12381
C	-4.98983	-1.47633	-2.74598
H	-3.38897	-2.32064	-1.58035
C	-5.95513	-0.47123	-2.83001
H	-6.82836	1.2459	-1.85967
H	-4.87934	-2.19794	-3.55031
H	-6.60184	-0.4082	-3.70078
C	-2.06437	1.79053	1.26727
C	-2.05563	3.03778	1.91895
C	-3.06449	0.84526	1.62857
C	-2.97718	3.36029	2.91282
H	-1.31086	3.77711	1.65097
C	-3.98827	1.19803	2.62974
C	-3.95154	2.43365	3.27143
H	-2.93038	4.33222	3.39559
H	-4.75125	0.48234	2.91437
H	-4.68314	2.6674	4.03961
Rh	0.17423	-0.65046	-0.63194
H	-1.18738	-0.97185	-1.24529
Cl	0.92338	0.1922	-2.69329
C	-0.02152	-1.65607	2.27489
C	1.22384	-1.71945	1.78366
H	-0.69101	-2.50709	2.22284
H	-0.39713	-0.7562	2.7564
H	1.5666	-2.6381	1.317
C	2.17675	-0.55639	1.7575
H	1.77689	0.26462	2.35963
H	3.15655	-0.82274	2.17586
N	2.30029	-0.09352	0.35175
H	2.30563	0.92351	0.34432
C	3.52039	-0.56235	-0.35686
H	3.39412	-0.2627	-1.40047
H	3.52141	-1.65269	-0.33929
C	4.81865	-0.02855	0.21386
C	5.73216	-0.87056	0.85254
C	5.14557	1.33576	0.11364
C	6.93201	-0.38768	1.3873
H	5.51507	-1.93377	0.922
C	6.32812	1.83475	0.64097
H	4.46487	2.01719	-0.39176
C	7.23166	0.97405	1.28514
H	7.61457	-1.07674	1.87066
H	6.58502	2.88613	0.55995
O	8.36603	1.56151	1.7694
C	9.32605	0.73606	2.4076

H	10.14138	1.39636	2.70736
H	8.9127	0.24669	3.29932
H	9.71624	-0.03259	1.72784

9^{L2}

Sum of electronic and thermal Free Energies= -3598.018467

S	-2.15337	-3.58462	-1.70998
C	-3.77868	-3.10274	-1.15273
C	-4.66119	-2.43042	-2.0197
C	-4.24226	-3.45951	0.12855
C	-5.96072	-2.11316	-1.61687
H	-4.32524	-2.17679	-3.02123
C	-5.53838	-3.13464	0.52956
H	-3.56638	-3.9772	0.79975
C	-6.40287	-2.45951	-0.33775
H	-6.62972	-1.60417	-2.30648
H	-5.87792	-3.41566	1.52314
H	-7.41419	-2.21666	-0.02341
P	1.7497	-1.49458	0.2801
P	2.31754	1.93463	-0.69585
C	2.44417	-2.79371	1.41405
C	3.32482	-2.47859	2.4605
C	2.20669	-4.14201	1.11153
C	3.94378	-3.49033	3.1954
H	3.52743	-1.44437	2.71772
C	2.8369	-5.15067	1.84094
H	1.51102	-4.40316	0.32311
C	3.70318	-4.82971	2.88617
H	4.61515	-3.22809	4.00835
H	2.63406	-6.18952	1.59791
H	4.18513	-5.61714	3.4587
C	3.26536	-1.33586	-0.77748
C	4.44652	-0.75016	-0.29313
C	3.29756	-1.99251	-2.01295
C	5.61866	-0.79288	-1.04462
H	4.45526	-0.26398	0.67737
C	4.47375	-2.03297	-2.76765
H	2.407	-2.49194	-2.37763
C	5.6343	-1.42845	-2.28995
H	6.52528	-0.33853	-0.65419
H	4.47847	-2.54503	-3.72559
H	6.54949	-1.46165	-2.87384
C	0.80089	2.84287	-1.26601
C	-0.26704	3.27917	-0.46686
C	0.74207	3.09197	-2.65036
C	-1.3572	3.94866	-1.03182
H	-0.26082	3.0988	0.60248
C	-0.33479	3.77626	-3.21236
H	1.54841	2.7436	-3.29109
C	-1.39049	4.20463	-2.40308
H	-2.17859	4.2597	-0.39346
H	-0.35539	3.964	-4.28217
H	-2.23663	4.72673	-2.8405
C	3.48353	3.34127	-0.36505
C	3.09042	4.68529	-0.25937
C	4.85192	3.03511	-0.26825
C	4.03652	5.68939	-0.04176
H	2.04269	4.95211	-0.3547
C	5.79504	4.03739	-0.04187
H	5.18036	2.00707	-0.38615
C	5.38975	5.36864	0.07318
H	3.71322	6.72381	0.03625
H	6.84795	3.77999	0.03282
H	6.1243	6.15097	0.24142
C	1.60617	0.01757	1.3669
C	1.08768	-0.27398	2.64775
C	1.8621	1.37714	1.03308
C	0.91115	0.71548	3.61089
H	0.8206	-1.29687	2.88944
C	1.71822	2.34899	2.04236
C	1.25866	2.03393	3.31838
H	0.52072	0.44822	4.58846
H	1.97108	3.37935	1.81476
H	1.16076	2.81327	4.06881
Rh	-0.4084	-2.11194	-0.73069
H	0.37866	-3.30194	-1.31276
Cl	-0.87899	-3.16652	1.39525
C	0.21752	-0.81477	-2.53425
C	-1.15787	-0.80961	-2.44896
H	0.69039	-1.42966	-3.29183
H	0.83395	-0.02768	-2.11474
H	-1.71461	-1.44521	-3.12672
C	-1.9714	0.1179	-1.55725
H	-1.85341	1.17303	-1.83159
H	-3.02692	-0.13939	-1.65934
N	-1.56202	-0.15819	-0.15706
H	-0.8732	0.52839	0.14085
C	-2.64823	-0.21248	0.8554
H	-2.18398	-0.57975	1.77425

H	-3.34813	-0.98393	0.53266
C	-3.36715	1.09882	1.09501
C	-4.58515	1.38345	0.47015
C	-2.83473	2.06823	1.96299
C	-5.25216	2.59523	0.67643
H	-5.03987	0.63733	-0.17695
C	-3.48182	3.27854	2.18118
H	-1.90448	1.8632	2.48863
C	-4.69802	3.55196	1.53431
H	-6.19817	2.7726	0.17845
H	-3.07947	4.02219	2.86187
O	-5.26083	4.76379	1.81698
C	-6.51	5.07715	1.22197
H	-6.77744	6.07024	1.58636
H	-6.4436	5.10146	0.12637
H	-7.28949	4.36271	1.51628

TS6^{L2}

Sum of electronic and thermal Free Energies= -3598.010744

S	2.50614	-2.88323	1.97347
C	4.08396	-2.62957	1.1827
C	5.13909	-2.06231	1.92365
C	4.33914	-3.05396	-0.13525
C	6.40815	-1.91387	1.3602
H	4.96885	-1.75725	2.9524
C	5.60749	-2.89639	-0.69254
H	3.53011	-3.48855	-0.71031
C	6.64734	-2.32577	0.04751
H	7.21114	-1.48264	1.95203
H	5.7849	-3.22883	-1.71184
H	7.63501	-2.21421	-0.39058
P	-1.60949	-1.65058	-0.24555
P	-2.72491	1.70461	0.60142
C	-2.21723	-2.99055	-1.37569
C	-3.06971	-2.73534	-2.4597
C	-1.91885	-4.32049	-1.04577
C	-3.60704	-3.7887	-3.20149
H	-3.30931	-1.71568	-2.7428
C	-2.46678	-5.37039	-1.7818
H	-1.23666	-4.53068	-0.2308
C	-3.30907	-5.10898	-2.8629
H	-4.25706	-3.57357	-4.04464
H	-2.21783	-6.3941	-1.5179
H	-3.72563	-5.92846	-3.44172
C	-3.08519	-1.59691	0.87196
C	-4.35979	-1.27095	0.37945
C	-2.9652	-2.03671	2.19436
C	-5.47837	-1.34658	1.20346
H	-4.48111	-0.96074	-0.65367
C	-4.08956	-2.11471	3.02178
H	-1.99492	-2.3346	2.5705
C	-5.34497	-1.76354	2.53208
H	-6.4574	-1.08782	0.80876
H	-3.97912	-2.45807	4.04656
H	-6.21923	-1.82618	3.17361
C	-1.36852	2.68849	1.40272
C	-0.25864	3.2632	0.75761
C	-1.4768	2.83338	2.79742
C	0.71339	3.95713	1.48527
H	-0.14422	3.17389	-0.31671
C	-0.52113	3.54763	3.52206
H	-2.31502	2.37549	3.31665
C	0.58101	4.10618	2.86708
H	1.56989	4.38062	0.96539
H	-0.63008	3.65379	4.59771
H	1.33359	4.64877	3.43128
C	-3.92109	3.021	0.07944
C	-3.99498	4.26697	0.72506
C	-4.88059	2.72391	-0.90646
C	-4.98456	5.19271	0.38243
H	-3.27405	4.52412	1.4949
C	-5.86041	3.65279	-1.25508
H	-4.84831	1.76821	-1.42339
C	-5.91745	4.89248	-0.61078
H	-5.02192	6.14929	0.89436
H	-6.58098	3.40577	-2.03069
H	-6.68226	5.61035	-0.87852
C	-1.58507	-0.13409	-1.3365
C	-0.95043	-0.38524	-2.57406
C	-1.99157	1.19516	-1.04017
C	-0.77561	0.61375	-3.52657
H	-0.57911	-1.38286	-2.78473
C	-1.81612	2.18293	-2.03288
C	-1.22715	1.90689	-3.26297
H	-0.29365	0.37634	-4.47024
H	-2.1617	3.19102	-1.83032
H	-1.11481	2.69555	-4.00175
Rh	0.52246	-2.02205	0.69809
H	-0.12766	-3.27967	1.29013

Cl	1.13035	-3.15256	-1.39562
C	0.14477	-0.72256	2.49494
C	1.53023	-0.51117	2.54973
H	-0.32153	-1.1936	3.35453
H	-0.47123	0.01184	1.98639
H	2.08711	-0.74986	3.44447
C	2.24136	0.30308	1.49849
H	2.22476	1.37166	1.77622
H	3.28697	0.00466	1.45267
N	1.61908	0.04821	0.1788
H	0.87932	0.72997	0.02364
C	2.55225	0.10164	-0.97803
H	1.9553	-0.15037	-1.85815
H	3.2725	-0.70744	-0.84804
C	3.26845	1.42367	-1.16568
C	4.59863	1.58708	-0.76756
C	2.61818	2.52702	-1.74722
C	5.26789	2.80595	-0.92173
H	5.13595	0.74316	-0.34053
C	3.26395	3.74712	-1.90421
H	1.59515	2.41965	-2.10216
C	4.59757	3.89519	-1.48909
H	6.30163	2.88807	-0.60683
H	2.76831	4.59671	-2.36401
O	5.14674	5.12891	-1.69197
C	6.50644	5.32346	-1.33765
H	6.73976	6.35858	-1.5926
H	6.67281	5.17145	-0.26328
H	7.17072	4.65451	-1.89973

10^{L2}

Sum of electronic and thermal Free Energies= -3598.034050

S	-2.2482	-2.63641	-2.10802
C	-3.94451	-2.59573	-1.51782
C	-4.97205	-2.14013	-2.35607
C	-4.24047	-3.10926	-0.24825
C	-6.29447	-2.17469	-1.91182
H	-4.74079	-1.76906	-3.35056
C	-5.57109	-3.15691	0.17607
H	-3.43184	-3.43891	0.40085
C	-6.59638	-2.6867	-0.647
H	-7.08896	-1.81521	-2.5596
H	-5.8008	-3.55493	1.16031
H	-7.62765	-2.72214	-0.30762
P	1.6912	-1.59565	0.33495
P	2.44232	1.75334	-0.783
C	2.36658	-2.85168	1.52595
C	3.30226	-2.51408	2.51747
C	2.02823	-4.20011	1.34709
C	3.88762	-3.50304	3.30802
H	3.56979	-1.4773	2.69253
C	2.62293	-5.18773	2.13374
H	1.27899	-4.47025	0.61335
C	3.55251	-4.84422	3.11491
H	4.60389	-3.2226	4.07533
H	2.34202	-6.22647	1.98665
H	4.00757	-5.61446	3.73137
C	3.14641	-1.51826	-0.80785
C	4.40383	-1.08458	-0.3551
C	3.03578	-2.02867	-2.10528
C	5.51528	-1.1366	-1.19252
H	4.51896	-0.7046	0.65481
C	4.15214	-2.07979	-2.94535
H	2.07657	-2.39244	-2.45233
C	5.39135	-1.63011	-2.49511
H	6.48196	-0.80099	-0.82677
H	4.04773	-2.47643	-3.95131
H	6.25922	-1.67177	-3.14706
C	0.94739	2.68492	-1.37457
C	-0.09479	3.18597	-0.57918
C	0.87409	2.87948	-2.76682
C	-1.17355	3.865	-1.15498
H	-0.07302	3.05271	0.49682
C	-0.19068	3.57326	-3.34082
H	1.6596	2.48027	-3.40365
C	-1.22056	4.06649	-2.53521
H	-1.97349	4.23018	-0.51758
H	-0.22173	3.71908	-4.41699
H	-2.05638	4.598	-2.98134
C	3.65249	3.13577	-0.50995
C	3.31346	4.49801	-0.48558
C	5.00638	2.78156	-0.37621
C	4.29713	5.4747	-0.31322
H	2.2782	4.80014	-0.60765
C	5.98683	3.75651	-0.19459
H	5.29334	1.73528	-0.42888
C	5.63478	5.10761	-0.16215
H	4.01517	6.52403	-0.29814
H	7.02743	3.46197	-0.08992

H	6.39866	5.86841	-0.02921
C	1.63616	-0.03187	1.35485
C	1.10962	-0.24978	2.64655
C	1.97786	1.29313	0.97194
C	1.01312	0.77844	3.57988
H	0.77212	-1.24513	2.91916
C	1.90707	2.30559	1.94922
C	1.44523	2.06054	3.23997
H	0.61619	0.57041	4.56919
H	2.21875	3.31104	1.68555
H	1.40818	2.86827	3.96567
Rh	-0.35421	-2.0921	-0.52427
H	0.39653	-3.33371	-1.05477
Cl	-1.12837	-3.18534	1.61988
C	-0.2316	-1.05611	-2.34664
C	-1.73848	-0.85487	-2.49882
H	0.17842	-1.63641	-3.17732
H	0.3062	-0.10677	-2.27615
H	-2.09683	-0.58347	-3.49991
C	-2.27713	0.12375	-1.4526
H	-2.06332	1.14323	-1.79414
H	-3.36297	0.04038	-1.3653
N	-1.64662	-0.1377	-0.13205
H	-0.938	0.57459	0.02439
C	-2.5711	-0.12374	1.03531
H	-1.98496	-0.46034	1.89331
H	-3.32403	-0.89383	0.86179
C	-3.23388	1.21007	1.31414
C	-4.52699	1.49169	0.86368
C	-2.56727	2.20861	2.04614
C	-5.14025	2.72598	1.10287
H	-5.08307	0.72781	0.32545
C	-3.15789	3.44175	2.29395
H	-1.57467	2.00741	2.44274
C	-4.45146	3.71116	1.81865
H	-6.14671	2.89925	0.74041
H	-2.64851	4.20836	2.8694
O	-4.94703	4.94862	2.11648
C	-6.26311	5.26335	1.69203
H	-6.4566	6.28056	2.03633
H	-6.35653	5.2296	0.5986
H	-7.00477	4.5858	2.13442

11[1,2]

Sum of electronic and thermal Free Energies= -3598.075706

C	-3.55292	1.99077	3.61264
C	-3.36109	0.71019	4.1329
C	-2.8307	-0.29536	3.32445
C	-2.48852	-0.03552	1.98797
C	-2.67254	1.26204	1.46208
C	-3.20659	2.26357	2.28882
H	-3.96127	2.77935	4.23863
H	-3.61427	0.49516	5.16701
H	-2.66169	-1.28333	3.74106
H	-3.33361	3.26868	1.89863
P	-1.80334	-1.35063	0.86702
P	-2.14463	1.55895	-0.29462
Cl	-0.01877	0.73348	-2.99115
C	2.11702	-1.10998	-0.04238
H	3.19205	-0.92685	0.05983
H	1.82376	-1.8085	0.74569
N	1.34034	0.14709	0.13918
H	1.19236	0.28298	1.13604
C	2.04502	1.36279	-0.37122
H	2.2819	1.18491	-1.42098
H	1.31912	2.17861	-0.35934
C	3.27874	1.74109	0.4236
C	4.56945	1.41755	-0.00751
C	3.15429	2.42563	1.6463
C	5.70142	1.74257	0.74857
H	4.70547	0.90171	-0.95484
C	4.26428	2.75784	2.41157
H	2.1659	2.71498	1.99869
C	5.55055	2.41224	1.96765
H	6.68199	1.46825	0.37713
H	4.16719	3.29195	3.35182
O	6.57744	2.77715	2.79195
C	7.90178	2.45612	2.39742
H	8.5518	2.83099	3.19016
H	8.04388	1.37191	2.29649
H	8.17308	2.94101	1.4507
C	0.30397	-2.08904	-1.48144
H	0.01108	-2.32961	-2.50519
H	0.08365	-2.94326	-0.83017
C	1.77524	-1.7227	-1.40105
H	2.01067	-1.01974	-2.20247
C	-0.86835	-2.45145	2.01927
C	-0.99365	-3.84746	1.94536
C	0.0601	-1.90459	2.92406

C	-0.2133	-4.67459	2.7556
H	-1.70657	-4.29232	1.25939
C	0.83818	-2.73202	3.73304
H	0.1635	-0.82766	3.01394
C	0.7041	-4.12138	3.64971
H	-0.32752	-5.75341	2.68564
H	1.54893	-2.29352	4.42599
H	1.31066	-4.76577	4.27929
C	-3.27393	-2.38429	0.41902
C	-3.25863	-3.09242	-0.79369
C	-4.38781	-2.51159	1.26464
C	-4.33017	-3.9146	-1.14585
H	-2.41294	-2.98696	-1.4656
C	-5.46303	-3.32423	0.90356
H	-4.43191	-1.96676	2.20121
C	-5.43619	-4.02922	-0.30074
H	-4.30272	-4.45461	-2.08803
H	-6.32322	-3.40049	1.56413
H	-6.27504	-4.65957	-0.5814
C	-3.72389	1.63845	-1.25118
C	-4.96411	1.93939	-0.66847
C	-3.65824	1.38189	-2.63158
C	-6.11978	1.98487	-1.44977
H	-5.03771	2.12787	0.3973
C	-4.81609	1.44329	-3.40932
H	-2.70199	1.13333	-3.08576
C	-6.04752	1.74026	-2.82173
H	-7.07573	2.20964	-0.98438
H	-4.75361	1.24702	-4.47567
H	-6.94828	1.77617	-3.42811
C	-1.56107	3.31072	-0.284
C	-1.91842	4.20042	-1.30682
C	-0.64651	3.74113	0.69497
C	-1.37702	5.48692	-1.34901
H	-2.6182	3.8896	-2.0744
C	-0.11097	5.02858	0.65474
H	-0.35878	3.07074	1.50032
C	-0.4745	5.90562	-0.37131
H	-1.66486	6.16156	-2.15168
H	0.59205	5.34483	1.41984
H	-0.05328	6.9058	-0.40948
Rh	-0.74533	-0.3438	-0.88959
H	-1.93383	-0.83789	-1.72839
S	2.83139	-3.24224	-1.70052
C	4.44678	-2.52326	-2.00937
C	5.53576	-2.89664	-1.20842
C	4.65504	-1.6261	-3.06955
C	6.80978	-2.38393	-1.46327
H	5.37714	-3.58584	-0.38461
C	5.92536	-1.09852	-3.30598
H	3.8245	-1.35118	-3.71304
C	7.00785	-1.47806	-2.50661
H	7.64553	-2.68657	-0.8377
H	6.07211	-0.40382	-4.12858
H	7.99805	-1.07529	-2.70135

TS7^{L2}

Sum of electronic and thermal Free Energies= -3598.047932

C	-4.59967	1.39681	3.31204
C	-4.42257	0.07648	3.73437
C	-3.61816	-0.78844	2.99446
C	-2.9882	-0.34478	1.82223
C	-3.19338	0.97287	1.37611
C	-3.98905	1.84144	2.14033
H	-5.21136	2.07869	3.89594
H	-4.89898	-0.27395	4.64546
H	-3.46631	-1.80559	3.34176
H	-4.11906	2.87121	1.82144
P	-1.85456	-1.42403	0.8198
P	-2.37551	1.45936	-0.2153
Cl	0.03183	1.29742	-2.57027
C	2.12803	-1.13058	-0.10889
H	3.21696	-1.01595	-0.04708
H	1.8574	-1.98718	0.51529
N	1.43305	0.06141	0.42184
H	1.30299	-0.06681	1.42146
C	2.12933	1.35347	0.19422
H	2.21608	1.49498	-0.88485
H	1.45241	2.13814	0.54538
C	3.47905	1.48303	0.87268
C	4.67372	1.30197	0.16992
C	3.56985	1.77589	2.24491
C	5.92024	1.39359	0.79868
H	4.64173	1.08517	-0.89465
C	4.79683	1.87367	2.88824
H	2.65925	1.94049	2.81824
C	5.9845	1.67969	2.16594
H	6.81862	1.23833	0.21355
H	4.86703	2.10793	3.94594

O	7.14163	1.797	2.8855
C	8.37145	1.62958	2.2003
H	9.15466	1.77309	2.94615
H	8.4642	0.62405	1.77021
H	8.49536	2.37128	1.40003
C	0.27644	-1.89961	-1.73179
H	0.12535	-2.1327	-2.79052
H	0.08313	-2.81418	-1.16457
C	1.72083	-1.42775	-1.55901
H	1.88122	-0.55037	-2.18674
C	-0.75172	-2.18088	2.09485
C	-0.19028	-3.45305	1.89272
C	-0.32966	-1.4308	3.20621
C	0.75146	-3.96654	2.78597
H	-0.49301	-4.05101	1.03913
C	0.61458	-1.94518	4.09627
H	-0.74704	-0.44474	3.38532
C	1.15687	-3.21499	3.88997
H	1.16976	-4.9539	2.61426
H	0.92371	-1.35315	4.95298
H	1.8912	-3.61417	4.5831
C	-2.95443	-2.81342	0.28701
C	-3.48453	-2.78371	-1.01153
C	-3.33874	-3.85207	1.15225
C	-4.37716	-3.76972	-1.43581
H	-3.19177	-1.98354	-1.68448
C	-4.22834	-4.83765	0.72465
H	-2.93286	-3.90584	2.15732
C	-4.75011	-4.79836	-0.57022
H	-4.77625	-3.73298	-2.44526
H	-4.51096	-5.63781	1.40289
H	-5.44111	-5.568	-0.90233
C	-3.7738	1.62444	-1.42123
C	-5.11669	1.74803	-1.03259
C	-3.46168	1.60532	-2.79234
C	-6.12568	1.85426	-1.99244
H	-5.38895	1.74961	0.01671
C	-4.47354	1.72815	-3.74572
H	-2.42644	1.49141	-3.10223
C	-5.80737	1.84959	-3.35072
H	-7.16106	1.93968	-1.67401
H	-4.21508	1.71861	-4.80094
H	-6.59375	1.93392	-4.09604
C	-1.86633	3.20389	0.11711
C	-2.18215	4.25963	-0.74625
C	-1.07143	3.46755	1.24496
C	-1.72032	5.55169	-0.48224
H	-2.78761	4.07724	-1.62726
C	-0.61868	4.75798	1.51173
H	-0.81258	2.65969	1.92175
C	-0.9412	5.80536	0.64557
H	-1.97333	6.35977	-1.16331
H	-0.01125	4.94617	2.39209
H	-0.58428	6.81092	0.84888
Rh	-0.80848	-0.17468	-0.75463
H	-1.09886	-1.24061	-1.884
S	2.84253	-2.77322	-2.25079
C	4.36716	-1.8795	-2.55761
C	5.56035	-2.33651	-1.98018
C	4.40216	-0.76187	-3.4075
C	6.76832	-1.69015	-2.25032
H	5.53536	-3.19625	-1.31764
C	5.60804	-0.10483	-3.65444
H	3.48876	-0.41257	-3.87929
C	6.79577	-0.56867	-3.08108
H	7.68657	-2.05954	-1.80147
H	5.62108	0.76121	-4.31065
H	7.7348	-0.06278	-3.28702

12^{L2}

Sum of electronic and thermal Free Energies= -3598.109412

C	5.24584	1.12563	2.97299
C	4.67271	2.39595	2.87454
C	3.56348	2.60031	2.05352
C	3.01815	1.53473	1.32526
C	3.61233	0.26172	1.40005
C	4.71823	0.06326	2.23831
H	6.09789	0.96089	3.62619
H	5.08149	3.22403	3.44663
H	3.11096	3.58599	1.99788
H	5.15369	-0.92722	2.33117
P	1.52787	1.65654	0.22455
P	2.82464	-1.08566	0.39183
Cl	0.19466	-2.66709	-1.01218
C	-2.26083	0.64955	-1.26666
H	-3.31836	0.63788	-0.98074
H	-1.97781	1.69724	-1.41023
N	-1.45283	0.11708	-0.13175
H	-1.39319	0.88061	0.54048

C	-2.12627	-1.01785	0.58775
H	-2.33824	-1.79399	-0.14795
H	-1.37409	-1.43851	1.25817
C	-3.36566	-0.63983	1.37173
C	-4.64802	-0.98176	0.93332
C	-3.25177	0.02392	2.60658
C	-5.787	-0.67946	1.6871
H	-4.77103	-1.50595	-0.00985
C	-4.37012	0.33383	3.36852
H	-2.26596	0.28853	2.98485
C	-5.64999	-0.02256	2.91314
H	-6.76079	-0.96443	1.30631
H	-4.28247	0.83367	4.32793
O	-6.68652	0.30878	3.74013
C	-7.99613	-0.07686	3.35655
H	-8.65629	0.25013	4.16167
H	-8.30495	0.40576	2.42
H	-8.08131	-1.16523	3.24077
C	-0.79806	0.28809	-3.34334
H	-0.72897	-0.23907	-4.30003
H	-0.76282	1.36658	-3.53975
C	-2.07704	-0.09527	-2.60013
H	-2.08424	-1.17586	-2.43607
C	0.38989	2.83627	1.0795
C	-0.45628	3.67524	0.33416
C	0.21755	2.78011	2.47344
C	-1.43512	4.44684	0.96602
H	-0.3438	3.73823	-0.74359
C	-0.75794	3.55579	3.10254
H	0.85223	2.13276	3.07038
C	-1.58759	4.39043	2.35078
H	-2.07592	5.0915	0.3718
H	-0.87035	3.50584	4.18151
H	-2.34987	4.98939	2.8414
C	2.19108	2.64017	-1.20394
C	2.53107	1.94903	-2.37723
C	2.44353	4.02022	-1.13434
C	3.10972	2.62085	-3.4559
H	2.34187	0.88158	-2.4329
C	3.0136	4.69131	-2.21597
H	2.1854	4.57789	-0.23882
C	3.34922	3.99282	-3.37891
H	3.3695	2.0701	-4.35575
H	3.19644	5.76019	-2.15066
H	3.79441	4.51706	-4.21992
C	4.08141	-1.54656	-0.88171
C	5.42872	-1.15934	-0.82186
C	3.64264	-2.3251	-1.96734
C	6.3217	-1.55552	-1.81905
H	5.7863	-0.54361	-0.0049
C	4.54211	-2.72241	-2.95703
H	2.59737	-2.61644	-2.0262
C	5.88362	-2.34061	-2.88505
H	7.36122	-1.24797	-1.75849
H	4.19233	-3.32801	-3.78771
H	6.58034	-2.64995	-3.65855
C	2.81593	-2.5039	1.57177
C	3.58391	-3.66116	1.39103
C	1.97724	-2.40643	2.69458
C	3.5147	-4.7039	2.3192
H	4.22757	-3.75892	0.52264
C	1.91976	-3.44126	3.62434
H	1.3602	-1.51971	2.82415
C	2.68732	-4.59517	3.43695
H	4.10623	-5.60288	2.16246
H	1.26739	-3.35214	4.48971
H	2.63436	-5.40834	4.15551
Rh	0.77491	-0.40671	-0.21204
H	0.07134	0.01458	-2.73685
S	-3.48715	0.32489	-3.74457
C	-4.87398	-0.55904	-3.0306
C	-6.00618	0.1557	-2.61642
C	-4.88036	-1.96115	-2.95273
C	-7.12962	-0.52105	-2.13559
H	-6.00136	1.24008	-2.67305
C	-5.99627	-2.6318	-2.4514
H	-4.0171	-2.52314	-3.2953
C	-7.12599	-1.91447	-2.04642
H	-8.00356	0.04417	-1.82433
H	-5.98959	-3.71707	-2.39356
H	-7.999	-2.44094	-1.67134

TS3$^{L2'}$

Sum of electronic and thermal Free Energies= -3598.022174

S	4.09326	0.02549	-0.2257
C	5.02797	1.40085	-0.87575
C	4.72162	1.99262	-2.11413
C	6.1495	1.86438	-0.16407
C	5.5138	3.02792	-2.61187

H	3.85021	1.64427	-2.65873
C	6.9473	2.89055	-0.67572
H	6.39689	1.404	0.78768
C	6.62948	3.47878	-1.89971
H	5.26309	3.4784	-3.56766
H	7.81378	3.23084	-0.11475
H	7.24547	4.28197	-2.29585
P	1.15024	-1.3945	0.58858
C	2.4407	-2.61704	1.13857
C	2.47272	-3.95683	0.72009
C	3.35062	-2.19883	2.12162
C	3.39547	-4.85033	1.26738
H	1.78534	-4.3086	-0.04107
C	4.26729	-3.09487	2.67213
H	3.35051	-1.16411	2.4466
C	4.29474	-4.42304	2.24518
H	3.40897	-5.88171	0.92545
H	4.96817	-2.74868	3.42646
H	5.01398	-5.11912	2.66805
C	-0.0397	-1.68202	1.98378
C	-0.47853	-2.97378	2.31562
C	-0.41215	-0.61744	2.81178
C	-1.30685	-3.1817	3.41587
H	-0.15682	-3.82371	1.7216
C	-1.23846	-0.8229	3.919
H	-0.03871	0.37453	2.59207
C	-1.69625	-2.1046	4.21788
H	-1.6418	-4.18683	3.65438
H	-1.51565	0.01718	4.55064
H	-2.33828	-2.26877	5.0782
C	0.48363	-2.16986	-0.96855
C	1.51232	-2.50234	-1.87432
C	-0.85923	-2.40619	-1.35097
C	1.24602	-3.14656	-3.0769
H	2.53888	-2.24596	-1.63248
C	-1.09962	-3.08995	-2.55915
C	-0.06844	-3.47354	-3.4094
H	2.06449	-3.39024	-3.74772
H	-2.12635	-3.30149	-2.8407
H	-0.29252	-3.99551	-4.33524
Rh	1.91643	0.91032	0.30951
H	2.45519	1.02213	1.83477
Cl	1.2031	1.06473	-2.0686
C	2.84268	2.51341	1.62326
C	2.33247	3.02227	0.39701
H	3.91513	2.40072	1.71706
H	2.32851	2.7472	2.55561
H	3.01502	3.32247	-0.38912
C	0.87737	3.44383	0.32514
H	0.62513	4.33111	0.9227
H	0.60487	3.63268	-0.71088
N	0.12569	2.23327	0.78437
H	0.0035	2.29093	1.79491
C	-1.21879	2.02273	0.1786
H	-1.53712	1.02224	0.48105
H	-1.07267	2.00438	-0.89772
C	-2.24696	3.04432	0.60909
C	-2.50006	4.20061	-0.13644
C	-2.97861	2.85495	1.79378
C	-3.4393	5.15032	0.27678
H	-1.96912	4.36157	-1.07155
C	-3.91777	3.78521	2.21901
H	-2.82329	1.95018	2.37719
C	-4.15329	4.94418	1.4616
H	-3.61115	6.03249	-0.33417
H	-4.49076	3.63575	3.12722
O	-5.09915	5.79447	1.95604
C	-5.37975	6.98186	1.23679
H	-6.139	7.50961	1.8165
H	-4.48755	7.61811	1.13856
H	-5.77581	6.76683	0.23563
P	-2.33141	-1.72385	-0.43512
C	-3.5303	-3.14146	-0.57002
C	-4.79774	-3.04809	-1.16471
C	-3.18303	-4.34937	0.06026
C	-5.69029	-4.12333	-1.12003
H	-5.09518	-2.13447	-1.66956
C	-4.06903	-5.42446	0.09441
H	-2.20796	-4.45071	0.52654
C	-5.33218	-5.31415	-0.49206
H	-6.66707	-4.02573	-1.58669
H	-3.7744	-6.34858	0.58195
H	-6.02808	-6.14817	-0.45747
C	-3.00828	-0.48106	-1.63459
C	-4.1693	0.21228	-1.24034
C	-2.38613	-0.10606	-2.83501
C	-4.7228	1.20525	-2.04758
H	-4.6445	-0.02434	-0.29149

C	-2.93144	0.90286	-3.63293
H	-1.46201	-0.57865	-3.1437
C	-4.10527	1.5521	-3.25133
H	-5.62549	1.71809	-1.7276
H	-2.42782	1.18065	-4.55439
H	-4.52823	2.332	-3.87803

$5^{L2'}$

Sum of electronic and thermal Free Energies= -3598.034525

S	-3.98417	0.0101	0.04666
C	-5.0221	1.11677	0.99681
C	-4.83495	1.29721	2.37763
C	-6.10388	1.75623	0.36814
C	-5.70542	2.11054	3.10392
H	-3.99796	0.81027	2.86494
C	-6.98041	2.5567	1.10432
H	-6.26071	1.61249	-0.6975
C	-6.78269	2.74054	2.47429
H	-5.54542	2.24482	4.17107
H	-7.81561	3.03969	0.6033
H	-7.46243	3.36596	3.04692
P	-0.98086	-1.45889	-0.88633
C	-2.18888	-2.53863	-1.8099
C	-2.12831	-3.94206	-1.82024
C	-3.12464	-1.90409	-2.63942
C	-2.9867	-4.68504	-2.62946
H	-1.41991	-4.46231	-1.18427
C	-3.97859	-2.64844	-3.45616
H	-3.20287	-0.82223	-2.63621
C	-3.91425	-4.04044	-3.45168
H	-2.92974	-5.76966	-2.61694
H	-4.70094	-2.13542	-4.08494
H	-4.58337	-4.62109	-4.08019
C	0.3767	-1.55909	-2.15012
C	1.06226	-2.74604	-2.44904
C	0.60274	-0.43785	-2.9567
C	1.96236	-2.79831	-3.51242
H	0.89436	-3.63433	-1.84976
C	1.50429	-0.48718	-4.02359
H	0.05472	0.47718	-2.75751
C	2.19094	-1.66764	-4.30073
H	2.48188	-3.72666	-3.73224
H	1.66118	0.39344	-4.63903
H	2.89047	-1.71292	-5.13021
C	-0.51578	-2.51011	0.58323
C	-1.61745	-3.16971	1.16845
C	0.75011	-2.6201	1.21613
C	-1.47751	-3.98825	2.28442
H	-2.60598	-3.04077	0.74135
C	0.87139	-3.48378	2.32055
C	-0.21667	-4.17173	2.85003
H	-2.35124	-4.48252	2.70129
H	1.84401	-3.60562	2.78557
H	-0.08311	-4.82476	3.70784
Rh	-1.86243	0.93078	-0.21364
H	-2.75256	2.52666	-2.22774
Cl	-1.26556	0.9377	2.05338
C	-3.05574	3.22108	-1.42605
C	-2.33611	2.94577	-0.11259
H	-4.13626	3.11251	-1.31113
H	-2.8401	4.23183	-1.80434
H	-2.92379	3.20255	0.76886
C	-0.88733	3.41181	-0.04571
H	-0.67179	4.36235	-0.5572
H	-0.57053	3.49331	0.99489
N	-0.13001	2.26497	-0.64689
H	-0.07768	2.39904	-1.65513
C	1.25486	2.04686	-0.14489
H	1.5581	1.04999	-0.47475
H	1.19582	2.01968	0.94443
C	2.24023	3.08379	-0.6356
C	2.50405	4.25527	0.07977
C	2.91022	2.8975	-1.85721
C	3.39247	5.22279	-0.39839
H	2.01814	4.41813	1.03797
C	3.7966	3.84642	-2.34836
H	2.74511	1.98262	-2.4217
C	4.04256	5.02036	-1.62114
H	3.57312	6.11517	0.18869
H	4.32222	3.69898	-3.28598
O	4.93262	5.88838	-2.18292
C	5.23268	7.08636	-1.4879
H	5.96127	7.61695	-2.10286
H	4.34196	7.71511	-1.35948
H	5.67239	6.88359	-0.50445
P	2.22888	-1.58577	0.72421
C	3.6343	-2.80499	0.81914
C	4.33065	-3.11753	1.99887
C	4.04906	-3.41438	-0.37644

C	5.38721	-4.02969	1.98637
H	4.05838	-2.63189	2.9304
C	5.10187	-4.33085	-0.3887
H	3.55166	-3.15754	-1.30568
C	5.7725	-4.64401	0.79409
H	5.91187	-4.2572	2.91024
H	5.40533	-4.79081	-1.32465
H	6.59633	-5.35195	0.78547
C	2.5489	-0.57412	2.24589
C	3.71974	0.20921	2.2398
C	1.6767	-0.46037	3.33785
C	4.02268	1.05451	3.30568
H	4.40486	0.15043	1.39675
C	1.97646	0.39678	4.40141
H	0.75257	-1.02507	3.3588
C	3.14899	1.15131	4.39345
H	4.93734	1.64149	3.28415
H	1.28264	0.47414	5.23447
H	3.3791	1.81466	5.22286

$6^{L2'}$

Sum of electronic and thermal Free Energies= -3598.078653

S	-2.87091	-0.46374	-1.12048
C	-3.14271	-1.63103	-2.44673
C	-2.94702	-1.25242	-3.78824
C	-3.6669	-2.9094	-2.18148
C	-3.26315	-2.12947	-4.82605
H	-2.53946	-0.27033	-3.99906
C	-3.98589	-3.7825	-3.22394
H	-3.82653	-3.21364	-1.15126
C	-3.78442	-3.39685	-4.55098
H	-3.10854	-1.81686	-5.8563
H	-4.38997	-4.76629	-2.99749
H	-4.03354	-4.07514	-5.36292
Rh	-0.47169	-0.21413	-0.74689
H	0.01275	-3.5585	-0.18799
Cl	-0.2173	0.88828	-2.9579
C	-0.1928	-3.37296	-1.24874
C	0.17224	-1.97898	-1.72867
H	-1.25757	-3.56872	-1.40676
H	0.36781	-4.13182	-1.82088
H	-0.23073	-1.8324	-2.73121
C	1.657	-1.59795	-1.68528
H	2.31849	-2.39797	-1.33559
H	2.00687	-1.28204	-2.66659
N	1.74348	-0.40896	-0.7696
H	2.02827	-0.72668	0.15209
C	2.67467	0.67352	-1.18022
H	2.47485	1.52542	-0.52523
H	2.39304	0.97136	-2.19115
C	4.13648	0.28867	-1.08931
C	4.8916	-0.03079	-2.21997
C	4.78105	0.25378	0.15954
C	6.2441	-0.37797	-2.12664
H	4.42411	0.00139	-3.20073
C	6.11972	-0.09272	0.27382
H	4.22472	0.51123	1.05752
C	6.86366	-0.40966	-0.87302
H	6.79647	-0.61193	-3.02883
H	6.62003	-0.11232	1.23648
O	8.17473	-0.72438	-0.65664
C	8.98805	-1.02235	-1.77987
H	9.98349	-1.23106	-1.38421
H	8.62424	-1.90402	-2.32252
H	9.04641	-0.17394	-2.47347
C	-1.24498	0.28737	2.59554
C	-1.54861	-0.04308	3.92956
C	-1.97281	0.93082	4.82997
C	-2.11282	2.25312	4.40278
C	-1.83139	2.58793	3.07805
C	-1.38959	1.61827	2.15541
H	-1.45189	-1.07161	4.26347
H	-2.19991	0.65719	5.85832
H	-2.45108	3.01958	5.09603
H	-1.97551	3.61151	2.74982
P	-1.04946	1.99119	0.375
P	-0.59876	-1.04063	1.45832
C	-1.60883	-2.49539	2.0133
C	-1.09508	-3.55271	2.78041
C	-2.98121	-2.48694	1.70717
C	-1.93066	-4.58482	3.21606
H	-0.04772	-3.57873	3.0539
C	-3.81011	-3.51553	2.15306
H	-3.38616	-1.68972	1.09277
C	-3.28918	-4.56974	2.90524
H	-1.51454	-5.39726	3.80449
H	-4.86756	-3.4891	1.90817
H	-3.9375	-5.37066	3.24913
C	1.08186	-1.36251	2.20401

C	1.82236	-2.49527	1.81382
C	1.68601	-0.45974	3.09471
C	3.10313	-2.72989	2.3129
H	1.39969	-3.206	1.11461
C	2.97059	-0.69474	3.59101
H	1.15649	0.42915	3.41388
C	3.68236	-1.83058	3.20653
H	3.64655	-3.61437	1.99486
H	3.41235	0.01453	4.2823
H	4.68043	-2.01193	3.59235
C	-2.58416	2.84827	-0.22043
C	-2.59624	3.27923	-1.55945
C	-3.74373	3.01677	0.5531
C	-3.72519	3.89802	-2.09016
H	-1.74042	3.09063	-2.20182
C	-4.87089	3.64184	0.01438
H	-3.78815	2.65595	1.57333
C	-4.86473	4.08966	-1.30421
H	-3.71868	4.21472	-3.1291
H	-5.75344	3.77073	0.63121
H	-5.74486	4.5691	-1.7231
C	0.20726	3.36432	0.36908
C	0.76914	3.67279	-0.88214
C	0.60695	4.11761	1.48805
C	1.6703	4.728	-1.01779
H	0.51887	3.06245	-1.74755
C	1.51036	5.17301	1.34632
H	0.22137	3.89245	2.47749
C	2.03749	5.48972	0.09474
H	2.0893	4.95044	-2.00025
H	1.79513	5.75531	2.21969
H	2.73813	6.31414	-0.00651

TS4$^{L2'}$

Sum of electronic and thermal Free Energies= -3598.023100

S	1.27277	-1.34083	-2.54133
C	2.13411	-2.88298	-2.33547
C	3.13331	-3.03919	-1.35849
C	1.92202	-3.91601	-3.26395
C	3.91615	-4.18876	-1.32965
H	3.27858	-2.25584	-0.62638
C	2.7066	-5.07061	-3.22656
H	1.15318	-3.80431	-4.02093
C	3.70728	-5.20936	-2.2616
H	4.68827	-4.29068	-0.56945
H	2.53563	-5.86168	-3.95126
H	4.3208	-6.10579	-2.23507
Rh	0.52913	-0.48111	-0.33925
H	-1.74408	0.36471	-2.90556
Cl	0.49949	-2.73855	0.67388
C	-1.58277	-0.65593	-3.25923
C	-1.15161	-1.59012	-2.15222
H	-0.85867	-0.62792	-4.0748
H	-2.54196	-1.01312	-3.66599
H	-0.90832	-2.58499	-2.51357
C	-2.11282	-1.70599	-0.98692
H	-3.07785	-2.04326	-1.43149
H	-1.77419	-2.49703	-0.31505
N	-2.23379	-0.48034	-0.20571
H	-2.53854	0.2941	-0.78823
C	-3.11772	-0.58271	0.96769
H	-2.96789	0.32334	1.56445
H	-2.75784	-1.42512	1.56733
C	-4.59676	-0.7521	0.66323
C	-5.1985	-2.01234	0.59516
C	-5.40592	0.37106	0.41516
C	-6.55519	-2.16597	0.28752
H	-4.60263	-2.9001	0.79613
C	-6.75456	0.24057	0.11067
H	-4.96744	1.36518	0.47079
C	-7.33988	-1.03343	0.04517
H	-6.98262	-3.16123	0.24764
H	-7.38235	1.10794	-0.07091
O	-8.67373	-1.05723	-0.25149
C	-9.32313	-2.31405	-0.32415
H	-10.36792	-2.10384	-0.54867
H	-8.90417	-2.93898	-1.11852
H	-9.26548	-2.85824	0.62377
C	1.87109	2.5852	0.28151
C	2.33704	3.89137	0.0719
C	3.28693	4.44817	0.92643
C	3.78842	3.7026	1.99634
C	3.32441	2.40742	2.21757
C	2.35565	1.84378	1.37099
H	1.97555	4.46577	-0.77457
H	3.64849	5.45647	0.74783
H	4.54335	4.12715	2.65203
H	3.72407	1.82362	3.04076
P	1.65338	0.15	1.60184

P	0.65663	1.75745	-0.86921
C	1.23667	2.44497	-2.4939
C	0.74068	3.63189	-3.05872
C	2.30624	1.79444	-3.13024
C	1.28698	4.14018	-4.23929
H	-0.06745	4.17141	-2.57867
C	2.85311	2.30799	-4.30707
H	2.69617	0.87406	-2.71112
C	2.34239	3.47849	-4.86829
H	0.88744	5.05719	-4.66257
H	3.67584	1.78587	-4.78702
H	2.7648	3.87411	-5.78798
C	-0.91129	2.68602	-0.51379
C	-1.92134	2.82179	-1.48203
C	-1.16142	3.17091	0.77973
C	-3.13379	3.44122	-1.17183
H	-1.75736	2.4639	-2.49298
C	-2.37476	3.78661	1.09046
H	-0.40978	3.06823	1.55453
C	-3.36387	3.92906	0.11591
H	-3.89508	3.54442	-1.93963
H	-2.54344	4.15763	2.09718
H	-4.30429	4.41611	0.3566
C	3.12492	-0.83597	2.11939
C	3.04844	-1.80354	3.13124
C	4.33719	-0.6747	1.4257
C	4.1612	-2.58431	3.44799
H	2.12081	-1.95302	3.67203
C	5.44989	-1.45034	1.75124
H	4.41594	0.06169	0.63112
C	5.36457	-2.41012	2.76295
H	4.08273	-3.33273	4.23148
H	6.3822	-1.30565	1.21169
H	6.22954	-3.01792	3.01349
C	0.63465	0.29151	3.14916
C	-0.26645	-0.74795	3.44385
C	0.69323	1.397	4.01309
C	-1.06714	-0.6869	4.58517
H	-0.33208	-1.59892	2.77148
C	-0.12141	1.45854	5.14612
H	1.3703	2.21879	3.80918
C	-1.00052	0.41593	5.43891
H	-1.75186	-1.50246	4.80083
H	-0.06286	2.32372	5.80105
H	-1.63143	0.46433	6.32207

TS6$^{L2'}$

Sum of electronic and thermal Free Energies= -3598.004381

S	-2.47086	-3.4503	-1.5993
C	-4.10261	-2.83079	-1.23274
C	-4.95397	-2.40197	-2.26645
C	-4.58929	-2.84568	0.08771
C	-6.25418	-1.97727	-1.98526
H	-4.60373	-2.42449	-3.29483
C	-5.89234	-2.42984	0.35986
H	-3.92843	-3.17704	0.88321
C	-6.7273	-1.98755	-0.67163
H	-6.90026	-1.64915	-2.79565
H	-6.25751	-2.45074	1.38327
H	-7.74128	-1.66433	-0.45388
P	1.50925	-1.6431	0.31617
C	2.281	-2.9196	1.42019
C	3.27893	-2.59016	2.35169
C	1.94822	-4.26843	1.23396
C	3.93032	-3.5874	3.07781
H	3.5441	-1.55342	2.52885
C	2.6078	-5.26365	1.9564
H	1.1556	-4.53574	0.54556
C	3.59846	-4.92805	2.87935
H	4.69497	-3.31361	3.79952
H	2.33076	-6.30263	1.80599
H	4.10399	-5.70457	3.44648
C	2.83097	-1.57477	-0.9802
C	4.15048	-1.20693	-0.66839
C	2.544	-2.01375	-2.27817
C	5.14452	-1.23388	-1.64264
H	4.40762	-0.90037	0.33993
C	3.54305	-2.04588	-3.25495
H	1.54088	-2.34896	-2.51857
C	4.84143	-1.64693	-2.9433
H	6.15699	-0.93488	-1.38668
H	3.30244	-2.38865	-4.25728
H	5.61789	-1.66937	-3.70251
C	1.58224	-0.10216	1.37145
C	1.08898	-0.3315	2.67619
C	1.97567	1.21457	1.01459
C	1.06391	0.67634	3.63483
H	0.71893	-1.31861	2.93699
C	1.98038	2.20454	2.01944

C	1.5411	1.9481	3.31445
H	0.68791	0.46009	4.63048
H	2.33831	3.19822	1.77048
H	1.55748	2.73715	4.06004
Rh	-0.65756	-2.16038	-0.42766
H	0.06924	-3.4113	-0.98183
Cl	-1.17061	-3.20365	1.7316
C	-1.45061	-1.57666	-2.93679
C	-0.79655	-0.67039	-2.09978
H	-2.48901	-1.42497	-3.20249
H	-0.88784	-2.22351	-3.60149
H	0.24879	-0.44651	-2.29004
C	-1.63426	0.33068	-1.31281
H	-1.29618	1.36515	-1.44161
H	-2.67747	0.27763	-1.64464
N	-1.59067	-0.10379	0.11155
H	-0.83897	0.38855	0.58927
C	-2.83033	0.04531	0.90612
H	-2.64606	-0.47665	1.84928
H	-3.61458	-0.50897	0.39053
C	-3.27402	1.47321	1.15243
C	-4.37264	2.01568	0.4802
C	-2.604	2.29111	2.07969
C	-4.80056	3.32858	0.7051
H	-4.92341	1.39751	-0.225
C	-3.01047	3.5983	2.31513
H	-1.75814	1.89177	2.63608
C	-4.11581	4.12701	1.62735
H	-5.66274	3.70763	0.16818
H	-2.50422	4.22724	3.04079
O	-4.44238	5.41767	1.9344
C	-5.58518	5.98572	1.31345
H	-5.67468	6.99749	1.71228
H	-5.47186	6.03854	0.22244
H	-6.49759	5.42213	1.5505
P	2.41226	1.7003	-0.73266
C	3.88619	2.79786	-0.45617
C	4.1102	3.93361	-1.25187
C	4.89475	2.40906	0.44499
C	5.29753	4.65912	-1.14438
H	3.35334	4.26041	-1.95642
C	6.0784	3.13958	0.55513
H	4.74859	1.54172	1.08116
C	6.28733	4.26668	-0.24164
H	5.44517	5.53776	-1.76786
H	6.8376	2.82577	1.26681
H	7.20979	4.83398	-0.15805
C	1.08706	2.91559	-1.20569
C	0.98449	3.17194	-2.58679
C	0.17026	3.54132	-0.34678
C	0.02722	4.05562	-3.08685
H	1.65739	2.66778	-3.27655
C	-0.80524	4.40584	-0.84872
H	0.19595	3.34739	0.71839
C	-0.87306	4.67392	-2.21683
H	-0.02473	4.24699	-4.15617
H	-1.51462	4.86213	-0.16534
H	-1.62989	5.35008	-2.6039

$10^{L2'}$

Sum of electronic and thermal Free Energies= -3598.026483

S	2.62569	-3.0339	1.67185
C	4.26229	-2.46417	1.1881
C	5.17398	-1.92584	2.10404
C	4.64676	-2.69339	-0.14091
C	6.46161	-1.58899	1.6817
H	4.89278	-1.77809	3.1423
C	5.94344	-2.37014	-0.54492
H	3.92373	-3.09696	-0.84653
C	6.85041	-1.81177	0.35891
H	7.16444	-1.16521	2.39365
H	6.23855	-2.54601	-1.57534
H	7.85558	-1.55638	0.03653
P	-1.47241	-1.71632	-0.25022
C	-2.22428	-3.01448	-1.34232
C	-3.23438	-2.71558	-2.27086
C	-1.84651	-4.3522	-1.15984
C	-3.8582	-3.7337	-2.99328
H	-3.53105	-1.6871	-2.44864
C	-2.47772	-5.3677	-1.87857
H	-1.03923	-4.59181	-0.47844
C	-3.48382	-5.0633	-2.79588
H	-4.6333	-3.48397	-3.71256
H	-2.16554	-6.39751	-1.73189
H	-3.9668	-5.8557	-3.36083
C	-2.73538	-1.71383	1.10273
C	-4.10409	-1.57442	0.81715
C	-2.34382	-1.95921	2.42296
C	-5.05053	-1.63728	1.83586

H	-4.43482	-1.42512	-0.20524
C	-3.29456	-2.02266	3.44561
H	-1.29469	-2.11455	2.64271
C	-4.64704	-1.85282	3.15724
H	-6.10509	-1.52633	1.59952
H	-2.97383	-2.21261	4.46611
H	-5.38664	-1.90352	3.95125
C	-1.63344	-0.17847	-1.29865
C	-1.0909	-0.3885	-2.58714
C	-2.13003	1.10911	-0.96617
C	-1.11024	0.60801	-3.55807
H	-0.64181	-1.35022	-2.82379
C	-2.16806	2.08719	-1.98166
C	-1.67744	1.8484	-3.2619
H	-0.69618	0.40691	-4.54182
H	-2.59146	3.06006	-1.75407
H	-1.72552	2.62946	-4.01564
Rh	0.70232	-2.13469	0.31947
H	0.0403	-3.36276	1.01186
Cl	1.26104	-3.27588	-1.8642
C	1.92337	-1.74295	2.84438
C	1.0253	-0.87811	1.98393
H	2.74155	-1.22745	3.36234
H	1.3655	-2.33013	3.57829
H	0.16792	-0.4948	2.53947
C	1.78588	0.21548	1.21117
H	1.46787	1.23067	1.47236
H	2.86203	0.15733	1.40629
N	1.57771	-0.07396	-0.23701
H	0.77918	0.45849	-0.57151
C	2.71395	0.16157	-1.15531
H	2.41973	-0.25945	-2.12172
H	3.55388	-0.43584	-0.79681
C	3.12647	1.61348	-1.29642
C	4.24239	2.12117	-0.6261
C	2.39063	2.49833	-2.10447
C	4.62085	3.46366	-0.73471
H	4.84391	1.45506	-0.01211
C	2.74835	3.8353	-2.2247
H	1.52809	2.12954	-2.65547
C	3.86906	4.32885	-1.53696
H	5.49745	3.81461	-0.20272
H	2.18868	4.51688	-2.85753
O	4.14258	5.65439	-1.72354
C	5.28033	6.2007	-1.07709
H	5.31535	7.25271	-1.3644
H	5.20086	6.12852	0.0156
H	6.20624	5.70772	-1.40028
P	-2.68	1.57829	0.76072
C	-4.00402	2.82428	0.38942
C	-3.84315	4.2143	0.49372
C	-5.27344	2.32162	0.05088
C	-4.91642	5.07591	0.25083
H	-2.8779	4.62864	0.7662
C	-6.34017	3.18176	-0.20336
H	-5.42743	1.24711	-0.00633
C	-6.16487	4.56438	-0.10298
H	-4.77235	6.14957	0.33671
H	-7.31113	2.77335	-0.46988
H	-6.99738	5.23587	-0.29269
C	-1.287	2.64707	1.36071
C	-1.20714	2.80297	2.75671
C	-0.32345	3.28467	0.56318
C	-0.21061	3.58909	3.33579
H	-1.93226	2.29964	3.39136
C	0.68551	4.05853	1.14281
H	-0.34827	3.17638	-0.51583
C	0.74079	4.21693	2.52871
H	-0.17096	3.70157	4.41572
H	1.4292	4.52856	0.5062
H	1.52527	4.81956	2.97776

TS8^{L2}

Sum of electronic and thermal Free Energies= -3598.059424

C	5.48083400	0.41217300	-2.99068300
C	5.06121900	-0.86694100	-3.35622300
C	3.97258900	-1.45705700	-2.71074800
C	3.29726000	-0.77384100	-1.69261600
C	3.72272600	0.51927700	-1.32305800
C	4.81285500	1.10399800	-1.97808100
H	6.31766400	0.87917100	-3.50183500
H	5.57025000	-1.40120000	-4.15318300
H	3.63290500	-2.44288800	-3.01321400
H	5.12525900	2.10920400	-1.71257400
P	1.81692400	-1.46282400	-0.82564800
P	2.77309600	1.38092500	0.00846500
S	-1.60655300	-0.57462700	-0.13862000
C	-2.15971200	-1.26813500	1.40749000
C	-1.46868100	-1.17700200	2.62859200

C	-3.39809500	-1.94339100	1.39318300
C	-1.99731500	-1.74435800	3.79111400
H	-0.51283500	-0.66504500	2.65722400
C	-3.91640500	-2.51138700	2.55502500
H	-3.94725700	-2.02772800	0.45956200
C	-3.22022100	-2.41440700	3.76372400
H	-1.44344400	-1.65977600	4.72274100
H	-4.86914100	-3.03242400	2.51416100
H	-3.62585100	-2.85734400	4.66858300
Rh	0.64398400	0.44075100	-0.03650700
H	0.87421600	-0.03158100	1.41043700
Cl	0.17402600	1.31794200	-2.42440000
C	-0.40555600	2.23880500	0.75938600
C	-1.71734300	1.91617800	0.35328700
H	0.10976400	2.94422400	0.11191000
H	-0.23226000	2.36871900	1.82644400
H	-1.95667000	2.05102600	-0.69802000
C	-2.88010600	1.89575000	1.29779800
H	-2.98254800	2.93282300	1.66030100
H	-2.62852500	1.29321100	2.19150100
N	-4.12313100	1.52085800	0.64680500
H	-4.00185700	0.61410100	0.20170500
C	-5.26966100	1.47843300	1.55084100
H	-5.13283100	0.76917100	2.38769700
H	-5.35972900	2.47477400	2.01091300
C	-6.55224200	1.13915000	0.81772900
C	-6.80562000	1.63725000	-0.46328600
C	-7.53429100	0.33819600	1.41860500
C	-7.99920100	1.35562600	-1.13296500
H	-6.04667500	2.24386900	-0.94726700
C	-8.73073300	0.05301800	0.77046500
H	-7.35716300	-0.07153300	2.41048100
C	-8.97137300	0.56164900	-0.51342400
H	-8.15610300	1.75585600	-2.12789500
H	-9.49067100	-0.56850800	1.23324200
O	-10.17304200	0.22260500	-1.07285600
C	-10.46100700	0.70140600	-2.37515500
H	-11.45131700	0.31775400	-2.62689000
H	-10.48095600	1.79870600	-2.41059300
H	-9.73505700	0.33544800	-3.11319200
C	2.51158500	-2.55971300	0.48555600
C	3.85424500	-2.96192400	0.51716400
C	1.63943200	-3.01761900	1.48750500
C	4.31597600	-3.80533700	1.53087200
H	4.54436800	-2.61822300	-0.24627800
C	2.10178300	-3.86615600	2.49209100
H	0.59986800	-2.70481500	1.48627400
C	3.44199800	-4.26047000	2.51789000
H	5.36018900	-4.10481700	1.54598600
H	1.41418200	-4.21333100	3.25794600
H	3.80249700	-4.91654600	3.30513000
C	1.05095500	-2.63814800	-2.01499700
C	1.28612500	-4.02144700	-1.94488100
C	0.20724600	-2.13045500	-3.01755900
C	0.69909800	-4.88172600	-2.87382200
H	1.92296600	-4.42983600	-1.16766600
C	-0.37334400	-2.99896200	-3.94230200
H	0.01107400	-1.06305300	-3.06707300
C	-0.13027900	-4.37195200	-3.87421100
H	0.88847700	-5.94967500	-2.81123700
H	-1.02456000	-2.59724000	-4.71314200
H	-0.58970100	-5.04377200	-4.59410200
C	3.75214300	1.07710800	1.54559300
C	5.11975800	0.76614100	1.51571400
C	3.11163900	1.19797400	2.78875500
C	5.82936000	0.57896400	2.70356200
H	5.63401300	0.66267400	0.56604700
C	3.82464200	1.02071600	3.97436300
H	2.05027100	1.42136900	2.82451300
C	5.18503700	0.70816900	3.93433100
H	6.88604700	0.33010600	2.66434300
H	3.31495400	1.11873200	4.92853000
H	5.73819800	0.56152900	4.85758000
C	3.02200900	3.17925100	-0.31293500
C	3.75926800	3.99492800	0.56015700
C	2.43812400	3.74896500	-1.45923600
C	3.91693200	5.35549500	0.28810200
H	4.21332100	3.57445000	1.45043600
C	2.60509100	5.10822800	-1.72406800
H	1.84136800	3.12968000	-2.12411700
C	3.34297000	5.91421200	-0.85416000
H	4.48995400	5.97564600	0.97163800
H	2.14945200	5.53707100	-2.61193100
H	3.46671400	6.97307800	-1.06354700

13^{L2}

Sum of electronic and thermal Free Energies= -3598.069576

C	4.05707200	3.97233600	-1.89486800
C	4.90555100	2.93706800	-2.28668500

C	4.62032900	1.62193400	-1.91490900	H	-5.76248200	0.68512100	0.82637800
C	3.48822000	1.32652700	-1.14509000	C	-9.01829100	0.59370000	-0.16697000
C	2.62626300	2.37511000	-0.75604500	H	-10.00795700	-1.16938900	-0.94714100
C	2.92035000	3.69113000	-1.13491400	H	-7.77220100	2.15153200	0.62033700
H	4.26772200	4.99531100	-2.19298500	O	-10.05334400	1.48384600	-0.24369800
H	5.78215900	3.14871200	-2.89229700	C	-11.29387300	1.02351400	-0.75067300
H	5.27056900	0.81646900	-2.24248800	H	-11.96823300	1.88127700	-0.72666900
H	2.24776900	4.49549600	-0.85344200	H	-11.20318900	0.66614900	-1.78500500
P	3.02578000	-0.39860900	-0.65109400	H	-11.71328900	0.21899300	-0.13204400
P	1.10660700	1.94819400	0.21318700	C	4.05093800	-0.72596400	0.85285300
S	-0.34426500	-2.47381800	-0.72583300	C	5.19675000	0.00917600	1.19053200
C	-0.45287100	-3.54914500	0.72094100	C	3.65336900	-1.78084100	1.69102100
C	-0.21979300	-3.11658000	2.03259200	C	5.93056300	-0.30676000	2.33652900
C	-0.76251700	-4.89583800	0.48104100	H	5.51914200	0.83225900	0.56084700
C	-0.31330500	-4.02193700	3.09123900	C	4.39316400	-2.10174800	2.82871500
H	0.04073500	-2.07916100	2.21129600	H	2.75577600	-2.34562400	1.45636600
C	-0.84606900	-5.79717100	1.54339300	C	5.53326200	-1.36400500	3.15552500
H	-0.93448200	-5.23285600	-0.53656100	H	6.81334100	0.27511000	2.58697500
C	-0.62522600	-5.36172600	2.85095900	H	4.07362000	-2.92304400	3.46397400
H	-0.13461200	-3.67777100	4.10615100	H	6.10517200	-1.60890600	4.04610800
H	-1.08407900	-6.83857500	1.34664800	C	3.81009200	-1.47319600	-1.93103100
H	-0.69037400	-6.06328500	3.67762200	C	5.05411800	-2.09628600	-1.73890500
Rh	0.60708600	-0.23662500	-0.25836600	C	3.11557600	-1.68348100	-3.13537400
H	0.81614200	-0.51617400	1.24395900	C	5.59944500	-2.90577500	-2.73726000
Cl	0.14359600	0.18428700	-2.77921100	H	5.59764600	-1.95594200	-0.81050400
C	-1.46812100	-0.15627900	0.12871200	C	3.67013000	-2.49104500	-4.12906200
C	-1.91302100	-1.38672800	-0.63499200	C	4.90994100	-3.10337600	-3.93449600
H	-1.90208100	0.75738000	-0.28048700	H	6.56217200	-3.38297000	-2.57549800
H	-1.69714700	-0.23434600	1.19505400	H	3.12505500	-2.64437400	-5.05616300
H	-2.01587700	-1.14333000	-1.69650900	H	5.33490500	-3.73532600	-4.70959200
C	-3.13632100	-2.15813600	-0.14180800	C	1.56125000	2.28578200	1.97173800
H	-3.00933000	-2.42039000	0.91560700	C	2.70625400	3.00741100	2.33508400
H	-3.21915200	-3.11376400	-0.69648300	C	0.70343300	1.81866700	2.98124800
N	-4.32587600	-1.32088500	-0.25830900	C	2.98981700	3.25412600	3.68114800
H	-4.46113900	-1.04719300	-1.22939800	H	3.38202900	3.37655900	1.57092500
C	-5.54382100	-1.96644200	0.23094500	C	0.98242400	2.07591400	4.32227300
H	-5.74756400	-2.93770300	-0.25931400	H	-0.17939000	1.24708600	2.71176500
H	-5.38108600	-2.19586600	1.29453600	C	2.12919800	2.79205600	4.67600500
C	-6.75408300	-1.06991400	0.07536200	H	3.88565600	3.80761000	3.94809800
C	-7.95874700	-1.56151500	-0.42765800	H	0.30798000	1.71149100	5.09196100
C	-6.69883500	0.28303200	0.45191200	H	2.35053300	2.98492400	5.72187100
C	-9.09162000	-0.74891500	-0.54985900	C	-0.09789000	3.28852900	-0.17631000
H	-8.02480700	-2.60267000	-0.73548500	C	-0.29469900	4.38004800	0.68551500
C	-7.81049100	1.10542100	0.33338500	C	-0.82968500	3.21605200	-1.37426400

C	-1.20322600	5.38606600	0.35125000
H	0.25623300	4.44918200	1.61710000
C	-1.73419700	4.22737900	-1.70001700
H	-0.68749800	2.36835900	-2.04032000
C	-1.92406800	5.31194600	-0.84127500
H	-1.34747200	6.22492200	1.02641200
H	-2.29511200	4.16112200	-2.62784700
H	-2.63316300	6.09412000	-1.09804900
H	2.14725700	-1.21326600	-3.28771300

TS9^{L2}

Sum of electronic and thermal Free Energies=-3598.040626

C	4.31764900	3.80446100	-1.91510700
C	5.12942400	2.70916100	-2.21276100
C	4.75713800	1.42816300	-1.79934600
C	3.57057900	1.23365800	-1.08333400
C	2.75365900	2.34147600	-0.78128800
C	3.13149600	3.62207300	-1.20098500
H	4.59764100	4.79853700	-2.25153300
H	6.04480400	2.84796700	-2.78082100
H	5.37769400	0.57449800	-2.05411200
H	2.48911900	4.47178800	-0.99040500
P	2.94321700	-0.42776300	-0.55571000
P	1.18900500	1.99509600	0.14081000
S	-0.32590100	-2.41067900	-0.80367900
C	-0.40587700	-3.45919700	0.66672800
C	-0.03437400	-3.01124900	1.94082600
C	-0.82100300	-4.78724700	0.49109600
C	-0.09854000	-3.88228600	3.03061300
H	0.31473000	-1.99050200	2.06135500
C	-0.87996500	-5.65281900	1.58419300
H	-1.09372300	-5.13758300	-0.49967700
C	-0.52197900	-5.20132200	2.85603300
H	0.18989700	-3.52826900	4.01643900
H	-1.20305800	-6.67978800	1.43999000
H	-0.56609600	-5.87662100	3.70568600
Rh	0.59888200	-0.15305800	-0.33467000
H	-0.30078900	-0.21330500	0.97762600
Cl	0.10248000	0.16879000	-3.01758700
C	-1.58543300	-0.16213400	0.16808200
C	-1.90474300	-1.37030900	-0.70992500
H	-1.90484100	0.78099200	-0.27524900
H	-2.06550700	-0.25605700	1.14761500
H	-1.95464700	-1.04233300	-1.75258000
C	-3.13708000	-2.19102300	-0.33008300
H	-3.02724100	-2.57365300	0.69233300
H	-3.20810200	-3.07510800	-0.99239200
N	-4.32369000	-1.34310200	-0.36321200
H	-4.45495900	-0.96615700	-1.29965300
C	-5.54581200	-2.02972900	0.05587900
H	-5.76900200	-2.92777900	-0.55077200
H	-5.37237900	-2.39490700	1.07911800
C	-6.74604100	-1.10667500	0.03649400
C	-7.96826800	-1.52076700	-0.49322900
C	-6.66560100	0.18761900	0.57797000
C	-9.09424500	-0.68976600	-0.48265200
H	-8.05439600	-2.51446400	-0.92708200
C	-7.77003000	1.02780900	0.59293300
H	-5.71581300	0.53143200	0.97578000
C	-8.99607000	0.59300100	0.06488100
H	-10.02491200	-1.04903000	-0.90591300
H	-7.71245600	2.02919900	1.00768500
O	-10.02230200	1.49365500	0.12933400
C	-11.28189700	1.11002700	-0.39470900
H	-11.94588700	1.96257000	-0.24207200
H	-11.22476800	0.88638200	-1.46818100
H	-11.69189600	0.23656300	0.12948000
C	3.89348000	-0.80273400	0.98738500
C	4.92821700	0.00756800	1.47440900
C	3.54144800	-1.95563700	1.71000400
C	5.59511800	-0.32649300	2.65640000
H	5.21932000	0.90110000	0.93264300
C	4.21522100	-2.29334100	2.88199000
H	2.73447500	-2.58955900	1.35491800
C	5.24347300	-1.47682300	3.36134300
H	6.39228900	0.31486500	3.02207400
H	3.93294100	-3.19158700	3.42406400
H	5.76412700	-1.73614200	4.27881900
C	3.66835800	-1.60815100	-1.77490400
C	4.87915700	-2.28108500	-1.53968800
C	2.98079400	-1.82630500	-2.98092500
C	5.39740700	-3.15334000	-2.49821100
H	5.41615600	-2.13098800	-0.60888400
C	3.50855300	-2.69934000	-3.93387900
C	4.71310200	-3.36403100	-3.69681200
H	6.33395000	-3.66935500	-2.30499100
H	2.96949600	-2.85979000	-4.86322600
H	5.11657900	-4.04580000	-4.44064900
C	1.60443100	2.37687500	1.90313000

C	2.72630600	3.13659200	2.26591500
C	0.75162400	1.90846900	2.91533600
C	2.98815100	3.41995000	3.60869100
H	3.40113300	3.50857800	1.50230700
C	1.00789000	2.20092100	4.25393200
H	-0.11195100	1.30574700	2.65228700
C	2.12993200	2.95561400	4.60485700
H	3.86507700	4.00442900	3.87262200
H	0.33537000	1.83295000	5.02357900
H	2.33463300	3.17609300	5.64861000
C	0.03335100	3.35119600	-0.32977800
C	-0.16697500	4.48006100	0.48171800
C	-0.65907200	3.24253900	-1.54861700
C	-1.04177100	5.48977600	0.07642300
H	0.35424300	4.57449100	1.42833000
C	-1.52926300	4.25914900	-1.94485000
H	-0.51427900	2.36418900	-2.17677100
C	-1.72342200	5.38132000	-1.13676700
H	-1.19107900	6.35824800	0.71192400
H	-2.05939900	4.16711000	-2.88845800
H	-2.40616200	6.16701500	-1.44861300
H	2.04216300	-1.30852800	-3.17038300

14^{L2}

Sum of electronic and thermal Free Energies= -3598.112459

C	-6.36178	-1.09624	-1.48991
C	-6.4698	0.26587	-1.20457
C	-5.38057	0.9572	-0.66998
C	-4.17518	0.29023	-0.41582
C	-4.06484	-1.08024	-0.71426
C	-5.16136	-1.76735	-1.24919
H	-7.2042	-1.63238	-1.91682
H	-7.39607	0.79438	-1.41163
H	-5.46219	2.0219	-0.47279
H	-5.06792	-2.81938	-1.50078
P	-2.65099	1.1162	0.25823
P	-2.39533	-1.83329	-0.44797
S	0.88159	1.43957	0.54569
C	1.32096	2.56752	-0.79123
C	1.46824	3.92824	-0.49457
C	1.48034	2.11014	-2.10706
C	1.77656	4.83377	-1.51169
H	1.34135	4.27129	0.52817
C	1.79917	3.02199	-3.11563
H	1.34639	1.054	-2.32622
C	1.94469	4.38173	-2.82198
H	1.88743	5.88903	-1.27683
H	1.92742	2.67021	-4.13609
H	2.18835	5.0864	-3.61247
Rh	-0.87041	-0.18633	-0.25545
H	1.15814	-0.69207	2.15321
Cl	0.84455	-1.66724	-1.1772
C	2.21411	-0.59811	1.88613
C	2.44644	0.43668	0.76666
H	2.54952	-1.57977	1.54538
H	2.77752	-0.33205	2.78548
H	2.55221	-0.08373	-0.18485
C	3.67269	1.32426	1.01821
H	3.6416	1.71561	2.04201
H	3.68067	2.19466	0.34206
N	4.86826	0.49489	0.87912
H	4.91897	0.14216	-0.08108
C	6.11942	1.17644	1.20256
H	6.22724	2.15171	0.69418
H	6.10036	1.39988	2.27955
C	7.31876	0.31257	0.86526
C	8.49215	0.87748	0.36428
C	7.28448	-1.0814	1.04768
C	9.60971	0.09671	0.0503
H	8.54362	1.95275	0.20749
C	8.38056	-1.87369	0.73107
H	6.37603	-1.53931	1.42647
C	9.55261	-1.28979	0.2274
H	10.50021	0.57507	-0.33984
H	8.3528	-2.95202	0.85816
O	10.57057	-2.15499	-0.06382
C	11.7706	-1.62056	-0.59559
H	12.43059	-2.47175	-0.77052
H	11.59805	-1.09854	-1.5461
H	12.25492	-0.92914	0.10642
C	-3.08134	1.45679	2.03
C	-4.37233	1.30246	2.55785
C	-2.04919	1.87537	2.88759
C	-4.62739	1.57155	3.90492
H	-5.1855	0.9682	1.92279
C	-2.30811	2.15052	4.22989
H	-1.03877	1.97908	2.50471
C	-3.59837	1.9994	4.74352
H	-5.63328	1.44364	4.29581

H	-1.49806	2.47491	4.87733
H	-3.7978	2.20771	5.79098
C	-2.73457	2.79027	-0.52403
C	-3.33009	3.89996	0.0938
C	-2.20257	2.93279	-1.81582
C	-3.40438	5.12397	-0.57513
H	-3.73369	3.81102	1.09738
C	-2.28193	4.15486	-2.48266
C	-2.88461	5.25254	-1.86395
H	-3.86743	5.97666	-0.08632
H	-1.86296	4.25199	-3.47991
H	-2.94266	6.20591	-2.38175
C	-2.5224	-2.74675	1.15132
C	-3.7308	-2.9295	1.8377
C	-1.33114	-3.2359	1.71812
C	-3.74979	-3.58319	3.07275
H	-4.65912	-2.55841	1.4154
C	-1.35722	-3.89364	2.94699
H	-0.38998	-3.08695	1.19538
C	-2.56531	-4.0641	3.63007
H	-4.69242	-3.71203	3.59781
H	-0.43099	-4.26478	3.3775
H	-2.58115	-4.5663	4.59331
C	-2.31263	-3.16765	-1.71435
C	-2.71211	-4.48302	-1.43109
C	-1.85908	-2.85171	-3.00359
C	-2.67102	-5.4631	-2.42519
H	-3.04498	-4.74744	-0.43274
C	-1.82748	-3.83072	-3.99533
H	-1.50464	-1.8474	-3.21403
C	-2.23163	-5.13782	-3.70832
H	-2.97609	-6.48045	-2.19209
H	-1.4685	-3.57768	-4.98854
H	-2.19388	-5.90213	-4.47971
H	-1.71773	2.08168	-2.28558

TS10^{L2}

Sum of electronic and thermal Free Energies= -3598.055475

C	3.06364	2.34598	3.79361
C	3.09895	1.03365	4.27112
C	2.67286	-0.01299	3.45703
C	2.20644	0.22681	2.15351
C	2.17093	1.54995	1.67748
C	2.59561	2.60057	2.507
H	3.39509	3.16754	4.423
H	3.45857	0.82607	5.27531
H	2.71716	-1.02859	3.83463
H	2.55919	3.62277	2.14315
P	1.63067	-1.15416	1.04508
P	1.43169	1.90139	0.01701
S	1.40454	-2.4509	-2.10012
C	-0.21008	-3.14962	-2.41399
C	-0.68984	-3.22959	-3.7362
C	-0.99505	-3.72065	-1.3946
C	-1.90767	-3.84928	-4.02533
H	-0.08621	-2.81192	-4.53624
C	-2.21527	-4.33026	-1.68327
H	-0.63942	-3.68873	-0.37074
C	-2.67908	-4.39773	-3.00024
H	-2.25287	-3.90205	-5.05469
H	-2.80124	-4.76518	-0.87764
H	-3.62681	-4.87963	-3.22417
Rh	1.21357	-0.19171	-1.10631
H	-0.4236	-0.22113	-1.23454
Cl	3.67194	-0.06239	-1.39209
C	0.82291	0.60119	-3.08827
C	-0.4885	0.24221	-2.66056
H	1.37541	-0.07719	-3.72763
H	1.09903	1.64981	-3.15419
H	-0.86828	-0.71984	-2.99889
C	-1.58041	1.28975	-2.52153
H	-1.92664	1.499	-3.54358
H	-1.16191	2.23566	-2.13344
N	-2.72141	0.7994	-1.7611
H	-2.45154	0.70265	-0.78551
C	-3.90166	1.66317	-1.82566
H	-3.68301	2.71405	-1.56148
H	-4.24233	1.67365	-2.87154
C	-5.00286	1.14764	-0.92204
C	-5.72824	2.01445	-0.10286
C	-5.32831	-0.22011	-0.88798
C	-6.75584	1.55523	0.72933
H	-5.49204	3.07617	-0.10757
C	-6.34116	-0.69425	-0.0644
H	-4.76666	-0.91155	-1.50914
C	-7.0646	0.19134	0.75113
H	-7.29478	2.26181	1.34985
H	-6.59726	-1.7488	-0.03571
O	-8.03732	-0.3745	1.52599

C	-8.79572	0.47303	2.37307
H	-9.50576	-0.17353	2.89139
H	-8.1621	0.97881	3.11413
H	-9.3493	1.22974	1.80169
C	2.52324	3.14013	-0.78834
C	2.00194	3.96923	-1.79843
C	3.8991	3.18931	-0.51869
C	2.83077	4.84861	-2.49559
H	0.94219	3.941	-2.03901
C	4.72424	4.07269	-1.2143
H	4.32964	2.52374	0.21541
C	4.19522	4.90603	-2.19909
H	2.40826	5.48532	-3.27144
H	5.78739	4.09638	-0.99326
H	4.84228	5.58876	-2.74211
C	-0.04913	2.89263	0.55091
C	-1.18566	2.19403	0.99179
C	-0.05027	4.29403	0.63792
C	-2.30334	2.87297	1.47847
H	-1.18469	1.10761	0.97784
C	-1.16777	4.97406	1.12547
H	0.82036	4.85858	0.3265
C	-2.29863	4.26742	1.54076
H	-3.1767	2.31114	1.80288
H	-1.14731	6.05569	1.18785
H	-3.16765	4.79912	1.91682
C	2.96958	-2.40604	1.19703
C	2.68569	-3.76063	0.96527
C	4.29748	-2.02392	1.43895
C	3.70341	-4.71372	1.00917
H	1.67298	-4.07371	0.74197
C	5.31159	-2.98118	1.48503
H	4.5467	-0.97971	1.57959
C	5.01769	-4.32729	1.27272
H	3.46762	-5.75684	0.82494
H	6.33382	-2.66869	1.67609
H	5.81012	-5.07023	1.30318
C	0.22297	-1.90494	1.99031
C	-1.08867	-1.65973	1.56389
C	0.41822	-2.69315	3.13761
C	-2.18065	-2.15498	2.27889
H	-1.24873	-1.10605	0.64405
C	-0.67089	-3.19368	3.84946
H	1.42207	-2.94255	3.46155
C	-1.97262	-2.91841	3.42763
H	-3.18742	-1.95274	1.92692
H	-0.50176	-3.80552	4.73109
H	-2.81835	-3.31115	3.98376

15^{L2}

Sum of electronic and thermal Free Energies=-3598.080769

C	-3.88760300	-1.14457400	4.01974900
C	-3.27211400	0.05913900	4.37198200
C	-2.50287800	0.74819900	3.43671900
C	-2.33761700	0.24732500	2.13624700
C	-2.98150300	-0.95018200	1.77336300
C	-3.74437400	-1.64465600	2.72707600
H	-4.47787600	-1.69096300	4.74950600
H	-3.38354000	0.45580800	5.37687900
H	-2.01344700	1.67207200	3.72680900
H	-4.21831200	-2.58286000	2.45591200
P	-1.31136900	1.14401600	0.86244700
P	-2.81298300	-1.51091000	0.02469400
S	-0.11567000	1.21398900	-2.58012500
C	0.69179800	2.70866200	-2.02942300
C	0.00494500	3.93341800	-1.93941700
C	2.08190200	2.70811800	-1.80733600
C	0.68295900	5.11158000	-1.61972200
H	-1.06219400	3.95641500	-2.13172500
C	2.75711900	3.88657200	-1.48886300
H	2.62846600	1.77529700	-1.90414000
C	2.06134900	5.09466200	-1.38852500
H	0.13267900	6.04725300	-1.56008400
H	3.83207600	3.86232900	-1.32858400
H	2.58877400	6.01427300	-1.15021400
Rh	-1.11936100	-0.25254900	-0.97270900
H	1.85932500	0.03823700	-0.03799300
Cl	-1.15471100	-1.83301800	-2.84305200
C	0.29713800	-1.45551400	-0.00506600
C	1.70728700	-1.00323500	-0.34537700
H	0.08683300	-2.45168500	-0.39748500
H	0.11978500	-1.44497400	1.07563500
H	1.86403100	-1.04885800	-1.42537900
C	2.75910800	-1.88398800	0.35316300
H	2.65266200	-2.92227600	0.01180300
H	2.57028400	-1.89417400	1.44593600
N	4.11024400	-1.43977100	0.02219500
H	4.22609300	-0.46855300	0.30457800
C	5.16165200	-2.24421200	0.63951200

H	5.08553100	-2.29159200	1.74377400
H	5.02401100	-3.27753300	0.28736700
C	6.54402500	-1.75493000	0.25910600
C	7.57118900	-1.68301200	1.20033700
C	6.83485600	-1.38489100	-1.06514000
C	8.86192800	-1.26929600	0.85138400
H	7.36951300	-1.95582700	2.23398000
C	8.10738700	-0.96636700	-1.42878700
H	6.03989300	-1.41911700	-1.80353900
C	9.13302100	-0.90926800	-0.47218900
H	9.63225800	-1.22693400	1.61258800
H	8.33654400	-0.67863000	-2.44999900
O	10.35051000	-0.48723000	-0.93132300
C	11.42533800	-0.42390100	-0.01106400
H	12.29115200	-0.07888200	-0.57897500
H	11.22396800	0.28539700	0.80291400
H	11.64849800	-1.40781300	0.42268900
C	-4.43253700	-1.10301300	-0.76621800
C	-4.49568400	-1.03311400	-2.17009400
C	-5.58932600	-0.83572300	-0.01619100
C	-5.70092000	-0.72069900	-2.80200500
H	-3.60286700	-1.22292800	-2.75985300
C	-6.78739400	-0.51688900	-0.65624000
H	-5.56197500	-0.86469800	1.06705000
C	-6.84734600	-0.46129100	-2.04970100
H	-5.73578800	-0.67449800	-3.88657100
H	-7.67320000	-0.30963400	-0.06248900
H	-7.78143200	-0.21212800	-2.54525100
C	-2.74919000	-3.34331000	0.12653400
C	-1.96277900	-3.96351200	1.11254000
C	-3.39674800	-4.14065600	-0.82866300
C	-1.84199700	-5.35229700	1.14962800
H	-1.44975800	-3.36567000	1.85891300
C	-3.27129500	-5.52921800	-0.78805600
H	-3.99684900	-3.67998300	-1.60487400
C	-2.49608100	-6.13849000	0.19942800
H	-1.23465200	-5.81826300	1.92024400
H	-3.77897400	-6.13389300	-1.53365100
H	-2.39965700	-7.21994300	0.22736200
C	-2.27795000	2.69291400	0.61117800
C	-2.23031200	3.77186500	1.50797200
C	-3.15356300	2.75222900	-0.48343000
C	-3.04178300	4.88884700	1.30925100
H	-1.54742600	3.75243100	2.35098200
C	-3.96913600	3.86848500	-0.67492800
H	-3.18347600	1.93352600	-1.19525000
C	-3.91368100	4.93838100	0.21945100
H	-2.98958500	5.72168600	2.00463900
H	-4.63961800	3.90238000	-1.52843100
H	-4.54356500	5.80999400	0.06631700
C	0.19046300	1.62881400	1.81170400
C	0.91036000	2.78396700	1.46469100
C	0.69933100	0.79120000	2.82040800
C	2.09802000	3.09950300	2.12694600
H	0.55385500	3.43986100	0.67921600
C	1.88918300	1.10935400	3.47477700
H	0.16428400	-0.10717000	3.10789400
C	2.59108100	2.26638000	3.13122600
H	2.63808800	3.99663900	1.84142200
H	2.26443500	0.45260700	4.25431900
H	3.51693000	2.51483600	3.64202700

TS11^{L2}

Sum of electronic and thermal Free Energies= -3598.045425

C	-3.85643	-2.89037	3.29997
C	-4.06337	-1.59387	3.77352
C	-3.46738	-0.50958	3.12627
C	-2.67121	-0.71019	1.99108
C	-2.47385	-2.01973	1.50629
C	-3.05953	-3.10281	2.17343
H	-4.32214	-3.73528	3.79968
H	-4.69305	-1.42416	4.64247
H	-3.63451	0.49671	3.49739
H	-2.91768	-4.11082	1.79648
P	-1.82331	0.69215	1.09253
P	-1.42651	-2.15569	-0.01582
S	-2.07314	1.74266	-2.49854
C	-1.63892	3.40745	-2.03042
C	-0.5564	3.76835	-1.21799
C	-2.421	4.43051	-2.59963
C	-0.263	5.11106	-0.97544
H	0.06974	2.99057	-0.8011
C	-2.13172	5.76921	-2.34513
H	-3.25222	4.16677	-3.24593
C	-1.05065	6.11875	-1.53284
H	0.58851	5.36877	-0.35189
H	-2.75023	6.54422	-2.79179
H	-0.82048	7.16283	-1.3448
Rh	-1.72584	-0.1207	-1.08837

H	1.24935	1.09853	-1.09638
Cl	-2.60842	-1.29617	-3.05546
C	0.04958	0.44392	-2.77219
C	1.31091	1.02572	-2.18759
H	-0.18444	0.74802	-3.78498
H	-0.03206	-0.63397	-2.68023
H	1.51391	2.03092	-2.56653
C	2.48307	0.08174	-2.53521
H	2.6431	0.07207	-3.6212
H	2.19787	-0.95	-2.2548
N	3.72449	0.50121	-1.8906
H	3.55863	0.62069	-0.89221
C	4.7965	-0.48468	-2.06508
H	4.4811	-1.50755	-1.78474
H	5.03218	-0.52446	-3.13899
C	6.02915	-0.11327	-1.27322
C	6.63957	-1.02583	-0.41201
C	6.59623	1.16757	-1.38962
C	7.79052	-0.69594	0.3134
H	6.21629	-2.0219	-0.30149
C	7.73462	1.51402	-0.67623
H	6.1222	1.89408	-2.04293
C	8.34288	0.58159	0.18032
H	8.23594	-1.43381	0.97054
H	8.17837	2.50065	-0.76414
O	9.4594	1.01944	0.83532
C	10.11954	0.11727	1.70696
H	10.97706	0.65864	2.11031
H	9.47017	-0.19632	2.53517
H	10.47448	-0.77547	1.17527
C	-1.92137	-3.71094	-0.85647
C	-0.95254	-4.50772	-1.48618
C	-3.27614	-4.03916	-1.01227
C	-1.32898	-5.62244	-2.23519
H	0.09932	-4.25819	-1.39997
C	-3.64789	-5.16294	-1.74829
H	-4.04304	-3.40944	-0.57296
C	-2.67658	-5.95651	-2.36269
H	-0.56636	-6.22432	-2.72209
H	-4.70001	-5.40702	-1.85798
H	-2.96948	-6.82313	-2.94812
C	0.23649	-2.57714	0.69226
C	1.27851	-1.64626	0.60633
C	0.46692	-3.78892	1.36633
C	2.52517	-1.91238	1.1797
H	1.09859	-0.7051	0.09984
C	1.71062	-4.05697	1.93557
H	-0.32285	-4.53053	1.43519
C	2.74236	-3.11787	1.84516
H	3.32227	-1.17763	1.11051
H	1.87551	-4.99923	2.45021
H	3.70987	-3.32711	2.29292
C	-2.96581	2.11312	1.4066
C	-2.81407	2.97938	2.5012
C	-4.06402	2.28611	0.54912
C	-3.74198	3.99742	2.73069
H	-1.97136	2.86665	3.17461
C	-4.99103	3.30082	0.78574
H	-4.18029	1.63418	-0.31075
C	-4.83187	4.15983	1.875
H	-3.60847	4.66348	3.57865
H	-5.83368	3.42395	0.11167
H	-5.55105	4.95418	2.05369
C	-0.39435	1.05032	2.23168
C	0.43641	2.15058	1.96465
C	-0.09147	0.24326	3.33796
C	1.53654	2.43288	2.77396
H	0.20543	2.80839	1.13745
C	1.00828	0.52891	4.15049
H	-0.71397	-0.61077	3.5754
C	1.82762	1.62075	3.87103
H	2.16259	3.29094	2.55017
H	1.2194	-0.10667	5.00536
H	2.68273	1.84069	4.50369

16^{L2}

Sum of electronic and thermal Free Energies= -3598.102400

C	-3.78329	-1.93944	4.03634
C	-2.79256	-1.11272	4.57349
C	-2.01237	-0.31974	3.7326
C	-2.21586	-0.34309	2.34569
C	-3.2181	-1.16697	1.80718
C	-3.9932	-1.96904	2.65831
H	-4.38387	-2.56627	4.68961
H	-2.62128	-1.09425	5.64614
H	-1.23132	0.30254	4.15837
H	-4.7469	-2.62919	2.23969
P	-1.2416	0.68656	1.13557
P	-3.39429	-1.14928	-0.03614

S	0.06092	0.99468	-2.47182
C	0.91953	2.55573	-2.23422
C	0.45423	3.48166	-1.29386
C	1.96173	2.91735	-3.10207
C	1.03907	4.74805	-1.21056
H	-0.37268	3.22135	-0.64389
C	2.54978	4.17645	-3.0029
H	2.30206	2.22177	-3.86349
C	2.09276	5.09741	-2.05679
H	0.66581	5.4595	-0.47901
H	3.35404	4.44378	-3.68023
H	2.54723	6.08171	-1.98947
Rh	-1.65074	-0.06727	-0.94923
H	2.23719	0.2045	-0.58607
Cl	-2.1644	-1.17499	-3.07406
C	1.42957	-0.25618	-2.54706
C	2.60217	-0.03572	-1.59085
H	1.76899	-0.31227	-3.58632
H	0.8974	-1.18481	-2.32357
H	3.20707	0.81355	-1.92274
C	3.51716	-1.26891	-1.53502
H	3.71552	-1.63363	-2.55469
H	2.99456	-2.09318	-1.00776
N	4.80292	-0.92637	-0.93602
H	4.64987	-0.52974	-0.00839
C	5.72901	-2.05199	-0.83261
H	5.36061	-2.86524	-0.17877
H	5.8075	-2.4929	-1.83726
C	7.1044	-1.61908	-0.36465
C	7.81902	-2.365	0.57275
C	7.71771	-0.4729	-0.90239
C	9.11511	-2.00827	0.9641
H	7.36362	-3.25096	1.01191
C	9.00073	-0.10131	-0.52482
H	7.16344	0.13031	-1.61494
C	9.71383	-0.87286	0.40717
H	9.63679	-2.61579	1.69477
H	9.47977	0.78138	-0.94002
O	10.97426	-0.43172	0.70225
C	11.7391	-1.17211	1.63898
H	12.70256	-0.66473	1.71177
H	11.2646	-1.18682	2.62977
H	11.90148	-2.20672	1.30721
C	-5.01319	-0.32269	-0.36615
C	-5.34777	-0.0692	-1.70946
C	-5.8901	0.09209	0.64731
C	-6.54555	0.57271	-2.02356
H	-4.65912	-0.36659	-2.49666
C	-7.0856	0.7416	0.32474
H	-5.646	-0.08381	1.68982
C	-7.4169	0.98068	-1.0091
H	-6.79387	0.76115	-3.0645
H	-7.75484	1.06029	1.11976
H	-8.34651	1.48637	-1.25777
C	-3.69646	-2.92126	-0.43636
C	-2.59126	-3.75282	-0.67402
C	-4.98722	-3.47004	-0.46481
C	-2.774	-5.11395	-0.91322
H	-1.59609	-3.31933	-0.69704
C	-5.16694	-4.83326	-0.71107
H	-5.85383	-2.83441	-0.30828
C	-4.06171	-5.65697	-0.93162
H	-1.91178	-5.74828	-1.10199
H	-6.17141	-5.24762	-0.7367
H	-4.20314	-6.71638	-1.12723
C	-1.80156	2.39624	1.58904
C	-1.43647	3.06207	2.77104
C	-2.71926	3.0101	0.72219
C	-1.97383	4.31358	3.0728
H	-0.72436	2.61231	3.45575
C	-3.25968	4.26087	1.02799
H	-3.00072	2.49379	-0.19233
C	-2.88745	4.91481	2.20297
H	-1.67985	4.81921	3.98838
H	-3.96872	4.7213	0.34613
H	-3.30526	5.88889	2.44133
C	0.48212	0.55228	1.79339
C	1.36297	1.64457	1.82376
C	0.96848	-0.71414	2.1649
C	2.68705	1.4798	2.23875
H	1.02152	2.62857	1.5218
C	2.28971	-0.87697	2.57999
H	0.30884	-1.57639	2.13337
C	3.15386	0.22158	2.62288
H	3.35162	2.33887	2.2614
H	2.64364	-1.86135	2.8742
H	4.18043	0.09769	2.95665

TS8$^{L2'}$

Sum of electronic and thermal Free Energies= -3598.046655

C	-4.07169	-2.45375	-3.30423
C	-4.8247	-1.28364	-3.21192
C	-4.50224	-0.31996	-2.2543
C	-3.42797	-0.52151	-1.38042
C	-2.66774	-1.70598	-1.47195
C	-2.99658	-2.66421	-2.43788
H	-4.30964	-3.19825	-4.05839
H	-5.65335	-1.11204	-3.89274
H	-5.07325	0.6018	-2.20045
H	-2.39692	-3.56382	-2.53279
P	-2.9029	0.72959	-0.13037
P	-1.26172	-1.90736	-0.28746
S	-0.20181	2.46775	1.4336
C	0.84245	3.65661	0.61035
C	1.33567	4.71304	1.39787
C	1.18858	3.5972	-0.74776
C	2.14959	5.69622	0.83325
H	1.07699	4.76006	2.45182
C	2.01673	4.57888	-1.29845
H	0.82306	2.78239	-1.36059
C	2.4979	5.63283	-0.51731
H	2.52415	6.50935	1.45656
H	2.28458	4.51646	-2.34964
H	3.13849	6.3943	-0.95437
Rh	-0.63084	0.25511	0.32085
H	-1.03271	-0.07341	1.7755
Cl	-0.09823	0.65223	-2.19952
C	1.56025	0.79965	1.81786
C	1.51889	-0.26642	0.90359
H	1.23325	0.66026	2.84048
H	2.25041	1.61692	1.64947
H	1.32545	-1.24723	1.3378
C	2.49748	-0.23687	-0.25478
H	2.38694	0.70057	-0.80677
H	2.26516	-1.03989	-0.97127
N	3.88265	-0.29977	0.24525
H	4.02523	-1.17674	0.74617
C	4.87983	-0.20021	-0.82418
H	4.77754	-0.99024	-1.59369
H	4.69235	0.75124	-1.34522
C	6.29445	-0.21673	-0.28282
C	7.2951	-0.97442	-0.89079
C	6.64433	0.55637	0.83626
C	8.61479	-0.96576	-0.42362
H	7.05068	-1.58687	-1.75608
C	7.94605	0.57388	1.31784
H	5.87495	1.13987	1.32788
C	8.94409	-0.18549	0.6869
H	9.36362	-1.56807	-0.92835
H	8.2204	1.17034	2.18082
O	10.19673	-0.09501	1.23123
C	11.24212	-0.83325	0.62935
H	12.13907	-0.61964	1.2141
H	11.04458	-1.91137	0.65465
H	11.40878	-0.52753	-0.41165
C	-4.01417	0.45519	1.315
C	-5.10728	-0.42139	1.28768
C	-3.73031	1.15667	2.50013
C	-5.90178	-0.59612	2.42439
H	-5.34117	-0.97311	0.3833
C	-4.53091	0.98624	3.62815
H	-2.88168	1.83401	2.5373
C	-5.61747	0.10714	3.59419
H	-6.74293	-1.28303	2.39078
H	-4.30298	1.53712	4.5362
H	-6.23684	-0.02864	4.47643
C	-3.43984	2.36006	-0.79132
C	-4.62715	2.97539	-0.36134
C	-2.64173	2.99917	-1.75466
C	-5.01366	4.20586	-0.89508
H	-5.24898	2.50249	0.39101
C	-3.03666	4.22846	-2.28209
H	-1.72236	2.52634	-2.08556
C	-4.21954	4.83434	-1.8552
H	-5.93315	4.67316	-0.55457
H	-2.4106	4.71561	-3.02384
H	-4.51899	5.79499	-2.26503
C	-1.9706	-2.94323	1.07454
C	-2.96393	-3.90493	0.82727
C	-1.47587	-2.80657	2.38011
C	-3.45067	-4.70559	1.86127
H	-3.36791	-4.02665	-0.1722
C	-1.95622	-3.61553	3.41184
H	-0.723	-2.05444	2.59217
C	-2.9464	-4.56499	3.15553
H	-4.22585	-5.43826	1.65408
H	-1.56172	-3.495	4.41669

H	-3.3265	-5.18856	3.95997
C	-0.08715	-3.06234	-1.11293
C	0.35716	-4.22937	-0.47021
C	0.41249	-2.74948	-2.39053
C	1.27652	-5.0733	-1.09641
H	-0.01588	-4.48911	0.51452
C	1.32329	-3.60362	-3.01195
H	0.10546	-1.8289	-2.87632
C	1.75779	-4.76539	-2.3691
H	1.61003	-5.97355	-0.58784
H	1.69961	-3.35304	-3.99965
H	2.46962	-5.4254	-2.85681

$13^{L2'}$

Sum of electronic and thermal Free Energies= -3598.055494

C	1.21582	-2.63958	4.05893
C	2.0111	-1.54967	4.41312
C	2.36682	-0.60476	3.44957
C	1.93533	-0.74083	2.12367
C	1.122	-1.83653	1.76841
C	0.77036	-2.77986	2.74355
H	0.92612	-3.37174	4.80714
H	2.34524	-1.42708	5.43943
H	2.96744	0.25444	3.73218
H	0.12786	-3.61365	2.47918
P	2.34408	0.48415	0.8003
P	0.51798	-1.97164	0.01811
S	0.74176	2.08204	-2.46407
C	0.46628	3.79033	-1.96229
C	1.16888	4.77311	-2.67219
C	-0.38272	4.14709	-0.90749
C	1.0175	6.11796	-2.33069
H	1.82313	4.4849	-3.48975
C	-0.53396	5.49618	-0.58383
H	-0.89777	3.37602	-0.34167
C	0.16274	6.48116	-1.28886
H	1.56271	6.87821	-2.88339
H	-1.19392	5.77553	0.23264
H	0.04137	7.52819	-1.0259
Rh	0.59374	0.13617	-0.88864
H	1.66145	-0.43735	-1.83893
Cl	-1.21779	1.12881	0.72085
C	-0.9373	1.39982	-2.87724
C	-0.74739	-0.08615	-2.56189
H	-1.20884	1.64288	-3.91214
H	-1.63942	1.87768	-2.19172
H	-0.1386	-0.52506	-3.35928
C	-2.05454	-0.87987	-2.55513
H	-1.82054	-1.94823	-2.43671
H	-2.49028	-0.78661	-3.57786
N	-3.02753	-0.50142	-1.54648
H	-2.97727	0.48371	-1.31271
C	-4.37984	-0.9315	-1.83982
H	-4.69536	-0.68356	-2.8758
H	-4.39806	-2.0327	-1.78768
C	-5.41289	-0.3783	-0.87623
C	-5.06734	0.21182	0.3418
C	-6.77779	-0.46921	-1.19863
C	-6.04607	0.69922	1.21816
H	-4.02145	0.30863	0.61762
C	-7.75985	0.00167	-0.33805
H	-7.07471	-0.9157	-2.1454
C	-7.39804	0.59293	0.88195
H	-5.73448	1.15901	2.14913
H	-8.81376	-0.0671	-0.58961
O	-8.43619	1.03391	1.65952
C	-8.12312	1.66299	2.88966
H	-9.07742	1.95249	3.33446
H	-7.59922	0.98245	3.5747
H	-7.50719	2.56014	2.74285
C	4.03926	-0.00143	0.24313
C	4.92496	-0.75497	1.02803
C	4.45447	0.41972	-1.03087
C	6.19784	-1.07586	0.55138
H	4.62202	-1.09798	2.01205
C	5.72998	0.10695	-1.50126
H	3.77036	0.9822	-1.65931
C	6.60412	-0.6435	-0.71173
H	6.87053	-1.66496	1.16876
H	6.03657	0.44114	-2.48844
H	7.59437	-0.89441	-1.0816
C	2.63848	2.05755	1.72035
C	3.92515	2.57077	1.94925
C	1.52201	2.76384	2.20119
C	4.09325	3.76292	2.65688
H	4.79734	2.04344	1.579
C	1.69995	3.94998	2.91286
H	0.52291	2.38363	2.00492
C	2.9825	4.45266	3.14327

H	5.09439	4.14935	2.82693
H	0.83022	4.48562	3.28248
H	3.1154	5.37942	3.69471
C	1.68375	-3.16359	-0.78268
C	2.52573	-4.0078	-0.04524
C	1.69269	-3.25379	-2.18436
C	3.36126	-4.91902	-0.69601
H	2.53627	-3.95575	1.03825
C	2.51763	-4.17292	-2.83121
H	1.05716	-2.5965	-2.76897
C	3.3574	-5.00621	-2.088
H	4.015	-5.55975	-0.11083
H	2.50992	-4.23233	-3.91597
H	4.00675	-5.71627	-2.59228
C	-1.03348	-2.94823	0.18292
C	-1.11912	-4.285	-0.24059
C	-2.14718	-2.34173	0.78758
C	-2.29778	-5.00828	-0.05041
H	-0.27046	-4.76601	-0.71363
C	-3.31761	-3.07586	0.98328
H	-2.09428	-1.30153	1.09022
C	-3.39661	-4.40559	0.56427
H	-2.35323	-6.04129	-0.38233
H	-4.17507	-2.59508	1.44396
H	-4.31353	-4.96946	0.713

TS9$^{L2'}$

Sum of electronic and thermal Free Energies= -3598.038417

C	-2.86016	-4.8963	0.02418
C	-3.70588	-4.29343	0.95559
C	-3.47918	-2.97424	1.3548
C	-2.40229	-2.25213	0.82846
C	-1.5499	-2.86257	-0.11255
C	-1.78414	-4.18346	-0.50889
H	-3.0454	-5.91626	-0.30095
H	-4.55114	-4.84285	1.36019
H	-4.15511	-2.49699	2.058
H	-1.14922	-4.64623	-1.25782
P	-2.05093	-0.48292	1.23746
P	-0.14308	-1.83517	-0.73388
S	-0.91792	2.82704	-0.2482
C	-2.30461	3.77331	-0.91035
C	-2.50783	5.052	-0.37664
C	-3.15492	3.26957	-1.90011
C	-3.55904	5.83839	-0.84597
H	-1.84519	5.42492	0.39755
C	-4.19992	4.07025	-2.36429
H	-3.0183	2.25927	-2.27843
C	-4.40363	5.34895	-1.8433
H	-3.71495	6.83035	-0.43343
H	-4.86223	3.68265	-3.13222
H	-5.2218	5.96164	-2.20935
Rh	-0.77927	0.34928	-0.5807
H	0.748	0.79201	-0.66127
Cl	-2.83606	-0.1728	-2.37202
C	0.53706	1.41181	-2.0753
H	-0.19353	1.11926	-2.83456
C	1.94003	1.09983	-2.59681
H	2.15028	1.76373	-3.4504
H	1.94869	0.07288	-3.00044
N	2.99227	1.32893	-1.60491
H	2.83899	0.70961	-0.81175
C	4.34018	1.08973	-2.12344
H	4.45264	0.08648	-2.57875
H	4.50844	1.80997	-2.93884
C	5.39437	1.26747	-1.04977
C	5.40088	2.40263	-0.23317
C	6.39942	0.31071	-0.85175
C	6.37518	2.59222	0.74878
H	4.62114	3.14603	-0.36277
C	7.38065	0.4832	0.1182
H	6.41366	-0.58591	-1.46653
C	7.37542	1.62813	0.92588
H	6.34522	3.48599	1.36068
H	8.15862	-0.25655	0.27294
O	8.37777	1.70748	1.85277
C	8.42838	2.85253	2.68685
H	9.30185	2.71966	3.32866
H	8.54658	3.77398	2.10301
H	7.53068	2.94136	3.31458
C	-1.18636	-0.53453	2.87108
C	-1.19211	-1.65335	3.71665
C	-0.48542	0.61592	3.27149
C	-0.5127	-1.62131	4.93719
H	-1.7201	-2.55488	3.4227
C	0.18085	0.65035	4.49578
H	-0.45519	1.48029	2.61358
C	0.17142	-0.47062	5.33091
H	-0.51982	-2.49842	5.57889

H	0.71454	1.54897	4.79366
H	0.6981	-0.44769	6.28086
C	-3.69846	0.23275	1.65917
C	-4.09944	0.46989	2.98408
C	-4.57407	0.54985	0.60606
C	-5.35884	1.00983	3.25267
H	-3.43346	0.23601	3.80732
C	-5.83221	1.0842	0.88546
H	-4.26397	0.37475	-0.42245
C	-6.2274	1.31694	2.20484
H	-5.65763	1.19035	4.28181
H	-6.50197	1.32454	0.06495
H	-7.2063	1.73888	2.41578
C	1.2661	-2.37112	0.34577
C	1.63844	-3.72334	0.44203
C	1.95944	-1.42408	1.11128
C	2.68787	-4.11167	1.27306
H	1.11177	-4.47639	-0.13535
C	3.01259	-1.81412	1.94315
H	1.64957	-0.38425	1.06651
C	3.37933	-3.15635	2.02418
H	2.96557	-5.15963	1.33552
H	3.53876	-1.06612	2.52954
H	4.19709	-3.46052	2.67152
C	0.29482	-2.51501	-2.38783
C	1.62293	-2.82699	-2.72234
C	-0.70578	-2.64387	-3.3667
C	1.94208	-3.27808	-4.00447
H	2.41175	-2.72455	-1.98489
C	-0.37898	-3.1046	-4.64228
H	-1.72294	-2.34284	-3.1404
C	0.94124	-3.42387	-4.96491
H	2.97453	-3.51505	-4.24859
H	-1.16055	-3.20019	-5.38875
H	1.19049	-3.77723	-5.96167
C	0.33973	2.86035	-1.63813
H	1.26128	3.27887	-1.21998
H	-0.04147	3.52194	-2.42465

TS10$^{L2'}$

Sum of electronic and thermal Free Energies= -3598.055320

C	-4.08126	3.67482	1.81136
C	-4.54883	2.53986	2.48011
C	-3.90275	1.31775	2.31236
C	-2.77288	1.21027	1.48414
C	-2.30417	2.35203	0.81364
C	-2.96988	3.57891	0.97826
H	-4.58915	4.62757	1.92919
H	-5.4231	2.60538	3.12148
H	-4.28402	0.43585	2.81715
H	-2.62256	4.45633	0.44137
P	-1.91979	-0.41713	1.20008
P	-0.86541	2.19416	-0.3373
S	0.08378	-2.56794	-0.49744
C	-1.04799	-3.56779	-1.4498
C	-0.9186	-3.72532	-2.84396
C	-2.02706	-4.34112	-0.79344
C	-1.75695	-4.58644	-3.55524
H	-0.12254	-3.19542	-3.36701
C	-2.84566	-5.2191	-1.50126
H	-2.13584	-4.25087	0.28222
C	-2.72438	-5.3391	-2.88699
H	-1.63602	-4.68669	-4.63096
H	-3.58319	-5.81158	-0.96562
H	-3.36732	-6.02033	-3.43863
Rh	-0.39509	-0.12496	-0.60727
H	-1.49101	-0.33451	-1.78232
Cl	1.49542	0.08815	0.98264
C	-0.50073	-0.13719	-2.91243
C	0.82028	0.17824	-2.49911
H	-1.11151	0.65863	-3.33109
H	-0.6937	-1.12184	-3.32895
H	1.09581	1.23069	-2.50921
C	1.98114	-0.75773	-2.73299
H	2.27424	-0.65974	-3.79361
H	1.64664	-1.79759	-2.58757
N	3.14214	-0.41722	-1.91935
H	2.85675	-0.41493	-0.93795
C	4.22431	-1.38401	-2.11102
H	3.88835	-2.42758	-1.96427
H	4.545	-1.3175	-3.16341
C	5.40875	-1.12587	-1.2051
C	5.98962	-2.16294	-0.47456
C	5.97659	0.15386	-1.09389
C	7.11105	-1.95687	0.33643
H	5.55974	-3.15994	-0.53124
C	7.08671	0.37963	-0.29088
H	5.5239	0.9768	-1.63879
C	7.66517	-0.67763	0.42834

H	7.52827	-2.7905	0.88926
H	7.52779	1.36723	-0.20003
O	8.7591	-0.35474	1.18742
C	9.37196	-1.38514	1.94057
H	10.20944	-0.9219	2.46632
H	8.6815	-1.81861	2.6762
H	9.75321	-2.18922	1.29686
C	-3.37627	-1.5316	0.97741
C	-3.92046	-2.27788	2.03432
C	-4.00083	-1.58076	-0.27764
C	-5.07015	-3.04682	1.83728
H	-3.44392	-2.26586	3.0088
C	-5.15405	-2.33963	-0.46958
H	-3.56832	-1.03701	-1.11226
C	-5.69213	-3.07536	0.58842
H	-5.47776	-3.62309	2.6633
H	-5.62006	-2.37201	-1.45012
H	-6.58542	-3.67471	0.43719
C	-1.24415	-0.86337	2.85281
C	-0.64113	-2.12209	3.01529
C	-1.27138	0.02365	3.938
C	-0.10854	-2.4905	4.24906
H	-0.56103	-2.79292	2.16655
C	-0.72919	-0.34892	5.16911
H	-1.70671	1.01018	3.83124
C	-0.153	-1.60798	5.32992
H	0.35624	-3.46569	4.35948
H	-0.75567	0.35088	5.99933
H	0.26896	-1.89645	6.28833
C	-1.51462	3.09944	-1.81663
C	-0.96469	4.29255	-2.30279
C	-2.63779	2.55982	-2.46761
C	-1.52839	4.92994	-3.41246
H	-0.106	4.73307	-1.81238
C	-3.20175	3.19892	-3.56962
H	-3.0754	1.63711	-2.10287
C	-2.6495	4.38855	-4.04454
H	-1.09143	5.85662	-3.77541
H	-4.07731	2.77018	-4.05359
H	-3.0879	4.88837	-4.90336
C	0.44648	3.28758	0.34419
C	1.66952	3.37752	-0.34888
C	0.28931	3.99962	1.54417
C	2.69017	4.19907	0.12374
H	1.84149	2.78786	-1.24552
C	1.32238	4.80706	2.02464
H	-0.63058	3.92207	2.11627
C	2.51905	4.91769	1.31207
H	3.62732	4.25941	-0.42684
H	1.18856	5.34558	2.96059
H	3.32074	5.54763	1.68641

15$^{L2'}$

Sum of electronic and thermal Free Energies= -3598.057788

C	2.92438	-4.85572	-0.02783
C	3.83864	-4.22831	0.82238
C	3.65047	-2.89634	1.18344
C	2.53825	-2.17283	0.72004
C	1.61461	-2.80911	-0.13011
C	1.82518	-4.14735	-0.50646
H	3.07537	-5.88848	-0.32818
H	4.70503	-4.77107	1.18919
H	4.38169	-2.40395	1.817
H	1.13281	-4.62892	-1.18993
P	2.3174	-0.37061	1.12015
P	0.18165	-1.84548	-0.79302
S	0.83457	2.80081	0.48507
C	1.90038	3.71243	-0.62321
C	1.34852	4.67032	-1.49729
C	3.30068	3.57438	-0.5972
C	2.1641	5.4501	-2.31975
H	0.27186	4.80969	-1.51273
C	4.11304	4.34662	-1.42724
H	3.74788	2.86684	0.09062
C	3.55041	5.28697	-2.29461
H	1.7135	6.18668	-2.98022
H	5.19193	4.21968	-1.38668
H	4.18582	5.89188	-2.93554
Rh	0.5133	0.46362	-0.33142
H	1.46032	0.89233	-1.8399
Cl	-1.1011	0.37737	1.47113
C	0.57152	1.24843	-2.55746
C	-0.7643	1.01161	-1.96266
H	0.79601	0.62952	-3.42967
H	0.83747	2.29626	-2.70457
H	-1.26437	0.12608	-2.35344
C	-1.76276	2.13194	-1.78775
H	-2.06916	2.48705	-2.78735
H	-1.30005	2.98291	-1.26495

N	-2.95768	1.61866	-1.11799
H	-2.68551	1.32938	-0.17696
C	-4.03822	2.60121	-1.02774
H	-3.75215	3.50907	-0.46604
H	-4.26465	2.93548	-2.05143
C	-5.28186	2.00288	-0.40577
C	-5.85299	2.53971	0.74695
C	-5.90052	0.88122	-0.98473
C	-7.01	1.99619	1.3186
H	-5.38855	3.40134	1.22026
C	-7.04776	0.32664	-0.43356
H	-5.46353	0.44192	-1.87706
C	-7.61205	0.88345	0.72607
H	-7.41874	2.44329	2.21711
H	-7.53482	-0.53313	-0.88351
O	-8.74224	0.26738	1.1906
C	-9.35372	0.79153	2.35642
H	-10.22617	0.16465	2.5494
H	-8.68114	0.74906	3.22333
H	-9.68168	1.8296	2.21222
C	4.05423	0.2277	0.89106
C	4.84079	0.7287	1.93709
C	4.59702	0.18971	-0.40426
C	6.141	1.17972	1.69095
H	4.43941	0.77304	2.94345
C	5.89737	0.62651	-0.64602
H	3.99466	-0.17838	-1.23063
C	6.67357	1.12716	0.40329
H	6.73587	1.57052	2.51157
H	6.30162	0.58687	-1.6535
H	7.68472	1.47646	0.21532
C	2.05056	-0.30884	2.93962
C	1.79152	0.9498	3.51019
C	2.05539	-1.44425	3.76221
C	1.57886	1.06616	4.88311
H	1.73505	1.82796	2.87316
C	1.82938	-1.32146	5.13464
H	2.22681	-2.42846	3.34098
C	1.59853	-0.06699	5.69888
H	1.37963	2.04425	5.31122
H	1.83236	-2.20997	5.75985
H	1.42342	0.02627	6.76703
C	0.21141	-2.30957	-2.5846
C	-0.92332	-2.77635	-3.26316
C	1.40432	-2.12867	-3.30753
C	-0.86444	-3.05798	-4.63085
H	-1.85274	-2.92793	-2.72532
C	1.46191	-2.41644	-4.66993
H	2.29631	-1.77144	-2.80014
C	0.32461	-2.88059	-5.33686
H	-1.75244	-3.42085	-5.14028
H	2.39369	-2.27835	-5.21097
H	0.36812	-3.10254	-6.39911
C	-1.34096	-2.64455	-0.13757
C	-2.57079	-1.99359	-0.34272
C	-1.32132	-3.85788	0.56496
C	-3.75533	-2.56888	0.11562
H	-2.61473	-1.025	-0.83015
C	-2.51014	-4.42322	1.03053
H	-0.38384	-4.36323	0.76611
C	-3.72864	-3.78484	0.80129
H	-4.69347	-2.0447	-0.04077
H	-2.47801	-5.36101	1.57793
H	-4.65191	-4.22421	1.16817

TS11$^{L2'}$

Sum of electronic and thermal Free Energies= -3598.039930

C	-4.97147	3.43513	-0.22252
C	-5.6253	2.20219	-0.3068
C	-4.88952	1.02063	-0.29109
C	-3.49085	1.05359	-0.18494
C	-2.83571	2.29099	-0.09123
C	-3.58456	3.47865	-0.11887
H	-5.54163	4.35891	-0.24701
H	-6.70623	2.16357	-0.39566
H	-5.40472	0.06917	-0.37075
H	-3.07768	4.43731	-0.07359
P	-2.45816	-0.50037	-0.21961
P	-0.98889	2.25804	-0.01047
S	0.91985	-1.96845	-0.50928
C	-0.00387	-3.48686	-0.31152
C	-0.79811	-3.9736	-1.36742
C	0.17282	-4.30404	0.81934
C	-1.41069	-5.22448	-1.28097
H	-0.92298	-3.37056	-2.25972
C	-0.45521	-5.54781	0.90961
H	0.82212	-3.97169	1.62229
C	-1.25234	-6.01387	-0.13788
H	-2.01358	-5.58243	-2.11146

H	-0.30601	-6.1602	1.79516
H	-1.72949	-6.98786	-0.07349
Rh	-0.24102	0.09782	-0.30045
Cl	1.95852	1.10476	-0.83567
C	2.29904	-1.29256	2.20367
H	2.20972	-2.37094	2.40499
H	2.48841	-0.82623	3.2025
N	3.39991	-1.04489	1.3017
H	3.23281	-0.23845	0.7024
C	4.6956	-0.99157	1.96539
H	4.7745	-0.16699	2.70291
H	4.80255	-1.92013	2.54957
C	5.84316	-0.88436	0.98498
C	6.83337	0.08424	1.13776
C	5.95089	-1.77858	-0.09376
C	7.92242	0.16864	0.26185
H	6.76322	0.79636	1.95708
C	7.02369	-1.71128	-0.97196
H	5.16815	-2.51926	-0.24518
C	8.02073	-0.73688	-0.79804
H	8.66124	0.94262	0.40924
H	7.11091	-2.39807	-1.80793
O	9.03857	-0.75554	-1.71438
C	10.05941	0.22766	-1.60217
H	10.75499	0.0455	-2.42584
H	9.65408	1.2483	-1.69463
H	10.60516	0.14224	-0.64825
C	0.95406	-0.69095	1.88125
H	1.01258	0.38688	1.77407
C	-0.17575	-1.1934	2.73235
H	0.18625	-1.3353	3.76309
H	-1.00732	-0.49102	2.75507
H	-0.55653	-2.16238	2.39872
C	-3.07514	-1.29446	-1.77422
C	-4.25626	-2.04954	-1.84547
C	-2.35006	-1.05656	-2.95287
C	-4.70089	-2.5534	-3.06895
H	-4.82412	-2.26296	-0.94578
C	-2.79978	-1.55561	-4.1759
H	-1.42112	-0.49508	-2.89894
C	-3.9764	-2.30568	-4.23642
H	-5.61327	-3.14244	-3.10744
H	-2.22539	-1.3653	-5.07817
H	-4.32414	-2.69951	-5.18715
C	-3.23448	-1.48264	1.14441
C	-3.78664	-0.83235	2.26213
C	-3.19067	-2.88625	1.13893
C	-4.29072	-1.56413	3.33758
H	-3.82989	0.251	2.2958
C	-3.70086	-3.61532	2.21456
H	-2.76206	-3.41786	0.29712
C	-4.25144	-2.95899	3.31659
H	-4.71653	-1.04187	4.19039
H	-3.65788	-4.69973	2.18585
H	-4.64608	-3.52885	4.1528
C	-0.51071	3.56828	-1.21579
C	-0.43449	4.9238	-0.86221
C	-0.26836	3.19422	-2.5455
C	-0.13825	5.88867	-1.82711
H	-0.59129	5.22865	0.16798
C	0.02105	4.16057	-3.508
H	-0.27691	2.14281	-2.81296
C	0.08527	5.50927	-3.15139
H	-0.07695	6.93499	-1.54079
H	0.21419	3.85741	-4.53292
H	0.32038	6.26027	-3.90031
C	-0.5692	2.99181	1.63095
C	0.78948	3.22131	1.91909
C	-1.52865	3.25693	2.61918
C	1.16899	3.71943	3.16495
H	1.54149	2.99697	1.16691
C	-1.1411	3.75087	3.8675
H	-2.58122	3.08706	2.41776
C	0.20611	3.98603	4.14244
H	2.22055	3.89747	3.37245
H	-1.8962	3.95468	4.62189
H	0.50538	4.37249	5.11256

3^{L2}-Br

Sum of electronic and thermal Free Energies= -5709.289

C	-4.68328900	-1.23215400	2.98150500
C	-4.63756600	0.14324000	3.20579800
C	-3.67636600	0.92376900	2.56044200
C	-2.75733800	0.33366500	1.68583900
C	-2.80419600	-1.05632100	1.45706800
C	-3.76806400	-1.82953400	2.11265100
H	-5.43719800	-1.84106900	3.47191900
H	-5.35513600	0.61291300	3.87204800
H	-3.65322500	1.99670300	2.72222900

H	-3.82840700	-2.89622900	1.92261800	H	9.31299100	-1.27526900	1.46536300
P	-1.46648400	1.32148400	0.80439900	C	-2.31000600	-3.26539700	-0.43633400
P	-1.54492400	-1.75982900	0.29833500	C	-1.55243600	-4.43651400	-0.61263000
S	-0.57859000	2.10591100	-2.44684800	C	-3.62499100	-3.22395900	-0.93288400
C	0.91931700	2.94406000	-1.94602200	C	-2.10379400	-5.54738800	-1.25269900
C	0.83708400	4.30436600	-1.59350900	H	-0.53450800	-4.48961900	-0.24129900
C	2.18938700	2.33584700	-1.94808900	C	-4.17118100	-4.34152100	-1.56486300
C	1.98200500	5.02942900	-1.25764900	H	-4.20241700	-2.30978700	-0.85508200
H	-0.13622500	4.78469000	-1.58253200	C	-3.41609200	-5.50474800	-1.72556600
C	3.32869600	3.05851800	-1.59229000	H	-1.50591600	-6.44566800	-1.37748900
H	2.28887000	1.29146100	-2.22444900	H	-5.18926300	-4.29540800	-1.94024800
C	3.23312600	4.41016900	-1.24735100	H	-3.84558600	-6.37068700	-2.22116800
H	1.89145300	6.07941100	-0.99102300	C	-0.28161900	-2.45788000	1.46282900
H	4.29554100	2.56129700	-1.59162000	C	1.01794000	-1.93847800	1.48332200
H	4.12288500	4.97224200	-0.97750300	C	-0.61394900	-3.47943300	2.37093800
Rh	-0.96639700	0.10272000	-1.10839200	C	1.97029600	-2.42780900	2.38149800
H	0.51486000	0.13229700	-0.66436900	H	1.27631800	-1.13394800	0.80501000
C	-0.94517400	-1.23247500	-3.11210400	C	0.33503400	-3.96893900	3.26604200
C	0.39198000	-1.03700200	-2.93089900	H	-1.61398300	-3.90080600	2.37569000
H	-1.52830300	-0.53584600	-3.70007800	C	1.63104700	-3.44465400	3.27244700
H	-1.43165000	-2.16412200	-2.84240100	H	2.97113300	-2.00664900	2.38015800
H	0.83846400	-0.14006000	-3.34930300	H	0.06292900	-4.75941700	3.95970300
C	1.36669400	-2.07790000	-2.44898600	H	2.36870200	-3.82715600	3.97224000
H	1.66642500	-2.66751000	-3.32996200	C	-2.12426200	3.03950600	0.73760800
H	0.87229900	-2.78943400	-1.76365100	C	-1.70739800	4.00410000	1.66946400
N	2.57853600	-1.47457700	-1.90889700	C	-3.07249700	3.38704400	-0.23896200
H	2.33840400	-0.87226200	-1.12489400	C	-2.24148500	5.29378300	1.63311100
C	3.59177700	-2.44592200	-1.49814700	H	-0.96528300	3.75841000	2.42037100
H	3.22501900	-3.15666500	-0.73471000	C	-3.60121300	4.67698200	-0.26529400
H	3.83535200	-3.05160700	-2.38388000	H	-3.38875300	2.64923000	-0.96805000
C	4.84139500	-1.76324100	-0.98418300	C	-3.18853700	5.63215400	0.66648800
C	5.43974500	-2.15027300	0.21503900	H	-1.91045300	6.03146400	2.35853000
C	5.44643800	-0.72950900	-1.72028800	H	-4.33218600	4.93569400	-1.02567400
C	6.61136100	-1.54285900	0.68343600	H	-3.60044000	6.63718700	0.63649000
H	4.99107100	-2.94831300	0.80244700	C	-0.08169100	1.43151800	2.02254300
C	6.60590700	-0.11344200	-1.27083900	C	1.15097500	1.94808300	1.59008800
H	4.98786600	-0.40888600	-2.65066600	C	-0.22477400	1.03827200	3.36074400
C	7.19912000	-0.51772100	-0.06349400	C	2.21588600	2.06837500	2.48183200
H	7.04599200	-1.87319800	1.61957700	H	1.28202300	2.25591500	0.55870900
H	7.07963500	0.68153800	-1.83809200	C	0.84708900	1.15570800	4.24925700
O	8.33781200	0.14981800	0.28857500	H	-1.16690100	0.63433300	3.71461800
C	8.99078400	-0.22590300	1.48922300	C	2.06773600	1.67047600	3.81316100
H	9.86914800	0.41652000	1.56991500	H	3.16013300	2.47265900	2.12945100
H	8.34965100	-0.07007300	2.36699300	H	0.72383200	0.84081300	5.28157200

H	2.89980600	1.76157900	4.50573900
Br	-3.57766300	0.20218500	-1.83568900

TS8^{L2}-Br

Sum of electronic and thermal Free Energies= -5709.275

C	4.76972500	3.52231800	-1.37755500
C	5.51204800	2.35683800	-1.56521200
C	4.97143600	1.11847000	-1.21157500
C	3.68479200	1.03677700	-0.66799900
C	2.93422400	2.21659400	-0.47715400
C	3.48439200	3.45266800	-0.83520000
H	5.18211200	4.48498700	-1.66534600
H	6.50644700	2.40690300	-1.99917600
H	5.54328100	0.21090300	-1.37879300
H	2.89957900	4.35931100	-0.71483200
P	2.88005100	-0.56578700	-0.21850600
P	1.23082000	2.03250000	0.21543900
S	-0.12904900	-2.39764000	-1.06881800
C	-0.51212700	-3.48889000	0.28617000
C	-0.56851700	-3.11464500	1.64004800
C	-0.78987800	-4.83130100	-0.04491800
C	-0.88947900	-4.05140300	2.62624900
H	-0.35552100	-2.08642400	1.91235400
C	-1.09732100	-5.76189400	0.94431600
H	-0.75647700	-5.13725800	-1.08654200
C	-1.15199400	-5.37882000	2.28795100
H	-0.92977400	-3.73596600	3.66591100
H	-1.29990300	-6.79200900	0.66318600
H	-1.39509400	-6.10558900	3.05751100
Rh	0.55776900	-0.11862900	-0.38495700
H	0.39805300	-0.44804700	1.11097200
C	-1.62435300	0.40346400	-0.43734200
C	-2.04732900	-0.76501000	-1.09187800
H	-1.50426600	1.28287800	-1.06358300
H	-2.00474700	0.57918200	0.56577200
H	-1.92476500	-0.79017300	-2.17135200
C	-3.07635000	-1.69404200	-0.49468700
H	-2.81425100	-1.91959700	0.54546200
H	-3.08553100	-2.65193600	-1.03859300
N	-4.37966800	-1.01573900	-0.48827200
H	-4.65778800	-0.80070200	-1.44398800
C	-5.43391700	-1.81974200	0.13535500
H	-5.54100100	-2.82191500	-0.32043500
H	-5.12896400	-1.99635700	1.17740300
C	-6.77265700	-1.11215100	0.09821700
C	-6.87164100	0.25858600	0.35477300
C	-7.95381400	-1.81795200	-0.17321800
C	-8.10479700	0.91516500	0.34751900
H	-5.96383200	0.82125400	0.54950600
C	-9.19045100	-1.18297700	-0.17817500
H	-7.90402400	-2.88334200	-0.38599600
C	-9.27397800	0.19176900	0.08248300
H	-8.14034500	1.97998800	0.54669100
H	-10.10491400	-1.72747900	-0.39035700
O	-10.53114100	0.72845700	0.04874900
C	-10.67158000	2.11751500	0.29256700
H	-11.73890000	2.33197900	0.21566200
H	-10.32107800	2.39230200	1.29619900
H	-10.12957600	2.71778000	-0.45009900
C	3.49152900	-0.91758500	1.48809800
C	4.52686700	-0.19236100	2.09419300
C	2.89253900	-1.97122900	2.19878300
C	4.95253800	-0.51223700	3.38611000
H	5.00406000	0.62419200	1.56271100
C	3.32632000	-2.29356800	3.48352600
H	2.08344600	-2.53936600	1.75090600
C	4.35577800	-1.56286500	4.08232600
H	5.75239900	0.06221900	3.84489300
H	2.85444300	-3.11339500	4.01751300
H	4.68865800	-1.81080200	5.08624800
C	3.71488900	-1.84918100	-1.24024900
C	4.76071800	-2.63434400	-0.72531300
C	3.29414400	-2.04843300	-2.56603600
C	5.38399200	-3.59086700	-1.52761500
H	5.09021500	-2.50387200	0.29958500
C	3.92416500	-3.00691000	-3.36048600
H	2.48219300	-1.45181600	-2.97028100
C	4.96711200	-3.77891800	-2.84644300
H	6.19258600	-4.18990200	-1.11823700
H	3.58963700	-3.15211100	-4.38355300
H	5.45060300	-4.52719500	-3.46848000
C	1.43612900	2.32765200	2.02894600
C	2.47181400	3.12285000	2.54285200
C	0.49968500	1.77851500	2.91801000
C	2.56953900	3.35891200	3.91509200
H	3.20900700	3.55558400	1.87461000
C	0.59324600	2.02367100	4.28830400
H	-0.29706600	1.14924600	2.53499400
C	1.63017900	2.81191500	4.79041400

H	3.38189100	3.96980400	4.29852900
H	-0.14022500	1.59164200	4.96295000
H	1.70786600	2.99582100	5.85814400
C	0.30665700	3.52423100	-0.35196900
C	-0.17751100	4.48205700	0.55345500
C	0.05815500	3.69218700	-1.72621800
C	-0.88788200	5.59231400	0.09248700
H	-0.00165600	4.36847800	1.61705100
C	-0.64785300	4.80703900	-2.17763400
H	0.39656000	2.93761300	-2.43085700
C	-1.12161500	5.75942100	-1.27257500
H	-1.25635700	6.32541500	0.80446000
H	-0.83272500	4.92460500	-3.24151000
H	-1.67406800	6.62429800	-1.62910800
Br	0.68038100	0.41456000	-3.04636600

13^{L2}-Br

Sum of electronic and thermal Free Energies= -5709.288834

C	-3.93396300	-3.00022000	-3.08909600
C	-4.79930400	-1.90925100	-3.01425400
C	-4.54651400	-0.87781800	-2.10747400
C	-3.42983200	-0.92590600	-1.26386300
C	-2.55291500	-2.02949500	-1.34515300
C	-2.81377900	-3.05879600	-2.25775000
H	-4.11923200	-3.79809600	-3.80237300
H	-5.66425000	-1.85206900	-3.66890800
H	-5.20960600	-0.01893200	-2.07059400
H	-2.12913100	-3.89787100	-2.33329400
P	-3.00575600	0.42684100	-0.06933000
P	-1.06736700	-2.04673300	-0.23992700
S	0.38461200	2.14222300	1.39598000
C	0.37078100	3.81034100	0.71154700
C	0.40056100	4.86697600	1.63185200
C	0.31406700	4.07138600	-0.66291700
C	0.38107400	6.18631200	1.17700100
H	0.44259600	4.65372900	2.69573700
C	0.30601400	5.39508300	-1.10533000
H	0.26863800	3.24739200	-1.36915400
C	0.33811100	6.45201400	-0.19252800
H	0.40483500	7.00279900	1.89318000
H	0.26642900	5.59807700	-2.17185500
H	0.32745800	7.47888300	-0.54706600
Rh	-0.58870600	0.13246500	0.26860200
H	-0.82613500	-0.26648800	1.74051700
C	1.48057100	-0.13591100	0.61518700
C	1.93135100	1.31480400	0.70156200
H	1.93048600	-0.65013600	-0.23417600
H	1.69610700	-0.68093800	1.53864900
H	2.02603800	1.72436500	-0.30867600
C	3.16134300	1.64235000	1.54958600
H	3.02089300	1.23579000	2.55968400
H	3.24642900	2.74166500	1.65876600
N	4.35330300	1.02769300	0.97402800
H	4.48378300	1.35716200	0.01953000
C	5.57192600	1.28794500	1.73992600
H	5.77483500	2.36699400	1.88020600
H	5.41020000	0.87997300	2.74883400
C	6.78221600	0.63282000	1.10864400
C	7.98322600	1.32526900	0.95448200
C	6.73055000	-0.70380000	0.67706700
C	9.11636400	0.71907400	0.39989800
H	8.04660000	2.36384600	1.27140100
C	7.84243400	-1.32039000	0.12085000
H	5.79673200	-1.24944000	0.77134100
C	9.04683000	-0.61276900	-0.01944600
H	10.03002200	1.29262900	0.29598000
H	7.80714400	-2.35172200	-0.21569000
O	10.08264700	-1.30955200	-0.57746900
C	11.32002800	-0.64127100	-0.75033000
H	11.99586200	-1.36737900	-1.20543800
H	11.22378300	0.22691600	-1.41570500
H	11.74108800	-0.30953400	0.20810400
C	-4.04049500	0.04988700	1.41722800
C	-5.23129500	-0.69061600	1.36567300
C	-3.61026900	0.55248500	2.65565500
C	-5.97524400	-0.91916400	2.52495900
H	-5.57953000	-1.09524500	0.42076400
C	-4.35961900	0.33158300	3.81145700
H	-2.67882800	1.10734200	2.71384400
C	-5.54322700	-0.40640000	3.74905300
H	-6.89217000	-1.49945700	2.46990200
H	-4.01343300	0.72880900	4.76141700
H	-6.12292300	-0.58531200	4.65023600
C	-3.82554900	1.92254400	-0.78123500
C	-4.98321800	2.48679200	-0.22318100
C	-3.24718300	2.52472600	-1.91268700
C	-5.55808700	3.62599800	-0.79110800
H	-5.43913100	2.04000200	0.65337000
C	-3.83219300	3.65705400	-2.47847800

C	-4.98692900	4.21128300	-1.92115800	C	-0.12696500	-3.01553500	2.00932100
H	-6.45336200	4.05286600	-0.34742500	C	-0.77409400	-4.80839100	0.51259300
H	-3.37753000	4.11063300	-3.35472500	C	-0.19261700	-3.90117200	3.08703100
H	-5.43595700	5.09689300	-2.36237800	H	0.17098900	-1.98201600	2.15453900
C	-1.58702400	-3.06380800	1.21443900	C	-0.83168900	-5.68948000	1.59349000
C	-2.71924400	-3.88964100	1.19220500	H	-0.99480900	-5.15816000	-0.49127200
C	-0.79302200	-3.03195600	2.37248200	C	-0.54481900	-5.23698400	2.88269300
C	-3.05340300	-4.66322700	2.30685100	H	0.03972200	-3.54555900	4.08700400
H	-3.34690600	-3.93041600	0.30852300	H	-1.09962200	-6.72874800	1.42623400
C	-1.12196400	-3.81337000	3.47875300	H	-0.58900400	-5.92364900	3.72315900
H	0.07865100	-2.38619200	2.40789200	Rh	0.58118500	-0.15058600	-0.26311000
C	-2.25600100	-4.62907500	3.45008300	H	-0.32654700	-0.21124300	1.04248800
H	-3.93972500	-5.29069700	2.27783000	C	-1.61027300	-0.15127700	0.22827100
H	-0.49656500	-3.77895700	4.36622100	C	-1.93267900	-1.36612900	-0.63914800
H	-2.51705200	-5.23099700	4.31583900	H	-1.92694900	0.78964000	-0.22157800
C	0.15652300	-3.13489100	-1.08997200	H	-2.09145000	-0.23538400	1.20823900
C	0.36664500	-4.46301800	-0.68317600	H	-1.99512400	-1.04429300	-1.68312700
C	0.88880800	-2.62674400	-2.17667500	C	-3.15788400	-2.19012400	-0.24356500
C	1.28706400	-5.26902800	-1.35584900	H	-3.03775100	-2.56584600	0.78017900
H	-0.18330000	-4.87276400	0.15640000	H	-3.23057000	-3.07853000	-0.89979800
C	1.80502500	-3.44008200	-2.84368500	N	-4.34771100	-1.34666700	-0.27139200
H	0.74257900	-1.59637700	-2.48922300	H	-4.48882600	-0.97571900	-1.20877400
C	2.00731400	-4.76041400	-2.43712400	C	-5.56384700	-2.03367000	0.16407400
H	1.44028700	-6.29401100	-1.02998200	H	-5.79236100	-2.93454500	-0.43631500
H	2.36528600	-3.03408600	-3.68100200	H	-5.37821500	-2.39438200	1.18674500
H	2.72516900	-5.38860800	-2.95725000	C	-6.76573500	-1.11256700	0.15481200
H	-2.33687800	2.10918200	-2.33647400	C	-7.99358200	-1.53092200	-0.35828200
Br	-0.02746100	0.83017700	-2.32596900	C	-6.68093600	0.18412400	0.68985500
TS9^{L2}-Br				C	-9.12079300	-0.70177100	-0.33743700
Sum of electronic and thermal Free Energies= -5709.258387				H	-8.08329900	-2.52660300	-0.78682500
C	4.34325100	3.77230700	-1.80098500	C	-7.78655000	1.02249100	0.71480900
C	5.15237400	2.67114500	-2.08212400	H	-5.72695500	0.53118400	1.07459700
C	4.77015200	1.39488700	-1.66183000	C	-9.01819500	0.58340600	0.20359400
C	3.57543300	1.21168700	-0.95748700	H	-10.05593700	-1.06436600	-0.74779200
C	2.76052600	2.32625900	-0.67225700	H	-7.72569700	2.02567700	1.12472900
C	3.14923200	3.60150300	-1.09634000	O	-10.04507000	1.48258600	0.27703600
H	4.63137900	4.76241600	-2.14218600	C	-11.31074700	1.09441200	-0.22875500
H	6.07403600	2.80114600	-2.64204100	H	-11.97421700	1.94645000	-0.07113100
H	5.38998800	0.53646200	-1.90194400	H	-11.26736000	0.86616400	-1.30189500
H	2.51019500	4.45631500	-0.89676800	H	-11.71219700	0.22254900	0.30463000
P	2.93304900	-0.44141600	-0.42158700	C	3.83341200	-0.78295900	1.15943900
P	1.18825000	1.98983800	0.23995400	C	4.87107100	0.02206300	1.64900600
S	-0.34979200	-2.39986400	-0.74225400	C	3.44233700	-1.90802800	1.90526500
C	-0.42786300	-3.46508300	0.71721700	C	5.50161700	-0.28921200	2.85690700

H	5.19290500	0.89377600	1.08932400
C	4.08038200	-2.22384800	3.10307500
H	2.63281700	-2.53721900	1.54768800
C	5.11119400	-1.41220500	3.58511500
H	6.30109600	0.34818800	3.22446300
H	3.76801900	-3.10094100	3.66301600
H	5.60378900	-1.65395900	4.52267700
C	3.70489500	-1.64941500	-1.58648400
C	4.90397100	-2.31709500	-1.28418500
C	3.06917100	-1.90192000	-2.81387400
C	5.45984500	-3.21605600	-2.19577800
H	5.40338600	-2.14179700	-0.33728400
C	3.63342700	-2.80141500	-3.71992800
C	4.82559200	-3.46047700	-3.41518100
H	6.38691700	-3.72646700	-1.94938900
H	3.13248200	-2.98664500	-4.66584300
H	5.25817100	-4.16305300	-4.12236000
C	1.61628200	2.32543500	2.00996600
C	2.74529800	3.06907800	2.38354200
C	0.76359900	1.84357600	3.01567100
C	3.01483400	3.32284900	3.73070400
H	3.41937000	3.45166400	1.62444700
C	1.02772000	2.10607800	4.35896400
H	-0.10607000	1.25387000	2.74346600
C	2.15710600	2.84452700	4.72066400
H	3.89718100	3.89524500	4.00294900
H	0.35532800	1.72784900	5.12375000
H	2.36772000	3.04182300	5.76787800
C	0.05351000	3.38149500	-0.18299200
C	-0.08957900	4.50308700	0.65099000
C	-0.68392900	3.31243900	-1.37746600
C	-0.94977400	5.54206200	0.29163000
H	0.46489100	4.56890400	1.58070200
C	-1.54011200	4.35713800	-1.72846400
H	-0.58143200	2.44466800	-2.02665800
C	-1.67636200	5.47114600	-0.89793700
H	-1.05314200	6.40383400	0.94511000
H	-2.10413200	4.29344500	-2.65459400
H	-2.34819000	6.27928700	-1.17397100
H	2.14193700	-1.38899100	-3.05961200
Br	0.12122000	0.20733300	-3.05691700

$14^{L,2}$-Br

Sum of electronic and thermal Free Energies= -5709.332118

C	-6.70097900	-0.27963100	0.49920900
C	-6.48669400	0.97830600	1.06897900
C	-5.18848800	1.46490700	1.21503200
C	-4.09331800	0.69390600	0.80110900
C	-4.30627800	-0.57944700	0.24638200
C	-5.61668200	-1.05433400	0.08822800
H	-7.71265000	-0.65263000	0.36722000
H	-7.33085200	1.58525300	1.38355300
H	-5.02854900	2.45428500	1.63229700
H	-5.78834700	-2.02363400	-0.36983200
P	-2.33884600	1.29534700	0.86291900
P	-2.79460200	-1.52826800	-0.26567000
S	0.92929000	1.42582600	-0.09571800
C	1.26808400	2.17421000	-1.70528400
C	1.46091100	3.56082800	-1.75345800
C	1.31293400	1.41495000	-2.88160600
C	1.70190600	4.18858000	-2.97732000
H	1.42103500	4.14131800	-0.83712700
C	1.56562100	2.05123800	-4.09799500
H	1.13831800	0.34381400	-2.83591200
C	1.75797700	3.43433200	-4.15036200
H	1.84917400	5.26441500	-3.01031600
H	1.60436800	1.46116200	-5.00944500
H	1.94942800	3.92207200	-5.10212600
Rh	-1.01456300	-0.13628000	-0.26236800
H	1.36716500	-1.06759800	1.42273200
C	2.20668500	-0.37666800	1.52857800
C	2.44589900	0.38676000	0.22646600
H	3.11173800	-0.94157800	1.76657600
H	2.00091900	0.30628300	2.36074600
H	2.48988100	-0.32314300	-0.60530300
C	3.70351000	1.26418500	0.26468400
H	3.66768400	1.91175600	1.15104400
H	3.72769500	1.93072300	-0.61459900
N	4.89763300	0.42516200	0.36461800
H	4.95898100	-0.17475100	-0.45603700
C	6.13729100	1.19448000	0.48166100
H	6.26799200	1.93148900	-0.33342500
H	6.06449700	1.78239200	1.40883800
C	7.35363000	0.29459500	0.53505300
C	8.48976800	0.56887200	-0.22657800
C	7.37663700	-0.83519200	1.37078600
C	9.63075400	-0.23897200	-0.16399100
H	8.49450800	1.43170700	-0.88875100
C	8.49691400	-1.65112700	1.44232100

H	6.49379600	-1.07349500	1.95587100
C	9.63576400	-1.35673400	0.67586900
H	10.49208500	0.00832400	-0.77335700
H	8.51844400	-2.52604900	2.08430800
O	10.68609100	-2.21987400	0.81834400
C	11.85991700	-1.97426400	0.06332600
H	12.56015400	-2.76947600	0.32469700
H	11.66371300	-2.00845300	-1.01652500
H	12.30850200	-1.00355300	0.31286100
C	-2.00338800	1.52389700	2.66594700
C	-2.72902300	0.82377600	3.64165400
C	-0.92154900	2.32357400	3.07519700
C	-2.38977600	0.92884100	4.99190000
H	-3.56235500	0.19252200	3.35105100
C	-0.58785900	2.42971800	4.42503400
H	-0.33794900	2.86424700	2.33677300
C	-1.32095100	1.73281300	5.38833700
H	-2.96429400	0.38053400	5.73320500
H	0.24777600	3.05650800	4.72374500
H	-1.05850600	1.81437900	6.43919600
C	-2.48543600	3.02266500	0.21678000
C	-2.80996600	4.12989900	1.01674000
C	-2.30544800	3.21039300	-1.16252700
C	-2.95840700	5.39481100	0.44501500
H	-2.93433400	4.00946400	2.08824800
C	-2.45794500	4.47496900	-1.73240400
C	-2.78527900	5.56926200	-0.92964000
H	-3.20659100	6.24442000	1.07520800
H	-2.31005800	4.60493000	-2.80047800
H	-2.89895500	6.55532500	-1.37133400
C	-2.70254300	-2.92926300	0.93940600
C	-3.66379100	-3.14540800	1.93798100
C	-1.59608400	-3.79406500	0.86108900
C	-3.52749900	-4.20748400	2.83575500
H	-4.52334000	-2.48964700	2.02199000
C	-1.47046900	-4.85675200	1.75457200
H	-0.83112900	-3.61790900	0.10991900
C	-2.43350600	-5.06716800	2.74474200
H	-4.28005000	-4.35970500	3.60468600
H	-0.61102300	-5.51708300	1.68034700
H	-2.32840200	-5.89293200	3.44293700
C	-3.32371700	-2.31877600	-1.84349700
C	-3.97417300	-3.56025700	-1.88547400
C	-3.09774600	-1.62248600	-3.03996500
C	-4.40621200	-4.08764100	-3.10444400
H	-4.13359100	-4.12206100	-0.97026900
C	-3.53594300	-2.14864100	-4.25426700
H	-2.55762900	-0.68123700	-3.00977700
C	-4.19154900	-3.38168800	-4.28881600
H	-4.90434900	-5.05291400	-3.12708000
H	-3.35182800	-1.60314200	-5.17544100
H	-4.52443900	-3.79525700	-5.23670200
H	-2.03486800	2.35686900	-1.77852000
Br	0.36661300	-1.88212800	-1.59076200

TS10^{L2}-Br

Sum of electronic and thermal Free Energies= -5709.274672

C	-3.90086300	-1.80285600	3.56743600
C	-3.86164400	-0.46147200	3.94831000
C	-3.11038400	0.45152800	3.20721300
C	-2.39801800	0.03656500	2.07410200
C	-2.46370800	-1.31323700	1.67300500
C	-3.20190700	-2.22611500	2.43682800
H	-4.48281500	-2.51812700	4.14135500
H	-4.41647500	-0.12376200	4.81881400
H	-3.08773100	1.49593000	3.50236500
H	-3.25175200	-3.26781400	2.13684300
P	-1.35272700	1.20138300	1.08177500
P	-1.51764900	-1.81873600	0.16362800
S	-1.29714000	2.36257900	-2.29016900
C	0.28501500	3.19511000	-2.27545600
C	1.17274800	3.07451300	-3.36215400
C	0.63440900	4.07892600	-1.23571500
C	2.37630000	3.78119600	-3.39255100
H	0.89548800	2.44097200	-4.19953000
C	1.83766900	4.78471300	-1.26692600
H	-0.05591600	4.21941700	-0.40999700
C	2.71838200	4.63399500	-2.34151800
H	3.04268600	3.67138800	-4.24423900
H	2.08348800	5.46302600	-0.45364400
H	3.65307300	5.18730000	-2.36619200
Rh	-1.19326700	0.20690700	-1.08742600
H	0.42940000	0.15180300	-1.24328300
C	-0.90590400	-0.76379000	-3.02201500
C	0.43101700	-0.44307400	-2.66252500
H	-1.43754100	-0.11169100	-3.70441100
H	-1.23758400	-1.79759900	-2.98546900
H	0.84720700	0.47120600	-3.07846400
C	1.46963700	-1.52753700	-2.44204200

H	1.72576200	-1.91188100	-3.43988500
H	1.02747300	-2.37434500	-1.88798700
N	2.69109500	-1.00890900	-1.84553700
H	2.48964700	-0.63216000	-0.92208800
C	3.75824400	-2.00318300	-1.73278600
H	3.44055800	-2.91734400	-1.19858300
H	4.01440500	-2.32099600	-2.75477600
C	4.98211900	-1.43193100	-1.04738300
C	5.69820200	-2.18224000	-0.11327500
C	5.44336300	-0.13893200	-1.34895700
C	6.84982500	-1.68265600	0.50540300
H	5.35746400	-3.18316400	0.14188100
C	6.57997400	0.37563800	-0.73972400
H	4.88995000	0.46396000	-2.06225000
C	7.29530600	-0.39497000	0.19051600
H	7.37809800	-2.29821100	1.22403200
H	6.94008900	1.37347100	-0.96941500
O	8.39984100	0.20115400	0.73077200
C	9.17250200	-0.53916700	1.66043200
H	10.00149400	0.10897800	1.94931300
H	8.59228500	-0.80080700	2.55532300
H	9.57303200	-1.45909400	1.21465300
C	-2.48514300	-3.15417200	-0.65110000
C	-1.81107900	-4.11630800	-1.42450900
C	-3.88933700	-3.16321600	-0.63627400
C	-2.52185600	-5.07593300	-2.14571600
H	-0.72596100	-4.12888700	-1.45608000
C	-4.59507100	-4.13085900	-1.35239300
H	-4.43071200	-2.40504800	-0.08526700
C	-3.91705000	-5.08808100	-2.10773300
H	-1.98325100	-5.81297000	-2.73436100
H	-5.68075100	-4.12479300	-1.32742000
H	-4.47167500	-5.83531700	-2.66790000
C	-0.08290100	-2.72973800	0.91177100
C	1.11392700	-2.03691900	1.14206300
C	-0.17905800	-4.06489600	1.34148500
C	2.19386700	-2.66007500	1.77156700
H	1.19568800	-0.99785100	0.84538900
C	0.89997000	-4.68844500	1.96740300
H	-1.09292900	-4.62577800	1.17818500
C	2.09021400	-3.98933800	2.18155000
H	3.11195000	-2.10358400	1.93412700
H	0.80930600	-5.72242700	2.28814600
H	2.92906000	-4.47821500	2.66882300
C	-2.11070600	2.85472800	1.37142700
C	-1.58231800	3.75928800	2.30642500
C	-3.24996500	3.21406200	0.63147700
C	-2.19115200	5.00019600	2.50713300
H	-0.69663900	3.50122600	2.87695200
C	-3.85464200	4.45255700	0.84339300
H	-3.65163200	2.52634100	-0.10552400
C	-3.32857900	5.34765300	1.77742600
H	-1.77271500	5.69258800	3.23227600
H	-4.73350000	4.72123600	0.26466400
H	-3.79974200	6.31443600	1.93191300
C	0.23429300	1.27797400	2.03679500
C	1.38330200	1.73783800	1.37098100
C	0.34365000	0.88592000	3.37942200
C	2.60964100	1.80506500	2.03311700
H	1.31980600	2.04431700	0.33195000
C	1.57381900	0.94887500	4.03870400
H	-0.52606600	0.51943900	3.91379500
C	2.70861400	1.40700000	3.36877100
H	3.48680400	2.16140100	1.50096700
H	1.64239000	0.63359500	5.07609400
H	3.66498000	1.45179100	3.88197300
Br	-3.79497400	0.20497700	-1.40014600

15^{L2}-Br

Sum of electronic and thermal Free Energies= -5709.299441

C	-3.62177800	-0.75189800	4.30922300
C	-2.92702000	0.43141400	4.57153500
C	-2.18543100	1.04203600	3.56229100
C	-2.12843800	0.48279900	2.27631100
C	-2.85557600	-0.69046200	2.00402600
C	-3.58770700	-1.30757400	3.03185400
H	-4.18918900	-1.23907300	5.09678800
H	-2.95379200	0.87203600	5.56385800
H	-1.63155100	1.94859100	3.78297900
H	-4.12399700	-2.22940700	2.82968000
P	-1.13278900	1.26693800	0.90890700
P	-2.83822400	-1.32214300	0.27013700
S	-0.10571400	1.10524700	-2.58653400
C	0.79082800	2.58388000	-2.13827700
C	0.16170600	3.84110300	-2.07629800
C	2.18837300	2.53083000	-1.97856600
C	0.90370400	5.00112900	-1.84467100
H	-0.91144500	3.90334000	-2.22110700
C	2.92752300	3.69146900	-1.74850100

H	2.68963000	1.57082900	-2.05307100
C	2.28955100	4.93297900	-1.67573000
H	0.39726000	5.96228300	-1.80529600
H	4.00676500	3.62635700	-1.63543300
H	2.86647800	5.83802700	-1.50631300
Rh	-1.11883500	-0.22747800	-0.86975600
H	1.88857600	-0.02266800	-0.03811000
C	0.27611000	-1.45459300	0.10616100
C	1.69354400	-1.07215500	-0.28747500
H	0.01705400	-2.45878500	-0.23337100
H	0.12926700	-1.39088000	1.18976000
H	1.82449800	-1.17583700	-1.36688100
C	2.73402600	-1.94743100	0.43463000
H	2.62391800	-2.99151600	0.11302600
H	2.53904800	-1.93549200	1.52630800
N	4.08897100	-1.51380000	0.10473900
H	4.20650300	-0.54098700	0.38139200
C	5.13458900	-2.31645200	0.73435500
H	5.04672600	-2.36173400	1.83784000
H	5.00261400	-3.35064800	0.38266000
C	6.51972200	-1.82390300	0.36837200
C	7.53571300	-1.74506300	1.32114300
C	6.82398600	-1.45482700	-0.95315000
C	8.82814900	-1.32494600	0.98636400
H	7.32363600	-2.01719100	2.35288200
C	8.09832900	-1.02996000	-1.30286700
H	6.03784100	-1.49456700	-1.70066500
C	9.11246000	-0.96528800	-0.33454900
H	9.58947800	-1.27726400	1.75628400
H	8.33772400	-0.74273100	-2.32187700
O	10.33256100	-0.53647800	-0.78011800
C	11.39613400	-0.46483500	0.15259800
H	12.26634800	-0.11529500	-0.40572900
H	11.18076000	0.24456800	0.96289300
H	11.62034300	-1.44658000	0.59062400
C	-4.47469800	-0.81369500	-0.42716200
C	-4.62558700	-0.75440800	-1.82439200
C	-5.56194800	-0.46480400	0.39077700
C	-5.84608600	-0.36956900	-2.38284000
H	-3.79068800	-1.01577400	-2.46851900
C	-6.77603500	-0.07515700	-0.17555700
H	-5.46771300	-0.48562500	1.47048600
C	-6.92237400	-0.02832100	-1.56295700
H	-5.94769400	-0.33318400	-3.46359700
H	-7.60647400	0.19420900	0.47093200
H	-7.86855400	0.27636700	-2.00123500
C	-2.91870300	-3.14870900	0.44570900
C	-2.08506500	-3.79976900	1.37114300
C	-3.73465200	-3.91963500	-0.39514100
C	-2.08125000	-5.19138000	1.46113600
H	-1.44261300	-3.22313600	2.02890300
C	-3.72674600	-5.31130900	-0.30140900
H	-4.37516500	-3.43612800	-1.12374600
C	-2.90222500	-5.95050900	0.62506600
H	-1.43469700	-5.68115900	2.18357300
H	-4.36464000	-5.89512700	-0.95838200
H	-2.89683200	-7.03440200	0.69416000
C	-2.02665800	2.85603000	0.64147800
C	-1.87398700	3.96606800	1.48714200
C	-2.95621700	2.91870100	-0.40738200
C	-2.63612600	5.11630300	1.28323400
H	-1.14832700	3.94382600	2.29349500
C	-3.72290700	4.06835100	-0.60326800
H	-3.06661400	2.07435800	-1.08020100
C	-3.56321000	5.16878100	0.24014700
H	-2.50292800	5.97238100	1.93843900
H	-4.43680700	4.10376800	-1.42072700
H	-4.15501200	6.06606000	0.08339200
C	0.44280200	1.70621600	1.75527400
C	1.19747200	2.81174800	1.32937600
C	0.96758300	0.87618600	2.76238700
C	2.43634200	3.08614600	1.91145200
H	0.82837800	3.46053200	0.54380200
C	2.20857500	1.15217200	3.33574900
H	0.40625300	0.01654000	3.11136800
C	2.94618900	2.25987900	2.91304200
H	3.00275100	3.94475400	1.56502800
H	2.59555200	0.50167900	4.11480000
H	3.91188600	2.47576300	3.36098400
Br	-1.34118800	-1.96907000	-2.75505900

TS11^{L2}-Br

Sum of electronic and thermal Free Energies= -5709.264331

C	-2.81102600	-1.22760400	4.51541000
C	-1.89302700	-0.20472900	4.76865800
C	-1.31674300	0.49287800	3.70888600
C	-1.64975800	0.17656800	2.38314000
C	-2.59420000	-0.83123000	2.13057100
C	-3.16220200	-1.53658500	3.20272700

H	-3.25073700	-1.78281800	5.33894800	C	11.39643900	-0.68690200	1.47092300
H	-1.61857700	0.04154400	5.79040400	H	12.36440000	-0.21485500	1.29439800
H	-0.59066500	1.27233600	3.91574600	H	10.94127800	-0.24868900	2.36914000
H	-3.87282800	-2.33325400	3.00636300	H	11.54513100	-1.76217500	1.63607800
P	-0.90732000	1.05971100	0.91760200	C	-4.74684900	-0.45484800	0.20079900
P	-3.03294300	-1.13801300	0.35910700	C	-5.35863900	-0.48604200	-1.06590000
S	-0.19051000	0.88701900	-2.74782100	C	-5.43744200	0.12803000	1.27465300
C	0.71726800	2.38298400	-2.37000300	C	-6.63796900	0.03955200	-1.24111700
C	0.03767600	3.51538400	-1.88590100	H	-4.82060000	-0.90558500	-1.91107000
C	2.07083600	2.51512500	-2.72591900	C	-6.71622400	0.65987200	1.08948300
C	0.69971200	4.73388000	-1.73490300	H	-4.98477700	0.17335900	2.25882700
H	-1.01489100	3.43538400	-1.64351500	C	-7.32097300	0.61407700	-0.16621200
C	2.73393900	3.73229200	-2.56191800	H	-7.09751100	0.00593300	-2.22486200
H	2.60085000	1.66739300	-3.14438800	H	-7.23620500	1.10911000	1.93110300
C	2.05435000	4.84484200	-2.06158300	H	-8.31580000	1.02701400	-0.30847600
H	0.15365700	5.59769600	-1.36566700	C	-3.26444000	-2.96453500	0.29737800
H	3.78185600	3.81244400	-2.83797000	C	-2.15331400	-3.77400400	0.02175500
H	2.56981800	5.79404700	-1.94512800	C	-4.50164100	-3.56965800	0.56182500
Rh	-1.49014600	-0.07591000	-0.99063000	C	-2.27103700	-5.16274900	0.03335600
H	2.25536400	0.21875500	-0.83520000	H	-1.20343300	-3.31165900	-0.22485000
C	0.71844200	-1.07924400	-1.60993100	C	-4.61833200	-4.96147600	0.56709300
C	2.15875200	-0.66010900	-1.48204300	H	-5.37752000	-2.95717100	0.75080800
H	0.44780200	-1.63169800	-2.50286900	C	-3.50393100	-5.75949000	0.30701000
H	0.33794500	-1.56344400	-0.70922300	H	-1.40405000	-5.77868900	-0.18744500
H	2.57030700	-0.39002100	-2.45727700	H	-5.58284300	-5.41931000	0.76785500
C	3.01644700	-1.79284900	-0.88463900	H	-3.59727200	-6.84178300	0.30647200
H	2.99355000	-2.66672000	-1.54924400	C	-1.61370800	2.75639400	1.14369200
H	2.57775700	-2.12018700	0.07778900	C	-1.13355100	3.68446100	2.08053600
N	4.40357900	-1.35828600	-0.75259500	C	-2.74782000	3.08320400	0.38374400
H	4.43686900	-0.53845200	-0.14921300	C	-1.76975000	4.91548400	2.24564700
C	5.28908700	-2.38438600	-0.20357300	H	-0.25413600	3.45780500	2.67438800
H	4.93275600	-2.79499000	0.76118300	C	-3.38683400	4.31218700	0.55563600
H	5.28361200	-3.22962200	-0.90785300	H	-3.11880900	2.37157500	-0.34960000
C	6.70144000	-1.86657800	-0.02889300	C	-2.89756200	5.23162400	1.48504600
C	7.42734000	-2.11815700	1.13557900	H	-1.38284400	5.62786700	2.96895300
C	7.32580200	-1.12728000	-1.04837800	H	-4.26247000	4.55018300	-0.04116200
C	8.74187200	-1.66517700	1.29625000	H	-3.39057000	6.19079700	1.61538700
H	6.96507100	-2.68217800	1.94274800	C	0.86741600	1.19699200	1.41886900
C	8.62669100	-0.66529600	-0.90531500	C	1.65373400	2.30152100	1.05216800
H	6.76715500	-0.90852500	-1.95318500	C	1.48468700	0.12502900	2.08748800
C	9.34690900	-0.93388100	0.26960500	C	3.01405200	2.34062300	1.36581600
H	9.27137900	-1.88252800	2.21642900	H	1.21178900	3.13284900	0.51587200
H	9.11274800	-0.09378400	-1.68972300	C	2.84368400	0.16757200	2.40079500
O	10.61939800	-0.43626100	0.31258800	H	0.90171400	-0.74350700	2.37646200

C	3.61370400	1.27761600	2.04322800
H	3.60238600	3.20484900	1.07246500
H	3.29923600	-0.66586900	2.92803800
H	4.67076200	1.31217400	2.29111200
Br	-2.39971600	-1.51518800	-2.93822800

16^{L2}-Br

Sum of electronic and thermal Free Energies= -5709.320959

C	0.35983000	2.86624000	4.12309000
C	1.04094100	1.75090400	4.61840600
C	1.53422400	0.78814900	3.73919900
C	1.35240700	0.93156100	2.35656800
C	0.68520000	2.06219100	1.85679600
C	0.18231600	3.02093500	2.74893200
H	-0.03819800	3.61011700	4.80731700
H	1.17679200	1.62627400	5.68896100
H	2.04422700	-0.08563800	4.13255600
H	-0.36244000	3.87925700	2.36769600
P	1.95729700	-0.29848200	1.10016000
P	0.49199600	2.17446200	0.01478800
S	1.30705100	-2.01206300	-2.08946300
C	2.78702500	-2.97700400	-1.75741000
C	4.00900000	-2.28952400	-1.74681800
C	2.77967800	-4.36989600	-1.60648600
C	5.20382100	-2.98517400	-1.56946200
H	4.01733900	-1.21087000	-1.86208900
C	3.98180100	-5.05837200	-1.42724200
H	1.84954800	-4.92568900	-1.62718300
C	5.19660400	-4.37260800	-1.40489500
H	6.14085000	-2.43633700	-1.55091800
H	3.96277300	-6.13827100	-1.30826500
H	6.12808200	-4.91275200	-1.26414900
Rh	1.02900800	0.18296100	-0.89703400
H	-1.56824100	-1.82752800	-2.27101500
C	-0.03320100	-3.10186000	-1.43395100
C	-1.33419400	-2.30879900	-1.31412700
H	0.28360800	-3.48420800	-0.45969800
H	-0.14590700	-3.94000900	-2.12887800
H	-1.18620500	-1.49723100	-0.59456800
C	-2.51126000	-3.17395200	-0.85774700
H	-2.25704700	-3.68421700	0.08203100
H	-2.70710700	-3.97134600	-1.60224400
N	-3.67666300	-2.32985700	-0.60703300
H	-3.88454500	-1.78178800	-1.43953700
C	-4.87419600	-3.06891700	-0.21056400
H	-5.18965400	-3.82203600	-0.95745400
H	-4.61707300	-3.63587300	0.69673000
C	-6.03306400	-2.13772400	0.07754400
C	-7.29980300	-2.36399300	-0.45981100
C	-5.86115200	-1.02013800	0.91286200
C	-8.38081700	-1.52000700	-0.17851300
H	-7.45762800	-3.21684700	-1.11610200
C	-6.91969100	-0.16939900	1.20038600
H	-4.87746300	-0.82055600	1.32682500
C	-8.19111200	-0.41524400	0.65661000
H	-9.34858000	-1.73043900	-0.61827500
H	-6.79191000	0.69338100	1.84654700
O	-9.16549300	0.47915100	1.00053400
C	-10.46925700	0.28003200	0.48091300
H	-11.08088800	1.09152000	0.87878700
H	-10.48116900	0.32524300	-0.61603400
H	-10.89263900	-0.68067900	0.80239100
C	1.55709700	3.60036600	-0.48514700
C	1.66694700	3.88112900	-1.85925300
C	2.28254700	4.37812300	0.42961000
C	2.47071400	4.93199500	-2.29859900
H	1.13276900	3.26193400	-2.57500900
C	3.09344400	5.42412500	-0.01881700
H	2.22345100	4.17243800	1.49282000
C	3.18629500	5.70629800	-1.38143900
H	2.54320500	5.13980200	-3.36245400
H	3.65132000	6.01640600	0.70134000
H	3.81619500	6.52092600	-1.72809700
C	-1.23195700	2.80192900	-0.16339600
C	-2.28453800	1.87370900	-0.16784300
C	-1.52662300	4.17072800	-0.23745000
C	-3.60789600	2.30821400	-0.22454400
H	-2.06406300	0.81141100	-0.14638900
C	-2.85359100	4.60266200	-0.30226100
H	-0.72326600	4.90037100	-0.25764600
C	-3.89465200	3.67403100	-0.29153500
H	-4.41324400	1.57916200	-0.22710200
H	-3.07021000	5.66544100	-0.36618700
H	-4.92602100	4.01150600	-0.34419600
C	3.79584200	-0.13037300	1.27252900
C	4.53560100	-0.64980400	2.34691100
C	4.45865000	0.63681100	0.30204600
C	5.90775500	-0.41443500	2.44058600
H	4.04719500	-1.25028900	3.10799500

C	5.83036400	0.87729500	0.40055700
H	3.88500800	1.04151000	-0.52850800
C	6.55777900	0.34974000	1.46855700
H	6.46919700	-0.82746300	3.27407300
H	6.32788600	1.47535600	-0.35766800
H	7.62598900	0.53257300	1.54495700
C	1.55295100	-1.92486800	1.87659900
C	2.39346900	-3.04074600	1.73769300
C	0.30738700	-2.09453400	2.50676100
C	2.00637300	-4.28763100	2.23594900
H	3.35055100	-2.94337100	1.23718100
C	-0.07610900	-3.33977700	3.00345900
H	-0.36495200	-1.24883700	2.61240100
C	0.77441300	-4.44094700	2.87233200
H	2.67215200	-5.13798300	2.12003900
H	-1.03888400	-3.44864700	3.49478900
H	0.47645100	-5.41052300	3.26112000
Br	-0.11081200	0.86977200	-3.09867800