Supporting Information

Mechanistic insights into the selective cyclization of indolines with alkynes and alkenes to produce six- and seven-membered 1,7-fused indolines via Rh(III) catalysis: a theoretical study

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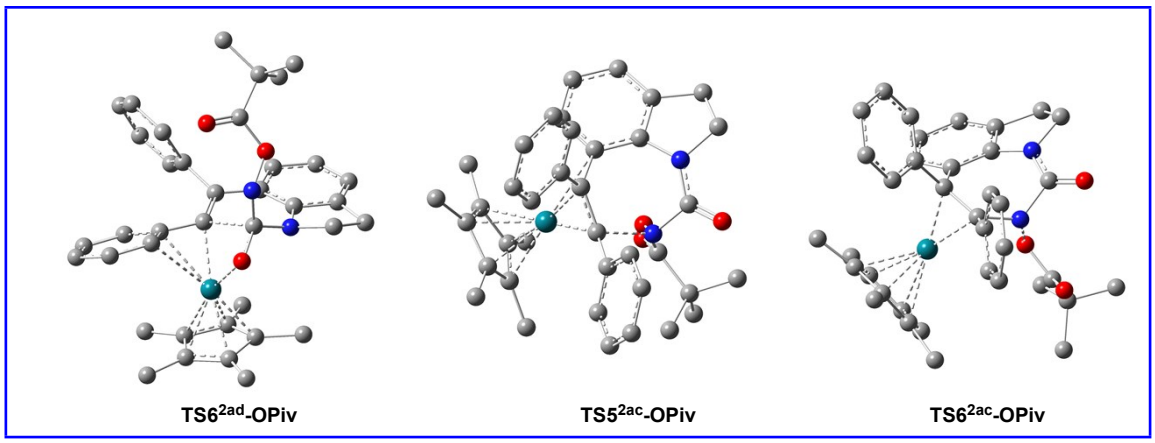

Fig. S1 Optimized structures of transition states **TS6^{2ad}-OPiv**, **TS5^{2ac}-OPiv**, and **TS6^{2ac}-OPiv**. The hydrogen atoms not participating in the reaction have been omitted for clarity. The relative free energies for the three transition states are 8.4, 21.3, and 10.2 kcal/mol, respectively, which indicates that the seven-membered ring product could not be obtained.

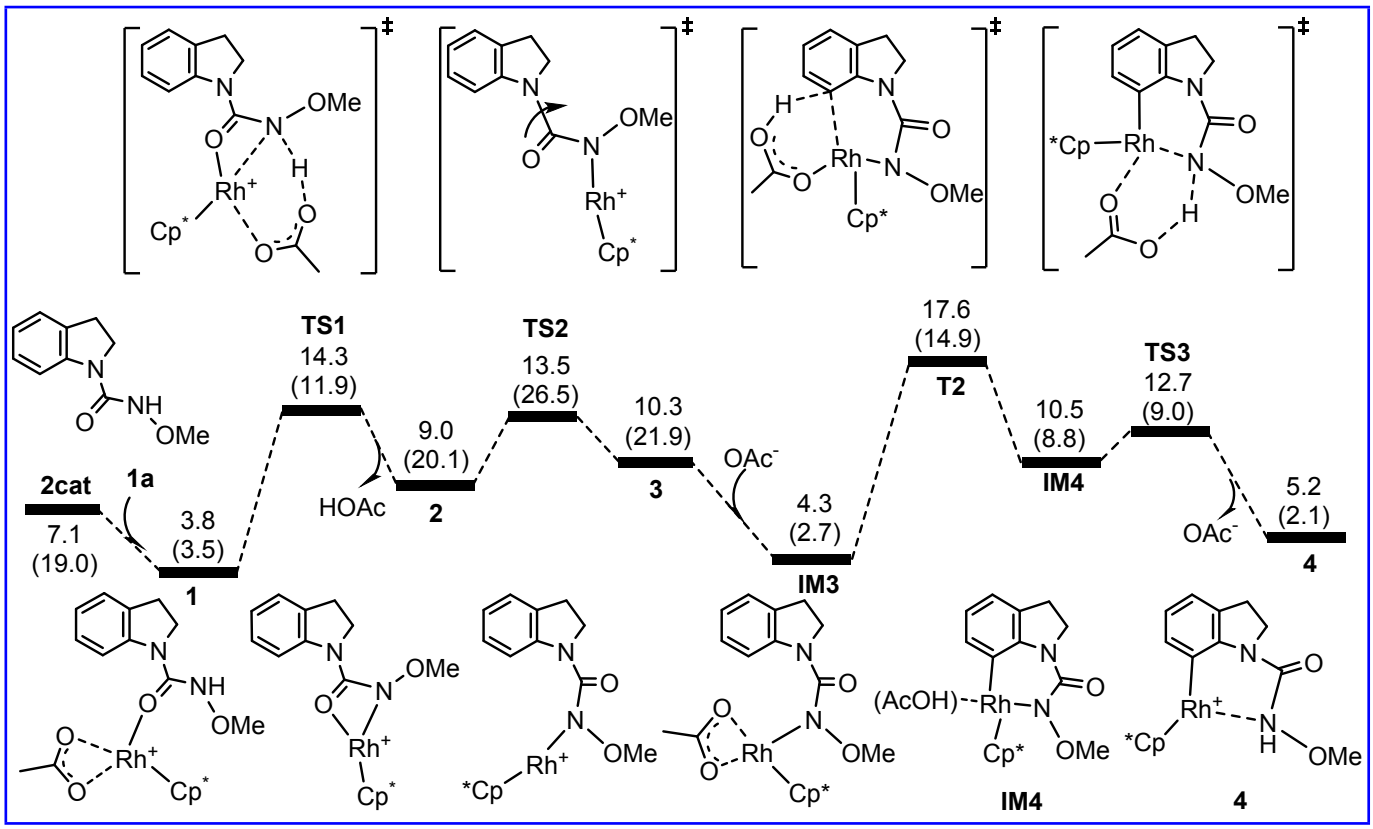

Fig. S2 Free energy diagram from **2cat** to **4** in dimethylformamide solvent. The relative free energies and relative enthalpic energies (in parentheses) are given in kcal/mol.

Cartesian coordinates and SCF energies in solution for all of the calculated structures

1a

Sum of electronic and thermal Free Energies= -648.026219

C	-5.21266	-2.0015	-0.30889
C	-3.76688	-2.0015	-0.30889
C	-3.06819	-0.81106	-0.30889
C	-3.79469	0.39143	-0.30876
C	-5.18465	0.39143	-0.30864
C	-5.9112	-0.81103	-0.30863
C	-4.49004	-4.20669	-0.30921
C	-3.3399	-3.39505	-0.30903
H	-1.9694	-0.79452	-0.30903
H	-3.24872	1.34667	-0.30874
H	-5.73065	1.34664	-0.3084
H	-7.00996	-0.79433	-0.30843
H	-4.49004	-4.82447	-1.18285
H	-2.75731	-3.59439	0.56604
N	-5.63966	-3.39521	-0.30912
H	-2.75719	-3.59418	-1.18407
H	-4.49011	-4.82476	0.56423
C	-7.04016	-3.84186	-0.30912
O	-7.37038	-5.04028	-0.30922
N	-7.96627	-2.83642	-0.30901
H	-7.69144	-1.88931	-0.30881
O	-9.2964	-3.11993	-0.30903
C	-10.04426	-1.90108	-0.30886
H	-9.80087	-1.33317	-1.18245
H	-11.09064	-2.12466	-0.30888
H	-9.80085	-1.33339	0.56486

cat

Sum of electronic and thermal Free Energies= -956.385250

C	1.54976	-2.10573	-0.86756
C	1.95383	-0.98417	-1.71169
C	3.3017	-0.62923	-1.3594
C	3.70276	-1.44807	-0.24742
C	2.61903	-2.38784	0.02826
C	2.65972	-3.43981	1.09381
H	1.67002	-3.85996	1.28095
H	3.32526	-4.25941	0.79563
H	3.03131	-3.02994	2.03687
C	0.23207	-2.81066	-0.95941
H	-0.59845	-2.10338	-1.03002
H	0.21374	-3.44445	-1.85543
H	0.05977	-3.45223	-0.0929
C	1.14881	-0.3949	-2.82638
H	1.37452	0.66699	-2.93271
H	1.37909	-0.90767	-3.77028
H	0.07888	-0.49177	-2.63296
C	4.12637	0.42739	-2.02541
H	4.92095	0.78613	-1.36753
H	4.59633	0.0164	-2.92813
H	3.50516	1.27972	-2.30425
C	5.03674	-1.44405	0.43437
H	5.72166	-2.15086	-0.05216
H	5.49768	-0.45462	0.40328
H	4.94567	-1.7368	1.48333
C	2.12629	2.61731	-0.10709
O	2.3797	1.68439	0.76138
O	1.70321	2.46245	-1.25968
C	0.39884	0.04529	2.3533
O	1.58769	-0.36426	2.54692
O	-0.01838	0.17849	1.15824
C	2.37524	4.02118	0.44202
H	2.61645	4.70284	-0.37632
H	1.45645	4.37404	0.92377
H	3.17017	4.02311	1.19049
C	-0.49488	0.40259	3.51186
H	-0.34214	1.45813	3.76114
H	-1.5417	0.26112	3.23671
H	-0.2411	-0.19645	4.38861
Rh	1.96171	-0.30879	0.37133

IM1

Sum of electronic and thermal Free Energies= -1604.381199

C	3.50494	0.19403	-0.17278
C	4.86989	0.3882	0.10898

C	5.38745	1.6685	0.24141
C	4.53686	2.77262	0.0995
C	3.18277	2.5724	-0.16565
C	2.64459	1.28525	-0.29379
C	4.39251	-1.94277	0.31434
C	5.56605	-0.94919	0.2054
H	6.44323	1.81066	0.45725
H	4.93033	3.77935	0.20168
H	2.51898	3.42581	-0.27007
H	1.58765	1.17042	-0.48611
H	4.52505	-2.85725	-0.26091
H	6.24385	-1.0214	1.06093
N	3.22391	-1.19354	-0.21435
H	6.16037	-1.14206	-0.69731
H	4.20206	-2.22868	1.35656
C	2.17029	-1.9553	-0.69879
O	2.19789	-3.17714	-0.57624
N	1.04875	-1.31359	-1.25856
H	1.11431	-0.36587	-1.64543
O	0.50272	-2.09495	-2.31072
C	-0.50752	-2.99565	-1.85968
H	-1.33612	-2.45344	-1.396
H	-0.86285	-3.47654	-2.77565
H	-0.08758	-3.75009	-1.18975
C	0.02694	0.70834	2.35273
C	-1.3521	0.34213	2.04469
C	-1.41363	-1.11485	1.93027
C	-0.08918	-1.60751	2.04015
C	0.80396	-0.47534	2.31287
C	2.2641	-0.60344	2.61073
H	2.81464	0.30327	2.35661
H	2.40341	-0.80113	3.68167
H	2.71106	-1.43307	2.06022
C	0.50416	2.11001	2.57644
H	0.21206	2.74446	1.73375
H	0.07076	2.52289	3.49442
H	1.59147	2.1518	2.6636
C	-2.52997	1.2592	2.05902
H	-3.19293	1.0245	1.22328
H	-3.07907	1.14079	3.00289
H	-2.21848	2.30243	1.9752
C	-2.66979	-1.90507	1.73965
H	-2.46293	-2.89535	1.32814
H	-3.16963	-2.04326	2.70726
H	-3.34769	-1.38404	1.06187
C	0.35576	-3.0359	1.99128
H	0.56165	-3.39487	3.00832
H	-0.41255	-3.6808	1.56216
H	1.27003	-3.16234	1.40589
C	-2.47114	-0.43685	-1.59939
O	-1.20248	-0.65854	-1.37916
O	-3.28542	0.00637	-0.78705
C	0.65654	1.76348	-1.77242
O	1.38895	0.90682	-2.27613
O	0.11259	1.69125	-0.58729
C	-2.88151	-0.79014	-3.02489
H	-3.95489	-0.6451	-3.15275
H	-2.33346	-0.15961	-3.73136
H	-2.614	-1.8272	-3.24873
C	0.3182	3.04499	-2.52013
H	-0.70119	2.96616	-2.91278
H	0.34209	3.90517	-1.84612
H	1.00987	3.19133	-3.35083
Rh	-0.20425	-0.13779	0.32987

T1

Sum of electronic and thermal Free Energies= -1604.372144

C	3.76107	-0.3184	-0.02761
C	5.04897	-0.88267	-0.07256
C	6.17678	-0.07431	-0.11971
C	6.02192	1.31635	-0.10496
C	4.74156	1.86817	-0.03626
C	3.59459	1.06763	0.00749
C	3.51423	-2.60125	0.47674
C	4.94215	-2.38945	-0.05376
H	7.16755	-0.52051	-0.15533
H	6.89463	1.96209	-0.13456
H	4.61674	2.94682	-0.00805
H	2.62333	1.53941	0.05399
H	3.00988	-3.4777	0.06775
H	5.69265	-2.8727	0.57839
N	2.80089	-1.3692	0.06111
H	5.04804	-2.80305	-1.06629
H	3.50228	-2.6863	1.57035
C	1.42584	-1.37409	0.27313
O	0.93018	-2.24861	0.99594
N	0.60816	-0.44713	-0.36997
H	0.59145	0.48866	0.57498
O	1.28373	0.29875	-1.35856

C	1.22904	-0.34853	-2.62772
H	0.19526	-0.4157	-2.9803
H	1.8055	0.29262	-3.29913
H	1.69212	-1.34272	-2.58578
C	-3.04401	-0.279	1.20831
C	-3.64613	-0.46894	-0.0747
C	-3.13819	-1.70299	-0.60593
C	-2.3041	-2.34154	0.41395
C	-2.22806	-1.45603	1.51922
C	-1.53093	-1.70268	2.81944
H	-1.20542	-0.76466	3.27491
H	-2.21592	-2.1954	3.52232
H	-0.65184	-2.32982	2.67384
C	-3.27724	0.88103	2.11817
H	-3.42001	1.79266	1.53795
H	-4.16887	0.6942	2.73238
H	-2.42673	1.03726	2.78302
C	-4.60783	0.46394	-0.74533
H	-4.60015	0.33183	-1.82948
H	-5.62862	0.27004	-0.39204
H	-4.34784	1.50146	-0.53216
C	-3.49962	-2.30511	-1.92699
H	-2.68839	-2.92066	-2.32239
H	-4.38351	-2.94769	-1.81918
H	-3.7331	-1.53552	-2.66531
C	-1.702	-3.70758	0.32271
H	-2.30631	-4.41901	0.90042
H	-1.67069	-4.06373	-0.7097
H	-0.68478	-3.69933	0.71746
C	-1.67842	2.30325	-1.40991
O	-1.32615	1.0898	-1.72777
O	-2.2366	2.64449	-0.35877
C	0.44701	2.64682	1.06177
O	0.20655	1.38556	1.49314
O	1.22383	2.89843	0.16419
C	-1.29072	3.34074	-2.45435
H	-1.9911	4.17807	-2.42858
H	-0.29578	3.71572	-2.19061
H	-1.24202	2.90964	-3.45616
C	-0.37943	3.6677	1.79764
H	0.11647	4.63795	1.75788
H	-1.33739	3.73397	1.27127
H	-0.56328	3.36978	2.83197
Rh	-1.42661	-0.40579	-0.28934

IM2

Sum of electronic and thermal Free Energies= -1604.385085

C	-3.7516	-0.35126	0.03422
C	-5.0193	-0.95655	0.10694
C	-6.16998	-0.18439	0.1941
C	-6.0585	1.21048	0.19075
C	-4.7983	1.80261	0.09085
C	-3.62866	1.03892	0.00595
C	-3.44781	-2.6169	-0.51139
C	-4.86652	-2.45883	0.06106
H	-7.14522	-0.66158	0.25096
H	-6.94966	1.82829	0.25163
H	-4.70796	2.88485	0.06785
H	-2.67385	1.53955	-0.07027
H	-2.90572	-3.48426	-0.133
H	-5.61874	-2.95521	-0.55879
N	-2.76125	-1.37043	-0.09267
H	-4.93158	-2.89219	1.06881
H	-3.4638	-2.68169	-1.60642
C	-1.38841	-1.34106	-0.31476
O	-0.87793	-2.20212	-1.04311
N	-0.58192	-0.39661	0.32133
H	-0.44751	1.14379	-1.29916
O	-1.25602	0.33879	1.32088
C	-1.25237	-0.34872	2.57206
H	-0.22967	-0.45696	2.94441
H	-1.82619	0.2901	3.24796
H	-1.7452	-1.32545	2.4896
C	3.08095	-0.23703	-1.21459
C	3.67076	-0.42207	0.07607
C	3.1592	-1.65579	0.60505
C	2.33846	-2.29765	-0.42484
C	2.27328	-1.41513	-1.53503
C	1.59896	-1.6604	-2.84849
H	1.23671	-0.72533	-3.28256
H	2.30956	-2.10467	-3.55804
H	0.74461	-2.32561	-2.7291
C	3.29362	0.92953	-2.12185
H	3.54269	1.82416	-1.55129
H	4.1109	0.70941	-2.82218
H	2.393	1.14467	-2.69932
C	4.6119	0.51775	0.76737
H	4.5077	0.44973	1.85301
H	5.65042	0.27299	0.51048

H	4.41632	1.55147	0.48086
C	3.51374	-2.25489	1.92952
H	2.70597	-2.88087	2.31532
H	4.40716	-2.88557	1.83155
H	3.72728	-1.48217	2.67083
C	1.73257	-3.66037	-0.32576
H	2.39182	-4.39552	-0.8058
H	1.60204	-3.96442	0.71561
H	0.75661	-3.67861	-0.81173
C	1.60632	2.20598	1.51455
O	1.41389	0.97076	1.87551
O	1.93674	2.56827	0.37655
C	-0.39379	3.02569	-1.50739
O	-0.06512	1.78314	-1.93492
O	-1.22188	3.22786	-0.64466
C	1.35083	3.2253	2.61513
H	1.99702	4.09474	2.47716
H	0.3106	3.55756	2.52926
H	1.49412	2.79467	3.6081
C	0.40034	4.09516	-2.20952
H	-0.11763	5.05074	-2.12623
H	1.36527	4.16296	-1.69696
H	0.57609	3.84227	-3.25764
Rh	1.45216	-0.36685	0.2665

IM3

Sum of electronic and thermal Free Energies= -1375.348117

C	3.48602	-0.50198	-0.08795
C	4.84494	-0.81982	-0.25068
C	5.82453	-0.0676	0.38409
C	5.44222	1.00037	1.2051
C	4.08727	1.29016	1.38157
C	3.08867	0.54659	0.74276
C	3.54752	-2.62161	-1.09134
C	4.96821	-2.02688	-1.15386
H	6.87514	-0.31567	0.25547
H	6.19736	1.59198	1.71411
H	3.7886	2.10234	2.03853
H	2.04634	0.78819	0.90107
H	3.22067	-3.09683	-2.01782
H	5.72892	-2.74158	-0.82709
N	2.69777	-1.44579	-0.79741
H	5.21884	-1.72384	-2.17964
H	3.45817	-3.35854	-0.28343
C	1.32243	-1.6528	-0.72964
O	0.87314	-2.80254	-0.64566
N	0.47651	-0.55683	-0.82486
O	1.11191	0.60453	-1.31575
C	1.04025	0.65045	-2.73986
H	-0.00197	0.63269	-3.07356
H	1.5072	1.59786	-3.02036
H	1.59543	-0.18179	-3.19029
C	-2.05801	-0.5794	1.98401
C	-3.22681	-0.29896	1.18504
C	-3.37802	-1.35798	0.24399
C	-2.31234	-2.33273	0.48028
C	-1.51517	-1.86578	1.56783
C	-0.39062	-2.60601	2.22136
H	0.28887	-1.92599	2.74035
H	-0.78984	-3.30981	2.96332
H	0.18719	-3.16407	1.48214
C	-1.55283	0.28011	3.09942
H	-1.25056	1.26574	2.73344
H	-2.33681	0.41192	3.85507
H	-0.68421	-0.16711	3.58516
C	-4.11671	0.89617	1.33799
H	-4.49573	1.22212	0.36862
H	-4.96671	0.6523	1.98854
H	-3.57715	1.7297	1.79397
C	-4.48166	-1.49048	-0.75494
H	-4.23681	-2.22062	-1.52894
H	-5.39735	-1.82983	-0.25258
H	-4.66784	-0.53029	-1.23721
C	-2.14839	-3.63945	-0.22851
H	-2.54694	-4.45151	0.39387
H	-2.69116	-3.64973	-1.17567
H	-1.09376	-3.8273	-0.43342
C	-2.52826	1.91584	-1.69832
O	-1.46371	1.47958	-1.06067
O	-3.58613	1.302	-1.81609
C	-2.3396	3.28516	-2.34172
H	-3.29087	3.6378	-2.74096
H	-1.93758	4.00386	-1.62323
H	-1.61204	3.20837	-3.15666
Rh	-1.37751	-0.39651	-0.07285

T2

Sum of electronic and thermal Free Energies= -1375.325011

Rh	-0.68986	-0.19055	0.03827
N	0.06792	1.69752	-0.35867

C	-0.44255	-1.73481	-1.53393
C	-1.23515	-2.35167	-0.47719
C	-2.43938	-1.60844	-0.35282
C	-2.43101	-0.54063	-1.33742
C	-1.21792	-0.65788	-2.09375
O	-1.72385	0.74058	1.69051
O	0.14222	1.06036	2.90064
C	-1.10356	1.17328	2.71041
C	-1.91369	1.89796	3.76878
H	-1.5784	1.59856	4.76427
H	-1.73539	2.97398	3.66963
H	-2.97977	1.70304	3.64691
O	-0.92944	2.48992	-0.98729
C	1.30403	2.00543	-0.86307
C	2.31837	0.01652	0.33465
C	1.22466	-0.49137	1.07461
C	3.58636	-0.60918	0.32851
C	1.48553	-1.69443	1.79286
H	0.64053	0.34119	1.89185
C	3.78325	-1.77643	1.03992
C	2.71866	-2.3281	1.78608
H	0.68803	-2.09812	2.41216
H	4.75516	-2.26458	1.0347
H	2.8785	-3.22939	2.37076
O	1.58081	2.97852	-1.56537
C	-0.83915	0.20468	-3.25929
H	-1.0578	1.25481	-3.05479
H	0.2243	0.12346	-3.49202
H	-1.40198	-0.10306	-4.14986
C	-3.53955	0.43657	-1.58574
H	-3.13511	1.41266	-1.86149
H	-4.19801	0.09166	-2.39409
H	-4.15163	0.56932	-0.69042
C	-3.54499	-1.83518	0.63302
H	-3.72284	-0.92982	1.22219
H	-4.47672	-2.09174	0.11523
H	-3.3092	-2.64734	1.32359
C	-0.87893	-3.61589	0.24721
H	-1.3729	-3.67901	1.21989
H	-1.18937	-4.49058	-0.3395
H	0.19694	-3.69152	0.41588
C	0.84362	-2.28088	-2.08001
H	1.46567	-2.70719	-1.28941
H	0.64412	-3.07247	-2.81431
H	1.42704	-1.50448	-2.57975
C	-1.1564	3.68272	-0.24235
H	-0.2554	4.30391	-0.22397
H	-1.95386	4.21177	-0.77334
H	-1.48359	3.45242	0.77782
C	4.523	0.16315	-0.57622
C	3.72364	1.44906	-0.90234
N	2.34678	1.13804	-0.47176
H	5.48237	0.39036	-0.10138
H	4.74442	-0.4073	-1.48758
H	4.09552	2.3154	-0.34275
H	3.72893	1.71804	-1.95887

IM4

Sum of electronic and thermal Free Energies= -1375.332389

Rh	-0.65244	-0.18366	0.03641
N	0.37958	1.46505	-0.6613
C	-0.85446	-1.83038	-1.35234
C	-1.51358	-2.28606	-0.1392
C	-2.61217	-1.4139	0.08903
C	-2.72884	-0.48646	-1.03168
C	-1.67509	-0.76672	-1.92664
O	-0.51231	0.51278	2.01128
O	-0.82309	0.68898	4.23148
C	-0.52031	1.18088	3.04541
C	-0.1561	2.63974	3.07793
H	-0.92399	3.2082	3.60918
H	0.78056	2.7584	3.63216
H	-0.03378	3.0174	2.06386
O	-0.57535	2.32828	-1.28663
C	1.51518	1.36002	-1.44983
C	2.33042	-0.34534	0.18018
C	1.15672	-0.65489	0.87951
C	3.6001	-0.78207	0.58766
C	1.32717	-1.38872	2.06905
H	-1.03704	-0.26922	4.11848
C	3.73319	-1.52496	1.75345
C	2.58734	-1.81376	2.50687
H	0.4546	-1.63675	2.67128
H	4.71006	-1.87121	2.08187
H	2.67471	-2.38069	3.42997
O	1.80866	2.10221	-2.38754
C	-1.4088	-0.0715	-3.22784
H	-1.53038	1.00886	-3.12779
H	-0.3907	-0.25468	-3.57646

H	-2.09905	-0.43438	-4.00028
C	-3.79009	0.56018	-1.20739
H	-3.38135	1.45327	-1.68763
H	-4.61865	0.19222	-1.8271
H	-4.21127	0.8637	-0.24514
C	-3.54446	-1.42986	1.2628
H	-3.63133	-0.43065	1.70066
H	-4.54853	-1.74795	0.95576
H	-3.19986	-2.11113	2.04319
C	-1.12079	-3.48686	0.66966
H	-1.50125	-3.42946	1.69265
H	-1.52396	-4.40429	0.22104
H	-0.03539	-3.59266	0.72927
C	0.25892	-2.54173	-2.06253
H	0.92955	-3.03788	-1.35714
H	-0.142	-3.30557	-2.74264
H	0.85939	-1.8461	-2.65301
C	-0.31832	3.68467	-0.94779
H	0.64815	4.00847	-1.34421
H	-1.12133	4.26101	-1.4176
H	-0.34753	3.84176	0.13976
C	4.63459	-0.36438	-0.43578
C	3.83768	0.52745	-1.42789
N	2.42202	0.3823	-1.02089
H	5.47198	0.18234	0.0122
H	5.06381	-1.23822	-0.94063
H	4.12383	1.58186	-1.36717
H	3.96558	0.22037	-2.46886

oac

Sum of electronic and thermal Free Energies= -229.052718

H	-2.55927	-0.76262	-0.00012
O	-1.52786	1.2481	0.00004
C	-0.94406	0.18578	-0.00004
O	-1.61581	-0.99559	0.00001
C	0.57331	-0.00992	-0.00001
H	1.03879	0.81101	0.50427
H	0.81529	-0.92194	0.50453
H	0.92704	-0.05569	-1.00881

IM5

Sum of electronic and thermal Free Energies= -1146.296932

Rh	-0.69232	-0.18728	0.04126
N	0.07573	1.69588	-0.35805
C	-0.4753	-1.72922	-1.53426
C	-1.26275	-2.342	-0.47199
C	-2.45991	-1.58892	-0.33532
C	-2.45371	-0.5209	-1.31918
C	-1.24836	-0.64523	-2.08559
O	-0.92182	2.49582	-0.97738
C	1.30922	1.99464	-0.87482
C	2.31896	-0.00167	0.31366
C	1.22384	-0.50715	1.05308
C	3.58641	-0.62821	0.30853
C	1.4834	-1.71093	1.77088
C	3.78215	-1.79503	1.02106
C	2.71655	-2.34491	1.76671
H	0.68506	-2.11524	2.38878
H	4.75358	-2.28413	1.01667
H	2.87475	-3.24615	2.35193
O	1.58646	2.96663	-1.57852
C	-0.87314	0.21622	-3.25318
H	-1.07954	1.26798	-3.04428
H	0.1871	0.12527	-3.49669
H	-1.44773	-0.0842	-4.13872
C	-3.55674	0.46572	-1.55488
H	-3.14754	1.437	-1.84031
H	-4.23064	0.12424	-2.35191
H	-4.15416	0.60776	-0.65106
C	-3.55813	-1.80991	0.66008
H	-3.73507	-0.90057	1.24316
H	-4.49273	-2.07318	0.15076
H	-3.31567	-2.61571	1.35577
C	-0.91113	-3.6109	0.24653
H	-1.39195	-3.66909	1.22616
H	-1.24007	-4.48163	-0.336
H	0.16602	-3.69941	0.39992
C	0.80066	-2.28484	-2.09467
H	1.42618	-2.71927	-1.31136
H	0.58702	-3.07209	-2.82965
H	1.3864	-1.51212	-2.5974
C	-1.1324	3.69033	-0.2306
H	-0.22655	4.30465	-0.22096
H	-1.93088	4.2255	-0.7539
H	-1.4516	3.46282	0.79281
C	4.52378	0.14171	-0.5975
C	3.72557	1.4276	-0.92648
N	2.34877	1.11953	-0.49371
H	5.48323	0.36914	-0.12289
H	4.74505	-0.43076	-1.50761

H	4.09893	2.2953	-0.36998
H	3.73041	1.69338	-1.98388

4a

Sum of electronic and thermal Free Energies= -234.505638

C	-0.25348	-0.13489	2.01093
C	0.16162	1.01597	1.77726
C	-0.86876	-1.24632	2.76606
H	-1.81871	-1.51454	2.29348
H	-0.23706	-2.13933	2.68662
C	-1.0899	-0.88721	4.24533
H	-1.75	-0.02054	4.34306
H	-1.55106	-1.72861	4.77222
H	-0.1446	-0.64886	4.7423
C	0.49327	2.44324	1.95466
H	-0.03089	3.03098	1.1944
H	1.56249	2.5875	1.76151
C	0.13248	2.94143	3.36541
H	0.6656	2.38074	4.13974
H	0.39715	3.99877	3.4645
H	-0.94113	2.84347	3.55057

IM6[4a]

Sum of electronic and thermal Free Energies= -1380.772162

Rh	0.60453	-0.18536	-0.08107
N	-0.31434	1.4438	-1.07827
C	2.80129	-0.7258	0.59165
C	2.15677	-1.9014	0.05
C	1.9033	-1.65058	-1.3423
C	2.3417	-0.31792	-1.63038
C	2.92732	0.24618	-0.43868
O	0.63764	2.51748	-1.11632
C	-1.54945	1.94514	-0.68541
C	-2.38488	-0.40778	-0.57346
C	-1.20636	-1.14046	-0.39927
C	-3.64736	-1.01125	-0.7182
C	-1.36598	-2.53593	-0.37665
C	-3.76893	-2.39308	-0.70489
C	-2.61121	-3.15898	-0.53155
H	-0.50798	-3.17144	-0.19211
H	-4.74023	-2.86867	-0.81445
H	-2.6746	-4.24343	-0.49543
O	-1.832	3.14252	-0.55475
C	3.62045	1.57465	-0.35887
H	2.98972	2.36364	-0.77344
H	3.85694	1.84285	0.67399
H	4.56644	1.558	-0.91535
C	2.33445	0.31873	-2.98642
H	2.52242	1.39016	-2.91862
H	3.11417	-0.12295	-3.62065
H	1.3741	0.17776	-3.48901
C	1.43685	-2.63979	-2.3679
H	0.97075	-2.13876	-3.21936
H	2.28798	-3.22026	-2.74852
H	0.70891	-3.3452	-1.96416
C	2.07984	-3.22702	0.7517
H	1.33943	-3.89117	0.30078
H	3.04729	-3.74516	0.70137
H	1.83031	-3.11582	1.81066
C	3.30591	-0.61375	1.99924
H	2.56951	-0.97995	2.72038
H	4.21836	-1.20988	2.12828
H	3.54386	0.41824	2.2644
C	0.48096	3.28688	-2.30821
H	-0.44263	3.87002	-2.27531
H	1.34444	3.9602	-2.33631
H	0.48602	2.64251	-3.19555
C	-4.69894	0.06863	-0.87999
C	-3.95009	1.35544	-0.45274
N	-2.53195	0.98339	-0.55252
H	-5.02831	0.13475	-1.92574
H	-5.59176	-0.10598	-0.27178
H	-4.15175	2.22122	-1.08479
H	-4.19515	1.63551	0.58067
C	-0.1732	-0.47002	1.59635
C	0.27671	0.77735	1.34309
C	-0.78848	-1.58144	2.35148
H	-1.73843	-1.84967	1.87891
H	-0.15678	-2.47446	2.27204
C	-1.00962	-1.22233	3.83075
H	-1.66972	-0.35567	3.92848
H	-1.47079	-2.06373	4.35764
H	-0.06433	-0.98399	4.32772
C	0.60835	2.20462	1.52048
H	0.0842	2.79236	0.76023
H	1.67758	2.34888	1.32733
C	0.24757	2.70282	2.93124
H	0.78069	2.14212	3.70557
H	0.51224	3.76016	3.03033
H	-0.82604	2.60485	3.1164

T3[4a]

Sum of electronic and thermal Free Energies= -1380.748417

Rh	-0.65773	0.06422	-0.06262
N	0.33925	-1.71681	-0.64946
C	-2.88096	0.65017	0.50264
C	-2.31607	1.70373	-0.30549
C	-2.05981	1.17154	-1.61927
C	-2.39621	-0.20892	-1.59277
C	-2.92164	-0.53582	-0.27705
O	-0.55334	-2.80995	-0.38887
C	1.61067	-2.06304	-0.21419
C	2.3406	0.30335	-0.57369
C	1.15412	1.02454	-0.3736
C	3.54227	0.90932	-0.98415
C	1.2274	2.40006	-0.68429
C	3.58321	2.26649	-1.26354
C	2.40507	3.01298	-1.11787
H	0.34923	3.01971	-0.54626
H	4.5062	2.74259	-1.58367
H	2.40681	4.07894	-1.32884
O	1.97143	-3.19135	0.13534
C	-3.53631	-1.85001	0.10473
H	-2.8619	-2.6748	-0.1323
H	-3.75266	-1.89348	1.17519
H	-4.4835	-2.00879	-0.42725
C	-2.36466	-1.14198	-2.76551
H	-2.40391	-2.18168	-2.44091
H	-3.22685	-0.96181	-3.42097
H	-1.45799	-1.01157	-3.36168
C	-1.60511	1.9505	-2.81786
H	-1.25228	1.28567	-3.60974
H	-2.42748	2.54982	-3.23048
H	-0.78649	2.63433	-2.57647
C	-2.32247	3.16036	0.06091
H	-1.60737	3.73777	-0.53011
H	-3.31399	3.59256	-0.13209
H	-2.09993	3.32193	1.11803
C	-3.38344	0.8252	1.90576
H	-2.72164	1.46993	2.49121
H	-4.37876	1.28841	1.90963
H	-3.46365	-0.13048	2.4288
C	-0.40201	-3.83696	-1.36993
H	0.53939	-4.37297	-1.22984
H	-1.24633	-4.5167	-1.21237
H	-0.44758	-3.41962	-2.38293
C	4.62473	-0.14936	-1.06246
C	3.99181	-1.35547	-0.32343
N	2.55297	-1.04748	-0.31858
H	4.84633	-0.40021	-2.10836
H	5.56529	0.16567	-0.60055
H	4.16158	-2.31721	-0.8088
H	4.36399	-1.43415	0.70632
C	0.65666	0.64492	1.64497
C	0.07022	-0.46464	1.84266
C	1.36278	1.75867	2.3533
C	0.47774	2.95646	2.72603
H	2.22147	2.104	1.77269
H	1.75585	1.30595	3.27317
H	1.05093	3.67442	3.32187
H	0.11995	3.47483	1.83365
H	-0.38877	2.63951	3.31499
C	-0.19877	-1.69358	2.62337
C	0.56812	-1.72713	3.95585
H	0.06533	-2.56195	2.00869
H	-1.27853	-1.77042	2.80414
H	0.33983	-2.64987	4.49864
H	1.64777	-1.69755	3.78213
H	0.29976	-0.8806	4.59636

IM7[4a]

Sum of electronic and thermal Free Energies= -1380.789872

Rh	1.05897	-0.19205	-0.18534
N	0.71855	0.22486	1.85279
C	1.97697	-1.77199	-1.53311
C	2.3269	-0.5131	-2.08704
C	3.2345	0.16851	-1.15696
C	3.38745	-0.64123	-0.02681
C	2.5338	-1.82145	-0.19719
O	0.85419	-0.94176	2.66595
C	-0.16553	1.11197	2.41245
C	-0.19853	2.38087	0.24604
C	-0.63544	1.48866	-0.76283
C	0.3864	3.63417	-0.07084
C	-0.37421	1.88958	-2.10602
C	0.60081	3.9907	-1.38487
C	0.22852	3.09709	-2.41663
H	-0.70649	1.22711	-2.89967
H	1.03748	4.95511	-1.6322
H	0.38243	3.37703	-3.45448

O	-0.61142	1.08578	3.55742
C	2.52696	-3.01251	0.71097
H	2.46117	-2.70457	1.75633
H	1.67257	-3.6605	0.50586
H	3.44345	-3.60401	0.57991
C	4.2762	-0.39744	1.15338
H	3.82596	-0.77726	2.07135
H	5.23749	-0.9118	1.02128
H	4.48517	0.66536	1.29653
C	3.88261	1.49159	-1.43474
H	4.3984	1.87948	-0.55341
H	4.62284	1.40439	-2.24087
H	3.14707	2.23977	-1.74938
C	2.0587	-0.04541	-3.48636
H	1.89364	1.03391	-3.52342
H	2.91749	-0.27137	-4.13264
H	1.18349	-0.5362	-3.91846
C	1.24695	-2.8857	-2.21932
H	0.65169	-2.51933	-3.05886
H	1.96298	-3.6188	-2.61339
H	0.57089	-3.40836	-1.54064
C	1.59827	-0.6909	3.86058
H	1.0073	-0.11739	4.57693
H	1.83334	-1.68026	4.26612
H	2.5285	-0.15386	3.63724
C	0.62966	4.38824	1.2204
C	-0.22988	3.59534	2.23818
N	-0.40342	2.26723	1.60888
H	1.69309	4.35694	1.49317
H	0.33657	5.44028	1.16325
H	0.22843	3.47821	3.22021
H	-1.20963	4.06733	2.37614
C	-1.57571	0.3385	-0.47767
C	-0.89788	-0.79838	-0.23515
C	-3.09252	0.60427	-0.46139
C	-3.63984	0.64075	-1.85776
H	-3.27061	1.57687	0.05857
H	-3.58192	-0.20434	0.13413
H	-4.74007	0.83345	-1.8464
H	-3.15014	1.44944	-2.45298
H	-3.46138	-0.3319	-2.37754
C	-1.42316	-2.23689	-0.07274
C	-1.8544	-2.79688	-1.39606
H	-2.27843	-2.21684	0.64568
H	-0.60806	-2.85763	0.37258
H	-2.23543	-3.84034	-1.27871
H	-2.66945	-2.17582	-1.8411
H	-0.99897	-2.81658	-2.11435

T4[4ad]

Sum of electronic and thermal Free Energies= -1380.777872

Rh	-0.93948700	-0.15661100	-0.16197900
N	1.77371900	1.83520000	1.39260900
C	-2.85714200	-1.16881600	-0.05793800
C	-1.86045500	-2.18754700	0.27655400
C	-1.23467900	-1.82730000	1.49903700
C	-1.78361000	-0.56423500	1.91335300
C	-2.82151500	-0.17273800	0.97423200
O	0.96454400	2.41639000	2.43070400
C	2.02757400	0.58871900	1.71708100
C	2.21256400	-0.57225600	-0.53322300
C	1.09714300	-0.05617500	-1.29287300
C	2.86698200	-1.75547000	-0.97409600
C	0.67954400	-0.84201800	-2.42456200
C	2.40929800	-2.47763000	-2.05525100
C	1.28605400	-2.03243300	-2.78302400
H	-0.10703000	-0.42710200	-3.04388800
H	2.92209200	-3.39006400	-2.35137100
H	0.93505500	-2.58780900	-3.64658100
O	1.79519500	-0.10122300	2.73349000
C	-3.77329500	0.97173600	1.15102800
H	-3.28058200	1.83252500	1.60957500
H	-4.19718900	1.29447300	0.19680700
H	-4.60810800	0.68383600	1.80351700
C	-1.40646500	0.16894700	3.16025000
H	-1.92653800	-0.28460100	4.01662400
H	-0.32753700	0.12364500	3.33446100
H	-1.68992300	1.22149800	3.11055100
C	-0.18126600	-2.59344900	2.24245900
H	0.24708400	-3.38446900	1.62136600
H	0.62302400	-1.92514300	2.56865700
H	-0.61402700	-3.07270600	3.13051900
C	-1.60607500	-3.42871500	-0.52315700
H	-0.57749000	-3.77691500	-0.40668100
H	-2.27359800	-4.23782500	-0.19805900
H	-1.78103300	-3.26301600	-1.58894200
C	-3.86507900	-1.27402000	-1.16316800
H	-3.44232700	-1.74748100	-2.05262700
H	-4.72115600	-1.88266100	-0.84115700

H	-4.24706200	-0.29295200	-1.45423500
C	1.17168600	3.80861900	2.40366300
H	0.89200800	4.25263300	1.43586100
H	0.53314500	4.22926100	3.18768500
H	2.21876900	4.07262000	2.61199700
C	4.06325600	-2.00346000	-0.08755900
C	3.80490600	-1.05477000	1.10032600
N	2.77072900	-0.10190200	0.62107300
H	4.16086700	-3.04767600	0.22541700
H	4.98887600	-1.73661500	-0.61405700
H	3.40682900	-1.57214300	1.97674900
H	4.69573800	-0.50002000	1.40763200
C	0.61337200	1.37027200	-1.25888400
C	-0.74963000	1.47959000	-1.21025500
C	1.61144800	2.48801200	-1.49375000
C	1.93474900	2.62964700	-2.99386000
H	2.51612000	2.28702100	-0.92028900
H	1.20782200	3.42625300	-1.10335100
H	2.67845300	3.41904200	-3.14592600
H	2.34513600	1.70076200	-3.40353900
H	1.04592200	2.88900200	-3.57935900
C	-1.61764900	2.66614600	-1.48905000
C	-2.38158400	2.53874200	-2.82085800
H	-1.00826500	3.58099800	-1.51191900
H	-2.34134900	2.79418300	-0.67591900
H	-3.01826600	3.41368600	-2.98791200
H	-1.69074500	2.45683100	-3.66625000
H	-3.01765000	1.64760900	-2.82449100

IM8[4ad]

Sum of electronic and thermal Free Energies= -1380.784016

Rh	0.63055	-0.05004	0.09446
N	-1.91203	-0.14957	-3.37125
C	2.63695	0.4242	1.03197
C	1.84663	-0.15457	2.05669
C	1.61117	-1.5647	1.7161
C	2.19275	-1.82008	0.47148
C	2.75886	-0.55945	-0.02341
O	-0.97746	-0.26975	-4.44627
C	-1.38145	-0.66227	-2.21375
C	-2.17074	-0.48056	0.1728
C	-1.62115	0.71071	0.71298
C	-2.82456	-1.43567	0.99603
C	-1.69393	0.84051	2.13112
C	-2.89231	-1.2547	2.36054
C	-2.30391	-0.1056	2.93754
H	-1.27551	1.73978	2.57225
H	-3.40607	-1.97808	2.98888
H	-2.36065	0.04907	4.01094
O	-0.19054	-0.84674	-1.97008
C	3.62946	-0.43559	-1.236
H	3.24871	-1.03889	-2.06021
H	3.68743	0.59786	-1.58482
H	4.6514	-0.77105	-1.01035
C	2.23633	-3.11844	-0.2764
H	1.75385	-3.03162	-1.25439
H	3.27243	-3.43734	-0.44481
H	1.72966	-3.91526	0.27301
C	0.86612	-2.51645	2.60297
H	0.74027	-3.49425	2.1329
H	1.39922	-2.66649	3.55046
H	-0.13058	-2.13318	2.84878
C	1.5239	0.45483	3.38941
H	0.54721	0.12714	3.75421
H	2.27159	0.16148	4.13883
H	1.51525	1.54692	3.34347
C	3.30482	1.7657	1.06046
H	2.76069	2.47474	1.68839
H	4.32231	1.67608	1.4639
H	3.38601	2.1967	0.06052
C	0.01776	0.7496	-4.3992
H	0.64434	0.6459	-3.51053
H	0.6214	0.60188	-5.30027
H	-0.43175	1.75216	-4.42523
C	-3.40198	-2.52021	0.10974
C	-3.36433	-1.86098	-1.29116
N	-2.33065	-0.81253	-1.16478
H	-2.77219	-3.41974	0.13799
H	-4.41318	-2.81822	0.40063
H	-3.10081	-2.54063	-2.10192
H	-4.33108	-1.40372	-1.53526
C	-1.21273	1.88574	-0.14881
C	0.04969	1.78554	-0.57659
C	-2.24613	2.94769	-0.47878
C	-2.65102	3.8551	0.69529
H	-3.14487	2.44478	-0.86327
H	-1.86661	3.56396	-1.30121
H	-3.40698	4.58346	0.3815
H	-3.0751	3.27459	1.52105

H	-1.78843	4.40824	1.08267
C	0.81427	2.70758	-1.48909
C	1.09322	4.10164	-0.89659
H	0.249	2.81777	-2.42488
H	1.75791	2.23803	-1.78177
H	1.66819	4.71289	-1.60147
H	0.16489	4.63487	-0.67241
H	1.66448	4.03344	0.03421

IM9[4ad]

Sum of electronic and thermal Free Energies= -1609.839049

Rh	-0.80937	-0.18382	-0.11908
N	3.12898	-1.64451	-0.85654
C	-2.96068	-0.72461	0.04816
C	-2.88229	0.68142	-0.1845
C	-2.3852	0.89886	-1.5536
C	-2.06002	-0.34376	-2.10017
C	-2.32875	-1.37161	-1.07866
O	2.68604	-2.95371	-1.18076
C	2.11765	-0.8313	-0.80356
C	1.67785	1.47815	-0.05578
C	0.80027	1.29567	1.04642
C	1.8319	2.73909	-0.68144
C	0.04412	2.43906	1.43617
C	1.08958	3.82196	-0.25828
C	0.17157	3.66756	0.80606
H	-0.62684	2.32966	2.28315
H	1.20682	4.79076	-0.73816
H	-0.40839	4.51941	1.14808
O	0.86363	-1.0939	-1.0135
C	-2.19582	-2.84511	-1.31737
H	-1.23287	-3.0748	-1.78093
H	-2.25927	-3.40965	-0.38397
H	-2.99167	-3.20689	-1.98234
C	-1.41695	-0.64713	-3.41781
H	-0.43087	-1.09763	-3.25389
H	-2.02026	-1.35573	-3.99737
H	-1.28425	0.25415	-4.02075
C	-2.23201	2.25338	-2.17764
H	-1.76343	2.19145	-3.16229
H	-3.20822	2.73896	-2.3021
H	-1.61715	2.91237	-1.55468
C	-3.45792	1.76499	0.67848
H	-2.85672	2.67622	0.62381
H	-4.47562	2.01923	0.35264
H	-3.51175	1.46099	1.72662
C	-3.64124	-1.40691	1.19604
H	-3.66157	-0.77474	2.08649
H	-4.68085	-1.6434	0.93318
H	-3.14908	-2.34509	1.4617
C	3.82173	-3.79299	-1.20097
H	4.32237	-3.82783	-0.22335
H	3.45368	-4.79139	-1.45558
H	4.55357	-3.47077	-1.95503
C	2.86176	2.61142	-1.78524
C	3.44175	1.1865	-1.5651
N	2.5064	0.53697	-0.62028
H	2.39041	2.7024	-2.77233
H	3.63914	3.37944	-1.7278
H	3.50576	0.59448	-2.47971
H	4.44473	1.22565	-1.1253
C	0.87969	0.07822	1.94506
C	0.00044	-0.87276	1.61428
C	1.93693	0.05255	3.03382
C	1.68855	1.03059	4.19425
H	2.90785	0.28497	2.57438
H	2.01974	-0.96753	3.42536
H	2.50223	0.98287	4.92642
H	1.62435	2.06333	3.8364
H	0.75219	0.79887	4.71374
C	-0.19679	-2.22545	2.24415
C	-0.85447	-2.18122	3.63585
H	0.78024	-2.72259	2.32376
H	-0.79149	-2.86123	1.57966
H	-0.9938	-3.19269	4.03407
H	-0.23794	-1.62247	4.34616
H	-1.83402	-1.69457	3.59883
H	4.69892	-0.7442	-0.88547
O	5.50281	-0.15685	-2.93208
C	6.05177	0.08651	-1.88113
O	5.53164	-0.28534	-0.68386
C	7.35979	0.81681	-1.71
H	7.74668	1.10361	-2.68686
H	7.21304	1.70532	-1.08874
H	8.08068	0.17513	-1.19469

T5[4ad]

Rh	-1.49970600	-0.29004100	-0.14398400
N	2.65266400	-1.21337000	-0.44561600
C	-3.54779000	-1.14556000	-0.08431700

C	-3.65437800	0.24165500	-0.40916900
C	-3.09564300	0.44677400	-1.75701000
C	-2.55268600	-0.76387000	-2.19027800
C	-2.74573100	-1.75633700	-1.11816400
O	2.42781400	-2.58377000	-0.69913300
C	1.54594400	-0.53246200	-0.55685600
C	0.72330900	1.72959200	-0.06566100
C	-0.20884200	1.50265800	0.98121100
C	0.73925600	2.93915700	-0.79762700
C	-1.15847900	2.54086400	1.20516600
C	-0.19016200	3.92497900	-0.53311100
C	-1.16140900	3.71817100	0.47191700
H	-1.87634900	2.39632600	2.00686300
H	-0.17812500	4.85653200	-1.09380300
H	-1.88873300	4.49451600	0.68921800
O	0.37460800	-0.99474300	-0.83417700
C	-2.38170900	-3.20430600	-1.24297800
H	-1.36385000	-3.31494000	-1.62571400
H	-2.43398800	-3.71601400	-0.27931900
H	-3.06430100	-3.71882400	-1.93266100
C	-1.78561100	-1.05088900	-3.44415900
H	-0.76654700	-1.36920900	-3.19640000
H	-2.25891100	-1.85613000	-4.01838700
H	-1.71929700	-0.17190800	-4.08928600
C	-3.09507300	1.76783800	-2.46502700
H	-2.56304700	1.71359400	-3.41719800
H	-4.12015800	2.09917200	-2.67295900
H	-2.61737000	2.54475000	-1.85803400
C	-4.44744800	1.27300200	0.33739000
H	-3.99992500	2.26510400	0.23944100
H	-5.47197700	1.33065800	-0.05415800
H	-4.51156900	1.03729300	1.40237700
C	-4.20577100	-1.85314400	1.06076400
H	-4.40733900	-1.17459200	1.89240700
H	-5.16508700	-2.27961700	0.73944100
H	-3.59145600	-2.67354200	1.43761400
C	3.62290100	-3.30077800	-0.42134900
H	3.86240600	-3.28319400	0.65185300
H	3.41974300	-4.33124900	-0.72503300
H	4.47367600	-2.89959700	-0.98178700
C	1.86551000	2.88644400	-1.80860400
C	2.62356200	1.58340000	-1.43350400
N	1.73247300	0.88313900	-0.47291200
H	1.47271300	2.84208800	-2.83228900
H	2.51968800	3.76198000	-1.75340100
H	2.81583800	0.93378700	-2.28977100
H	3.58208400	1.79258800	-0.95020100
C	-0.03172900	0.38941500	1.99374600
C	-0.74814600	-0.70125500	1.70214700
C	0.92595400	0.61135700	3.15041900
C	0.45420400	1.65017500	4.18143300
H	1.89405300	0.93081500	2.74031100
H	1.10500700	-0.34708200	3.65006400
H	1.20351800	1.78662000	4.96879800
H	0.28355000	2.62491800	3.71286900
H	-0.48294800	1.33916700	4.65599300
C	-0.82028400	-2.00191900	2.45708600
C	-1.60309300	-1.91614300	3.78066500
H	0.20232400	-2.34579300	2.66712600
H	-1.26279600	-2.77865900	1.82380600
H	-1.64772800	-2.89506000	4.27106600
H	-1.13081000	-1.21429500	4.47420400
H	-2.62910700	-1.57352100	3.61515000
H	3.96986858	-0.67403936	-0.08807792
O	6.21467800	-1.20726000	-1.07656900
C	6.09981000	-0.32456900	-0.24511500
O	4.95205900	0.02506200	0.34199100
C	7.26072500	0.51255800	0.25468400
H	8.17684500	0.21450000	-0.25475000
H	7.06338800	1.57459800	0.07946000
H	7.37548200	0.38023300	1.33504900

IM10[4ad]

Sum of electronic and thermal Free Energies= -1609.832690

Rh	-1.8752	-0.14735	-0.03769
N	4.75201	-1.50483	0.21312
C	-3.61777	0.97604	-0.71743
C	-3.64717	-0.21042	-1.5677
C	-3.75846	-1.32186	-0.71421
C	-3.84151	-0.85504	0.6744
C	-3.84099	0.58276	0.64923
O	4.99002	-2.75279	-0.38901
C	3.61202	-0.83644	-0.25445
C	2.57204	1.42457	-0.25947
C	1.29946	1.33767	0.35252
C	2.94756	2.52954	-1.04313
C	0.43555	2.42073	0.08067
C	2.06398	3.56735	-1.29878
C	0.78869	3.49725	-0.73162

H	-0.53346	2.42416	0.56018
H	2.36634	4.41806	-1.90378
H	0.07797	4.30515	-0.88281
O	2.61296	-1.44846	-0.60004
C	-4.13059	1.50694	1.79186
H	-3.78259	1.10065	2.74039
H	-3.65826	2.48173	1.64413
H	-5.21384	1.67564	1.8638
C	-4.18741	-1.72208	1.84641
H	-3.93037	-1.23243	2.78661
H	-5.26622	-1.93428	1.8497
H	-3.65976	-2.67823	1.80753
C	-3.7565	-2.76934	-1.09811
H	-3.08292	-3.34096	-0.45329
H	-4.76111	-3.19584	-0.98297
H	-3.44184	-2.91755	-2.13302
C	-3.49251	-0.19139	-3.05989
H	-2.59964	0.36945	-3.35541
H	-3.39943	-1.20123	-3.46592
H	-4.35642	0.28173	-3.5434
C	-3.53954	2.37891	-1.23652
H	-2.83929	2.45408	-2.07244
H	-4.52548	2.70326	-1.59533
H	-3.2206	3.07898	-0.46179
C	4.48631	-3.7966	0.44858
H	3.40124	-3.7163	0.55545
H	4.74298	-4.72356	-0.07044
H	4.96384	-3.77802	1.43558
C	4.38008	2.38139	-1.5029
C	4.91337	1.29327	-0.55061
N	3.70069	0.54199	-0.14666
H	4.42999	2.04619	-2.54783
H	4.95561	3.30823	-1.42572
H	5.63606	0.63313	-1.03479
H	5.38406	1.74638	0.33129
C	0.88239	0.28138	1.33047
C	-0.31639	-0.3569	1.32335
C	1.90164	0.06599	2.4562
C	2.02092	1.28345	3.39254
H	2.89412	-0.13573	2.04321
H	1.64089	-0.81411	3.04635
H	2.75725	1.09796	4.18343
H	2.33626	2.1765	2.84357
H	1.06208	1.51288	3.8685
C	-0.6495	-1.43814	2.35393
C	-1.06767	-0.93322	3.7481
H	0.20925	-2.11644	2.46024
H	-1.46749	-2.05944	1.97605
H	-1.2971	-1.78042	4.40581
H	-0.27865	-0.34546	4.22485
H	-1.96368	-0.31505	3.67256
H	5.62364	-0.99147	0.25624
O	-0.42784	0.64202	-1.55747
C	-0.2596	-0.51811	-2.04821
O	-0.89378	-1.50436	-1.55991
C	0.71947	-0.73064	-3.17869
H	0.82775	0.18073	-3.76966
H	1.69793	-0.98354	-2.75534
H	0.3996	-1.56177	-3.81044

T6[4ad]

Sum of electronic and thermal Free Energies= -1609.775731

Rh	1.16929	0.09218	-0.32105
C	3.17488	0.81326	0.67604
C	2.91346	1.51034	-0.54622
C	2.94446	0.53875	-1.63161
C	3.14015	-0.74224	-1.05543
C	3.23205	-0.58815	0.39101
O	-2.34192	3.3432	0.31003
C	-1.27453	1.45716	-0.70352
O	-0.27755	1.09401	-1.43918
C	3.5807	-1.68752	1.3488
H	2.92359	-2.54455	1.18777
H	3.46298	-1.36386	2.38604
H	4.62528	-2.00122	1.21751
C	3.28377	-2.04283	-1.78368
H	2.914	-2.86804	-1.17357
H	4.34151	-2.23071	-2.01088
H	2.73255	-2.03978	-2.72667
C	2.77461	0.87232	-3.08296
H	3.64905	1.41246	-3.46804
H	1.89329	1.50324	-3.23938
H	2.64566	-0.02931	-3.68538
C	2.82374	2.99538	-0.73904
H	3.79372	3.41503	-1.03748
H	2.51674	3.50671	0.17761
H	2.10618	3.24491	-1.52659
C	3.49973	1.44502	1.99595
H	3.02177	2.41793	2.12422

H	4.58457	1.6037	2.05975
H	3.21374	0.81114	2.8374
C	-2.97122	4.50943	-0.21471
H	-2.252	5.32755	-0.35461
H	-3.70688	4.80371	0.53745
H	-3.46895	4.30228	-1.1682
C	-1.11378	-0.48057	1.6642
C	-0.33847	0.5717	1.22735
C	-1.11802	-0.92293	3.12957
C	0.04607	-1.88839	3.44185
H	-1.0335	-0.05866	3.78929
H	-2.07113	-1.40189	3.37451
H	-0.04984	-2.28028	4.46093
H	1.00676	-1.3706	3.36606
H	0.08946	-2.72131	2.73629
C	0.20278	1.60903	2.20339
C	1.55347	1.30599	2.88663
H	1.82789	2.13725	3.54751
H	2.36981	1.17231	2.17296
H	1.4929	0.39604	3.48491
N	-1.40413	2.85729	-0.63218
H	-0.49432	3.28667	-0.47432
C	0.29547	-2.80384	-0.6099
O	0.1362	-1.59353	-1.04535
O	0.94026	-3.15989	0.385
C	-0.38637	-3.84606	-1.49972
H	-0.47505	-4.79373	-0.96552
H	0.22491	-4.00351	-2.39604
H	-1.36934	-3.49908	-1.82433
C	-2.68024	-0.53368	-0.27296
C	-2.03237	-1.20118	0.78662
C	-3.79938	-1.07664	-0.93323
C	-2.52088	-2.50254	1.07403
C	-4.24545	-2.34732	-0.62673
C	-3.57593	-3.07225	0.37787
H	-2.04011	-3.07787	1.85656
H	-5.10424	-2.77452	-1.13756
H	-3.90278	-4.0774	0.62676
C	-4.34489	-0.04617	-1.89926
C	-3.69394	1.26309	-1.39256
N	-2.4879	0.78358	-0.67727
H	-4.02429	-0.26306	-2.92667
H	-5.43708	0.01249	-1.89626
H	-3.40547	1.94454	-2.19502
H	-4.35727	1.79356	-0.6994
H	0.3044	2.53357	1.67444
H	-0.52851	1.74707	2.9722

IM11[4ad]

Sum of electronic and thermal Free Energies= -1609.841228

Rh	1.8558	-0.55575	-0.20131
N	-1.43111	1.56286	-0.97917
C	3.51799	-0.42841	-1.58942
C	3.26633	0.90265	-1.09513
C	3.43489	0.86051	0.32657
C	3.86089	-0.49089	0.70519
C	3.93053	-1.27863	-0.47864
O	-2.65766	1.58131	-1.69329
C	-1.10851	0.37399	-0.4518
C	-3.02499	-1.06695	-0.82481
C	-3.57096	-0.86202	0.44444
C	-3.62884	-1.81835	-1.83443
C	-4.83918	-1.44332	0.66169
C	-4.8705	-2.3843	-1.59223
C	-5.47426	-2.18229	-0.33565
H	-5.33679	-1.31535	1.61742
H	-5.37783	-2.9707	-2.35374
H	-6.45121	-2.61288	-0.13777
O	0.19084	0.49072	-0.73446
C	4.40066	-2.69678	-0.56928
H	5.49661	-2.73221	-0.51834
H	3.98508	-3.28485	0.25097
H	4.0987	-3.16012	-1.51147
C	4.22064	-0.9501	2.0818
H	3.79966	-1.94088	2.2657
H	5.31244	-0.99925	2.18565
H	3.84481	-0.26336	2.84267
C	3.27042	2.01948	1.2545
H	2.94116	1.69174	2.24331
H	4.24374	2.51449	1.37977
H	2.55556	2.75472	0.8707
C	2.8373	2.10016	-1.88407
H	2.03235	2.64115	-1.37451
H	3.68287	2.7884	-2.00614
H	2.49625	1.8163	-2.88241
C	3.44534	-0.86207	-3.01848
H	2.75365	-0.24227	-3.59175
H	4.43645	-0.77636	-3.48291
H	3.12886	-1.90428	-3.10372

C	-3.70447	2.17872	-0.91922
H	-3.41901	3.1783	-0.57843
H	-4.556	2.23815	-1.60075
H	-3.97245	1.55411	-0.06051
C	-2.69386	-1.84398	-3.02947
C	-1.53481	-0.88118	-2.61985
N	-1.80415	-0.56675	-1.20664
H	-2.31563	-2.85623	-3.2153
H	-3.17967	-1.50998	-3.95196
H	-0.54882	-1.33988	-2.72424
H	-1.55372	0.04015	-3.21226
C	-2.76564	-0.08245	1.38673
C	-1.58631	0.4775	0.97972
C	-3.29738	0.07129	2.79858
C	-3.18544	-1.20665	3.6533
H	-4.3531	0.36786	2.74336
H	-2.78376	0.88987	3.30702
H	-3.60068	-1.03934	4.65286
H	-3.72439	-2.04318	3.19961
H	-2.14113	-1.51214	3.76788
C	-0.71426	1.34439	1.87065
C	0.06807	0.59018	2.96195
H	-1.33324	2.11858	2.33847
H	-0.00421	1.88021	1.23838
H	0.71695	1.28583	3.5067
H	-0.5919	0.11755	3.69457
H	0.69144	-0.19797	2.53012
H	-0.70941	1.64007	-1.69639
O	0.61272	-2.00373	0.48452
C	0.9744	-3.06912	1.16304
O	2.11537	-3.32686	1.54449
C	-0.19485	-3.99935	1.45329
H	-1.00905	-3.44074	1.92295
H	-0.58553	-4.40268	0.51336
H	0.12507	-4.8186	2.09817

P1[4ad]

Sum of electronic and thermal Free Energies= -711.614315

C	1.44871	0.30382	-0.43176
C	3.72063	-0.25037	-0.99673
C	4.27652	0.75251	-0.20236
C	4.4446	-1.17252	-1.75988
C	5.69441	0.80843	-0.20097
C	5.82275	-1.08849	-1.74466
C	6.43803	-0.0871	-0.95659
H	6.21024	1.55093	0.39727
H	6.43408	-1.78144	-2.3156
H	7.5218	-0.0225	-0.93837
O	0.23471	0.03268	-0.67563
C	3.46674	-2.1181	-2.42493
C	2.06657	-1.59186	-1.98948
N	2.36942	-0.44398	-1.10098
H	3.57433	-2.12605	-3.51463
H	3.61326	-3.13949	-2.0628
H	1.45786	-1.24324	-2.82756
H	1.50965	-2.33677	-1.42023
C	3.34892	1.5774	0.54297
C	1.98566	1.34687	0.45766
C	3.93975	2.6782	1.40254
C	4.4428	3.888	0.58741
H	4.77715	2.26212	1.97552
H	3.21354	3.02505	2.13917
H	4.86967	4.64349	1.25467
H	5.21216	3.59893	-0.13343
H	3.62751	4.35317	0.02636
C	0.99992	2.14017	1.29302
C	0.65954	3.54193	0.7589
H	1.3865	2.22114	2.31428
H	0.08575	1.54604	1.41816
H	-0.07265	4.02355	1.41652
H	1.54492	4.1824	0.72607
H	0.22943	3.49308	-0.24411

T4[4ac]

Sum of electronic and thermal Free Energies= -1380.748782

Rh	-0.60891	-0.46322	0.11013
N	0.05633	-0.23894	1.57905
C	-2.61531	0.01102	-0.82737
C	-1.82499	-0.56775	-1.8521
C	-1.58953	-1.97788	-1.5115
C	-2.17111	-2.23326	-0.26688
C	-2.73722	-0.97263	0.22801
O	-0.81569	0.17216	2.63456
C	1.38145	-0.66227	2.21375
C	2.17074	-0.48056	-0.1728
C	1.62115	0.71071	-0.71298
C	2.82456	-1.43567	-0.99603
C	1.69393	0.84051	-2.13112
C	2.89231	-1.2547	-2.36054
C	2.30391	-0.1056	-2.93754

H	1.27551	1.73978	-2.57225
H	3.40607	-1.97808	-2.98888
H	2.36065	0.04907	-4.01094
O	1.7702	-0.70629	3.37936
C	-3.60782	-0.84877	1.44059
H	-3.22707	-1.45207	2.26481
H	-3.66579	0.18468	1.78941
H	-4.62976	-1.18423	1.21495
C	-2.21469	-3.53162	0.48099
H	-1.73221	-3.4448	1.45898
H	-3.25079	-3.85052	0.6494
H	-1.70802	-4.32843	-0.06841
C	-0.84448	-2.92963	-2.39837
H	-0.71863	-3.90743	-1.92831
H	-1.37758	-3.07967	-3.34586
H	0.15221	-2.54636	-2.64418
C	-1.50226	0.04165	-3.18482
H	-0.52557	-0.28604	-3.54961
H	-2.24995	-0.2517	-3.93424
H	-1.49361	1.13374	-3.13888
C	-3.28318	1.35252	-0.85587
H	-2.73906	2.06156	-1.48379
H	-4.30067	1.2629	-1.25931
H	-3.36437	1.78352	0.14407
C	-1.0793	-0.89012	3.5477
H	-0.17093	-1.18843	4.07585
H	-1.80666	-0.48341	4.25739
H	-1.51827	-1.75918	3.03788
C	3.40198	-2.52021	-0.10974
C	3.36433	-1.86098	1.29116
N	2.33065	-0.81253	1.16478
H	2.77219	-3.41974	-0.13799
H	4.41318	-2.81822	-0.40063
H	3.10081	-2.54063	2.10192
H	4.33108	-1.40372	1.53526
C	1.21273	1.88574	0.14881
C	-0.02805	1.37236	0.78118
C	2.24613	2.94769	0.47878
C	2.65102	3.8551	-0.69529
H	3.14487	2.44478	0.86327
H	1.86661	3.56396	1.30121
H	3.40698	4.58346	-0.3815
H	3.0751	3.27459	-1.52105
H	1.78843	4.40824	-1.08267
C	-0.79263	2.2944	1.69369
C	-1.07158	3.68846	1.10118
H	-0.22736	2.40459	2.62947
H	-1.73627	1.82485	1.98636
H	-1.64655	4.29971	1.80607
H	-0.14325	4.22169	0.87701
H	-1.64284	3.62026	0.17039

IM8[4ac]

Sum of electronic and thermal Free Energies= -1380.793443

Rh	0.74368	-0.07095	-0.08781
N	-0.31176	1.41905	0.50176
C	3.00244	-0.58424	-0.36422
C	2.1549	-1.72144	-0.61217
C	1.43621	-1.51235	-1.8675
C	1.67502	-0.19323	-2.25907
C	2.6364	0.40822	-1.30951
O	0.55063	2.5313	0.71007
C	-1.63811	2.05934	0.21747
C	-2.58064	-0.26501	-0.00453
C	-1.63641	-1.06094	0.673
C	-3.60899	-0.82045	-0.77585
C	-1.76897	-2.45832	0.47775
C	-3.71313	-2.19683	-0.94876
C	-2.77351	-3.01563	-0.31457
H	-1.07486	-3.11912	0.98809
H	-4.51751	-2.62448	-1.54046
H	-2.83377	-4.09554	-0.41698
O	-2.00217	3.22947	0.33183
C	3.32034	1.72856	-1.50436
H	2.67689	2.45023	-2.00951
H	3.63085	2.16811	-0.55321
H	4.22075	1.60651	-2.1227
C	1.14688	0.49626	-3.48277
H	1.89507	0.4934	-4.28652
H	0.24759	0.00576	-3.86252
H	0.89114	1.53943	-3.28064
C	0.56273	-2.53604	-2.52807
H	0.01964	-2.11248	-3.37629
H	1.15817	-3.37812	-2.90573
H	-0.18058	-2.94412	-1.8343
C	2.24336	-3.04759	0.08633
H	1.27819	-3.56066	0.0916
H	2.95804	-3.7043	-0.42878
H	2.57902	-2.94182	1.12034

C	4.10753	-0.50917	0.64698
H	3.86678	-1.06955	1.55473
H	5.03516	-0.93514	0.23999
H	4.32152	0.52091	0.93997
C	0.56796	3.40676	-0.41696
H	-0.36507	3.96931	-0.48905
H	1.40751	4.08556	-0.24056
H	0.73728	2.84543	-1.34336
C	-4.51289	0.29255	-1.26611
C	-4.11652	1.47349	-0.35098
N	-2.75342	1.12798	0.10549
H	-4.31235	0.52379	-2.32143
H	-5.57574	0.04791	-1.18236
H	-4.10061	2.44522	-0.84303
H	-4.78887	1.54182	0.51341
C	-0.75283	-0.52957	1.76227
C	0.10444	0.55081	1.66496
C	-0.82022	-1.29149	3.09387
C	0.40023	-2.15256	3.4543
H	-1.7139	-1.9237	3.07053
H	-0.9833	-0.56155	3.89622
H	0.25349	-2.63968	4.42494
H	0.57231	-2.93572	2.70963
H	1.30972	-1.5467	3.51512
C	0.61955	1.45478	2.73944
C	2.14223	1.60286	2.82293
H	0.2163	1.12646	3.70529
H	0.18507	2.442	2.54194
H	2.40873	2.3071	3.61788
H	2.62895	0.64748	3.03958
H	2.53456	1.98474	1.87842

T5[4ac]

Sum of electronic and thermal Free Energies= -1609.820031

Rh	1.19589	-0.09641	0.0342
N	-1.22542	1.3781	-0.68513
C	3.26679	0.63173	0.60952
C	3.31425	-0.78317	0.97104
C	3.08569	-1.53603	-0.19123
C	2.95987	-0.59697	-1.3063
C	3.17417	0.72102	-0.82927
O	-0.6606	2.23482	-1.67183
C	-2.62651	1.84075	-0.37346
C	-2.92321	-0.41709	0.65208
C	-1.64676	-0.82918	1.04796
C	-4.04425	-1.2599	0.63037
C	-1.53469	-2.20427	1.3452
C	-3.90139	-2.60176	0.94805
C	-2.62359	-3.06978	1.29152
H	-0.55673	-2.58204	1.62513
H	-4.75536	-3.27292	0.93825
H	-2.48152	-4.11923	1.53154
O	-3.02734	2.92547	-0.73891
C	3.35624	1.95387	-1.66657
H	2.70958	1.94802	-2.54845
H	3.13606	2.86346	-1.10295
H	4.39323	2.0381	-2.02236
C	2.80981	-1.00689	-2.74225
H	3.78932	-1.25432	-3.17434
H	2.16958	-1.88644	-2.83365
H	2.37891	-0.20285	-3.34524
C	3.09877	-3.03129	-0.31851
H	2.26961	-3.3762	-0.93916
H	4.0397	-3.37978	-0.76786
H	3.00733	-3.51164	0.65999
C	3.70996	-1.34202	2.30812
H	3.113	-2.21565	2.58638
H	4.76006	-1.66442	2.28426
H	3.62053	-0.60437	3.10707
C	3.68245	1.76866	1.50092
H	3.4619	1.57039	2.55203
H	4.76471	1.94347	1.42553
H	3.18394	2.7021	1.22605
C	-1.175	1.94495	-2.9785
H	-2.24485	2.16693	-3.04282
H	-0.62813	2.6255	-3.63321
H	-0.9614	0.90988	-3.25967
C	-5.27544	-0.46307	0.24692
C	-4.80403	1.00259	0.40465
N	-3.33158	0.90368	0.29511
H	-5.57085	-0.66931	-0.79024
H	-6.13974	-0.67912	0.8809
H	-5.17773	1.68754	-0.35651
H	-5.06526	1.40136	1.39094
C	-0.51822	0.12399	1.34881
C	-0.28913	1.31284	0.51066
C	-0.4567	0.27972	2.89568
C	0.8952	0.33843	3.60511
H	-0.99932	-0.56713	3.32501

H	-1.04897	1.16478	3.17336
H	0.74114	0.45107	4.68501
H	1.45153	-0.58381	3.4354
H	1.51678	1.17079	3.27054
C	-0.09045	2.67132	1.17896
C	0.42575	3.86056	0.3568
H	0.60349	2.49967	2.00344
H	-1.03853	2.97365	1.65522
H	0.67781	4.68335	1.03533
H	1.3202	3.59694	-0.21127
H	-0.32288	4.22127	-0.34916
H	-1.12912	0.27149	-1.13915
O	0.14473	-2.96291	-1.71844
C	-0.57891	-1.99021	-1.88425
O	-0.32982	-0.782	-1.42786
C	-1.85876	-2.12156	-2.70973
H	-2.42164	-2.98715	-2.35241
H	-2.49297	-1.23306	-2.66635
H	-1.59025	-2.31462	-3.75358

IM9[4ac]

Sum of electronic and thermal Free Energies= -1609.938841

Rh	2.52671	0.07315	-0.38739
N	-1.86579	0.05955	0.08203
C	2.44004	1.74262	1.05574
C	3.70074	1.01921	1.26571
C	4.4626	1.10723	0.07259
C	3.66029	1.82652	-0.90427
C	2.43767	2.27673	-0.26598
O	0.72064	-0.22756	-1.18041
C	-2.32786	1.30564	0.43511
C	-4.67104	0.65708	0.01625
C	-4.69165	-0.73078	-0.17307
C	-5.70952	1.4949	-0.41103
C	-5.82165	-1.23692	-0.85203
C	-6.80674	0.96753	-1.07854
C	-6.85133	-0.41368	-1.3022
H	-5.89761	-2.30494	-1.02405
H	-7.61802	1.6101	-1.40958
H	-7.70031	-0.85272	-1.81798
O	-1.57536	2.28233	0.50594
C	1.36702	3.11698	-0.89033
H	0.37887	2.86241	-0.50063
H	1.55637	4.17907	-0.68728
H	1.34463	2.9847	-1.97461
C	4.08371	2.15758	-2.30004
H	4.65023	3.09834	-2.30552
H	4.72556	1.37959	-2.71929
H	3.22219	2.28323	-2.95883
C	5.84589	0.5729	-0.13636
H	6.09344	0.50753	-1.19846
H	6.58018	1.23967	0.33389
H	5.93742	-0.42401	0.29817
C	4.1372	0.35728	2.53386
H	4.58523	-0.61297	2.30862
H	4.87542	0.98222	3.0533
H	3.29637	0.20288	3.21335
C	1.37937	1.94758	2.08949
H	1.32664	1.10083	2.77831
H	1.61977	2.83816	2.68623
H	0.39577	2.09699	1.63699
C	0.44026	-1.24293	-2.12109
H	1.06208	-2.13249	-1.97477
H	-0.61838	-1.53063	-2.03433
H	0.59614	-0.87496	-3.14789
C	-5.3993	2.92382	-0.02037
C	-4.24731	2.75168	0.99639
N	-3.68542	1.41031	0.71631
H	-5.07753	3.50419	-0.8955
H	-6.25536	3.44461	0.41865
H	-3.45669	3.4945	0.90757
H	-4.63318	2.76292	2.02246
C	-3.64087	-1.61406	0.37488
C	-2.35241	-1.21168	0.49597
C	-4.06959	-3.00911	0.81807
C	-3.84212	-4.11343	-0.23284
H	-5.13178	-2.98202	1.08369
H	-3.54603	-3.28544	1.73904
H	-4.19362	-5.08229	0.13912
H	-4.37143	-3.89993	-1.16651
H	-2.78097	-4.21195	-0.48171
C	-1.24907	-2.06101	1.09784
C	-0.76611	-3.16029	0.13258
H	-0.0179	-3.7977	0.61536
H	-1.60024	-3.79489	-0.18255
H	-0.31685	-2.72856	-0.7679
H	-0.88292	0.07866	-0.22301
O	4.6302	-2.21799	0.69061
C	3.84484	-2.61644	-0.17022

O	2.90519	-1.9105	-0.74912
C	3.88186	-4.05818	-0.66593
H	4.68787	-4.60563	-0.17593
H	2.92423	-4.54565	-0.45821
H	4.02363	-4.07692	-1.75091
H	-0.42167	-1.42947	1.34573
H	-1.61455	-2.52109	1.99207

P2^{4ac}

Sum of electronic and thermal Free Energies= -766.936086

N	-0.96387	-1.37656	-0.93534
C	0.14454	-2.05051	-0.41503
C	1.25188	0.10994	0.07511
C	0.2767	1.11292	-0.02045
C	2.62601	0.387	0.05205
C	0.7691	2.4281	-0.1733
C	3.07736	1.69014	-0.10265
C	2.13091	2.71479	-0.22177
H	0.06393	3.2484	-0.24886
H	4.1409	1.91169	-0.11897
H	2.45689	3.74398	-0.33931
O	0.29247	-3.25031	-0.60778
C	3.40593	-0.89929	0.22177
C	2.3253	-1.88855	0.71402
N	1.04103	-1.27848	0.30018
H	3.83563	-1.2215	-0.73605
H	4.23085	-0.80905	0.93437
H	2.39813	-2.8871	0.28577
H	2.3415	-1.97113	1.80686
C	-1.17073	0.83303	0.10083
C	-1.71289	-0.33465	-0.31989
C	-2.0402	1.91906	0.72685
C	-2.74961	2.83803	-0.28641
H	-1.41569	2.52901	1.38756
H	-2.79294	1.46446	1.37936
H	-3.32918	3.61111	0.23007
H	-2.03666	3.33842	-0.9487
H	-3.43584	2.27227	-0.9245
C	-3.18169	-0.692	-0.21817
C	-4.0336	-0.05816	-1.33447
H	-5.09316	-0.29456	-1.19416
H	-3.93056	1.03138	-1.34799
H	-3.72765	-0.43266	-2.31632
H	-1.53462	-2.05604	-1.42241
H	-3.2813	-1.75601	-0.27161
H	-3.55207	-0.35834	0.72862

IM1'

Sum of electronic and thermal Free Energies= -1604.388113

C	-2.49390400	0.00231700	-1.76094600
C	-2.01298500	-1.38141100	-1.68950600
C	-2.57074800	-1.98077500	-0.52843100
C	-3.29794500	-0.95118000	0.19790300
C	-3.30042800	0.25522900	-0.62307500
C	-4.04631500	1.50739500	-0.28110800
H	-3.70240600	2.35691900	-0.87466900
H	-5.11704200	1.36936300	-0.48060500
H	-3.91601000	1.74215400	0.77782800
C	-2.17570500	0.94072400	-2.88276700
H	-1.11381800	1.20129500	-2.87969300
H	-2.41762800	0.47369000	-3.84413000
H	-2.75000000	1.86591100	-2.80385100
C	-1.14325900	-2.05354100	-2.70502700
H	-0.45556200	-2.73773500	-2.20473100
H	-1.75159600	-2.61396700	-3.42694000
H	-0.55227900	-1.31982400	-3.25765100
C	-2.46412800	-3.41591800	-0.12165800
H	-2.52239600	-3.52465000	0.96349800
H	-3.30000300	-3.97807100	-0.55875600
H	-1.52121800	-3.84941000	-0.45154800
C	-4.09788200	-1.13560300	1.44710100
H	-5.16906100	-1.16144500	1.20570900
H	-3.84334200	-2.07078600	1.94971600
H	-3.90093400	-0.30550000	2.12969700
C	-1.45794100	1.68883700	2.36967400
O	-2.61538400	1.36485900	2.65479000
O	-0.76871700	1.29908800	1.33792400
C	-0.67718500	2.63514500	3.28186300
H	-0.01712300	3.28795400	2.70498400
H	-1.36485100	3.22540600	3.89042500
H	-0.04795300	2.03511000	3.94843300
Rh	-1.25901400	-0.29933200	0.08362300
C	3.51182900	0.04138300	-0.36918700
C	4.78105800	0.23460000	0.19330700
C	5.65669300	-0.83536500	0.32473500
C	5.25056600	-2.10421100	-0.10605700
C	3.97733900	-2.28338500	-0.65121100
C	3.08650800	-1.21411600	-0.79740400
C	3.74424900	2.38098100	-0.04722400
C	4.94796200	1.67525100	0.61773900

H	6.64192700	-0.68875900	0.75966700	C	1.98537000	3.12372000	0.64627200
H	5.92424000	-2.95013200	-0.00731700	H	2.89607600	3.71349800	0.81325800
H	3.65058500	-3.27117700	-0.96034900	H	1.55154000	3.44199700	-0.30399200
H	2.09317700	-1.37012100	-1.18985400	H	1.27798700	3.37580100	1.43847200
H	3.23376300	3.07925700	0.61959400	C	1.51762200	1.01733100	3.04241900
H	5.89741300	2.11425400	0.29721500	H	2.28921200	1.17392800	3.80651700
N	2.82589700	1.28427500	-0.42886700	H	0.88596700	1.90755700	3.01546100
H	4.89860800	1.76941900	1.70947200	H	0.89922900	0.17590100	3.36487400
H	4.06791500	2.93065400	-0.94397600	O	-2.00688700	-0.92481000	-2.09450600
C	1.54208800	1.48409000	-0.86014300	C	-4.09575700	-1.96890500	-2.50866400
O	0.74058400	0.57965400	-1.10988200	H	-3.99645000	-2.98348400	-2.10567800
N	1.23080700	2.84882300	-0.97713800	H	-5.14492700	-1.67497100	-2.43089800
H	1.97461700	3.42203700	-1.36613100	H	-3.77961400	-1.99026300	-3.55374400
O	0.05125300	3.11817600	-1.68090100	Rh	1.07647000	-0.07538500	-0.10626600
C	-0.83128900	3.87888300	-0.84407500	C	-1.35135500	1.66924200	-0.09585700
H	-0.38914300	4.85054700	-0.58995600	C	-1.78019200	3.00235600	-0.08346000
H	-1.72566600	4.04005000	-1.45088800	C	-1.36635400	3.84402800	-1.10523700
H	-1.07068300	3.32009500	0.06238500	C	-0.55378800	3.33280000	-2.14023300
O	-0.02468900	-1.31447600	1.40248400	C	-0.18906200	1.99057700	-2.14941800
C	0.59481800	-2.40571200	1.06364000	C	-0.58359200	1.08741500	-1.12273100
O	0.57355800	-2.95642200	-0.04535000	C	-3.07298100	1.75972700	1.48453900
C	1.45000200	-2.97906400	2.19114100	C	-2.69852100	3.21361000	1.10329700
H	2.45482100	-2.54978500	2.11508200	H	-1.68669400	4.88271500	-1.12857400
H	1.04180700	-2.72700000	3.17178800	H	-0.25429600	3.98729300	-2.95400000
H	1.53532400	-4.06187200	2.07635600	H	0.37474200	1.59311600	-2.98933100
T1'				H	-1.09186700	0.01922200	-1.50407300
Sum of electronic and thermal Free Energies= -1604.33684				H	-3.20470300	1.59629800	2.55487000
C	3.27176800	-0.38033100	0.00265500	H	-3.58520100	3.80686000	0.86519700
C	2.96277500	0.95477400	-0.45816500	N	-1.91789100	0.97896200	0.98264500
C	2.32156600	1.66443500	0.64342100	H	-2.17591800	3.71536800	1.92910200
C	2.14540700	0.74294800	1.70950300	H	-3.96991600	1.43681300	0.94556200
C	2.72880100	-0.53549500	1.31595500	C	-1.69973900	-0.35390000	1.21867100
C	2.79501300	-1.78132700	2.14409900	O	-0.63186900	-0.93924700	0.96763500
H	2.40855100	-2.62332300	1.56230500	N	-2.75436000	-0.97937300	1.88649400
H	3.82936000	-1.99370100	2.44247700	H	-3.57426600	-0.92018600	1.26967600
H	2.19847700	-1.68613400	3.05385700	O	-2.52489300	-2.35441700	2.10686200
C	4.01682400	-1.42992800	-0.75999300	C	-2.05559600	-2.55725900	3.43411400
H	5.07883800	-1.40495200	-0.48247900	H	-2.75717800	-2.15182300	4.17341800
H	3.61463500	-2.41981600	-0.54081900	H	-1.97918500	-3.64107800	3.54644500
H	3.94596800	-1.26457300	-1.83673600	H	-1.06346300	-2.11262500	3.58126900
C	3.43649000	1.57577000	-1.73732600	O	0.82715200	-1.43371400	-1.63306800
H	3.47439100	0.83981200	-2.54364200	C	0.86691600	-2.71373700	-1.36587300
H	2.77663900	2.38639900	-2.05378800	O	1.29588200	-3.22849200	-0.33065300
H	4.44550300	1.99113700	-1.61414500	C	0.31001000	-3.54596200	-2.51323900

H	0.35568800	-4.60771500	-2.26619500
H	-0.72083200	-3.23004100	-2.69518000
H	0.87612300	-3.35265100	-3.43007400
C	-3.21734700	-1.02331300	-1.68469400
O	-3.72131900	-0.45964800	-0.68523800

IM2'

Sum of electronic and thermal Free Energies= -1375.337792

C	2.98951200	0.55076200	0.21569000
C	2.73801800	-0.65908000	-0.57274800
C	2.08987100	-0.25412700	-1.79869800
C	1.79628600	1.13602300	-1.68259900
C	2.41288900	1.64193800	-0.45174000
C	2.36265500	3.07454500	-0.01204300
H	2.75832700	3.19604300	0.99857000
H	2.95086400	3.71585200	-0.68101700
H	1.33393700	3.44999300	-0.01145500
C	3.72592200	0.55339800	1.52004400
H	4.80633000	0.46459600	1.34452000
H	3.55350000	1.47389200	2.08254500
H	3.40829000	-0.29363500	2.13214400
C	3.35636300	-1.99509000	-0.28751100
H	3.10215400	-2.31491900	0.72528400
H	3.00764000	-2.75423400	-0.99249700
H	4.44916300	-1.93988100	-0.38350400
C	1.82183700	-1.12999900	-2.98523000
H	1.06924500	-0.69296400	-3.64547500
H	2.74030600	-1.26752200	-3.56984800
H	1.46351300	-2.11778400	-2.68778600
C	1.12065400	2.00621400	-2.69995500
H	1.86040200	2.58627100	-3.26704900
H	0.53869200	1.41775400	-3.41272700
H	0.44235000	2.71552000	-2.21795100
Rh	0.72509400	0.06959400	-0.04339300
C	-2.01912600	-1.13685700	-0.41162400
C	-2.98127200	-2.11928800	-0.68381400
C	-2.59226700	-3.42406500	-0.95726600
C	-1.22739400	-3.72169900	-0.94245000
C	-0.28572900	-2.72014000	-0.68429000
C	-0.64164300	-1.38265900	-0.43483300
C	-4.15441200	-0.13863900	-0.01428200
C	-4.37279100	-1.53216300	-0.64330400
H	-3.33206200	-4.19308700	-1.16224500
H	-0.89225400	-4.74020600	-1.11937100
H	0.76163100	-2.99818500	-0.64229300
H	-4.69021700	0.65108400	-0.54766700
H	-5.07424100	-2.13037100	-0.05403400
N	-2.69460800	0.08864100	-0.09796200
H	-4.79436400	-1.44158300	-1.65231100
H	-4.46999200	-0.12808800	1.03813000
C	-2.11726200	1.28362800	0.14735700
O	-0.90098900	1.52814100	0.08313800
N	-3.02223600	2.33729400	0.38736900
H	-3.82201200	2.08188900	0.95769000
O	-2.42619200	3.45515300	1.00113400
C	-2.21981900	4.48145900	0.03128300
H	-3.16312700	4.77842200	-0.44224700
H	-1.80550300	5.32150200	0.59366700
H	-1.50459100	4.16294200	-0.73403700
O	0.15928600	-0.27110500	1.94271900
C	0.70678600	-1.17263800	2.70159600
O	1.65988000	-1.90451300	2.41794200
C	0.02670700	-1.28095300	4.06838600
H	-0.20062200	-0.29011800	4.47063300
H	-0.92242200	-1.81651500	3.95525600
H	0.66315000	-1.83477000	4.76064800

Cat^{+}

Sum of electronic and thermal Free Energies= -727.716021

C	-1.50734	0.32905	-1.16761
C	-1.49645	-1.04287	-0.6275
C	-1.41636	-0.95141	0.7889
C	-1.3259	0.47039	1.13787
C	-1.4331	1.25097	-0.08486
C	-1.45291	2.75144	-0.1758
H	-1.12427	3.09323	-1.16852
H	-2.48989	3.11689	-0.00263
H	-0.80302	3.19776	0.58975
C	-1.58023	0.65733	-2.62123
H	-1.04389	-0.07119	-3.23724
H	-2.63252	0.64759	-2.94391
H	-1.1693	1.6505	-2.83568
C	-1.5903	-2.2874	-1.44187
H	-1.20687	-3.15071	-0.90371
H	-2.65131	-2.4867	-1.67841
H	-1.05189	-2.20598	-2.38567
C	-1.42081	-2.07136	1.77783
H	-0.76506	-1.86293	2.62775
H	-2.43266	-2.21624	2.16835
H	-1.09401	-3.0105	1.32228

C	-1.25828	1.03272	2.51856
H	-2.28428	1.17075	2.89067
H	-0.75497	0.35049	3.20079
H	-0.76111	2.00303	2.54263
C	2.85306	-0.01312	0.10397
O	2.18031	1.08404	-0.18202
O	2.17711	-1.10566	0.41641
C	4.34265	-0.00905	0.11418
H	4.72969	-1.0177	-0.15288
H	4.7258	0.80696	-0.57997
H	4.67748	0.24899	1.18093
Rh	0.37708	-0.0107	-0.07743

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Sum of electronic and thermal Free Energies= -1375.766674

C	-0.13263	-2.1977	-3.98956
C	-0.39747	-0.85055	-4.50582
C	0.73883	-0.43492	-5.27036
C	1.75498	-1.45895	-5.13348
C	1.17531	-2.57519	-4.38527
C	1.88093	-3.85977	-4.08751
H	1.37808	-4.42715	-3.30285
H	1.91333	-4.48531	-4.98769
H	2.91062	-3.67987	-3.7685
C	-1.11328	-3.04114	-3.2374
H	-1.78542	-2.43651	-2.62544
H	-1.73821	-3.59743	-3.94715
H	-0.6179	-3.76957	-2.59237
C	-1.6669	-0.07617	-4.35791
H	-1.4406	0.96679	-4.12653
H	-2.23912	-0.1162	-5.29329
H	-2.30028	-0.48052	-3.56597
C	0.84459	0.81588	-6.07984
H	1.88523	1.09248	-6.25903
H	0.37081	0.65074	-7.05606
H	0.34567	1.64698	-5.58114
C	3.09647	-1.46324	-5.79352
H	3.01287	-1.8939	-6.7997
H	3.49603	-0.45237	-5.89487
H	3.81673	-2.06361	-5.23392
C	3.8132	-1.64923	-3.49619
O	3.27736	-0.45738	-3.32772
O	3.31579	-2.70529	-3.1116
C	5.15738	-1.60854	-4.20752
H	5.37599	-2.58544	-4.64027
H	5.1809	-0.83431	-4.97784
H	5.93895	-1.36904	-3.47809
Rh	1.35588	-0.72409	-3.17656
C	3.97554	0.32247	-0.18082
C	4.86704	0.5118	0.88409
C	6.19507	0.12722	0.75097
C	6.62603	-0.43655	-0.45547
C	5.73301	-0.60004	-1.51555
C	4.3917	-0.21865	-1.39779
C	2.81033	1.59692	1.4623
C	4.15498	1.13486	2.06288
H	6.89228	0.26895	1.57142
H	7.66229	-0.73698	-0.57097
H	6.08045	-1.01879	-2.45463
H	3.72234	-0.31129	-2.24341
H	1.9468	1.39866	2.09629
H	4.7078	1.97092	2.49883
N	2.68786	0.80897	0.20526
H	3.99756	0.39674	2.85861
H	2.82171	2.66215	1.21054
C	1.48314	0.61848	-0.34954
O	1.34058	-0.06127	-1.39598
N	0.37732	1.16768	0.31901
H	0.50021	2.14856	0.56587
O	-0.80948	1.06526	-0.44153
C	-1.77497	0.27143	0.27897
H	-1.96665	0.72097	1.2557
H	-2.67772	0.30906	-0.33121
H	-1.42426	-0.7575	0.39556

TS1

Sum of electronic and thermal Free Energies= -1375.759098

C	-2.97584400	-0.89788000	1.11922100
C	-3.47182000	0.09001800	0.18942600
C	-3.27500300	-0.42230200	-1.15799700
C	-2.57970400	-1.66279500	-1.05203200
C	-2.37272000	-1.96023600	0.36186800
C	-1.80726300	-3.24563400	0.88444700
H	-1.54226400	-3.17896500	1.94085200
H	-2.54618200	-4.04971400	0.78052200
H	-0.91474700	-3.54583500	0.32994200
C	-3.10878500	-0.79657900	2.60694200
H	-2.69118200	0.14082700	2.98553700
H	-4.17047900	-0.81732700	2.87925800
H	-2.61908900	-1.62445800	3.12071000

C	-4.20459000	1.34671000	0.53863400
H	-5.28664900	1.16401100	0.54088200
H	-3.92545500	1.71420800	1.52833900
H	-4.00011600	2.13433600	-0.18965300
C	-3.69282900	0.28766300	-2.40522600
H	-3.39778200	-0.25924200	-3.30169600
H	-4.78189500	0.40678200	-2.42329000
H	-3.23854500	1.28243100	-2.44660500
C	-2.13580900	-2.53910700	-2.17913900
H	-2.87038800	-3.33935200	-2.33475400
H	-2.04093000	-1.98334800	-3.11317000
H	-1.17434400	-3.01067500	-1.96356900
C	-0.55428000	2.86813500	-0.80328700
O	0.08443000	2.98131000	0.28652800
O	-1.13373500	1.79825800	-1.19309900
C	-0.61428300	4.06608400	-1.72066200
H	-1.42492800	3.97066600	-2.44299700
H	-0.72519600	4.97811100	-1.13071300
H	0.33365400	4.13632300	-2.26496700
Rh	-1.33965800	-0.06387000	-0.13932600
C	3.64264600	-0.42366600	-0.24052300
C	4.86153600	0.16506000	0.10920600
C	6.03458900	-0.26897900	-0.49816900
C	5.96818200	-1.29112800	-1.45055700
C	4.73943300	-1.86235600	-1.79336100
C	3.55061100	-1.43559000	-1.19477000
C	3.18832700	1.05705900	1.58305400
C	4.64664900	1.26631500	1.11994000
H	6.98830600	0.18004500	-0.23740300
H	6.87730300	-1.64093300	-1.92906400
H	4.70188100	-2.65136500	-2.53779600
H	2.59731000	-1.86716600	-1.46691600
H	3.14571200	0.55034800	2.54954100
H	4.77241300	2.25028200	0.65302800
N	2.59376800	0.16722400	0.53678900
H	5.34076200	1.21606700	1.96308300
H	2.61429900	1.98076600	1.64991400
C	1.29042500	0.04917100	0.29132400
O	0.78406900	-0.53177600	-0.70937400
N	0.29759400	0.65521400	1.12608600
H	0.19887300	1.81769600	0.83620900
O	0.51771000	0.58300100	2.52398300
C	0.55496300	-0.75912300	3.01094900
H	1.42387100	-1.30818400	2.62744800
H	0.63553500	-0.66379700	4.09518600
H	-0.36101900	-1.29682900	2.75167800

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Sum of electronic and thermal Free Energies= -1146.701726

C	3.43119400	0.33250600	-0.41623100
C	3.04256200	0.44186600	0.95317200
C	2.50531600	-0.85009400	1.35105000
C	2.65912500	-1.77500400	0.23710500
C	3.21347900	-1.05371500	-0.84875500
C	3.54133200	-1.58202700	-2.20819400
H	3.32001900	-0.85146600	-2.99043900
H	4.61292200	-1.81178300	-2.26926100
H	2.99216200	-2.49815100	-2.43185900
C	4.06050700	1.39368800	-1.26187700
H	3.86221100	2.39472700	-0.87539200
H	5.14860100	1.25257300	-1.28334000
H	3.70490700	1.34927100	-2.29419000
C	3.17061500	1.63738700	1.84505800
H	4.00448700	1.49695500	2.54330800
H	3.36639900	2.54652800	1.27432000
H	2.26471000	1.79804400	2.43542900
C	2.01389200	-1.20236000	2.71619700
H	1.24862600	-1.98062300	2.68348200
H	2.84960200	-1.58561800	3.31722600
H	1.60477400	-0.33326500	3.23533500
C	2.27782600	-3.22294400	0.25728700
H	3.09833500	-3.82129000	0.67156700
H	1.39553400	-3.39726700	0.87704600
H	2.06385000	-3.59805400	-0.74509300
Rh	1.27625400	-0.07334400	-0.24630000
C	-3.51608900	-0.34376600	-0.05932800
C	-4.76497200	0.28727400	-0.07852600
C	-5.92623700	-0.47337900	-0.00573000
C	-5.82278000	-1.86467400	0.08718200
C	-4.56777800	-2.48043900	0.10196200
C	-3.39100700	-1.73115100	0.02879500
C	-3.09310000	2.00775800	0.01262900
C	-4.60307200	1.78066800	-0.21957800
H	-6.89989800	0.00726000	-0.02090500
H	-6.72183600	-2.46959800	0.14716100
H	-4.50010100	-3.56150600	0.17271800
H	-2.42069300	-2.20659200	0.03328500
H	-2.64453000	2.67893400	-0.71906400
H	-5.20343100	2.34431100	0.49984500

N	-2.48618900	0.64780000	-0.11618300
H	-4.90200400	2.11136300	-1.22127700
H	-2.88672400	2.39475000	1.01182600
C	-1.19108800	0.40479700	-0.32409200
O	-0.72568000	-0.77106800	-0.59309900
N	-0.16659500	1.32724400	-0.30765800
O	-0.36279700	2.47125800	0.47471600
C	0.20343000	3.61007600	-0.18017300
H	-0.30344600	3.81318800	-1.12985300
H	0.05913900	4.44222600	0.51085400
H	1.27333000	3.45993400	-0.36297600

TS2

Sum of electronic and thermal Free Energies= -1146.664941

C	2.69775523	1.33390572	0.55932197
C	3.11714623	0.83705272	-0.73052403
C	2.91511223	1.89613072	-1.70740503
C	2.29009823	2.98903572	-1.03777603
C	2.13405523	2.64268972	0.37152297
C	1.65127123	3.58804472	1.42902097
H	1.40904223	3.07408272	2.36059397
H	2.42945023	4.32778372	1.65389597
H	0.76280723	4.13445472	1.10305997
C	2.86148723	0.58451472	1.84495597
H	2.40364923	-0.40756528	1.79376997
H	3.92912123	0.44380872	2.05023997
H	2.42959723	1.12024472	2.69089097
C	3.78985023	-0.47173228	-1.00019103
H	4.87987623	-0.34920628	-0.96749603
H	3.51575623	-1.22588628	-0.25950803
H	3.52567823	-0.85113728	-1.98955003
C	3.26360623	1.79110372	-3.15714003
H	2.97641623	2.68681372	-3.70944703
H	4.34395323	1.65138272	-3.27507403
H	2.75578723	0.93338572	-3.60890303
C	1.86632123	4.28729172	-1.64628203
H	2.63869623	5.04645572	-1.46930603
H	1.71893823	4.20228172	-2.72393503
H	0.93708023	4.65183672	-1.20256903
Rh	0.98888123	1.19934072	-0.86133303
C	-3.52769600	0.37718200	0.13012100
C	-4.76744900	-0.25927600	0.24207200
C	-5.93008500	0.44098200	-0.06003000
C	-5.83235000	1.77430400	-0.47105400
C	-4.58352300	2.39164600	-0.58489200
C	-3.40497100	1.70118500	-0.28821400
C	-3.10883900	-1.76990300	1.09912300
C	-4.58718900	-1.69975400	0.65807000
H	-6.89981800	-0.04092400	0.02108700
H	-6.73286800	2.33247600	-0.70630600
H	-4.52199200	3.42544000	-0.90987200
H	-2.43686600	2.17244400	-0.38716700
H	-3.01546300	-1.74122000	2.18684000
H	-4.77690600	-2.37314600	-0.18606500
N	-2.49326100	-0.53386300	0.52185000
H	-5.25674400	-1.99904500	1.46882700
H	-2.58367300	-2.64984600	0.72883500
C	-1.19187100	-0.36883000	0.29372900
O	-0.26000791	-0.78799932	1.03617106
N	-0.70085741	0.39231373	-0.81505186
O	-1.37241360	0.21490363	-2.05008943
C	-1.29494859	-1.12592067	-2.53589877
H	-1.84129430	-1.82551865	-1.89122019
H	-1.76504851	-1.09695917	-3.52043739
H	-0.25512927	-1.45058601	-2.62939419

3

Sum of electronic and thermal Free Energies= -1146.675204

C	-3.46188400	-0.16443500	0.14781000
C	-4.78629300	0.28964000	0.04087600
C	-5.84027500	-0.61188200	0.11558200
C	-5.56471100	-1.96917100	0.31534600
C	-4.24488800	-2.40441300	0.45490500
C	-3.17335200	-1.50869300	0.38221500
C	-3.38483000	2.19353500	0.32003200
C	-4.80404600	1.79212400	-0.12494900
H	-6.86609400	-0.26440600	0.03426500
H	-6.37968300	-2.68275800	0.38115600
H	-4.04100400	-3.45511600	0.63692700
H	-2.15880400	-1.85968800	0.51290100
H	-2.95252200	3.02373600	-0.23900200
H	-5.57305600	2.28140500	0.47793800
N	-2.58573300	0.96108700	0.08161100
H	-4.98101600	2.07136600	-1.17170000
H	-3.35033900	2.44479900	1.38582800
C	-1.22710000	1.07701800	0.12114400
O	-0.65620800	2.07696700	0.56404500
N	-0.40819000	0.04846700	-0.40078200
O	-0.92791100	-0.91442800	-1.29135000
C	-1.25056600	-0.36594700	-2.59124000

H	-0.37289900	0.11450600	-3.03451500	C	3.35587500	-2.55547800	1.03157800
H	-1.55775500	-1.22570100	-3.18764200	C	2.12085600	-3.16284800	1.27707800
H	-2.07457600	0.34657500	-2.50826100	H	-0.03159400	-3.05119700	1.01721300
C	3.00298000	-0.79511100	1.25216000	H	4.26217100	-2.96250300	1.46414200
C	3.66254100	-0.89507600	-0.01524300	H	2.06854900	-4.08400300	1.85442900
C	3.53636300	0.36535300	-0.69125300	O	2.01135300	1.73364500	-2.79803500
C	2.81105700	1.28173200	0.17382000	C	-3.24561500	1.64306200	-1.26689400
C	2.46543900	0.55680000	1.38123100	H	-2.52106600	2.46589100	-1.22599000
C	1.79848000	1.14462700	2.58045600	H	-3.42447600	1.41634300	-2.32055700
H	1.42721900	0.37244200	3.25651500	H	-4.19634400	2.00283700	-0.85039300
H	2.52131600	1.75678600	3.13576200	C	-1.80492300	1.75351700	1.53702300
H	0.96407900	1.78367600	2.28155700	H	-1.42399900	2.53859300	0.88359300
C	2.91774500	-1.86087600	2.29599100	H	-2.73210100	2.11918400	1.98795700
H	2.98452200	-2.86112500	1.86397500	H	-1.08588200	1.59588800	2.35231100
H	3.75025600	-1.75028800	3.00327700	C	-1.49149200	-1.24373000	2.64535800
H	1.99035800	-1.79324200	2.86879600	H	-1.03970700	-0.41531900	3.18979300
C	4.34947000	-2.11292800	-0.55420400	H	-2.34834500	-1.59106100	3.23239800
H	4.30544100	-2.15608500	-1.64476300	H	-0.75987300	-2.05833000	2.61788000
H	5.40878500	-2.10167500	-0.26954100	C	-2.60493900	-3.20645500	0.38132300
H	3.91413600	-3.03387200	-0.16033900	H	-1.91114800	-3.65182500	1.09820300
C	4.10143200	0.70447500	-2.03340900	H	-3.62010400	-3.39528200	0.74696700
H	3.51124100	1.47102500	-2.53979200	H	-2.49755300	-3.73137800	-0.57823900
H	5.12030200	1.09614600	-1.91722600	C	-3.68178000	-1.46676000	-2.02186500
H	4.16038200	-0.17105200	-2.68339300	H	-3.15482400	-2.33175600	-2.44998600
C	2.53534100	2.72852800	-0.07019400	H	-4.67235700	-1.80026200	-1.71621000
H	3.21174800	3.33682400	0.54433500	H	-3.80810100	-0.71972600	-2.80767900
H	2.69764500	3.00248400	-1.11408700	C	0.23411400	3.38228000	-1.22142300
H	1.50554800	2.97202600	0.20305800	H	1.15540700	3.48225800	-1.78794900
Rh	1.46239500	-0.35017300	-0.29044100	H	-0.50518100	4.10906500	-1.56154400
TS3				H	0.41215900	3.51356000	-0.14343000
Sum of electronic and thermal Free Energies= -1375.334781				C	4.57998400	-0.65577700	-0.32271900
Rh	-0.64178200	-0.61360500	-0.64913200	C	3.99300700	0.05440600	-1.55625800
N	0.35816400	1.01357900	-0.98969400	N	2.54643100	0.13373100	-1.24135600
C	-2.95337900	-0.90481600	-0.83710700	H	4.89843300	0.06628300	0.43337400
C	-2.38159700	-1.73438500	0.23178700	H	5.44398700	-1.27552100	-0.57137400
C	-1.93285300	-0.85084000	1.27054400	H	4.38989700	1.05754200	-1.72815500
C	-2.07888900	0.48826400	0.78159300	H	4.15437600	-0.53200700	-2.46986600
C	-2.75485600	0.44997200	-0.51310200	H	0.68362143	1.25173856	0.28806281
O	-0.39634200	2.10373700	-1.46548000	O	-0.32276300	3.31183500	1.90401200
C	1.76532800	1.05441600	-1.81352700	C	0.44202900	2.46358700	2.30481700
C	2.20008800	-0.90450700	-0.31253700	O	0.92238200	1.47835100	1.50430300
C	0.89654900	-1.31084700	0.15354500	C	0.98234800	2.34550900	3.70754200
C	3.39936400	-1.46082500	0.18753500	H	0.57505800	3.14663200	4.32277900
C	0.91831400	-2.57246500	0.79509900	H	0.71323300	1.37323800	4.13088500

H	2.07482400	2.40252400	3.69253900

4

Sum of electronic and thermal Free Energies= -1146.701726

Rh	0.66468500	-0.15790400	-0.31935400
N	-0.45161300	1.63621500	-0.74554100
C	1.69413200	-0.19227500	1.55744300
C	1.68529800	-1.56109300	1.03925800
C	2.41368700	-1.53331200	-0.17566200
C	3.02127300	-0.18813300	-0.33060900
C	2.61877800	0.60665700	0.74581100
O	0.45805000	2.70314400	-0.88334700
C	-1.54543600	1.94939900	0.22700000
C	-2.32493600	-0.38837800	-0.15813000
C	-1.14160400	-1.07088300	-0.47354900
C	-3.59083100	-0.98741700	-0.15507700
C	-1.30691800	-2.41205800	-0.87602700
C	-3.71684200	-2.31149500	-0.55644600
C	-2.56609300	-3.01542600	-0.93629600
H	-0.43718300	-3.00380500	-1.14699800
H	-4.68794100	-2.79728400	-0.57049500
H	-2.64940800	-4.04969600	-1.25586900
O	-1.57659200	3.01089600	0.81036500
C	2.98771100	2.02728000	1.04229400
H	3.54562400	2.47856500	0.22072900
H	2.10159500	2.64196800	1.21929500
H	3.61532800	2.07329900	1.94016600
C	3.91794200	0.18971500	-1.46585200
H	4.08332200	1.26688200	-1.51281300
H	4.89478300	-0.29748900	-1.35406700
H	3.50709400	-0.13535100	-2.42664700
C	2.70389200	-2.68987300	-1.07898000
H	2.70527200	-2.39177600	-2.13070800
H	3.69856800	-3.09651900	-0.85486300
H	1.98179600	-3.49824800	-0.95066800
C	1.07452200	-2.74831900	1.71644400
H	0.79352700	-3.52519000	1.00395600
H	1.79755300	-3.18266400	2.41789200
H	0.18197100	-2.47539700	2.28237400
C	1.09120900	0.25775100	2.84716800
H	0.20597500	-0.32547500	3.10739300
H	1.82402300	0.13072200	3.65591100
H	0.81834300	1.31516100	2.81569800
C	-0.08153200	3.80411000	-1.64435900
H	-0.92319600	4.26576700	-1.12660400
H	0.74603300	4.51025700	-1.72115200
H	-0.36644300	3.46987200	-2.65112000
C	-4.63040500	0.00894700	0.31772900
C	-3.77594600	1.14043900	0.93947900
N	-2.45074000	0.95193000	0.30100400
H	-5.22453100	0.38299100	-0.52520200
H	-5.32771400	-0.41508800	1.04451000
H	-4.14248700	2.14679800	0.73530000
H	-3.67526200	1.02233000	2.02377200
H	-0.88008200	1.45190000	-1.66309200

5[4a]

Sum of electronic and thermal Free Energies= -1381.181016

Rh	0.66070000	-0.20055400	-0.10150500
N	-0.35809900	1.45541200	-1.20031300
C	2.84486800	-0.48797200	0.70025700
C	2.21287200	-1.75356800	0.31182500
C	2.03898400	-1.73098800	-1.11623100
C	2.37989800	-0.41640200	-1.56344500
C	2.93991900	0.33230500	-0.44004500
O	0.54263200	2.50971400	-1.44727200
C	-1.63144500	1.94180600	-0.60646600
C	-2.34584200	-0.44686200	-0.63493600
C	-1.14425000	-1.15821200	-0.52289000
C	-3.60284700	-1.05452100	-0.78548700
C	-1.27990900	-2.55476500	-0.61173700
C	-3.69527800	-2.43618000	-0.87679900
C	-2.51663600	-3.18357600	-0.79477500
H	-0.40871100	-3.18726800	-0.50140800
H	-4.65777100	-2.92513900	-0.99229000
H	-2.55887600	-4.26756700	-0.84694000
O	-1.78304100	3.10949200	-0.30434800
C	3.57824900	1.68383700	-0.54973100
H	2.93653800	2.38094000	-1.09180100
H	3.78901400	2.11363100	0.43140000
H	4.53086800	1.61095700	-1.08856200
C	2.39350300	0.04717200	-2.98739300
H	2.16387900	1.11270800	-3.05993100
H	3.39186600	-0.10018000	-3.41900400
H	1.68614000	-0.51259500	-3.60399300
C	1.70704400	-2.88572100	-2.01351100
H	0.89540900	-2.65635700	-2.70814100
H	2.59182600	-3.14298000	-2.60828100
H	1.42900600	-3.77676500	-1.44949500
C	2.12313600	-2.96092800	1.19691000

H	1.29729700	-3.61848700	0.91549200
H	3.04806500	-3.54811700	1.13164200
H	1.99109400	-2.68030400	2.24407300
C	3.33325100	-0.19121400	2.08375800
H	2.54990400	-0.35413200	2.82978800
H	4.16852600	-0.85589500	2.33468100
H	3.68745200	0.83607000	2.18134500
C	0.12623300	3.36556000	-2.53317700
H	-0.79174700	3.89826400	-2.28451200
H	0.94982800	4.07117300	-2.65244200
H	0.00915900	2.78312500	-3.45699500
C	-4.68960300	0.00110500	-0.79638400
C	-3.96929900	1.24715400	-0.23349600
N	-2.54315900	0.95935600	-0.50810500
H	-5.04772400	0.18291900	-1.81754600
H	-5.55714800	-0.27417600	-0.19152800
H	-4.25225600	2.18733700	-0.70751800
H	-4.11832500	1.34656000	0.84742400
C	-0.35863900	-0.15794600	2.02390600
C	0.11449200	0.97222600	1.83372700
C	-1.03639700	-1.29455400	2.67987700
C	-1.36638000	-0.98512900	4.15181000
H	-0.40357800	-2.18653700	2.61536600
H	-1.95011800	-1.53482400	2.12806200
H	-1.87067400	-1.84360600	4.60410200
H	-0.46039800	-0.77882700	4.72833600
H	-2.02799600	-0.11861100	4.23387000
C	0.54806300	2.37282500	2.01476200
C	0.04227000	2.95141700	3.35043700
H	0.18429200	2.98434700	1.18419800
H	1.64277500	2.41307400	1.97598400
H	0.39489900	3.98074100	3.45890500
H	-1.05022300	2.96193600	3.38129100
H	0.40822000	2.37137400	4.20201600
H	-0.56747300	0.99392100	-2.09257100

TS4[4a]

Sum of electronic and thermal Free Energies= -1381.17225

Rh	0.74474900	-0.06307500	-0.09469200
N	-0.34393000	1.86166600	-0.52973000
C	2.90541300	-0.63426100	0.45791600
C	2.29572500	-1.65903000	-0.37037800
C	2.08492600	-1.10869900	-1.69782700
C	2.42182300	0.26277500	-1.63537000
C	2.94164500	0.56490300	-0.29213000
O	0.54997900	2.93177400	-0.31999700
C	-1.64661100	2.09600600	0.14286800
C	-2.34326600	-0.17472700	-0.62577000
C	-1.19860500	-0.96698900	-0.41407200
C	-3.53245800	-0.66185400	-1.18713900
C	-1.29979300	-2.29287600	-0.89973700
C	-3.58741400	-1.96653300	-1.65787300
C	-2.44919600	-2.77552200	-1.52384900
H	-0.47171900	-2.97446300	-0.74752500
H	-4.49788100	-2.36260200	-2.09712100
H	-2.47430600	-3.80231600	-1.87593000
O	-1.85068800	3.08589800	0.81104300
C	3.58469500	1.85830900	0.10643800
H	3.03438100	2.71490900	-0.28391600
H	3.64030600	1.96453900	1.19179900
H	4.60876600	1.90759800	-0.28506400
C	2.39815000	1.24817600	-2.76342700
H	2.09193900	2.23795300	-2.41640000
H	3.40241200	1.35502600	-3.19203200
H	1.73011400	0.93484500	-3.56881600
C	1.64825100	-1.88268500	-2.90477200
H	1.37141100	-1.22256200	-3.72928300
H	2.46196600	-2.52729900	-3.25859100
H	0.78915900	-2.52437400	-2.69278600
C	2.24634500	-3.11550000	-0.01751900
H	1.54771800	-3.66942000	-0.64771100
H	3.23744100	-3.56169500	-0.17296700
H	1.97645800	-3.27919800	1.02770500
C	3.44565100	-0.86497000	1.83639400
H	2.76192700	-1.46168800	2.44620000
H	4.39399200	-1.41354900	1.77954100
H	3.64269700	0.07210500	2.36040100
C	0.17317100	4.13544800	-1.02232100
H	-0.75437100	4.55094700	-0.62866700
H	0.99987200	4.82361900	-0.83944800
H	0.09386800	3.94191700	-2.10088000
C	-4.60178900	0.41069500	-1.11642900
C	-4.01860000	1.40530000	-0.08397100
N	-2.56141000	1.14671200	-0.17357300
H	-4.74109700	0.89397600	-2.09165000
H	-5.57314600	0.02159800	-0.80213900
H	-4.22075300	2.45446900	-0.30069700
H	-4.36883700	1.18660100	0.93059900
C	-0.81993500	-0.82081600	1.54826400

C	-0.02117500	0.14104900	1.83341600
C	-1.63798300	-1.90234700	2.18602300
C	-0.87942400	-3.20833500	2.46596500
H	-2.53461200	-2.10639900	1.59519300
H	-1.96965000	-1.47067100	3.13969400
H	-1.53084300	-3.90804400	2.99762400
H	-0.55862400	-3.69213200	1.54003300
H	0.00236200	-3.02599100	3.08739800
C	0.40835000	1.08858300	2.89997000
C	-0.29369600	0.86308800	4.24895100
H	0.21747200	2.11005500	2.54742600
H	1.49508900	1.01311100	3.02017100
H	0.06381600	1.59317200	4.98073800
H	-1.37639700	0.98762100	4.15549500
H	-0.09237600	-0.13712500	4.64419100
H	-0.51438700	1.77870900	-1.53842500

6[4a]

Sum of electronic and thermal Free Energies= -1381.192376

Rh	-1.33561	0.06853	0.07348
C	-2.86848	1.72591	-0.66327
C	-3.50215	0.98492	0.34208
C	-3.47503	-0.41954	-0.07387
C	-2.93445	-0.49085	-1.42369
C	-2.48427	0.80867	-1.75023
O	1.52791	-0.9895	-2.11197
C	2.9296	-1.63439	-0.27334
O	3.63398	-2.62539	-0.27492
C	-1.87036	1.25286	-3.04355
H	-1.43127	0.41578	-3.59028
H	-1.09075	2.00348	-2.88615
H	-2.63086	1.70767	-3.69165
C	-2.92653	-1.70691	-2.30182
H	-2.13587	-1.65483	-3.05378
H	-3.88111	-1.80633	-2.83407
H	-2.78125	-2.62384	-1.7242
C	-4.2682	-1.50129	0.59209
H	-4.2484	-1.41506	1.68089
H	-3.92504	-2.49928	0.31299
H	-5.31885	-1.42042	0.28136
C	-4.14916	1.49526	1.5952
H	-5.2388	1.54658	1.47392
H	-3.80304	2.49941	1.85026
H	-3.94699	0.8452	2.45013
C	-2.64876	3.20833	-0.70674
H	-2.83297	3.6757	0.26289
H	-3.32791	3.6747	-1.43129
H	-1.62871	3.45731	-1.01417
C	2.23737	-1.41627	-3.29154
H	3.32207	-1.33802	-3.16681
H	1.90565	-0.73008	-4.07142
H	1.96629	-2.44414	-3.56125
C	0.49416	-0.36403	1.47011
C	-0.14358	-1.41639	0.6967
C	0.54701	-0.472	3.00293
C	-0.70865	0.0091	3.74327
H	0.75821	-1.50944	3.27808
H	1.40911	0.1076	3.35198
H	-0.5873	-0.12122	4.82331
H	-1.59189	-0.55284	3.42698
H	-0.90113	1.07008	3.55775
C	-0.39724	-2.87498	1.03703
C	-1.4202	-3.16896	2.14717
H	-1.64799	-4.23884	2.14313
H	-2.35115	-2.62504	1.9922
H	-1.0434	-2.92113	3.13979
N	1.80961	-1.81605	-1.00385
H	1.68779	-2.7961	-1.27696
C	2.49056	0.76798	0.30345
C	1.20715	0.83711	0.89109
C	3.2681	1.90612	0.05957
C	0.7281	2.14873	1.14647
C	2.74825	3.17479	0.29138
C	1.4616	3.29051	0.82607
H	-0.23051	2.25326	1.64074
H	3.34632	4.05969	0.09516
H	1.04853	4.27084	1.03991
C	4.65985	1.49619	-0.37651
C	4.72376	0.0179	0.06638
N	3.29383	-0.38166	0.07584
H	4.77673	1.58777	-1.46383
H	5.44402	2.09617	0.09078
H	5.28169	-0.63789	-0.60205
H	5.1352	-0.08274	1.07594
H	-0.74957	-3.37069	0.12305
H	0.55197	-3.35968	1.30986

TS5[4ad]

Sum of electronic and thermal Free Energies= -1381.176732

Rh	-1.33561000	0.06853000	0.07348000

C	-2.86848000	1.72591000	-0.66327000
C	-3.50215000	0.98492000	0.34208000
C	-3.47503000	-0.41954000	-0.07387000
C	-2.93445000	-0.49085000	-1.42369000
C	-2.48427000	0.80867000	-1.75023000
O	5.01055611	-2.22456205	-1.31377110
C	2.92960000	-1.63439000	-0.27334000
O	2.25709506	-2.40781135	0.38071749
C	-1.87036000	1.25286000	-3.04355000
H	-1.43127000	0.41578000	-3.59028000
H	-1.09075000	2.00348000	-2.88615000
H	-2.63086000	1.70767000	-3.69165000
C	-2.92653000	-1.70691000	-2.30182000
H	-2.13587000	-1.65483000	-3.05378000
H	-3.88111000	-1.80633000	-2.83407000
H	-2.78125000	-2.62384000	-1.72420000
C	-4.26820000	-1.50129000	0.59209000
H	-4.24840000	-1.41506000	1.68089000
H	-3.92504000	-2.49928000	0.31299000
H	-5.31885000	-1.42042000	0.28136000
C	-4.14916000	1.49526000	1.59520000
H	-5.23880000	1.54658000	1.47392000
H	-3.80304000	2.49941000	1.85026000
H	-3.94699000	0.84520000	2.45013000
C	-2.64876000	3.20833000	-0.70674000
H	-2.83297000	3.67570000	0.26289000
H	-3.32791000	3.67470000	-1.43129000
H	-1.62871000	3.45731000	-1.01417000
C	5.60903734	-3.19388166	-0.43110966
H	5.37510557	-2.99007913	0.61864992
H	6.68147815	-3.08705181	-0.59713907
H	5.29205579	-4.21054739	-0.69313656
C	0.49416000	-0.36403000	1.47011000
C	-0.14358000	-1.41639000	0.69670000
C	0.54701000	-0.47200000	3.00293000
C	-0.70865000	0.00910000	3.74327000
H	0.75821000	-1.50944000	3.27808000
H	1.40911000	0.10760000	3.35198000
H	-0.58730000	-0.12122000	4.82331000
H	-1.59189000	-0.55284000	3.42698000
H	-0.90113000	1.07008000	3.55775000
C	-0.39724000	-2.87498000	1.03703000
C	-1.42020000	-3.16896000	2.14717000
H	-1.64799000	-4.23884000	2.14313000
H	-2.35115000	-2.62504000	1.99220000
H	-1.04340000	-2.92113000	3.13979000
N	3.60140360	-2.26599946	-1.25861774
H	3.28977214	-3.23560674	-1.37119986
C	2.49056000	0.76798000	0.30345000
C	1.20715000	0.83711000	0.89109000
C	3.26810000	1.90612000	0.05957000
C	0.72810000	2.14873000	1.14647000
C	2.74825000	3.17479000	0.29138000
C	1.46160000	3.29051000	0.82607000
H	-0.23051000	2.25326000	1.64074000
H	3.34632000	4.05969000	0.09516000
H	1.04853000	4.27084000	1.03991000
C	4.65985000	1.49619000	-0.37651000
C	4.72376000	0.01790000	0.06638000
N	3.29383000	-0.38166000	0.07584000
H	4.77673000	1.58777000	-1.46383000
H	5.44402000	2.09617000	0.09078000
H	5.28169000	-0.63789000	-0.60205000
H	5.13520000	-0.08274000	1.07594000
H	-0.74957000	-3.37069000	0.12305000
H	0.55197000	-3.35968000	1.30986000

7[4ad]

Sum of electronic and thermal Free Energies= -1381.201487

Rh	1.21021	0.15138	-0.49866
C	2.39145	-0.73108	1.18973
C	3.24001	0.11976	0.43404
C	3.38269	-0.44043	-0.92588
C	2.58978	-1.59488	-1.00899
C	1.89822	-1.74468	0.27832
O	-3.12914	2.01271	-1.65786
C	-1.36134	0.48285	-1.81058
O	-0.04288	0.39012	-2.05553
C	1.03272	-2.90572	0.64387
H	0.435	-3.2456	-0.20428
H	0.36005	-2.67529	1.47107
H	1.67295	-3.74381	0.95214
C	2.41186	-2.50541	-2.18358
H	1.36078	-2.77013	-2.32668
H	2.97038	-3.43706	-2.03192
H	2.76996	-2.0474	-3.10711
C	4.24749	0.15033	-1.99454
H	4.192	1.24231	-1.99878
H	3.96622	-0.20643	-2.98684

H	5.29721	-0.12108	-1.82529
C	4.03822	1.27576	0.94613
H	5.06016	0.9418	1.16896
H	3.61841	1.69037	1.86401
H	4.11558	2.07709	0.20706
C	2.10252	-0.65413	2.65692
H	2.22275	0.36085	3.03973
H	2.7948	-1.30179	3.20903
H	1.08736	-0.98452	2.88439
C	-4.23202	2.38279	-2.49506
H	-3.95337	3.18805	-3.18544
H	-4.9987	2.74401	-1.80761
H	-4.6058	1.5258	-3.06339
C	-1.11468	0.92861	1.38996
C	-0.21028	1.48142	0.63325
C	-1.5594	1.86899	2.50301
C	-0.6276	1.90318	3.73381
H	-1.63812	2.8824	2.09804
H	-2.56436	1.58209	2.82851
H	-1.00031	2.63332	4.45814
H	0.39105	2.18912	3.46005
H	-0.5743	0.9361	4.24054
C	0.06529	2.94691	0.30971
C	1.0957	3.69197	1.17408
H	1.2539	4.69958	0.77666
H	2.06133	3.18067	1.17777
H	0.76666	3.79692	2.20969
N	-2.08753	1.48564	-2.44439
H	-1.49233	2.22979	-2.8056
C	-2.05752	-1.02382	0.20756
C	-1.64052	-0.43392	1.41739
C	-2.78759	-2.23001	0.17108
C	-1.95531	-1.1521	2.60033
C	-3.04663	-2.91775	1.33954
C	-2.60763	-2.37562	2.56564
H	-1.67672	-0.73368	3.56086
H	-3.6053	-3.84913	1.32288
H	-2.81401	-2.90223	3.4916
C	-3.19259	-2.50644	-1.26262
C	-2.99893	-1.1272	-1.93774
N	-1.99565	-0.47309	-1.05922
H	-2.5345	-3.25674	-1.72034
H	-4.21924	-2.86758	-1.35896
H	-2.62101	-1.18736	-2.95977
H	-3.9339	-0.55477	-1.93655
H	0.41449	3.00534	-0.73028
H	-0.88838	3.49284	0.33229

TS6[4ad]

Sum of electronic and thermal Free Energies= -1381.163853

Rh	1.14248	0.01652	-0.35248
C	3.20947	0.86876	0.44972
C	2.86414	1.41869	-0.82285
C	2.82274	0.3392	-1.79114
C	3.08119	-0.8717	-1.08536
C	3.27663	-0.56068	0.31725
O	-1.65183	3.34693	1.009
C	-1.14872	1.55059	-0.4665
O	-0.3252	1.08736	-1.35752
C	3.692	-1.56268	1.35391
H	2.98305	-2.39455	1.3674
H	3.72061	-1.12185	2.35335
H	4.69484	-1.95554	1.14038
C	3.21089	-2.23903	-1.6817
H	2.88248	-3.00225	-0.97508
H	4.26066	-2.43364	-1.93854
H	2.61874	-2.33718	-2.59406
C	2.57029	0.50882	-3.25887
H	3.43552	0.96296	-3.75926
H	1.70302	1.15366	-3.43452
H	2.37097	-0.45039	-3.74103
C	2.72445	2.8734	-1.1611
H	3.63628	3.25512	-1.63909
H	2.55016	3.48136	-0.26809
H	1.89654	3.03745	-1.8575
C	3.60442	1.68578	1.64376
H	2.87546	2.46685	1.87845
H	4.56026	2.18612	1.44206
H	3.73569	1.07267	2.53472
C	-2.1546	4.66081	0.79357
H	-1.34338	5.38937	0.65905
H	-2.71154	4.90926	1.70048
H	-2.81952	4.70237	-0.07627
C	-1.38372	-0.57501	1.50002
C	-0.41503	0.37401	1.23921
C	-1.69845	-1.04656	2.92104
C	-0.87993	-2.27939	3.3605
H	-1.52139	-0.22692	3.62413
H	-2.76467	-1.28495	2.99385

H	-1.14187	-2.55474	4.3886
H	0.19242	-2.08733	3.30847
H	-1.06503	-3.14197	2.71647
C	0.14361	1.2512	2.35542
C	1.06278	0.5896	3.40008
H	1.62044	1.35199	3.95544
H	1.77746	-0.08673	2.92823
H	0.49878	0.00714	4.12983
N	-0.95588	2.917	-0.15208
H	0.03837	3.10056	-0.0261
C	-2.87804	-0.13575	-0.41281
C	-2.33644	-1.06	0.49581
C	-4.02708	-0.38789	-1.1804
C	-2.99896	-2.31134	0.54892
C	-4.63225	-1.62851	-1.12196
C	-4.09324	-2.60101	-0.2557
H	-2.63513	-3.07064	1.23201
H	-5.51578	-1.84959	-1.71484
H	-4.55594	-3.58162	-0.19611
C	-4.3843	0.87445	-1.94088
C	-3.53827	1.96469	-1.22481
N	-2.49308	1.18938	-0.52144
H	-4.09292	0.7909	-2.99583
H	-5.45289	1.10677	-1.91177
H	-3.07789	2.67548	-1.91387
H	-4.1444	2.52337	-0.5011
H	0.70096	2.07252	1.88856
H	-0.69036	1.74153	2.87614

8[4ad]

Sum of electronic and thermal Free Energies= -1381.190035

Rh	-1.23661	-0.2027	-0.37135
C	-2.19395	1.4486	0.83089
C	-3.11139	0.37448	0.79451
C	-3.42651	0.10268	-0.61259
C	-2.73652	1.04759	-1.43388
C	-1.90532	1.836	-0.55127
O	2.87779	-2.53936	-0.8502
C	1.10111	-1.03216	-1.09018
O	-0.08177	-0.89845	-1.81891
C	-1.02702	2.97683	-0.9491
H	-0.69357	2.88763	-1.98432
H	-0.14928	3.05106	-0.30315
H	-1.58635	3.91753	-0.85799
C	-2.82483	1.18177	-2.92171
H	-1.86958	1.48807	-3.35327
H	-3.57321	1.93735	-3.19027
H	-3.11533	0.24135	-3.39391
C	-4.38842	-0.93867	-1.08445
H	-4.38761	-1.81656	-0.43463
H	-4.17009	-1.26201	-2.10397
H	-5.40634	-0.52699	-1.07618
C	-3.75675	-0.31113	1.9588
H	-4.76395	0.0938	2.1184
H	-3.19153	-0.16392	2.88021
H	-3.86023	-1.38598	1.794
C	-1.63278	2.14595	2.02965
H	-1.86181	1.61386	2.95305
H	-2.06332	3.15191	2.10657
H	-0.54665	2.25873	1.96133
C	4.15741	-2.62576	-1.47328
H	4.14138	-3.30922	-2.33037
H	4.82621	-3.0221	-0.70555
H	4.51505	-1.64332	-1.80165
C	1.17412	-0.73863	1.5028
C	0.64007	-1.3932	0.36737
C	1.0583	-1.33686	2.89385
C	0.00574	-0.70339	3.82352
H	0.86714	-2.40813	2.82107
H	2.04105	-1.24097	3.3676
H	0.05388	-1.1725	4.81028
H	-1.0053	-0.84836	3.43398
H	0.16852	0.3694	3.95365
C	0.13955	-2.84713	0.46019
C	-1.18488	-3.13686	1.18331
H	-1.35949	-4.21725	1.21134
H	-2.02987	-2.68467	0.6506
H	-1.20732	-2.77176	2.21232
N	1.92217	-2.02571	-1.78181
H	1.32812	-2.80934	-2.05325
C	2.25372	0.86324	0.03283
C	1.95224	0.45571	1.34946
C	3.03787	1.99804	-0.26775
C	2.5118	1.25174	2.39321
C	3.54835	2.74725	0.76721
C	3.27993	2.3634	2.10987
H	2.33905	0.98206	3.42883
H	4.1632	3.62138	0.57127
H	3.69609	2.95043	2.92158

C	3.12981	2.12185	-1.77715
C	2.40389	0.84585	-2.30118
N	1.83314	0.22922	-1.08243
H	2.63717	3.03344	-2.13362
H	4.16525	2.16495	-2.1275
H	1.60184	1.06732	-3.00988
H	3.0861	0.14209	-2.78305
H	0.02719	-3.22715	-0.55735
H	0.9423	-3.44613	0.90755

P1[4ad]

Sum of electronic and thermal Free Energies= -711.614315

C	1.44871	0.30382	-0.43176
C	3.72063	-0.25037	-0.99673
C	4.27652	0.75251	-0.20236
C	4.4446	-1.17252	-1.75988
C	5.69441	0.80843	-0.20097
C	5.82275	-1.08849	-1.74466
C	6.43803	-0.0871	-0.95659
H	6.21024	1.55093	0.39727
H	6.43408	-1.78144	-2.3156
H	7.5218	-0.0225	-0.93837
O	0.23471	0.03268	-0.67563
C	3.46674	-2.1181	-2.42493
C	2.06657	-1.59186	-1.98948
N	2.36942	-0.44398	-1.10098
H	3.57433	-2.12605	-3.51463
H	3.61326	-3.13949	-2.0628
H	1.45786	-1.24324	-2.82756
H	1.50965	-2.33677	-1.42023
C	3.34892	1.5774	0.54297
C	1.98566	1.34687	0.45766
C	3.93975	2.6782	1.40254
C	4.4428	3.888	0.58741
H	4.77715	2.26212	1.97552
H	3.21354	3.02505	2.13917
H	4.86967	4.64349	1.25467
H	5.21216	3.59893	-0.13343
H	3.62751	4.35317	0.02636
C	0.99992	2.14017	1.29302
C	0.65954	3.54193	0.7589
H	1.3865	2.22114	2.31428
H	0.08575	1.54604	1.41816
H	-0.07265	4.02355	1.41652
H	1.54492	4.1824	0.72607
H	0.22943	3.49308	-0.24411

TS5[4ac]

Sum of electronic and thermal Free Energies= -1381.153413

Rh	0.9818	0.04356	0.00622
C	2.71701	1.60762	0.43273
C	3.26719	0.45443	-0.15928
C	2.94626	-0.69433	0.70295
C	2.25431	-0.20351	1.86325
C	2.03525	1.19351	1.65278
O	-1.29811	-1.13701	1.80997
C	-2.97366	-1.61165	0.17046
O	-3.75581	-2.538	0.06983
C	1.33776	2.12939	2.5925
H	0.64993	1.60033	3.25517
H	0.77057	2.89311	2.0541
H	2.07184	2.64947	3.22135
C	1.91511	-0.99983	3.08766
H	1.08892	-0.55198	3.6433
H	2.7783	-1.0488	3.76412
H	1.6352	-2.02614	2.83802
C	3.55863	-2.05829	0.59022
H	3.87072	-2.29005	-0.42898
H	2.87808	-2.84383	0.92881
H	4.4547	-2.1105	1.22247
C	4.11244	0.38794	-1.39438
H	5.17723	0.40536	-1.12779
H	3.92644	1.23456	-2.05859
H	3.93495	-0.53012	-1.96002
C	2.84113	3.02283	-0.05007
H	3.0375	3.07044	-1.12436
H	3.6702	3.53437	0.45486
H	1.93594	3.60146	0.15261
C	-2.04904	-1.60241	2.94671
H	-3.12564	-1.45154	2.81571
H	-1.69178	-0.99822	3.78151
H	-1.84553	-2.66187	3.14494
C	-0.48949	-0.38712	-1.5625
C	-0.14734	-1.439	-0.69211
C	-0.60346	-0.49063	-3.08651
C	0.50813	0.20026	-3.89078
H	-0.64659	-1.54736	-3.36409
H	-1.57187	-0.06487	-3.3774
H	0.35851	0.03133	-4.96151
H	1.49313	-0.18877	-3.61747

H	0.51402	1.28206	-3.72958
C	0.15507	-2.87903	-1.04245
C	1.28775	-3.08542	-2.0648
H	1.53319	-4.14988	-2.12079
H	2.18748	-2.543	-1.77233
H	1.01013	-2.75854	-3.06772
N	-1.62077	-1.85801	0.64036
H	-1.55512	-2.86164	0.83062
C	-2.38739	0.79745	-0.28404
C	-1.11962	0.8288	-0.92083
C	-3.08532	1.9688	0.03627
C	-0.58243	2.12706	-1.14776
C	-2.50162	3.21632	-0.15718
C	-1.23374	3.29087	-0.73993
H	0.35215	2.20648	-1.68878
H	-3.04236	4.12142	0.10352
H	-0.77819	4.25685	-0.93165
C	-4.48463	1.62303	0.50116
C	-4.65394	0.18048	-0.02087
N	-3.2531	-0.30702	-0.08749
H	-4.55732	1.65802	1.59567
H	-5.24384	2.29691	0.09783
H	-5.23922	-0.47497	0.6239
H	-5.09448	0.16457	-1.02328
H	0.43691	-3.40365	-0.12108
H	-0.75278	-3.37104	-1.42044

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Sum of electronic and thermal Free Energies= -1381.169634

Rh	1.19211	-0.63335	-0.25461
C	2.79261	-2.18333	0.44634
C	2.99832	-0.9914	1.15471
C	3.22243	0.06923	0.15898
C	3.31896	-0.54241	-1.15647
C	2.96144	-1.8955	-0.98964
O	-0.82246	-1.17648	-2.00103
C	-2.66112	0.39768	-1.79586
O	-3.10882	1.05878	-2.70584
C	2.8778	-2.94115	-2.05988
H	2.788	-2.5002	-3.05539
H	2.02887	-3.61351	-1.90127
H	3.7811	-3.56479	-2.0561
C	3.80431	0.13279	-2.40553
H	3.40553	-0.33735	-3.30833
H	4.89923	0.08269	-2.47153
H	3.53322	1.19132	-2.42772
C	3.6915	1.45746	0.47259
H	3.46439	1.74448	1.50001
H	3.2541	2.19963	-0.20102
H	4.78162	1.50918	0.35084
C	3.02587	-0.78783	2.63828
H	4.04997	-0.59348	2.98099
H	2.66402	-1.66943	3.17187
H	2.40938	0.06394	2.93975
C	2.53012	-3.55172	1.00171
H	1.72199	-4.05995	0.46619
H	2.25668	-3.51396	2.05816
H	3.4224	-4.18453	0.91452
C	-0.8574	-1.49935	-3.40893
H	-1.84452	-1.29936	-3.8351
H	-0.64544	-2.56783	-3.44414
H	-0.0804	-0.94613	-3.94836
C	-0.56987	0.13885	0.69976
C	-0.33615	0.77744	-0.60001
N	-1.1335	0.21344	-1.77695
H	-0.82596	0.75229	-2.59788
C	-2.738	-1.13178	0.16476
C	-1.50029	-1.03855	0.81129
C	-3.68456	-2.12538	0.44528
C	-1.22173	-2.08203	1.72126
C	-3.38152	-3.13013	1.35386
C	-2.12862	-3.10685	1.98056
H	-0.27778	-2.05207	2.25476
H	-4.10157	-3.90989	1.58196
H	-1.8693	-3.88087	2.69591
C	-4.9485	-1.88233	-0.35256
C	-4.76517	-0.43574	-0.8639
N	-3.29156	-0.23448	-0.80164
H	-5.02796	-2.58839	-1.18854
H	-5.85567	-1.98435	0.24804
H	-5.11052	-0.26218	-1.88279
H	-5.24354	0.29134	-0.20103
C	-0.44063	0.96251	1.99455
C	1.00198	1.20542	2.32713
H	-0.94685	0.40104	2.81705
H	-0.9809	1.92932	1.84828
H	1.09617	1.8029	3.26624
H	1.54193	0.23838	2.47325
H	1.50798	1.7667	1.50434

C	-0.25231	2.29126	-0.87001
C	1.15723	2.7808	-0.71404
H	-0.93311	2.8116	-0.15323
H	-0.62476	2.48196	-1.90582
H	1.2185	3.87883	-0.90987
H	1.52936	2.58986	0.32188
H	1.83784	2.2601	-1.43079

TS6[4ac]

Sum of electronic and thermal Free Energies= -1381.160649

Rh	0.99273	-0.81067	-0.23351
C	2.04618	-2.62061	0.67578
C	2.49791	-1.47015	1.36786
C	3.10835	-0.59114	0.38255
C	3.1666	-1.29045	-0.89529
C	2.45963	-2.49856	-0.72892
O	-0.80103	-1.31649	-1.80371
C	-2.52682	0.52811	-1.98244
O	-2.86514	0.99514	-3.05186
C	2.25323	-3.56907	-1.75685
H	2.3494	-3.18469	-2.77476
H	1.27253	-4.04221	-1.65608
H	3.00324	-4.36061	-1.63239
C	3.91243	-0.82266	-2.10827
H	3.521	-1.26772	-3.0263
H	4.97282	-1.09947	-2.03885
H	3.87466	0.2648	-2.21518
C	3.88954	0.65093	0.68667
H	3.65003	1.05479	1.67052
H	3.72671	1.43278	-0.06077
H	4.96153	0.41365	0.67864
C	2.44118	-1.21148	2.8423
H	3.42779	-1.37724	3.29328
H	1.73925	-1.88235	3.34224
H	2.14465	-0.18337	3.06582
C	1.36859	-3.82459	1.25434
H	0.57039	-4.19035	0.60162
H	0.92771	-3.61289	2.23032
H	2.0847	-4.64645	1.38375
C	-0.66426	-1.7551	-3.1516
H	-1.58101	-1.56558	-3.72079
H	-0.50437	-2.8367	-3.09889
H	0.19866	-1.29427	-3.65183
C	-0.59652	0.41705	0.65101
C	-0.30319	0.91011	-0.68822
N	-1.04968	0.37507	-1.78658
H	-0.64733	0.7042	-2.66905
C	-2.91394	-0.61612	0.18584
C	-1.71036	-0.56312	0.89446
C	-3.98927	-1.43726	0.55313
C	-1.61773	-1.46055	1.98187
C	-3.86829	-2.29695	1.63512
C	-2.6596	-2.30898	2.34337
H	-0.70583	-1.45388	2.56854
H	-4.6925	-2.93836	1.93138
H	-2.53914	-2.97081	3.1952
C	-5.16179	-1.21031	-0.37656
C	-4.77165	0.08279	-1.12507
N	-3.29612	0.156	-0.95192
H	-5.27554	-2.05044	-1.07273
H	-6.10963	-1.09722	0.15549
H	-5.0096	0.08383	-2.18835
H	-5.22051	0.96818	-0.66455
C	-0.27194	1.32037	1.85527
C	0.99458	0.87619	2.52564
H	-1.13228	1.2759	2.5665
H	-0.17724	2.37104	1.48765
H	1.23041	1.53121	3.39919
H	0.89952	-0.17455	2.89305
H	1.8547	0.92054	1.81409
C	0.23097	2.29808	-1.08799
C	1.61474	2.19024	-1.65747
H	0.22689	2.94826	-0.17955
H	-0.47121	2.73979	-1.83621
H	2.00256	3.1968	-1.94764
H	2.31662	1.74841	-0.90899
H	1.61854	1.5398	-2.56576

8[4ac]

Sum of electronic and thermal Free Energies= -1381.294376

Rh	0.07639	0.59916	-1.84599
N	1.97695	0.03212	0.46079
C	-0.97519	-1.0043	-0.74121
C	-1.89461	0.06244	-1.13149
C	-1.97716	0.09516	-2.57367
C	-1.03726	-0.85046	-3.07324
C	-0.42852	-1.54924	-1.93361
O	1.67923	0.90298	-0.73726
C	2.31213	-1.30519	0.52242
C	4.58302	-0.80841	-0.28464

C	4.75071	0.5789	-0.20669
C	5.38832	-1.62614	-1.08835
C	5.76397	1.12026	-1.02719
C	6.37741	-1.06529	-1.88438
C	6.55342	0.32431	-1.85384
H	5.93843	2.191	-1.00983
H	7.00837	-1.68992	-2.51083
H	7.32104	0.7866	-2.46745
O	1.46115	-2.19212	0.614
C	0.56167	-2.6668	-2.03349
H	1.25257	-2.66863	-1.18828
H	0.03322	-3.6295	-2.05566
H	1.14718	-2.59407	-2.95346
C	-0.75609	-1.15713	-4.51124
H	-1.35304	-2.01749	-4.84086
H	-1.00025	-0.3112	-5.15674
H	0.29628	-1.40687	-4.66703
C	-2.88169	0.98974	-3.36552
H	-2.58277	1.03269	-4.41518
H	-3.91152	0.61228	-3.32807
H	-2.86178	2.00476	-2.96409
C	-2.69714	0.93273	-0.21923
H	-2.61282	1.97464	-0.5408
H	-3.7542	0.63764	-0.25123
H	-2.35598	0.85524	0.81484
C	-0.67198	-1.44369	0.65737
H	-0.73905	-0.60718	1.35754
H	-1.39548	-2.20373	0.97988
H	0.33163	-1.87021	0.72778
C	2.59736	1.95305	-0.97996
H	2.70702	2.17876	-2.04529
H	2.29121	2.88064	-0.47336
H	3.57356	1.65056	-0.57489
C	4.97924	-3.07201	-0.9037
C	4.09015	-3.01335	0.36163
N	3.66983	-1.59743	0.46719
H	4.41327	-3.42996	-1.77407
H	5.83123	-3.74528	-0.77077
H	3.20444	-3.6447	0.3167
H	4.66961	-3.2769	1.25401
C	3.98043	1.40357	0.74951
C	2.69335	1.11177	1.0593
C	4.72345	2.57034	1.39208
C	4.41781	3.94839	0.77621
H	5.79873	2.37819	1.31965
H	4.50742	2.60775	2.46548
H	5.02391	4.72818	1.2507
H	4.62879	3.96544	-0.29787
H	3.3649	4.21625	0.90346
C	1.86599	1.87935	2.07236
C	0.71335	2.71335	1.47992
H	0.18115	3.23913	2.27986
H	1.09154	3.46419	0.77887
H	-0.00901	2.0894	0.94709
H	0.96908	0.15878	0.31586
H	1.4458	1.14925	2.77818
H	2.5136	2.53716	2.65619

P2[4ac]

Sum of electronic and thermal Free Energies= -766.936086

N	-0.96387	-1.37656	-0.93534
C	0.14454	-2.05051	-0.41503
C	1.25188	0.10994	0.07511
C	0.2767	1.11292	-0.02045
C	2.62601	0.387	0.05205
C	0.7691	2.4281	-0.1733
C	3.07736	1.69014	-0.10265
C	2.13091	2.71479	-0.22177
H	0.06393	3.2484	-0.24886
H	4.1409	1.91169	-0.11897
H	2.45689	3.74398	-0.33931
O	0.29247	-3.25031	-0.60778
C	3.40593	-0.89929	0.22177
C	2.3253	-1.88855	0.71402
N	1.04103	-1.27848	0.30018
H	3.83563	-1.2215	-0.73605
H	4.23085	-0.80905	0.93437
H	2.39813	-2.8871	0.28577
H	2.3415	-1.97113	1.80686
C	-1.17073	0.83303	0.10083
C	-1.71289	-0.33465	-0.31989
C	-2.0402	1.91906	0.72685
C	-2.74961	2.83803	-0.28641
H	-1.41569	2.52901	1.38756
H	-2.79294	1.46446	1.37936
H	-3.32918	3.61111	0.23007
H	-2.03666	3.33842	-0.9487
H	-3.43584	2.27227	-0.9245
C	-3.18169	-0.692	-0.21817

C	-4.0336	-0.05816	-1.33447
H	-5.09316	-0.29456	-1.19416
H	-3.93056	1.03138	-1.34799
H	-3.72765	-0.43266	-2.31632
H	-1.53462	-2.05604	-1.42241
H	-3.2813	-1.75601	-0.27161
H	-3.55207	-0.35834	0.72862

5[2a]

Sum of electronic and thermal Free Energies= -1685.981483

Rh	-0.09789500	-0.52289500	0.83683200
N	0.00004100	-2.32193000	-0.50706700
C	1.34790900	0.33507600	2.46288300
C	-0.06208200	0.56825900	2.80116100
C	-0.65983600	-0.71009000	3.07593400
C	0.30274300	-1.71015000	2.74414500
C	1.57011300	-1.05390100	2.42140900
O	1.11759000	-3.13960700	-0.24511000
C	-0.16764500	-2.05260200	-1.96119500
C	-2.27606400	-0.93840000	-1.25790500
C	-2.03586600	-0.53111000	0.06132900
C	-3.53044200	-0.85532200	-1.88418300
C	-3.17045400	-0.07486000	0.75411600
C	-4.63021600	-0.40569800	-1.16527000
C	-4.44048800	-0.02618200	0.16750700
H	-3.07145800	0.29380000	1.76657600
H	-5.61037000	-0.34024600	-1.62805200
H	-5.28032700	0.34171000	0.74956800
O	0.64966600	-2.42297400	-2.77624100
C	2.87363500	-1.76364400	2.21746100
H	2.74393900	-2.66134000	1.61076500
H	3.61030100	-1.12583600	1.72601500
H	3.29049300	-2.06974500	3.18527200
C	0.12721700	-3.18408700	2.94039800
H	0.69088200	-3.75318500	2.19916300
H	0.50115700	-3.47354200	3.93097400
H	-0.92389700	-3.47832600	2.89005400
C	-1.98151000	-0.97107200	3.73471300
H	-2.58330200	-1.70843500	3.19758600
H	-1.80714300	-1.35973300	4.74553200
H	-2.57270400	-0.06042500	3.83989800
C	-0.66001200	1.90027300	3.13692500
H	-1.73566800	1.92163200	2.94844500
H	-0.50150400	2.12579700	4.19930800
H	-0.21067900	2.70654600	2.55640000
C	2.36445600	1.41631400	2.27404600
H	1.94209000	2.27636000	1.75042400
H	2.71616400	1.76836300	3.25203600
H	3.23137600	1.07065200	1.70939200
C	0.94651800	-4.49615800	-0.70842900
H	0.88382100	-4.53446700	-1.79588000
H	1.84284000	-5.01433900	-0.36401600
H	0.06182500	-4.95127500	-0.24308800
C	-3.41915200	-1.30808900	-3.32638600
C	-1.89172500	-1.32337700	-3.57407100
N	-1.32826900	-1.41330200	-2.20832800
H	-3.84965900	-2.30914400	-3.45519100
H	-3.93508700	-0.64156100	-4.02222100
H	-1.53764500	-2.16379800	-4.17145800
H	-1.54943200	-0.39600500	-4.04549100
C	-0.08343800	1.50254800	-0.50886800
C	0.89351000	0.75286900	-0.73535800
H	-0.83562600	-2.81147000	-0.16764400
C	-0.91258200	2.67075900	-0.41748500
C	-2.24207200	2.70537100	-0.88135900
C	-0.32804300	3.86086600	0.07313400
C	-2.96671700	3.89368700	-0.83459400
H	-2.69384100	1.80841700	-1.28415300
C	-1.05940900	5.04435600	0.10772100
H	0.70687800	3.85118200	0.40043000
C	-2.38327400	5.06224700	-0.33898800
H	-3.99032900	3.90906900	-1.19577600
H	-0.59553800	5.95283100	0.47923600
H	-2.95388700	5.98534200	-0.30974200
C	2.14472000	0.55425200	-1.44593400
C	2.94828600	-0.58696300	-1.30758900
C	2.57188300	1.59609400	-2.29763300
C	4.15449900	-0.68322700	-2.00089200
H	2.61838800	-1.40481800	-0.68150000
C	3.77589700	1.49044900	-2.98563300
H	1.95420900	2.48167300	-2.40985500
C	4.57283600	0.35098500	-2.83820200
H	4.76418600	-1.57495100	-1.89206700
H	4.09269100	2.29808900	-3.63835200
H	5.51149500	0.27045800	-3.37763500
C	5.44786900	3.47709800	0.20601800
H	4.35606600	3.50538900	0.23963300
H	5.79240400	3.98754400	-0.69542700
H	5.85899900	3.97697000	1.08522500

H	5.78630900	2.43896000	0.18317400

TS4[2a]

Sum of electronic and thermal Free Energies= -1685.979483

Rh	-0.70487700	-0.47588600	-0.60362400
N	-1.38933900	-1.11176100	1.45428700
C	-1.69553600	0.51310100	-2.42734900
C	-0.68549800	-0.45010000	-2.83798400
C	-1.15976600	-1.77981300	-2.49678900
C	-2.35622700	-1.61781400	-1.76167700
C	-2.70199100	-0.18993800	-1.72511700
O	-2.76126800	-0.82486700	1.60417500
C	-0.60009400	-0.64638600	2.62362900
C	1.38352200	-1.57364700	1.43406000
C	1.19478700	-1.24720700	0.07765900
C	2.41226200	-2.41135500	1.89346900
C	2.07132000	-1.90187900	-0.81858200
C	3.23571800	-3.05403700	0.97908000
C	3.04276300	-2.80299800	-0.38855700
H	2.02600000	-1.65195400	-1.87191700
H	4.02872900	-3.71668700	1.31211400
H	3.68860500	-3.27975200	-1.11962200
O	-1.11553900	-0.06983800	3.55400000
C	-4.00260100	0.35937500	-1.22184800
H	-4.27397700	-0.07615600	-0.25849000
H	-3.96328200	1.44393800	-1.10515300
H	-4.80740400	0.13070200	-1.93218100
C	-3.23533400	-2.70373500	-1.22187100
H	-3.69112100	-2.40484800	-0.27556000
H	-4.05245000	-2.90962500	-1.92457300
H	-2.69007800	-3.63801700	-1.07015300
C	-0.52282900	-3.07115000	-2.91363400
H	-0.98875200	-3.92673000	-2.42077100
H	-0.63138200	-3.21556200	-3.99527100
H	0.54510400	-3.09930300	-2.68321200
C	0.46281300	-0.15294400	-3.75564200
H	1.18406500	-0.97219800	-3.78137400
H	0.09050300	-0.01870900	-4.77942200
H	0.99487000	0.75954600	-3.47771200
C	-1.68364500	1.97432600	-2.75797400
H	-0.66591300	2.35272000	-2.87478300
H	-2.20543600	2.14512100	-3.70799100
H	-2.18002700	2.57073200	-1.99051000
C	-3.40516300	-1.63008700	2.61427300
H	-3.02305200	-1.39732200	3.60793700
H	-4.45963100	-1.35859400	2.54382400
H	-3.28957400	-2.69816500	2.38432900
C	2.41431300	-2.42195900	3.41028900
C	1.52909000	-1.20123700	3.76275100
N	0.69827100	-1.03418000	2.54577500
H	1.97769900	-3.35087500	3.79855200
H	3.41755700	-2.33135500	3.83374900
H	0.88420000	-1.34113200	4.63027200
H	2.13005300	-0.29924900	3.91777400
C	1.20426800	0.76688300	-0.05758600
C	0.05547600	1.26364600	0.27040700
H	-1.28292400	-2.12997700	1.37900000
C	2.50520100	1.19590100	-0.56663400
C	3.71948400	0.67054800	-0.08989700
C	2.54122700	2.25191400	-1.50048900
C	4.93257800	1.18774400	-0.53672200
H	3.70878500	-0.13058500	0.63937500
C	3.75845400	2.76106200	-1.94868300
H	1.60803000	2.67835300	-1.85466700
C	4.95698600	2.22794700	-1.46997400
H	5.86326200	0.78133300	-0.15297000
H	3.77059900	3.57406300	-2.66812800
H	5.90592700	2.62419400	-1.81797900
C	-0.56975700	2.45374300	0.81535400
C	-1.94516400	2.49749300	1.10597400
C	0.21881200	3.59570500	1.07704600
C	-2.52092600	3.65667400	1.62297400
H	-2.54606000	1.60904200	0.95382000
C	-0.36384100	4.74796300	1.59375200
H	1.28311800	3.57175100	0.86703100
C	-1.73554100	4.78514800	1.86415800
H	-3.58280700	3.67507600	1.84913600
H	0.25292800	5.62037500	1.78733900
H	-2.18574400	5.68660800	2.26824000

6[2a]

Sum of electronic and thermal Free Energies= -1685.999286

Rh	-1.11360400	0.13521800	-0.29996200
N	-0.95554800	0.31242700	1.88049300
C	-2.00326100	1.21821400	-2.12146600
C	-2.18781800	-0.18459500	-2.28471900
C	-3.12514900	-0.66640300	-1.25933700
C	-3.41657500	0.41198500	-0.41848600
C	-2.66052800	1.58857400	-0.89422900
O	-1.10002300	1.66305900	2.26726400

C	0.16385000	-0.36665600	2.59864800
C	0.20339400	-2.16899000	0.83637000
C	0.66061500	-1.62463100	-0.38834100
C	-0.21619400	-3.51338900	0.95281400
C	0.53441200	-2.47677000	-1.52116200
C	-0.32286900	-4.30562300	-0.17469100
C	0.03351300	-3.76516500	-1.42844500
H	0.90420700	-2.10623000	-2.47156000
H	-0.62901800	-5.34459600	-0.09445600
H	-0.02032000	-4.38873400	-2.31546900
O	0.68170200	0.12046400	3.57330800
C	-2.83169900	2.96927300	-0.34277500
H	-2.69153700	2.97658900	0.74032200
H	-2.11334800	3.66922800	-0.77065500
H	-3.84083000	3.34289800	-0.55931500
C	-4.34958300	0.43673100	0.75449300
H	-3.97266200	1.08244400	1.55307800
H	-5.32406200	0.84378200	0.45780200
H	-4.52615300	-0.56143600	1.16324000
C	-3.66647900	-2.06267800	-1.19496300
H	-4.20031600	-2.24790400	-0.26038700
H	-4.37158800	-2.23830600	-2.01677300
H	-2.87218300	-2.80994700	-1.28422800
C	-1.76699300	-0.97774000	-3.48271400
H	-1.63765100	-2.03460700	-3.24555700
H	-2.54400600	-0.90563900	-4.25558200
H	-0.83755900	-0.60223200	-3.91646900
C	-1.36206900	2.11430900	-3.14053800
H	-0.34120000	1.80638000	-3.38057000
H	-1.94332000	2.08021800	-4.06987000
H	-1.33669900	3.15440500	-2.81455800
C	-1.66823500	1.83177500	3.58323600
H	-0.99161600	1.47769800	4.35972200
H	-1.81445000	2.90927500	3.67131200
H	-2.64304700	1.32811600	3.65011300
C	-0.32644600	-3.87340600	2.42213000
C	0.53107500	-2.76964200	3.08855900
N	0.37593300	-1.63702000	2.13734300
H	-1.36507300	-3.82811000	2.77518100
H	0.05324500	-4.87411700	2.64031100
H	0.19659800	-2.46771900	4.08133900
H	1.58437500	-3.06205500	3.14674100
C	1.52195400	-0.37884000	-0.45409600
C	0.85044800	0.77676200	-0.26930800
H	-1.80954900	-0.18641300	2.16135100
C	2.96079000	-0.57438200	-0.78063600
C	3.63012400	-1.74461300	-0.37954900
C	3.67874100	0.38516100	-1.51778200
C	4.97667500	-1.93943200	-0.68428100
H	3.09728900	-2.50737100	0.18099700
C	5.02274800	0.18691500	-1.82418800
H	3.17735800	1.28587700	-1.85453200
C	5.67905400	-0.97392400	-1.40685100
H	5.47660600	-2.84638200	-0.35727900
H	5.55768800	0.93787100	-2.39792600
H	6.72628800	-1.12690400	-1.64875600
C	1.38035900	2.11037100	0.03339800
C	0.90309900	3.28496600	-0.57329500
C	2.39436500	2.23618600	1.00920200
C	1.43310700	4.53172200	-0.24646300
H	0.12136700	3.21499800	-1.31642800
C	2.91663800	3.48275000	1.34094300
H	2.76945800	1.34666100	1.50343600
C	2.44134000	4.63714600	0.71326200
H	1.05735600	5.42321200	-0.74042200
H	3.69589800	3.55343100	2.09390300
H	2.85009500	5.60899600	0.97236300

TS5[2ad]

Sum of electronic and thermal Free Energies= -1685.973665

Rh	-1.46313300	-0.27683500	0.12630100
C	-2.27857200	-1.04446600	-1.80975400
C	-3.30369700	-0.35880100	-1.07018400
C	-3.63771700	-1.16003300	0.12161500
C	-2.74115100	-2.22889400	0.18228600
C	-1.84227400	-2.13463700	-0.98704900
O	-0.21172387	-2.76767961	0.72387728
C	1.33673400	-1.21627600	1.62690300
O	1.55539459	-0.66052798	2.72926941
C	-0.84425300	-3.18490900	-1.35925000
H	-0.32998700	-3.57529600	-0.47755900
H	-0.09509200	-2.80793900	-2.05653900
H	-1.35818400	-4.02926600	-1.83761700
C	-2.65649200	-3.30799200	1.21804000
H	-1.63273400	-3.42879000	1.58451500
H	-2.96952800	-4.27090100	0.79661700
H	-3.29674800	-3.09635300	2.07630800
C	-4.74289300	-0.81937100	1.07268200
H	-4.71538000	0.23687300	1.35833100

H	-4.69567100	-1.41768500	1.98436400
H	-5.71705000	-1.00278000	0.60275000
C	-4.13569400	0.78163600	-1.56971000
H	-5.04087400	0.39132200	-2.05274700
H	-3.60055200	1.38339700	-2.30649300
H	-4.45263300	1.44118800	-0.75892900
C	-1.81346700	-0.72515400	-3.19691400
H	-1.90616600	0.34020900	-3.41774100
H	-2.42627400	-1.26853100	-3.92755000
H	-0.77209700	-1.01114200	-3.35184200
C	-1.40426812	-2.69886152	-0.06434930
H	-2.28587615	-2.52676951	0.56451145
H	-1.48354064	-3.67869821	-0.53833609
H	-1.34071810	-1.91377902	-0.82561028
C	1.11627500	1.23718200	-0.70477800
C	-0.14879900	1.22178500	-0.27051800
N	0.00038173	-1.53175638	1.37965812
H	-0.51748690	-1.51041400	2.25671048
C	2.09773700	-1.15199900	-0.77565900
C	1.63099600	0.01113100	-1.40460100
C	2.72025900	-2.17853900	-1.50975200
C	1.73952700	0.05058100	-2.80881200
C	2.81127100	-2.11462100	-2.89259600
C	2.29818400	-0.98998700	-3.54793600
H	1.40065700	0.94798900	-3.31736500
H	3.29584900	-2.91029900	-3.45058500
H	2.36983400	-0.90770900	-4.62792500
C	3.26743500	-3.22659300	-0.57158500
C	3.29726800	-2.47676600	0.77195900
N	2.21282200	-1.46012900	0.62377700
H	2.60541600	-4.10120000	-0.51956100
H	4.25942400	-3.58191300	-0.86126900
H	3.09080800	-3.11742400	1.62712100
H	4.25096400	-1.96675100	0.92798600
C	-1.08992500	2.06793000	0.43500800
C	-1.88094400	3.05604500	-0.22463300
C	-1.40667800	1.74661800	1.78832600
C	-2.90845900	3.69296100	0.44184200
H	-1.64423400	3.31254500	-1.25256800
C	-2.48315800	2.38424100	2.43589300
H	-0.74541000	1.09784100	2.34947000
C	-3.22852800	3.34586000	1.77321700
H	-3.47785500	4.46913900	-0.06116400
H	-2.69836000	2.14315600	3.47256300
H	-4.04130900	3.85494600	2.28193200
C	2.06783400	2.38351200	-0.58017600
C	3.44094900	2.18515400	-0.82032600
C	1.64985500	3.67651600	-0.21074500
C	4.35565800	3.22973900	-0.69028900
H	3.80139200	1.20494500	-1.11108200
C	2.56404400	4.71867900	-0.08410300
H	0.60216500	3.87926300	-0.02812000
C	3.92352400	4.50292800	-0.32223600
H	5.40870500	3.04447300	-0.88070900
H	2.21114700	5.70674100	0.19660600
H	4.63374500	5.31830200	-0.22548300

7[2ad]

Sum of electronic and thermal Free Energies= -1686.011126

Rh	1.2395	-0.44811	-0.28781
C	2.76691	0.54942	0.89967
C	3.40981	-0.30219	-0.04663
C	3.16341	-1.71421	0.34424
C	2.30206	-1.72184	1.43397
C	1.95961	-0.31972	1.73834
O	-3.71614	-1.90485	-2.02266
C	-1.83182	-1.37539	-0.69617
O	-0.57761	-1.42736	-0.75811
C	1.16608	0.09918	2.9314
H	0.32344	-0.57224	3.11019
H	0.78045	1.11366	2.83361
H	1.81114	0.06305	3.82035
C	1.74247	-2.90033	2.17011
H	0.65445	-2.83224	2.26616
H	2.15551	-2.95201	3.18454
H	1.97583	-3.84059	1.66759
C	3.74938	-2.88444	-0.38021
H	3.6105	-2.79552	-1.46243
H	3.30626	-3.82817	-0.05849
H	4.82999	-2.94073	-0.20029
C	4.39589	0.10101	-1.09788
H	5.4176	-0.04993	-0.72578
H	4.2935	1.15183	-1.37091
H	4.28975	-0.50069	-2.00474
C	2.9413	2.02731	1.07248
H	3.23522	2.51197	0.14005
H	3.72365	2.22575	1.81565
H	2.02049	2.49949	1.41951
C	-4.62845	-3.00515	-2.11702

H	-4.23105	-3.79383	-2.7666
H	-5.52866	-2.58379	-2.56739
H	-4.85753	-3.4243	-1.1315
C	-0.6979	1.74412	-0.92705
C	0.39798	1.0798	-1.32201
N	-2.50535	-2.33677	-1.43754
H	-1.88618	-2.72843	-2.14557
C	-2.1067	0.5623	0.85371
C	-1.24992	1.60154	0.45902
C	-2.79146	0.58277	2.07929
C	-1.03712	2.61502	1.41596
C	-2.56889	1.60086	2.99608
C	-1.66599	2.61565	2.66175
H	-0.38121	3.43791	1.15054
H	-3.10268	1.62159	3.94145
H	-1.48116	3.42865	3.35717
C	-3.76643	-0.56969	2.14377
C	-3.87634	-0.99422	0.66482
N	-2.57265	-0.55717	0.0837
H	-3.37649	-1.39047	2.7599
H	-4.73715	-0.28274	2.55563
H	-4.0013	-2.06754	0.53438
H	-4.69059	-0.474	0.15437
C	1.00816	1.1153	-2.73552
C	2.07385	1.97161	-3.01392
C	0.49553	0.29133	-3.73743
C	2.62628	2.00437	-4.29414
H	2.47727	2.62165	-2.22401
C	1.04865	0.32326	-5.01784
H	-0.34429	-0.38377	-3.51814
C	2.11378	1.17969	-5.29636
H	3.46586	2.67976	-4.51381
H	0.64452	-0.32681	-5.80749
H	2.54955	1.20565	-6.30568
C	-1.51393	2.66796	-1.8502
C	-2.6436	3.32328	-1.35941
C	-1.12364	2.84968	-3.17692
C	-3.38314	4.15958	-2.19541
H	-2.95148	3.1792	-0.31361
C	-1.86274	3.68697	-4.01304
H	-0.23321	2.3334	-3.56386
C	-2.99242	4.34179	-3.52257
H	-4.27393	4.67565	-1.80881
H	-1.55454	3.83038	-5.05895
H	-3.57564	5.00128	-4.18153

TS6^{2ad}

Sum of electronic and thermal Free Energies= -1685.944878

Rh	-1.42657	-0.38173	-0.06636
C	-3.03196	-0.5643	-1.67547
C	-3.42771	-1.38587	-0.57908
C	-2.37325	-2.34295	-0.34222
C	-1.35191	-2.15664	-1.36347
C	-1.74812	-1.04473	-2.17499
O	2.68011	0.88023	2.09408
C	1.1379	-0.96822	1.98717
O	0.27122	-1.62246	2.58981
C	-1.04913	-0.55742	-3.40473
H	0.02418	-0.75557	-3.3639
H	-1.19062	0.51475	-3.55794
H	-1.44884	-1.07148	-4.28865
C	-0.17826	-3.0562	-1.58276
H	0.65522	-2.53369	-2.05612
H	-0.46716	-3.88704	-2.2399
H	0.17422	-3.48204	-0.64138
C	-2.32698	-3.40378	0.71204
H	-2.35832	-4.39901	0.25194
H	-3.16876	-3.32783	1.40213
H	-1.40284	-3.32797	1.29548
C	-4.71244	-1.2738	0.18376
H	-5.50481	-1.83365	-0.32834
H	-5.04379	-0.23616	0.26755
H	-4.62272	-1.68086	1.19268
C	-3.83511	0.54466	-2.27987
H	-4.47515	1.03149	-1.54081
H	-4.4867	0.14789	-3.0694
H	-3.19938	1.30617	-2.73761
C	4.00335	0.8985	2.64094
H	3.9941	1.20722	3.69229
H	4.55039	1.63608	2.04966
H	4.48429	-0.08118	2.55388
C	1.1194	0.87779	-0.3174
C	0.25659	0.43661	0.71522
N	1.89812	-0.06639	2.7891
H	1.29244	0.41391	3.45475
C	2.448	-1.2073	-0.17535
C	2.09864	-0.01657	-0.86686
C	3.40593	-2.11023	-0.69868
C	2.76867	0.22169	-2.10545

C	4.02931	-1.84029	-1.89593
C	3.70414	-0.65826	-2.60798
H	2.52393	1.11929	-2.66128
H	4.76899	-2.5275	-2.29781
H	4.1945	-0.44828	-3.55242
C	3.52413	-3.29625	0.23652
C	2.67058	-2.87858	1.46093
N	1.94818	-1.66309	1.00262
H	3.12771	-4.20483	-0.23172
H	4.55903	-3.50996	0.51854
H	1.94823	-3.63491	1.77271
H	3.28831	-2.62553	2.32977
C	1.06191	2.26531	-0.87102
C	-0.09655	2.76901	-1.4833
C	2.19392	3.09393	-0.77768
C	-0.12403	4.06618	-1.9929
H	-0.97603	2.13538	-1.55428
C	2.15632	4.3995	-1.26735
H	3.09258	2.71451	-0.30305
C	1.00028	4.88757	-1.88019
H	-1.02317	4.43825	-2.47485
H	3.03293	5.03329	-1.17444
H	0.976	5.9006	-2.26962
C	-0.67162	1.24808	1.51877
C	-1.67061	0.4517	2.16698
C	-0.75782	2.66286	1.64652
C	-2.76746	1.06456	2.81496
H	-1.43647	-0.59582	2.36972
C	-1.814	3.23341	2.33212
H	0.01415	3.2921	1.22435
C	-2.84308	2.44265	2.88951
H	-3.50881	0.44476	3.3104
H	-1.85542	4.31338	2.44095
H	-3.66538	2.92043	3.4131

8[2ad]

Sum of electronic and thermal Free Energies= -1685.995550

Rh	1.23595	0.20875	-0.36793
C	2.19772	-1.46361	0.80218
C	3.11332	-0.38748	0.78473
C	3.42563	-0.08846	-0.61749
C	2.73626	-1.01906	-1.45543
C	1.90756	-1.82514	-0.5868
O	-2.87707	2.55805	-0.79832
C	-1.10257	1.05307	-1.06877
O	0.07981	0.93193	-1.80074
C	1.03038	-2.95952	-1.00494
H	0.69342	-2.85018	-2.03712
H	0.15493	-3.04866	-0.35785
H	1.59195	-3.90071	-0.93476
C	2.82228	-1.12486	-2.94561
H	1.86652	-1.42396	-3.38109
H	3.57105	-1.87427	-3.22984
H	3.11076	-0.1752	-3.40022
C	4.38541	0.96304	-1.07085
H	4.38374	1.82878	-0.40495
H	4.16585	1.30475	-2.08409
H	5.40403	0.55293	-1.07091
C	3.75954	0.27676	1.96079
H	4.76717	-0.13051	2.11151
H	3.19563	0.11199	2.88005
H	3.86217	1.35454	1.81587
C	1.64044	-2.18423	1.98892
H	1.86767	-1.66705	2.92119
H	2.07567	-3.18938	2.04813
H	0.55481	-2.30072	1.91959
C	-4.15693	2.65855	-1.41878
H	-4.14046	3.35902	-2.26202
H	-4.82483	3.04028	-0.6429
H	-4.51593	1.68332	-1.76655
C	-1.17321	0.70721	1.51766
C	-0.64041	1.38458	0.39534
N	-1.92244	2.06151	-1.74016
H	-1.32734	2.84949	-1.99625
C	-2.25589	-0.86353	0.01682
C	-1.95227	-0.48327	1.34104
C	-3.04101	-1.99158	-0.30588
C	-2.51056	-1.30035	2.36906
C	-3.55015	-2.76179	0.7142
C	-3.27948	-2.40573	2.06409
H	-2.33616	-1.05202	3.40976
H	-4.16572	-3.63143	0.50131
H	-3.69469	-3.00915	2.86418
C	-3.13542	-2.08407	-1.81738
C	-2.41024	-0.79749	-2.31596
N	-1.83679	-0.20687	-1.08578
H	-2.64336	-2.98808	-2.19341
H	-4.17139	-2.11997	-2.16697
H	-1.60974	-1.00409	-3.03084

H	-3.09331	-0.0836	-2.78146
C	-1.05325	1.28478	2.9402
C	-1.59086	0.58875	4.02324
C	-0.40706	2.50365	3.14592
C	-1.48285	1.11189	5.31161
H	-2.10092	-0.37179	3.86063
C	-0.29806	3.02661	4.43474
H	0.01688	3.05228	2.29245
C	-0.83594	2.33103	5.51752
H	-1.90713	0.56364	6.16525
H	0.21185	3.98746	4.59669
H	-0.75084	2.74328	6.53344
C	-0.1396	2.83581	0.51672
C	-0.9951	3.89631	0.21684
C	1.1692	3.09005	0.92655
C	-0.54162	5.2107	0.32614
H	-2.02664	3.69552	-0.10698
C	1.62267	4.40481	1.03689
H	1.84354	2.25433	1.16312
C	0.76758	5.46509	0.73664
H	-1.21568	6.04663	0.08919
H	2.65452	4.60497	1.36045
H	1.12489	6.50153	0.82281

P1[2ad]

Sum of electronic and thermal Free Energies= -1016.410577

C	0.67222	-1.61964	-0.20241
C	-1.22802	-0.12322	-0.0481
C	-0.46574	1.03634	-0.21913
C	-2.61425	-0.15757	0.13048
C	-1.20112	2.24576	-0.20288
C	-3.30441	1.04154	0.14176
C	-2.58126	2.24263	-0.02734
H	-0.68919	3.19403	-0.32708
H	-4.3822	1.06981	0.27619
H	-3.11623	3.18743	-0.0201
O	1.1127	-2.77211	-0.18982
C	-3.0407	-1.60895	0.27564
C	-1.70681	-2.41425	0.15436
N	-0.67788	-1.37863	-0.0424
H	-3.5287	-1.7944	1.2385
H	-3.75286	-1.90335	-0.50267
H	-1.47416	-2.99568	1.05072
H	-1.69815	-3.10413	-0.6939
C	0.97175	0.86327	-0.39284
C	1.50868	-0.40426	-0.38486
C	1.82738	2.13406	-0.5497
C	1.21851	3.38935	-0.54936
C	3.21104	2.03014	-0.69199
C	1.99312	4.54037	-0.69197
H	0.12756	3.47089	-0.43793
C	3.98613	3.18147	-0.83367
H	3.6911	1.04087	-0.6921
C	3.37743	4.43647	-0.83382
H	1.51321	5.5298	-0.69235
H	5.07711	3.09925	-0.94543
H	3.98798	5.34415	-0.94619
C	3.0054	-0.73208	-0.53969
C	3.57686	-0.79943	-1.81065
C	3.78974	-0.96156	0.59066
C	4.93223	-1.09686	-1.95118
H	2.95806	-0.61922	-2.70164
C	5.14575	-1.25812	0.45032
H	3.33954	-0.90834	1.59247
C	5.71704	-1.32594	-0.82034
H	5.38259	-1.15058	-2.95297
H	5.76402	-1.43861	1.34175
H	6.78569	-1.56038	-0.93138

TS5[2ac]

Sum of electronic and thermal Free Energies= -1685.967258

Rh	-0.99753	0.04454	-0.03324
C	-2.5304	1.70193	-0.76999
C	-3.16407	0.96094	0.23537
C	-3.13694	-0.44352	-0.18058
C	-2.59636	-0.51483	-1.5304
C	-2.14619	0.78469	-1.85694
O	1.25743	-0.92659	-1.84505
C	2.9296	-1.63439	-0.27334
O	3.63398	-2.62539	-0.27492
C	-1.53227	1.22887	-3.15026
H	-1.09319	0.3918	-3.69699
H	-0.75267	1.97949	-2.99287
H	-2.29278	1.68368	-3.79837
C	-2.58845	-1.73089	-2.40854
H	-1.79779	-1.67881	-3.1605
H	-3.54303	-1.83031	-2.94079
H	-2.44316	-2.64783	-1.83092
C	-3.93012	-1.52528	0.48538
H	-3.91032	-1.43904	1.57418

H	-3.58696	-2.52326	0.20627
H	-4.98076	-1.4444	0.17464
C	-3.81108	1.47128	1.48848
H	-4.90072	1.5226	1.36721
H	-3.46495	2.47543	1.74355
H	-3.60891	0.82122	2.34341
C	-2.31068	3.18434	-0.81346
H	-2.49488	3.65172	0.15618
H	-2.98983	3.65072	-1.53801
H	-1.29063	3.43333	-1.12089
C	1.96689	-1.35336	-3.02462
H	3.05159	-1.27511	-2.89989
H	1.63517	-0.66716	-3.8045
H	1.69581	-2.38123	-3.29433
C	0.49416	-0.36403	1.47011
C	0.19451	-1.44037	0.58999
N	1.53913	-1.75314	-0.73692
H	1.4173	-2.73319	-1.01003
C	2.49056	0.76798	0.30345
C	1.20715	0.83711	0.89109
C	3.2681	1.90612	0.05957
C	0.7281	2.14873	1.14647
C	2.74825	3.17479	0.29138
C	1.4616	3.29051	0.82607
H	-0.23051	2.25326	1.64074
H	3.34632	4.05969	0.09516
H	1.04853	4.27084	1.03991
C	4.65985	1.49619	-0.37651
C	4.72376	0.0179	0.06638
N	3.29383	-0.38166	0.07584
H	4.77673	1.58777	-1.46383
H	5.44402	2.09617	0.09078
H	5.28169	-0.63789	-0.60205
H	5.1352	-0.08274	1.07594
C	1.26673	-0.5007	2.79527
C	1.50513	0.6258	3.58307
C	1.72805	-1.75066	3.20799
C	2.20528	0.50238	4.78298
H	1.14197	1.61122	3.25704
C	2.42758	-1.87444	4.40872
H	1.54009	-2.63865	2.58729
C	2.66637	-0.74818	5.19615
H	2.39378	1.39036	5.40368
H	2.79083	-2.86017	4.73408
H	3.21834	-0.84525	6.1423
C	-0.79773	-2.60009	0.79522
C	-0.95233	-3.56951	-0.19615
C	-1.5418	-2.68141	1.9722
C	-1.8513	-4.6196	-0.01077
H	-0.36613	-3.50469	-1.12427
C	-2.44037	-3.73231	2.15821
H	-1.41996	-1.91755	2.75373
C	-2.59533	-4.70127	1.16693
H	-1.97366	-5.3834	-0.7924
H	-3.02661	-3.7964	3.08649
H	-3.30403	-5.52935	1.31289

7[2ac]

Sum of electronic and thermal Free Energies= -1685.973610

Rh	-1.11795	-0.63486	0.1376
C	-2.74229	-2.2172	-0.51869
C	-3.10001	-0.97269	-1.05526
C	-3.21189	-0.03321	0.06768
C	-3.07846	-0.78657	1.30916
C	-2.69741	-2.09585	0.94753
O	0.92798	-0.99179	2.21952
C	2.79877	0.42624	1.67223
O	3.45703	1.19431	2.34636
C	-2.43684	-3.24228	1.87721
H	-2.19556	-2.89794	2.8852
H	-1.61375	-3.87046	1.5247
H	-3.32378	-3.88522	1.95077
C	-3.39875	-0.29289	2.68918
H	-2.73046	-0.71807	3.44233
H	-4.42337	-0.57356	2.96548
H	-3.33907	0.79531	2.75744
C	-3.76049	1.35632	-0.04571
H	-3.56849	1.78452	-1.03149
H	-3.34207	2.02894	0.70597
H	-4.84942	1.33684	0.09491
C	-3.3458	-0.62339	-2.49256
H	-4.41698	-0.47143	-2.67483
H	-3.01109	-1.4184	-3.16253
H	-2.82934	0.29597	-2.78435
C	-2.49851	-3.50045	-1.25547
H	-1.58725	-3.99827	-0.90986
H	-2.40672	-3.34127	-2.33185
H	-3.32892	-4.19922	-1.09514
C	1.39931	-1.32293	3.54017

H	2.49227	-1.30394	3.59865
H	1.03598	-2.33636	3.71435
H	0.97443	-0.64223	4.28756
C	0.53508	0.36085	-0.78015
C	0.377	0.7668	0.76863
N	1.28793	0.3201	1.84616
H	1.05329	0.97431	2.59867
C	2.52185	-1.19965	-0.21544
C	1.29502	-0.93923	-0.86127
C	3.31869	-2.30576	-0.54243
C	0.88325	-1.9167	-1.80308
C	2.86805	-3.25587	-1.45073
C	1.62989	-3.06117	-2.07214
H	-0.02782	-1.72977	-2.36005
H	3.48122	-4.11748	-1.69745
H	1.26964	-3.77794	-2.80284
C	4.6494	-2.21239	0.17528
C	4.69066	-0.7306	0.60787
N	3.25405	-0.3653	0.67389
H	4.67514	-2.87906	1.04669
H	5.49503	-2.47501	-0.46462
H	5.15743	-0.54639	1.57535
H	5.18752	-0.10712	-0.14253
C	0.5059	1.18099	-2.03709
C	-0.54692	2.07634	-2.30294
C	1.54084	1.08009	-2.98345
C	-0.56126	2.84256	-3.46612
H	-1.3556	2.17363	-1.58752
C	1.52431	1.84659	-4.1497
H	2.37084	0.40366	-2.80686
C	0.47428	2.73032	-4.39752
H	-1.38564	3.52573	-3.64863
H	2.33747	1.75242	-4.86326
H	0.46048	3.32434	-5.30599
C	0.2634	2.17908	1.18732
C	-0.65836	2.5434	2.18668
C	1.13057	3.16731	0.68089
C	-0.73563	3.85717	2.64494
H	-1.30471	1.77912	2.60457
C	1.04869	4.48157	1.13585
H	1.86127	2.90434	-0.07598
C	0.11465	4.83078	2.11437
H	-1.45447	4.12222	3.41432
H	1.71967	5.23303	0.73162
H	0.05543	5.85544	2.46826

TS6^{2ac}

Sum of electronic and thermal Free Energies= -1685.966624

Rh	1.19211	-0.63335	-0.25461
C	2.79261	-2.18333	0.44634
C	2.99832	-0.9914	1.15471
C	3.22243	0.06923	0.15898
C	3.31896	-0.54241	-1.15647
C	2.96144	-1.8955	-0.98964
O	-0.3109	-1.03857	-1.55756
C	-2.66112	0.39768	-1.79586
O	-3.10882	1.05878	-2.70584
C	2.8778	-2.94115	-2.05988
H	2.788	-2.5002	-3.05539
H	2.02887	-3.61351	-1.90127
H	3.7811	-3.56479	-2.0561
C	3.80431	0.13279	-2.40553
H	3.40553	-0.33735	-3.30833
H	4.89923	0.08269	-2.47153
H	3.53322	1.19132	-2.42772
C	3.6915	1.45746	0.47259
H	3.46439	1.74448	1.50001
H	3.2541	2.19963	-0.20102
H	4.78162	1.50918	0.35084
C	3.02587	-0.78783	2.63828
H	4.04997	-0.59348	2.98099
H	2.66402	-1.66943	3.17187
H	2.40938	0.06394	2.93975
C	2.53012	-3.55172	1.00171
H	1.72199	-4.05995	0.46619
H	2.25668	-3.51396	2.05816
H	3.4224	-4.18453	0.91452
C	-0.34584	-1.36143	-2.96546
H	-1.33296	-1.16144	-3.39162
H	-0.13388	-2.42991	-3.00067
H	0.43116	-0.80821	-3.50489
C	-0.56987	0.13885	0.69976
C	-0.33615	0.77744	-0.60001
N	-1.1335	0.21344	-1.77695
H	-0.82596	0.75229	-2.59788
C	-2.738	-1.13178	0.16476
C	-1.50029	-1.03855	0.81129
C	-3.68456	-2.12538	0.44528
C	-1.22173	-2.08203	1.72126

C	-3.38152	-3.13013	1.35386
C	-2.12862	-3.10685	1.98056
H	-0.27778	-2.05207	2.25476
H	-4.10157	-3.90989	1.58196
H	-1.8693	-3.88087	2.69591
C	-4.9485	-1.88233	-0.35256
C	-4.76517	-0.43574	-0.8639
N	-3.29156	-0.23448	-0.80164
H	-5.02796	-2.58839	-1.18854
H	-5.85567	-1.98435	0.24804
H	-5.11052	-0.26218	-1.88279
H	-5.24354	0.29134	-0.20103
C	-0.44315	0.94646	1.96932
C	0.57137	1.90742	2.1409
C	-1.36768	0.79433	3.01998
C	0.664	2.6698	3.30341
H	1.28779	2.06934	1.34734
C	-1.27211	1.55334	4.18789
H	-2.17981	0.08269	2.93032
C	-0.25521	2.49396	4.34009
H	1.45881	3.40425	3.39871
H	-2.0036	1.40798	4.9774
H	-0.1805	3.0837	5.24837
C	-0.2542	2.25698	-0.86389
C	0.69526	2.75426	-1.77214
C	-1.18069	3.14979	-0.29987
C	0.72611	4.10989	-2.10203
H	1.41593	2.06892	-2.21036
C	-1.1426	4.50584	-0.62199
H	-1.92182	2.78232	0.40241
C	-0.19082	4.98901	-1.52265
H	1.4683	4.47976	-2.80302
H	-1.86108	5.18483	-0.17331
H	-0.165	6.0451	-1.77262

8[2ac]

Sum of electronic and thermal Free Energies= -1686.096505

Rh	-2.06308	-0.11624	-0.29484
N	1.24524	0.69472	-0.12388
C	-3.31866	0.7609	1.19608
C	-3.95082	0.96583	-0.09313
C	-4.2072	-0.32885	-0.63799
C	-3.8391	-1.34221	0.36694
C	-3.32068	-0.67517	1.4972
O	-1.16332	1.27875	-1.43026
C	0.97583	-0.5976	0.16388
C	3.32577	-1.29169	0.08002
C	4.07717	-0.11496	0.00793
C	3.83205	-2.54868	-0.26052
C	5.38867	-0.2683	-0.48732
C	5.13119	-2.66793	-0.74021
C	5.90298	-1.50907	-0.8621
H	6.0254	0.60443	-0.57452
H	5.53988	-3.63844	-1.0047
H	6.9205	-1.57294	-1.23428
O	-0.21473	-1.0573	0.08078
C	-2.83648	-1.28354	2.77529
H	-1.93195	-0.78849	3.13758
H	-3.60262	-1.18329	3.55376
H	-2.61615	-2.34589	2.65929
C	-4.01598	-2.81651	0.18742
H	-5.06067	-3.0942	0.3753
H	-3.77467	-3.12952	-0.83175
H	-3.38959	-3.38643	0.87556
C	-4.82889	-0.62796	-1.96377
H	-4.42575	-1.54462	-2.40116
H	-5.91027	-0.77203	-1.84163
H	-4.67639	0.18701	-2.67335
C	-4.17556	2.29546	-0.74477
H	-4.8352	2.20759	-1.60967
H	-4.63433	2.99713	-0.04207
H	-3.22035	2.71177	-1.08579
C	-2.89026	1.84743	2.1253
H	-2.56149	2.73292	1.57747
H	-3.7396	2.14112	2.75704
H	-2.08494	1.52333	2.7879
C	-0.72324	0.84547	-2.70816
H	-0.13296	-0.08415	-2.66696
H	-1.5641	0.68639	-3.39836
H	-0.08046	1.62586	-3.13678
C	2.78378	-3.61284	-0.02366
C	1.7264	-2.86871	0.82194
N	1.97505	-1.43024	0.546
H	2.36075	-3.96193	-0.9743
H	3.17421	-4.48862	0.50121
H	0.69898	-3.12153	0.57071
H	1.88731	-3.04362	1.89089
C	3.575	1.19633	0.48651
C	2.26972	1.54097	0.41764

H	0.4188	1.16503	-0.52177
C	4.62182	2.15559	1.08283
C	5.96281	1.77518	1.14206
C	4.22939	3.40474	1.56362
C	6.91098	2.64352	1.68259
H	6.27176	0.78999	0.76364
C	5.17788	4.27387	2.10344
H	3.17255	3.7048	1.51685
C	6.51849	3.89343	2.16312
H	7.96789	2.3435	1.72988
H	4.86824	5.25887	2.48206
H	7.26628	4.57794	2.58921
C	1.68491	2.89265	0.86771
C	1.53642	3.17056	2.22682
C	1.30379	3.83911	-0.08335
C	1.00628	4.39441	2.63468
H	1.83627	2.42387	2.97634
C	0.77439	5.06378	0.3245
H	1.42092	3.62031	-1.15458
C	0.62546	5.3415	1.68325
H	0.88862	4.61329	3.70592
H	0.47435	5.80999	-0.42558
H	0.20754	6.30642	2.00508

P2^{2ac}

Sum of electronic and thermal Free Energies= -1071.738311

N	-0.87434	-1.58276	-0.51597
C	0.35077	-2.10609	-0.09392
C	1.29447	0.17392	0.07821
C	0.2211	1.07342	0.02894
C	2.62061	0.56501	-0.15298
C	0.55623	2.40405	-0.30655
C	2.91728	1.88066	-0.48001
C	1.86604	2.80175	-0.56239
H	-0.23224	3.1466	-0.3632
H	3.943	2.19141	-0.65835
H	2.07079	3.83797	-0.81465
O	0.59354	-3.2995	-0.21744
C	3.53778	-0.62708	0.01774
C	2.62781	-1.6581	0.72417
N	1.24799	-1.19971	0.44185
H	3.87826	-0.99705	-0.9585
H	4.43008	-0.39981	0.60824
H	2.74159	-2.68027	0.36639
H	2.79009	-1.64347	1.80798
C	-1.16594	0.68288	0.36551
C	-1.64242	-0.55952	0.10733
H	-1.42796	-2.35477	-0.86422
C	-2.04805	1.7583	1.02655
C	-1.52828	3.0281	1.27934
C	-3.36663	1.46294	1.37245
C	-2.32679	4.00206	1.87852
H	-0.48846	3.26041	1.00722
C	-4.16582	2.43739	1.97092
H	-3.7765	0.46224	1.17312
C	-3.6461	3.70677	2.22411
H	-1.91698	5.00277	2.07838
H	-5.20555	2.20435	2.24316
H	-4.27552	4.47488	2.69648
C	-3.08253	-1.02243	0.39607
C	-3.52802	-1.13538	1.71336
C	-3.94157	-1.32869	-0.65931
C	-4.83205	-1.55514	1.97514
H	-2.85029	-0.8946	2.54519
C	-5.24634	-1.74765	-0.39764
H	-3.59068	-1.23956	-1.6976
C	-5.69163	-1.86104	0.91932
H	-5.18306	-1.64479	3.01344
H	-5.92355	-1.98865	-1.22996
H	-6.71979	-2.19193	1.12597

TS6^{2ad}-OPiv

Sum of electronic and thermal Free Energies= -1917.186996

Rh	2.04750600	-0.17166300	-0.39509900
C	3.67693600	0.43968400	1.01027700
C	4.28994000	0.12945900	-0.28590400
C	4.02081700	-1.22735700	-0.59109100
C	3.21606100	-1.77290600	0.49756500
C	3.06966600	-0.75010100	1.51316200
O	-2.57717500	-0.97918500	-1.53377100
C	-0.21859200	-1.11830100	-1.32529800
O	0.91294400	-1.05708400	-1.94393200
C	2.43476400	-0.94128700	2.85540800
H	1.56555400	-1.60083200	2.80382600
H	2.11399000	0.00775700	3.28870500
H	3.15647400	-1.39444000	3.54671100
C	2.80430300	-3.20361200	0.63280800
H	1.89464700	-3.30299900	1.22716400
H	3.60001200	-3.77086500	1.13347600
H	2.63247700	-3.66297100	-0.34235400

C	4.44706000	-1.99427900	-1.80477900
H	5.25300400	-2.69330000	-1.55106800
H	4.81310800	-1.33305500	-2.59192400
H	3.61758700	-2.57587200	-2.21640500
C	5.07715100	1.10630700	-1.10100300
H	6.06074200	1.27000200	-0.64298200
H	4.57702300	2.07767000	-1.15737000
H	5.23795000	0.74795200	-2.11900800
C	3.86297300	1.73023800	1.74613200
H	3.80931100	2.58919700	1.07441500
H	4.85010400	1.74302700	2.22524500
H	3.11376900	1.86546000	2.52865500
C	-0.86208800	0.48819700	1.00920700
C	0.05492100	0.54999100	-0.01133700
N	-1.31355900	-0.89510600	-2.15914700
H	-1.29615300	-0.07137500	-2.76261500
C	-1.02027300	-1.99683000	0.89274400
C	-1.25676800	-0.79702100	1.59329900
C	-1.43408900	-3.24595400	1.38908800
C	-1.96991100	-0.92103600	2.81347000
C	-2.08810800	-3.33342200	2.60568600
C	-2.35981800	-2.15298600	3.31880300
H	-2.22693500	-0.02666000	3.36569400
H	-2.41004300	-4.29624400	2.99226200
H	-2.89562000	-2.20088300	4.26098000
C	-1.03737100	-4.32302200	0.40248500
C	-0.74360900	-3.50959300	-0.87493000
N	-0.39833100	-2.15499500	-0.34549200
H	-0.14139400	-4.85683000	0.74476600
H	-1.81715800	-5.07100700	0.23792700
H	0.08717100	-3.89622000	-1.46834500
H	-1.63324000	-3.44946100	-1.51192700
C	-1.55049900	1.73587300	1.48450400
C	-1.36934600	2.20671500	2.79691200
C	-2.35331700	2.48241600	0.60746100
C	-1.98752400	3.38355000	3.22260900
H	-0.72635600	1.66224700	3.48250200
C	-2.97629800	3.65421100	1.03909300
H	-2.48036800	2.15568200	-0.41936400
C	-2.79906300	4.10736000	2.34735400
H	-1.83168200	3.73431300	4.23847600
H	-3.59645100	4.21629800	0.34713800
H	-3.28348100	5.01993500	2.68044500
C	0.64445000	1.76253900	-0.61897100
C	1.00178700	1.81589700	-1.99716700
C	1.00421900	2.89068900	0.18222400
C	1.65192400	2.93766600	-2.53558400
H	0.74345100	1.00236000	-2.65936500
C	1.62884200	3.99465700	-0.36543100
H	0.75931200	2.88171500	1.23659900
C	1.96247900	4.02521300	-1.73316900
H	1.88971200	2.95071900	-3.59471200
H	1.85960500	4.84765800	0.26607500
H	2.44895400	4.89915100	-2.15548000
C	-3.44164500	0.01268300	-1.95127000
O	-3.05331700	0.90745200	-2.67074200
C	-4.86610500	-0.23605700	-1.46721100
C	-4.88510300	-0.72347300	-0.00401400
H	-4.35003400	-1.66757300	0.11959600
H	-4.43871800	0.01412200	0.66933700
H	-5.92295800	-0.87725300	0.30623700
C	-5.65944300	1.07444200	-1.61126800
H	-5.62625000	1.44973100	-2.63635000
H	-6.70375600	0.89816300	-1.33818200
H	-5.26392300	1.85244400	-0.95154400
C	-5.46542000	-1.32335200	-2.39692000
H	-5.46084200	-0.99976300	-3.44214700
H	-4.91314700	-2.26404400	-2.32022400
H	-6.50299700	-1.51107200	-2.10501000

TS5^{2ac}-OPiv

Sum of electronic and thermal Free Energies= -1917.162063

Rh	-0.62764600	-1.12316100	-0.47705100
C	-1.46623800	-2.73257600	-1.98405200
C	-2.36025300	-2.62967500	-0.90974800
C	-1.59896300	-2.90876600	0.31413000
C	-0.26366800	-3.35361900	-0.06965900
C	-0.15485700	-3.15385900	-1.46128800
O	2.12586600	0.17368800	-0.54472100
C	1.82456600	2.30706400	0.50515400
O	2.43539700	2.87785600	1.38945400
C	1.03403200	-3.44980500	-2.32347300
H	1.96703000	-3.42090500	-1.75862000
H	1.12707500	-2.73220900	-3.14231100
H	0.93990000	-4.44787900	-2.77158900
C	0.74305600	-4.01110900	0.82674400
H	1.76534600	-3.84634600	0.47705800
H	0.58136400	-5.09685600	0.85014900
H	0.67199400	-3.65785600	1.85830900

C	-2.22294100	-3.11035900	1.66094800
H	-3.10474300	-2.48089200	1.79628800
H	-1.52753700	-2.90512600	2.47676100
H	-2.55018600	-4.15417600	1.76004300
C	-3.82533900	-2.31489600	-0.95234100
H	-4.41826600	-3.21419300	-0.74357700
H	-4.12951500	-1.94474800	-1.93387400
H	-4.10285600	-1.55939900	-0.21137300
C	-1.75400900	-2.53028600	-3.44149500
H	-0.98568100	-1.91800900	-3.92307700
H	-2.72052600	-2.04839700	-3.60302800
H	-1.77365100	-3.49396500	-3.96539600
C	-1.10491400	0.90305200	-0.01647400
C	-0.17618100	0.28920000	0.90107900
N	1.62911500	0.85103100	0.60455400
H	2.10339300	0.53472500	1.45023200
C	0.43015100	2.28215400	-1.57056700
C	-0.62874400	1.37755500	-1.36700800
C	0.66855800	2.90408000	-2.80241100
C	-1.39238600	1.07204200	-2.52081500
C	-0.08739200	2.56183300	-3.91688200
C	-1.11619700	1.62515600	-3.76943400
H	-2.24648000	0.41481600	-2.40411800
H	0.09808300	3.03347000	-4.87711500
H	-1.73270600	1.35831700	-4.62163900
C	1.75638700	3.94692100	-2.64892100
C	1.80680300	4.15424200	-1.11874300
N	1.28905600	2.86420500	-0.59757400
H	2.71555600	3.57047300	-3.02596900
H	1.53319100	4.87565800	-3.17904000
H	2.80125200	4.33773100	-0.71229500
H	1.14297800	4.96454400	-0.80050100
C	-2.44575100	1.42374300	0.41799200
C	-3.23813000	0.72333500	1.34683500
C	-2.94319800	2.63777100	-0.08789300
C	-4.47497900	1.21791700	1.75426200
H	-2.87529300	-0.21239000	1.75619900
C	-4.18332500	3.13180100	0.31968700
H	-2.35609900	3.20721000	-0.80080800
C	-4.95586800	2.42509700	1.24083300
H	-5.06724200	0.65706500	2.47144900
H	-4.54248200	4.07374000	-0.08413000
H	-5.92163500	2.80831600	1.55520900
C	-0.19857800	0.37995100	2.37962100
C	0.17929100	-0.72446900	3.16404100
C	-0.51125200	1.59014600	3.02991400
C	0.22101000	-0.63435700	4.55476400
H	0.43950700	-1.65259800	2.66727100
C	-0.46936000	1.67994900	4.41936600
H	-0.79988500	2.45533200	2.44271500
C	-0.10688600	0.56860800	5.18474900
H	0.50793400	-1.49851300	5.14636400
H	-0.71756900	2.61811200	4.90566500
H	-0.07622800	0.64109600	6.26758700
C	3.34249400	-0.57358900	-0.58443700
O	3.47606600	-1.12111600	-1.64123800
C	4.35541900	-0.63911100	0.57501000
C	3.73733500	-1.21144100	1.87551100
H	3.12451100	-0.50461500	2.44417100
H	3.14100900	-2.10830800	1.68420900
H	4.55329600	-1.49457000	2.54643200
C	5.46325000	-1.60901500	0.10566700
H	5.92547900	-1.26493800	-0.82121200
H	6.23392600	-1.66766700	0.87907900
H	5.07055500	-2.61373000	-0.06939900
C	4.98641900	0.75227300	0.82351200
H	5.42663500	1.15040500	-0.09592300
H	4.28651700	1.48827000	1.22248800
H	5.79412700	0.63939400	1.55268000

TS6^{2ac}-OPiv

Sum of electronic and thermal Free Energies= -1917.185613

Rh	-0.38159400	-1.01693400	-0.66574100
C	-0.68781900	-2.35476300	-2.49980000
C	-1.88905600	-2.35601300	-1.75361100
C	-1.55116500	-2.85338100	-0.42774200
C	-0.16625100	-3.34161600	-0.45114000
C	0.37026900	-2.99137300	-1.69443200
O	2.27614900	0.26650500	0.35467700
C	1.41936800	2.29282800	1.39569700
O	1.88801600	2.65764400	2.44963500
C	1.74097400	-3.29662600	-2.21440300
H	2.44371500	-3.51563800	-1.40801800
H	2.14429800	-2.47015100	-2.80641900
H	1.71112800	-4.17533400	-2.87201800
C	0.48584300	-4.14576100	0.63265200
H	0.11634500	-3.87170700	1.62321200
H	1.57222900	-4.03026100	0.63407800
H	0.27007800	-5.21367500	0.49620600

C	-2.54133400	-3.19849400	0.64176600
H	-3.49731800	-2.69549200	0.48874700
H	-2.17530800	-2.94952200	1.64060600
H	-2.73307600	-4.27969100	0.62286900
C	-3.26103400	-1.98116700	-2.22494300
H	-3.87324700	-2.87996200	-2.37140100
H	-3.22697800	-1.45228700	-3.17995600
H	-3.77983700	-1.33885900	-1.50853100
C	-0.50815000	-1.95044600	-3.93130000
H	0.41132500	-1.37611200	-4.07784400
H	-1.34373000	-1.34922200	-4.29462600
H	-0.43928000	-2.84015500	-4.57039900
C	-1.04993300	0.90472100	-0.16173500
C	-0.32453700	0.40196400	1.01831400
N	1.01384600	0.84626700	1.30431300
H	1.35840500	0.40640900	2.18420100
C	0.73829800	2.58173800	-0.97641100
C	-0.26093400	1.62912700	-1.22275200
C	1.30763500	3.37481800	-1.98213100
C	-0.62350900	1.47728900	-2.58401600
C	0.94047900	3.18407300	-3.30685800
C	-0.02941800	2.21701800	-3.60234500
H	-1.42315900	0.78482000	-2.81930400
H	1.37691700	3.78883800	-4.09592300
H	-0.34672400	2.06599000	-4.62909400
C	2.26010200	4.37971900	-1.36921500
C	1.88794300	4.33877100	0.12979800
N	1.23254800	3.01291600	0.28001300
H	3.30260700	4.07555000	-1.52445700
H	2.14549900	5.38261600	-1.78726400
H	2.73447400	4.40207500	0.81318400
H	1.16872500	5.12122500	0.39112100
C	-2.50958400	1.27216900	-0.09935500
C	-3.47404600	0.41599700	0.46210300
C	-2.94833900	2.51682500	-0.58687300
C	-4.81641500	0.78411200	0.52924200
H	-3.16438800	-0.54119700	0.86081300
C	-4.29299600	2.88562600	-0.52198500
H	-2.23422000	3.21164300	-1.01556700
C	-5.23524000	2.02103800	0.03371800
H	-5.53753900	0.10179500	0.96999300
H	-4.59995300	3.85448300	-0.90453200
H	-6.28140800	2.30642000	0.08323400
C	-0.94769300	0.07532000	2.35993500
C	-0.66812500	-1.13165500	3.01913300
C	-1.69929900	1.05444400	3.03274900
C	-1.15342200	-1.36838400	4.30618900
H	-0.04996100	-1.87460000	2.52719200
C	-2.19865800	0.80822400	4.31092000
H	-1.90444700	2.00413500	2.55000900
C	-1.92885900	-0.40329500	4.95075200
H	-0.92379500	-2.30564800	4.80396900
H	-2.78681400	1.57061400	4.81230800
H	-2.31082700	-0.58915800	5.94975100
C	3.11307100	-0.43173900	1.16507100
O	2.82666400	-0.67930800	2.32310800
C	4.45611000	-0.79494500	0.51193600
C	5.49595200	0.13457000	1.18917700
H	6.49054300	-0.09623900	0.79571600
H	5.28724300	1.18882200	0.98037300
H	5.50612500	-0.00934800	2.27198400
C	4.76522500	-2.26459500	0.86111600
H	4.05267800	-2.94677900	0.38565500
H	5.76543700	-2.52136200	0.50004700
H	4.73014100	-2.42721500	1.94014700
C	4.46921700	-0.57722800	-1.00976200
H	5.45364100	-0.85042100	-1.40125400
H	3.72317300	-1.19638900	-1.51409100
H	4.27960900	0.46655600	-1.27274900

6a

Sum of electronic and thermal Free Energies= -306.404599

C	-0.06823	0.4191	0.
O	1.16204	0.4191	0.
O	-0.69758	1.62132	0.
C	0.25481	2.68801	-0.00005
H	-0.26015	3.62594	-0.00204
H	0.86736	2.61929	0.87457
H	0.86987	2.61696	-0.87273
C	-1.05963	-0.75934	0.00007
H	-0.69296	-1.76455	0.00012
C	-2.39486	-0.52759	0.00005
H	-2.91879	-1.46054	-0.0019
H	-2.66032	0.02871	0.87468

5[6a]

Sum of electronic and thermal Free Energies= -1453.091917

C	-2.65654	0.51105	-1.07531
C	-2.60749	-0.93588	-0.78824
C	-2.56317	-1.09608	0.62441

C	-2.50474	0.24352	1.20419
C	-2.64614	1.21869	0.1494
C	-2.68131	2.70517	0.33621
H	-2.35831	3.23177	-0.56379
H	-3.69838	3.03999	0.57239
H	-2.03144	3.02031	1.15649
C	-2.73837	1.09218	-2.44944
H	-3.77549	1.05614	-2.80783
H	-2.41398	2.13387	-2.47086
H	-2.12955	0.5277	-3.16026
C	-2.76104	-2.01251	-1.81671
H	-2.24	-1.76269	-2.7437
H	-2.37597	-2.97029	-1.46273
H	-3.82269	-2.14759	-2.05985
C	-2.71465	-2.361	1.4127
H	-2.00162	-2.41894	2.23859
H	-3.72383	-2.40697	1.84012
H	-2.58752	-3.24788	0.79011
C	-2.45711	0.53879	2.6674
H	-3.48046	0.59826	3.06226
H	-1.93501	-0.24488	3.22014
H	-1.97038	1.49442	2.87287
Rh	-0.72941	-0.07884	-0.04546
C	2.11039	-1.08615	-0.01199
C	3.16294	-2.01735	0.02338
C	2.88495	-3.37175	0.08198
C	1.54451	-3.78668	0.10724
C	0.51866	-2.849	0.08194
C	0.75071	-1.45365	0.02163
C	4.14918	0.17438	-0.11461
C	4.50565	-1.32667	-0.00245
H	3.68961	-4.10062	0.10876
H	1.30943	-4.84579	0.14868
H	-0.50194	-3.21162	0.10846
H	4.54571	0.76232	0.71826
H	5.11847	-1.65238	-0.84829
N	2.66376	0.2189	-0.08939
H	5.08033	-1.52743	0.90726
H	4.51256	0.60667	-1.05397
C	1.95998	1.3672	-0.11848
O	0.70351	1.42459	-0.09422
N	2.68822	2.54293	-0.09763
H	3.60569	2.53186	-0.5301
O	1.98541	3.67636	-0.51536
C	1.74518	4.5467	0.60121
H	2.68495	4.86356	1.06503
H	1.23385	5.41028	0.17232
H	1.10454	4.06194	1.34441
C	0.5732	0.73276	-2.47578
O	0.49799	1.90559	-2.78629
O	1.74214	0.10826	-2.20051
C	2.91141	0.93428	-2.30045
H	3.75207	0.2869	-2.0506
H	3.01979	1.32947	-3.31383
H	2.85272	1.77318	-1.60214
C	-0.60529	-0.16113	-2.35954
H	-1.54579	0.33475	-2.57933
C	-0.54984	-1.45132	-2.02063
H	-1.45057	-2.05378	-1.95264
H	0.39499	-1.9378	-1.80279

TS3[6a]

Sum of electronic and thermal Free Energies= -1146.659611

Rh	-0.94747800	-0.00671100	-0.34267700
C	-3.17228400	-0.21736400	-0.69475200
C	-2.95594400	0.62116200	0.43317700
C	-2.34077800	-0.19333700	1.49896400
C	-2.15529300	-1.49816600	1.00130400
C	-2.58751200	-1.50643200	-0.39406900
O	-0.47798400	2.87503100	0.27846700
C	1.05444500	1.49047700	1.46847000
O	0.89265700	2.17831500	2.45674200
C	-2.69955000	-2.72987000	-1.25400400
H	-1.94934800	-3.47897500	-0.99400900
H	-2.59981300	-2.49516000	-2.31684800
H	-3.68491700	-3.19352400	-1.11613000
C	-1.64069700	-2.69203600	1.74499000
H	-2.46668700	-3.37469000	1.97892100
H	-1.17007200	-2.40898900	2.68819300
H	-0.90764800	-3.25077000	1.15766400
C	-2.07456000	0.30763600	2.88532200
H	-1.54596400	1.26517200	2.88026300
H	-1.48146200	-0.40134200	3.46593100
H	-3.02245800	0.46050600	3.41594800
C	-3.46111000	2.01717100	0.62199300
H	-4.43980700	1.99132600	1.11871700
H	-3.58428200	2.53490400	-0.33112300
H	-2.78240700	2.60581900	1.24023300
C	-3.91719300	0.13878000	-1.94534700

H	-3.86714900	1.20859600	-2.15833100
H	-4.97598600	-0.12677300	-1.83497100
H	-3.53958700	-0.40190300	-2.81688700
C	0.72022600	-0.26821500	-2.14904600
C	-0.40632300	0.63264200	-2.28691600
N	0.34073500	1.72681800	0.22715100
H	1.02709400	1.83739300	-0.53294500
C	1.87149000	-0.75421500	0.64085900
C	0.97211400	-1.13204500	-0.38904900
C	2.78916900	-1.67197500	1.18821100
C	1.00598000	-2.50561300	-0.74574100
C	2.80973100	-2.99575300	0.77799500
C	1.88339800	-3.42151200	-0.18136700
H	0.33451000	-2.85342500	-1.52442600
H	3.52319500	-3.69215600	1.20799800
H	1.86591600	-4.45682200	-0.50596300
C	3.63324700	-1.00116900	2.24476700
C	2.81555100	0.25344500	2.58625600
N	1.94934100	0.45443800	1.38918100
H	3.80240200	-1.63079900	3.12150000
H	4.61681400	-0.73527600	1.83814500
H	2.17682400	0.10453600	3.46260300
H	3.41697500	1.14695000	2.75642700
H	-1.18571700	0.30779500	-2.97115600
H	-0.22380500	1.70331300	-2.31964100
H	0.61152900	-1.20256200	-2.68310600
C	2.13631400	0.22016900	-2.34974100
O	2.97088800	-0.40405300	-2.95520700
O	2.35390500	1.44976900	-1.81613500
C	3.68451400	1.99154800	-2.02218900
H	3.68745600	2.95874700	-1.52208600
H	4.43107100	1.32421900	-1.58895200
H	3.87448800	2.10675300	-3.09006500
C	0.27713100	4.10309700	0.25827600
H	-0.48240000	4.88578000	0.23400400
H	0.88984100	4.20590400	1.15552200
H	0.88925200	4.16559900	-0.65037800

6[6a]

Sum of electronic and thermal Free Energies= -1453.090563

Rh	0.89907	0.0228	0.08435
C	3.08256	-0.10467	0.39402
C	2.35296	-0.66939	1.50931
C	1.69322	0.4349	2.23334
C	1.89689	1.60972	1.50236
C	2.70503	1.27152	0.31403
O	-0.19518	-0.60941	1.86329
C	-2.12201	-0.63456	0.5035
O	-2.90759	-1.49614	0.96482
C	3.23584	2.28817	-0.6488
H	2.4811	3.03701	-0.89931
H	3.58497	1.82901	-1.57548
H	4.08703	2.8143	-0.19762
C	1.41095	2.99177	1.81158
H	2.25382	3.64132	2.07733
H	0.7099	2.99936	2.64824
H	0.91545	3.44458	0.94651
C	0.92109	0.25583	3.50323
H	0.19886	-0.56135	3.41354
H	0.37804	1.16094	3.78163
H	1.59766	0.00357	4.32839
C	2.46561	-2.07872	1.99528
H	3.37134	-2.1905	2.60615
H	2.53074	-2.77703	1.15757
H	1.61118	-2.35608	2.61695
C	4.06219	-0.83659	-0.46873
H	3.68412	-1.82427	-0.74393
H	5.00448	-0.96473	0.07853
H	4.28727	-0.28324	-1.38301
C	-1.22852	-0.4156	2.83794
H	-1.8602	0.44174	2.57842
H	-0.69817	-0.20734	3.76842
H	-1.85113	-1.30998	2.94642
C	-0.4735	-0.51703	-2.33354
C	0.78992	-1.10562	-1.70495
N	-0.77045	-0.89894	0.60838
H	-0.61835	-1.84564	0.95357
C	-1.60903	1.31635	-0.88273
C	-0.65812	0.91888	-1.84485
C	-1.91889	2.66806	-0.64663
C	0.0453	1.97143	-2.48083
C	-1.22103	3.6695	-1.30232
C	-0.21559	3.31019	-2.21562
H	0.77383	1.71005	-3.24328
H	-1.46547	4.71446	-1.13588
H	0.32524	4.0819	-2.75431
C	-3.08329	2.76397	0.31284
C	-3.66454	1.33168	0.2912
N	-2.50949	0.49404	-0.14274

H	-2.74378	3.03468	1.32075
H	-3.82483	3.50562	0.00608
H	-4.01996	1.00011	1.26518
H	-4.47426	1.23194	-0.43554
H	-0.41194	-0.50819	-3.4289
H	-1.3447	-1.11827	-2.07371
H	1.69801	-0.83847	-2.24744
C	0.83412	-2.56648	-1.41366
O	1.85335	-3.18043	-1.12988
O	-0.37175	-3.17169	-1.48752
C	-0.37185	-4.58807	-1.2271
H	-0.05787	-4.78968	-0.19983
H	-1.39886	-4.91543	-1.38702
H	0.3059	-5.10386	-1.91031

7[6a]

Sum of electronic and thermal Free Energies= -1453.082243

Rh	-0.85355	-0.26447	0.39456
C	-3.03051	0.33536	0.18242
C	-2.8746	-0.54016	1.31143
C	-2.39518	-1.79823	0.81117
C	-2.38789	-1.72423	-0.65667
C	-2.78234	-0.42892	-1.04272
O	0.63495	-2.84842	0.33311
C	1.737	-1.33159	-1.1304
O	1.54739	-2.08482	-2.05844
C	-3.03386	0.06597	-2.43342
H	-2.62255	-0.6152	-3.18019
H	-2.60246	1.05521	-2.60502
H	-4.11455	0.1381	-2.61058
C	-2.05815	-2.87667	-1.55147
H	-2.84977	-3.63363	-1.48491
H	-1.11876	-3.34843	-1.25602
H	-1.97164	-2.57035	-2.59446
C	-2.25217	-3.06319	1.60078
H	-2.00535	-2.8619	2.64531
H	-1.47612	-3.70442	1.18334
H	-3.19823	-3.61946	1.58203
C	-3.27281	-0.22375	2.72214
H	-2.72226	-0.82649	3.4461
H	-4.34164	-0.43411	2.85521
H	-3.1122	0.82936	2.9619
C	-3.67253	1.68608	0.23117
H	-3.52214	2.235	-0.69857
H	-3.30092	2.28862	1.06214
H	-4.75463	1.56089	0.36825
C	1.7668	-3.71561	0.53048
H	2.38175	-3.77677	-0.37073
H	1.32908	-4.6921	0.7422
H	2.36131	-3.38995	1.3937
C	0.71457	1.53122	0.62311
C	0.12481	1.54441	-0.64243
N	1.00913	-1.50104	0.14049
H	1.59332	-1.21937	0.93325
C	2.97207	0.47189	0.03848
C	2.11703	1.17198	0.90907
C	4.36567	0.49991	0.16729
C	2.73468	1.76279	2.03396
C	4.94661	1.12325	1.26553
C	4.11465	1.72981	2.21661
H	2.11408	2.30206	2.74378
H	6.02552	1.14562	1.38488
H	4.55051	2.21424	3.08414
C	4.9952	-0.20153	-1.02006
C	3.81054	-0.33019	-2.01075
N	2.6128	-0.27389	-1.12459
H	5.82361	0.3656	-1.45149
H	5.38604	-1.18698	-0.73611
H	3.77682	0.51551	-2.70301
H	3.79022	-1.25624	-2.58347
H	0.27532	2.19215	1.36165
H	0.17349	0.67226	1.26296
H	0.63006	1.11713	-1.50112
C	-0.81652	2.63082	-1.03766
O	-1.23659	2.76836	-2.17133
O	-1.08307	3.49576	-0.03622
C	-1.80556	4.68792	-0.41261
H	-2.81193	4.44278	-0.75764
H	-1.84871	5.29719	0.48906
H	-1.27451	5.21235	-1.20931

TS4[6a]

Sum of electronic and thermal Free Energies= -1453.071774

Rh	0.94074	-0.39616	-0.20716
C	3.02423	0.33385	-0.17965
C	3.00054	-0.6753	-1.24811
C	2.65882	-1.92061	-0.68879
C	2.40505	-1.69692	0.73397
C	2.75387	-0.32688	1.06261
O	-0.3602	-2.82407	-0.56654

C	-1.61845	-1.50942	0.97272
O	-1.36972	-2.29426	1.86365
C	2.87705	0.25819	2.43276
H	2.43076	-0.39239	3.18654
H	2.39702	1.23759	2.5079
H	3.93955	0.3755	2.68121
C	2.05085	-2.7698	1.71108
H	2.9479	-3.36071	1.93963
H	1.29314	-3.44211	1.30494
H	1.66893	-2.35904	2.64638
C	2.61709	-3.24839	-1.37939
H	2.46313	-3.14285	-2.45563
H	1.81957	-3.87602	-0.98136
H	3.56737	-3.77676	-1.23165
C	3.32666	-0.38494	-2.67843
H	2.93517	-1.14937	-3.35204
H	4.41588	-0.35067	-2.81029
H	2.93578	0.58751	-2.98927
C	3.54209	1.73014	-0.33637
H	3.32332	2.33278	0.54587
H	3.12202	2.23319	-1.21043
H	4.63242	1.70538	-0.45976
C	-1.42074	-3.75969	-0.8367
H	-2.0284	-3.93678	0.05397
H	-0.90823	-4.67971	-1.12128
H	-2.04035	-3.41587	-1.675
C	-0.86624	1.39067	-0.90256
C	-0.22447	1.37491	0.47319
N	-0.83851	-1.52648	-0.27301
H	-1.42273	-1.22625	-1.0611
C	-3.06899	0.24953	-0.08962
C	-2.34749	1.05647	-0.98591
C	-4.47533	0.21422	-0.08889
C	-3.10749	1.70629	-1.97982
C	-5.19465	0.8863	-1.06496
C	-4.49508	1.61724	-2.03337
H	-2.58911	2.33409	-2.69941
H	-6.27999	0.85783	-1.07159
H	-5.03728	2.15234	-2.80615
C	-4.96784	-0.59809	1.09004
C	-3.70804	-0.70387	1.9773
N	-2.59191	-0.55013	1.00302
H	-5.797	-0.11765	1.61501
H	-5.31161	-1.59034	0.77062
H	-3.65973	0.1155	2.70062
H	-3.59514	-1.64919	2.50526
H	-0.68849	2.3535	-1.38445
H	-0.13351	0.32316	-1.34161
H	-0.84935	1.01444	1.285
C	0.47731	2.60193	0.93378
O	0.79056	2.81006	2.09329
O	0.73456	3.48886	-0.0617
C	1.28839	4.75248	0.35805
H	2.2697	4.61547	0.81735
H	1.37084	5.35125	-0.54826
H	0.62644	5.23479	1.0802

8[6a]

Sum of electronic and thermal Free Energies= -1453.077747

Rh	-0.89216	-0.23603	0.27917
C	-3.0229	0.4081	0.3228
C	-2.83126	-0.51072	1.43061
C	-2.45538	-1.76742	0.88869
C	-2.4825	-1.65003	-0.57803
C	-2.88551	-0.33593	-0.92078
O	0.53712	-2.88779	0.17053
C	1.76344	-1.35514	-1.17038
O	1.61072	-2.0717	-2.13356
C	-3.19607	0.18831	-2.28811
H	-2.85926	-0.49975	-3.06498
H	-2.73187	1.15958	-2.47785
H	-4.28139	0.30732	-2.39775
C	-2.24375	-2.78956	-1.51734
H	-3.10986	-3.46375	-1.50331
H	-1.36438	-3.36622	-1.22535
H	-2.10053	-2.44782	-2.54327
C	-2.27694	-3.04853	1.64239
H	-1.99936	-2.86981	2.68351
H	-1.5095	-3.67259	1.18489
H	-3.21712	-3.6148	1.64193
C	-3.07442	-0.18508	2.87349
H	-2.49738	-0.82914	3.53968
H	-4.13627	-0.32837	3.1104
H	-2.8263	0.85388	3.10116
C	-3.60237	1.78319	0.44316
H	-3.51244	2.33529	-0.49255
H	-3.12812	2.36423	1.23668
H	-4.67139	1.70546	0.67969
C	1.62631	-3.80659	0.37502

H	2.27377	-3.85507	-0.50349
H	1.14379	-4.77283	0.52879
H	2.19755	-3.53922	1.27357
C	0.69667	1.44699	0.66622
C	0.15825	1.4582	-0.65876
N	0.96702	-1.54931	0.05064
H	1.52295	-1.32369	0.88114
C	2.98321	0.4113	0.09972
C	2.11758	1.111	0.95953
C	4.37648	0.44202	0.25896
C	2.71479	1.70703	2.09089
C	4.93737	1.0635	1.36686
C	4.09019	1.6746	2.30106
H	2.0816	2.2473	2.78911
H	6.01417	1.08487	1.50425
H	4.51008	2.16203	3.17472
C	5.0351	-0.24785	-0.91858
C	3.87843	-0.35508	-1.94136
N	2.65908	-0.31751	-1.08493
H	5.87939	0.31906	-1.31815
H	5.41024	-1.23995	-0.63643
H	3.86226	0.50513	-2.61653
H	3.87264	-1.26855	-2.53406
H	0.30476	2.21587	1.32493
H	-0.63327	-1.49615	-0.0166
H	0.74016	1.05382	-1.47888
C	-0.70531	2.57922	-1.11656
O	-1.09693	2.69981	-2.26225
O	-0.96436	3.48581	-0.14515
C	-1.64721	4.68256	-0.57459
H	-2.6425	4.44868	-0.958
H	-1.71644	5.31214	0.31149
H	-1.07434	5.18118	-1.35893

TS5[6a]

Sum of electronic and thermal Free Energies= -1453.047240

Rh	1.00464	-0.22353	0.36537
C	2.76469	-0.50866	-0.85639
C	1.94272	-1.69581	-1.10357
C	1.8202	-2.36317	0.1306
C	2.70247	-1.69517	1.11435
C	3.32952	-0.60944	0.49495
O	-1.80742	-1.95686	-0.93942
C	-2.60498	0.15125	-1.84955
O	-2.90555	0.32832	-3.01358
C	4.35588	0.32264	1.0627
H	4.51252	0.14268	2.12801
H	4.06823	1.37142	0.93771
H	5.31933	0.17786	0.55862
C	2.88182	-2.17496	2.52117
H	3.45853	-3.10852	2.53698
H	1.92005	-2.38731	2.99886
H	3.41155	-1.4453	3.13568
C	1.08786	-3.6413	0.40554
H	0.31553	-3.83379	-0.34082
H	0.60871	-3.62575	1.38828
H	1.78449	-4.48957	0.39836
C	1.45307	-2.14727	-2.44714
H	2.2239	-2.74158	-2.95415
H	1.23062	-1.30174	-3.10601
H	0.56702	-2.78248	-2.3638
C	3.25747	0.43692	-1.90543
H	2.48401	0.67667	-2.63873
H	4.09949	-0.01867	-2.44404
H	3.6163	1.36671	-1.46084
C	-2.65132	-2.77253	-1.7775
H	-3.60442	-2.28299	-1.99632
H	-2.82259	-3.67173	-1.18513
H	-2.14153	-3.03203	-2.71274
C	-0.47524	1.35687	0.31565
C	0.74065	1.84799	0.87138
N	-1.43478	-0.74722	-1.57924
H	-1.04626	-0.95947	-2.50623
C	-2.84186	0.54902	0.61535
C	-1.57604	0.84297	1.15948
C	-3.97581	0.32784	1.40432
C	-1.4792	0.71343	2.56668
C	-3.85048	0.22439	2.78352
C	-2.58139	0.38896	3.35398
H	-0.53622	0.92563	3.05728
H	-4.71809	0.04239	3.40997
H	-2.46209	0.31788	4.43028
C	-5.20857	0.28744	0.52356
C	-4.69656	0.90695	-0.79898
N	-3.23922	0.6076	-0.75108
H	-5.55386	-0.74268	0.36846
H	-6.04385	0.85515	0.94012
H	-5.1271	0.48186	-1.70548
H	-4.83888	1.99152	-0.81637

H	-0.76704	1.75232	-0.65353
H	-0.49047	-0.37189	-0.85129
H	0.87942	1.93782	1.94494
C	1.6288	2.77653	0.12908
O	2.66607	3.22578	0.5827
O	1.17159	3.07856	-1.10923
C	1.94243	4.0572	-1.83478
H	2.94916	3.6857	-2.03931
H	1.40057	4.22443	-2.76491
H	2.01762	4.98294	-1.26079

9[6a]

Sum of electronic and thermal Free Energies= -1453.044927

Rh	0.9755	-0.24417	0.32886
C	2.75895	-0.50144	-0.87017
C	1.92615	-1.6671	-1.16484
C	1.78058	-2.372	0.04793
C	2.67135	-1.7561	1.05932
C	3.31252	-0.65772	0.48357
O	-1.80213	-1.86976	-1.09066
C	-2.59668	0.29458	-1.83398
O	-2.91128	0.57387	-2.97468
C	4.3467	0.24141	1.08821
H	4.49879	0.02043	2.14645
H	4.07153	1.29744	1.00052
H	5.30978	0.10475	0.58112
C	2.83673	-2.28894	2.44857
H	3.41089	-3.22411	2.43491
H	1.87035	-2.51616	2.90957
H	3.36287	-1.58403	3.09434
C	1.02834	-3.64814	0.27237
H	0.26247	-3.80568	-0.48854
H	0.53833	-3.65815	1.24978
H	1.7147	-4.50438	0.24515
C	1.43831	-2.06768	-2.52516
H	2.2	-2.66542	-3.04166
H	1.24131	-1.19798	-3.15978
H	0.53548	-2.68095	-2.46671
C	3.27313	0.47497	-1.87981
H	2.51535	0.73331	-2.62289
H	4.12799	0.03653	-2.41245
H	3.62043	1.39205	-1.40079
C	-2.66229	-2.61806	-1.97261
H	-3.61777	-2.11186	-2.13745
H	-2.82697	-3.56042	-1.44917
H	-2.17057	-2.80574	-2.9345
C	-0.46343	1.3718	0.39235
C	0.76233	1.81661	0.95218
N	-1.43283	-0.61639	-1.64497
H	-1.05497	-0.76298	-2.58812
C	-2.81537	0.51735	0.65642
C	-1.54781	0.7889	1.21023
C	-3.93827	0.23394	1.4413
C	-1.43438	0.57123	2.60565
C	-3.79731	0.04225	2.80965
C	-2.52506	0.18358	3.37993
H	-0.48894	0.76478	3.09935
H	-4.65701	-0.18997	3.43052
H	-2.39566	0.04437	4.44832
C	-5.17947	0.23975	0.57125
C	-4.68589	0.95427	-0.70974
N	-3.22616	0.6661	-0.69677
H	-5.51405	-0.78161	0.34892
H	-6.01704	0.76716	1.03366
H	-5.1223	0.58948	-1.63941
H	-4.8392	2.03599	-0.6502
H	-0.76352	1.81314	-0.55342
H	-0.92539	-0.38916	-0.92457
H	0.92876	1.83588	2.02507
C	1.65405	2.76602	0.23971
O	2.70679	3.17335	0.69715
O	1.18002	3.13689	-0.97166
C	1.95772	4.1327	-1.66663
H	2.94686	3.74465	-1.9206
H	1.39476	4.36424	-2.56996
H	2.0757	5.02335	-1.04638

TS6[6a]

Sum of electronic and thermal Free Energies= -1453.022283

Rh	1.05655	-0.20711	0.41848
C	2.76095	-0.49498	-0.86702
C	1.92064	-1.66968	-1.13512
C	1.8155	-2.37587	0.07523
C	2.69447	-1.72766	1.07132
C	3.33281	-0.62993	0.47223
O	-1.92146	-2.25147	-0.98194
C	-2.72348	0.21445	-1.81496
O	-3.08256	0.36636	-2.96357
C	4.37078	0.27963	1.05815
H	4.50346	0.09734	2.12649

H	4.10695	1.33403	0.92884
H	5.34057	0.11339	0.57309
C	2.88561	-2.23925	2.46592
H	3.50298	-3.14671	2.45933
H	1.93199	-2.50551	2.93211
H	3.38077	-1.50477	3.10339
C	1.07791	-3.65718	0.32249
H	0.29644	-3.8249	-0.42102
H	0.60851	-3.66674	1.31008
H	1.76716	-4.51062	0.28477
C	1.41027	-2.07604	-2.48591
H	2.16907	-2.65803	-3.02477
H	1.18646	-1.20839	-3.11606
H	0.52098	-2.70805	-2.41098
C	3.25785	0.46592	-1.90091
H	2.48553	0.72761	-2.62778
H	4.09392	0.013	-2.4508
H	3.62614	1.38415	-1.44026
C	-2.7308	-3.00982	-1.90925
H	-3.69843	-2.53482	-2.08789
H	-2.86879	-3.96631	-1.40515
H	-2.20206	-3.15739	-2.85762
C	-0.46341	1.32252	0.30397
C	0.75019	1.84753	0.86304
N	-1.49804	-0.67752	-1.61904
H	-1.09509	-0.785	-2.55985
C	-2.83763	0.53547	0.67259
C	-1.55008	0.81799	1.17118
C	-3.94005	0.28289	1.49524
C	-1.40469	0.64867	2.57091
C	-3.76458	0.13897	2.8657
C	-2.47583	0.29586	3.38972
H	-0.44524	0.85032	3.0328
H	-4.60742	-0.06602	3.518
H	-2.31399	0.19532	4.45821
C	-5.20718	0.26222	0.66478
C	-4.75593	0.93334	-0.65327
N	-3.29573	0.6345	-0.67946
H	-5.55003	-0.76473	0.48537
H	-6.02936	0.80672	1.1349
H	-5.22429	0.54314	-1.55659
H	-4.894	2.01789	-0.62138
H	-0.77311	1.7347	-0.65435
H	-0.70153	-0.33562	-0.93923
H	0.86111	1.98963	1.93492
C	1.62546	2.77678	0.10944
O	2.66192	3.2412	0.54949
O	1.16089	3.06154	-1.1337
C	1.92111	4.04017	-1.86886
H	2.92985	3.67557	-2.0761
H	1.3743	4.19814	-2.79801
H	1.99267	4.97071	-1.30207

10[6a]

Sum of electronic and thermal Free Energies= -1453.155938

Rh	0.88615	-0.27072	-0.03042
C	1.61566	-0.96409	2.0185
C	2.53468	-1.4105	1.03466
C	1.85477	-2.37202	0.16306
C	0.49782	-2.45158	0.57628
C	0.32294	-1.54172	1.70397
O	1.60635	0.48992	-1.79259
C	-1.38187	-0.27913	-2.09576
O	-1.22426	-1.03525	-3.04122
C	-0.90933	-1.43844	2.54457
H	-1.81971	-1.5533	1.95385
H	-0.96938	-0.48288	3.06703
H	-0.89913	-2.23235	3.30302
C	-0.56236	-3.33939	0.00097
H	-0.43012	-3.48808	-1.07305
H	-1.55982	-2.92624	0.16568
H	-0.53355	-4.32443	0.48308
C	2.5181	-3.19091	-0.89737
H	3.25716	-2.61327	-1.45786
H	1.79718	-3.60631	-1.60423
H	3.05206	-4.03089	-0.43432
C	3.97986	-1.02409	0.96394
H	4.54734	-1.55829	1.73636
H	4.10486	0.04845	1.13346
H	4.42209	-1.27462	-0.00209
C	1.95604	-0.08619	3.18403
H	2.5585	0.76949	2.86841
H	2.53386	-0.65887	3.91937
H	1.06305	0.28396	3.69179
C	1.97557	-0.4304	-2.7832
H	3.04841	-0.65782	-2.66346
H	1.7996	-0.01248	-3.78147
H	1.42608	-1.37789	-2.70325
C	-0.92004	2.33426	0.31658

C	0.43972	1.73629	0.72835
N	-0.25845	0.32895	-1.45747
H	-0.12279	1.29669	-1.73955
C	-2.83464	0.58991	-0.19742
C	-2.1536	1.5013	0.64069
C	-4.05115	0.00381	0.21006
C	-2.73085	1.72045	1.9079
C	-4.58793	0.25025	1.46598
C	-3.90956	1.11264	2.32923
H	-2.24266	2.43201	2.56884
H	-5.52816	-0.20678	1.75959
H	-4.31442	1.33789	3.3106
C	-4.62615	-0.86849	-0.88234
C	-3.81755	-0.44299	-2.11673
N	-2.56235	0.11789	-1.54314
H	-4.4785	-1.93246	-0.6562
H	-5.69841	-0.71213	-1.02471
H	-3.56835	-1.2519	-2.80135
H	-4.32322	0.35182	-2.674
H	-1.02234	3.27758	0.8699
H	-0.56223	1.25733	-0.66887
H	0.47862	1.56208	1.80107
C	1.67428	2.47231	0.30846
O	2.76585	2.32242	0.83616
O	1.4573	3.28977	-0.73638
C	2.61759	3.98131	-1.25015
H	3.3429	3.26	-1.63047
H	2.2454	4.61514	-2.0535
H	3.07757	4.58245	-0.46392

TS7[6a]

Sum of electronic and thermal Free Energies= -1453.132463

Rh	-1.2462	-0.60814	-0.01345
C	-2.97349	-0.21886	1.32657
C	-3.41328	-0.96178	0.19689
C	-3.13647	-0.1603	-0.99581
C	-2.60281	1.1074	-0.57824
C	-2.43905	1.05506	0.84088
O	-0.19329	-2.18717	0.43279
C	0.65072	0.79289	-1.81311
O	0.31849	0.92898	-2.98657
C	-1.92079	2.15025	1.71807
H	-1.22084	2.79848	1.18787
H	-1.4139	1.75443	2.60097
H	-2.75521	2.77185	2.06791
C	-2.29924	2.25487	-1.49145
H	-1.73886	1.93187	-2.37331
H	-1.72222	3.02883	-0.98193
H	-3.23321	2.71494	-1.8351
C	-3.46927	-0.53649	-2.4041
H	-3.46651	-1.61891	-2.54805
H	-2.76502	-0.09261	-3.11155
H	-4.4736	-0.17133	-2.65641
C	-4.08364	-2.2996	0.20394
H	-5.17304	-2.17	0.20691
H	-3.81698	-2.88384	1.08692
H	-3.82575	-2.88566	-0.68131
C	-3.09373	-0.61565	2.76446
H	-3.12219	-1.70089	2.88308
H	-4.02074	-0.21211	3.1908
H	-2.26319	-0.23067	3.36091
C	-0.62592	-3.27097	1.22555
H	0.24913	-3.8763	1.49487
H	-1.32529	-3.91675	0.67452
H	-1.11721	-2.94185	2.15324
C	2.71934	-0.22937	0.35667
C	2.4094	-1.49218	0.86687
N	0.42372	-0.34426	-1.04406
H	0.25774	-1.08471	-1.72836
C	1.79194	2.01678	0.11274
C	2.34634	1.01723	0.94144
C	1.67626	3.3458	0.56061
C	2.59397	1.3409	2.30297
C	1.99146	3.65419	1.87227
C	2.42904	2.63856	2.75349
H	3.00296	0.57918	2.95933
H	1.90074	4.67503	2.23306
H	2.67357	2.88897	3.78014
C	1.16328	4.19975	-0.57998
C	1.22089	3.2339	-1.79242
N	1.31417	1.87998	-1.1827
H	0.13943	4.54458	-0.38712
H	1.77417	5.09104	-0.7443
H	0.35366	3.27706	-2.44805
H	2.11167	3.41179	-2.40289
H	3.09413	-0.20543	-0.66568
H	0.47863	-0.95745	0.0103
H	2.01304	-1.58102	1.87336
C	2.98927	-2.7734	0.33264

O	2.94194	-3.81152	0.95158
O	3.52066	-2.61474	-0.88815
C	4.08623	-3.806	-1.48545
H	3.31762	-4.574	-1.59053
H	4.4582	-3.49269	-2.45932
H	4.89797	-4.18777	-0.86355

11[6a]

Sum of electronic and thermal Free Energies= -1453.165110

Rh	-1.56626	-0.20718	0.30823
C	-3.58581	0.69369	0.59782
C	-3.60662	-0.61943	1.1386
C	-3.25649	-1.53776	0.06081
C	-3.09261	-0.77697	-1.16436
C	-3.24674	0.60302	-0.82903
O	0.32373	-0.39406	1.52171
C	0.51906	0.64518	-1.67891
O	-0.10237	0.62831	-2.74282
C	-3.15525	1.73998	-1.79353
H	-2.31347	1.59791	-2.47714
H	-3.04028	2.69845	-1.28392
H	-4.07402	1.79011	-2.39191
C	-2.81823	-1.3143	-2.53384
H	-2.02606	-0.74014	-3.02194
H	-3.72778	-1.2445	-3.14284
H	-2.52019	-2.36397	-2.50482
C	-3.18998	-3.02338	0.18387
H	-2.8524	-3.33484	1.17458
H	-2.5298	-3.46484	-0.56476
H	-4.19325	-3.44322	0.02954
C	-3.95102	-1.01527	2.54089
H	-5.01184	-1.2872	2.60334
H	-3.77658	-0.20039	3.2459
H	-3.37097	-1.87995	2.87125
C	-3.86622	1.96774	1.32481
H	-3.76357	1.85352	2.40497
H	-4.89474	2.2897	1.11678
H	-3.20222	2.77175	0.99787
C	0.27853	-0.32237	2.94482
H	0.78637	-1.18545	3.3888
H	-0.76359	-0.30551	3.27273
H	0.77305	0.59811	3.26932
C	3.17361	-0.47977	-0.04347
C	3.5441	-1.53082	0.71097
N	0.3407	-0.34856	-0.67385
H	0.37014	-1.26374	-1.12268
C	2.26302	1.85486	-0.2673
C	3.06397	0.91195	0.40525
C	2.34063	3.22734	0.01995
C	3.84524	1.4056	1.47423
C	3.12646	3.68324	1.0681
C	3.86487	2.75394	1.81414
H	4.49856	0.71668	1.99968
H	3.18804	4.74397	1.29282
H	4.49809	3.09319	2.6276
C	1.507	4.00347	-0.97734
C	1.26917	2.95943	-2.08997
N	1.38189	1.66615	-1.37179
H	0.55779	4.33146	-0.53261
H	2.01673	4.89403	-1.35305
H	0.2978	3.0204	-2.57796
H	2.04588	3.01631	-2.85998
H	2.95558	-0.66519	-1.09124
H	1.10257	-0.35159	0.96205
H	3.76738	-1.43802	1.76926
C	3.68225	-2.91168	0.20092
O	4.04209	-3.84586	0.88943
O	3.35186	-3.03226	-1.10959
C	3.5334	-4.34808	-1.66386
H	2.90445	-5.07583	-1.14504
H	3.24678	-4.26794	-2.71221
H	4.57642	-4.66018	-1.57528

TS8[6a]

Sum of electronic and thermal Free Energies= -1453.116893

Rh	1.17466	-0.1171	0.24632
C	2.8783	-1.39838	0.90808
C	3.19804	-0.05296	1.22334
C	3.15696	0.69984	-0.02425
C	2.8839	-0.21751	-1.11933
C	2.66355	-1.50446	-0.54444
O	-0.01892	1.81112	1.46045
C	-0.46632	-0.89419	-1.52909
O	0.19265	-1.2052	-2.52257
C	2.35327	-2.75128	-1.30608
H	1.62022	-2.54773	-2.09272
H	1.96794	-3.53959	-0.65674
H	3.26629	-3.13058	-1.78275
C	2.83915	0.09679	-2.58124
H	1.95873	-0.35868	-3.04277

H	3.73748	-0.30125	-3.06866
H	2.81315	1.17254	-2.76475
C	3.45735	2.15465	-0.16193
H	3.14648	2.71878	0.71978
H	2.97873	2.58845	-1.04169
H	4.54164	2.28871	-0.27451
C	3.54965	0.50741	2.5666
H	4.63912	0.52221	2.69285
H	3.13134	-0.09163	3.37774
H	3.19373	1.53302	2.68365
C	2.78224	-2.53903	1.86735
H	2.64411	-2.19884	2.89474
H	3.70751	-3.12837	1.82944
H	1.95928	-3.21134	1.61232
C	0.21458	2.26719	2.79318
H	0.24575	3.36096	2.82975
H	1.16479	1.86229	3.14357
H	-0.58976	1.90303	3.43945
C	-2.3046	0.88604	-0.2436
C	-2.37378	2.06515	0.38648
N	-0.44251	0.24112	-0.65942
H	-0.22075	1.03543	-1.26264
C	-2.55855	-1.40489	-0.1347
C	-3.1387	-0.21152	0.36214
C	-3.00341	-2.66494	0.30292
C	-4.07677	-0.35733	1.40695
C	-3.93824	-2.77168	1.32188
C	-4.459	-1.60185	1.89148
H	-4.56123	0.53397	1.79324
H	-4.27835	-3.74667	1.65841
H	-5.2031	-1.66597	2.67871
C	-2.34301	-3.75706	-0.5087
C	-1.77877	-2.97361	-1.71021
N	-1.59108	-1.60351	-1.16962
H	-1.53924	-4.24468	0.05921
H	-3.04372	-4.53655	-0.81789
H	-0.82991	-3.34354	-2.09485
H	-2.49696	-2.94315	-2.53662
H	-1.98857	0.89815	-1.2749
H	-1.09337	2.0438	0.83802
H	-2.6287	2.15154	1.43841
C	-2.05652	3.36259	-0.25024
O	-2.11392	4.42487	0.33679
O	-1.68509	3.24574	-1.54975
C	-1.4363	4.49249	-2.22547
H	-0.61918	5.03598	-1.74455
H	-1.17339	4.22522	-3.24866
H	-2.3303	5.11981	-2.21182

12[6a]

Sum of electronic and thermal Free Energies= -1453.171170

Rh	1.6601	0.43267	0.10285
C	2.60224	-1.06583	1.4162
C	3.38933	0.15669	1.50735
C	3.87049	0.45802	0.20273
C	3.39848	-0.58975	-0.70853
C	2.66003	-1.55009	0.06121
O	1.09224	1.76226	0.21342
C	-0.66572	-0.92681	-1.90736
O	-0.09544	-1.13383	-2.97412
C	2.13272	-2.85318	-0.44874
H	1.80022	-2.76617	-1.48495
H	1.3026	-3.21943	0.1583
H	2.92886	-3.60694	-0.41152
C	3.68337	-0.69056	-2.17125
H	2.78859	-0.99865	-2.72027
H	4.46625	-1.44035	-2.34452
H	4.03331	0.25752	-2.58274
C	4.74252	1.60697	-0.19146
H	4.66749	2.43712	0.51318
H	4.49432	1.97909	-1.1882
H	5.7907	1.28308	-0.21354
C	3.65968	0.91612	2.76835
H	4.4686	0.43152	3.32895
H	2.78321	0.94539	3.42091
H	3.96991	1.94281	2.56691
C	1.92944	-1.74612	2.56265
H	1.61515	-1.03397	3.32839
H	2.6307	-2.44836	3.03301
H	1.05511	-2.31509	2.24077
C	1.65005	2.88831	0.9051
H	0.86373	3.63795	1.03449
H	2.45469	3.31236	0.29809
H	2.04173	2.60683	1.88876
C	-1.74256	0.46974	-0.28018
C	-1.54032	1.70147	0.40189
N	-0.48745	0.26783	-1.14317
H	-0.46448	1.05174	-1.79788
C	-2.11228	-1.72174	-0.06253

C	-2.36683	-0.52764	0.61755
C	-2.47221	-2.97638	0.42916
C	-2.9541	-0.64051	1.88889
C	-3.06405	-3.06522	1.68588
C	-3.28979	-1.89044	2.41642
H	-3.19799	0.25896	2.44428
H	-3.3572	-4.02778	2.09467
H	-3.75969	-1.94707	3.3928
C	-2.10181	-4.03921	-0.58796
C	-1.68377	-3.21597	-1.83841
N	-1.49396	-1.84167	-1.32011
H	-1.27798	-4.66708	-0.22623
H	-2.9344	-4.71044	-0.81468
H	-0.76687	-3.56125	-2.31601
H	-2.47288	-3.20659	-2.59668
H	-2.64793	0.60688	-0.86777
H	-0.59829	1.87793	0.19737
H	-1.48029	1.67593	1.48872
C	-2.11871	2.96535	-0.11448
O	-2.18738	3.99234	0.53279
O	-2.49797	2.87295	-1.41393
C	-3.03802	4.08111	-1.98567
H	-2.29812	4.88413	-1.95388
H	-3.29013	3.83088	-3.01564
H	-3.92804	4.39756	-1.43791

P[6a]

Sum of electronic and thermal Free Energies= -838.822245

C	0.31931	1.89362	0.06836
O	0.1856	3.10064	0.12477
C	-0.78416	-0.40562	-0.33341
C	-1.7696	-0.90691	0.69098
N	-0.7503	0.9445	0.07174
H	-1.6497	1.43461	0.09087
C	1.68368	-0.10222	-0.06505
C	0.61051	-0.96675	-0.23414
C	3.01422	-0.50767	0.00414
C	0.91887	-2.32884	-0.33658
C	3.30312	-1.86342	-0.10161
C	2.24492	-2.76846	-0.27321
H	0.11368	-3.04621	-0.46271
H	4.32751	-2.22129	-0.05212
H	2.45684	-3.82982	-0.35572
C	3.89769	0.70915	0.21165
C	2.92271	1.91822	0.07929
N	1.58404	1.29719	0.04262
H	4.36686	0.69037	1.20197
H	4.7056	0.77015	-0.52366
H	2.98097	2.61682	0.91655
H	3.0876	2.48442	-0.84283
H	-1.13579	-0.40984	-1.37179
H	-1.60888	-1.95862	0.80484
C	-3.17247	-0.70716	0.45043
O	-4.12744	-1.23241	0.99915
O	-3.37738	0.3097	-0.50881
C	-4.74941	0.61359	-0.76686
H	-5.24733	0.98752	0.13277
H	-4.7497	1.38103	-1.54388
H	-5.28956	-0.27231	-1.11195
H	-1.53251	-0.43734	1.62275

TS9[6a]

Sum of electronic and thermal Free Energies= -1453.035702

Rh	-2.27199	0.32902	-0.01662
C	-2.98512	-1.48841	0.8911
C	-3.12312	-1.66832	-0.53389
C	-4.00154	-0.63831	-0.97612
C	-4.57903	0.04272	0.20283
C	-3.97118	-0.48596	1.34453
O	2.43524	0.73492	1.94011
C	3.26547	1.758	-0.0811
O	3.43015	2.94818	-0.25953
C	-4.22864	-0.12919	2.77563
H	-4.73037	0.836	2.86721
H	-3.30091	-0.07997	3.35221
H	-4.86812	-0.88427	3.25048
C	-5.63103	1.1052	0.13138
H	-5.70774	1.66392	1.06595
H	-6.61222	0.65791	-0.07292
H	-5.42975	1.8192	-0.67227
C	-4.43881	-0.38801	-2.38556
H	-3.71174	-0.76295	-3.10875
H	-4.59439	0.6772	-2.57591
H	-5.39373	-0.89441	-2.57844
C	-2.47432	-2.72629	-1.37596
H	-3.13179	-3.59967	-1.47102
H	-1.53571	-3.07419	-0.93705
H	-2.26	-2.36462	-2.38444
C	-2.17421	-2.34405	1.81263
H	-1.30791	-2.77623	1.30721

H	-2.78727	-3.17419	2.18796
H	-1.8234	-1.77965	2.68015
C	2.9474	1.70028	2.88165
H	3.86523	2.17203	2.51817
H	3.15691	1.11587	3.77806
H	2.19267	2.46404	3.10275
C	1.43478	-0.67838	-0.99812
C	0.71725	0.1806	0.0125
N	2.07367	1.337	0.71206
H	1.54269	2.19733	0.89801
C	3.88233	-0.65371	-0.33488
C	2.69423	-1.3643	-0.51934
C	5.11878	-1.27466	-0.1347
C	2.77795	-2.75626	-0.36978
C	5.17706	-2.65643	0.00082
C	3.99061	-3.39282	-0.09657
H	1.88143	-3.3547	-0.50865
H	6.12568	-3.15957	0.16142
H	4.01732	-4.47326	0.00132
C	6.21784	-0.23098	-0.14301
C	5.51238	1.0045	-0.75457
N	4.07764	0.75093	-0.45906
H	6.57003	-0.01953	0.87447
H	7.08581	-0.53323	-0.73389
H	5.80833	1.96127	-0.32453
H	5.65188	1.05044	-1.83902
H	0.71322	-1.4361	-1.32552
H	1.64713	-0.06338	-1.87936
C	-0.31832	1.11389	-0.42247
O	-0.97944	1.79859	0.49993
O	0.03267	1.7209	-1.6133
C	-0.88431	2.68195	-2.14335
H	-0.41099	3.08472	-3.03876
H	-1.83198	2.19929	-2.41784
H	-1.07861	3.48364	-1.42678
H	0.53138	-0.2613	0.98705

13[6a]

Sum of electronic and thermal Free Energies= -1453.044449

Rh	2.04307	-0.49697	0.23386
C	2.78776	1.33534	1.10812
C	2.87977	1.5018	-0.31811
C	3.73294	0.45625	-0.78296
C	4.34188	-0.22233	0.3805
C	3.77268	0.32124	1.53751
O	-2.31812	-0.65251	1.86819
C	-3.23415	-1.71754	0.02164
O	-3.47805	-2.89605	-0.15321
C	4.07056	-0.03063	2.96147
H	4.54784	-1.00893	3.0443
H	3.16337	-0.04724	3.57141
H	4.74786	0.71051	3.40493
C	5.38366	-1.29274	0.28699
H	5.47024	-1.85656	1.21762
H	6.36489	-0.85141	0.07017
H	5.16423	-2.00076	-0.51694
C	4.11677	0.1914	-2.20469
H	3.36132	0.55573	-2.90377
H	4.26852	-0.8754	-2.38779
H	5.06173	0.69908	-2.43907
C	2.20969	2.55531	-1.14876
H	2.8654	3.42728	-1.26591
H	1.28306	2.90594	-0.68736
H	1.96983	2.18901	-2.14989
C	2.00401	2.19462	2.04891
H	1.13501	2.64144	1.56169
H	2.63474	3.01321	2.42028
H	1.66021	1.62799	2.91781
C	-2.91752	-1.53422	2.83708
H	-3.88197	-1.91982	2.49234
H	-3.05999	-0.91021	3.72012
H	-2.24443	-2.36659	3.07494
C	-1.25672	0.56787	-0.98932
C	-0.86971	-0.49893	0.19145
N	-2.02664	-1.31695	0.65239
H	-1.55972	-2.20782	0.85756
C	-3.69299	0.72356	-0.28198
C	-2.46279	1.34497	-0.51056
C	-4.87936	1.43594	-0.07824
C	-2.44921	2.74364	-0.40261
C	-4.84036	2.82147	0.01591
C	-3.6085	3.47116	-0.12628
H	-1.51719	3.27442	-0.57918
H	-5.74897	3.39328	0.17829
H	-3.55908	4.55337	-0.06227
C	-6.04784	0.47136	-0.03425
C	-5.44193	-0.82611	-0.6239
N	-3.98887	-0.6651	-0.36139
H	-6.39032	0.31259	0.99614

H	-6.90619	0.81681	-0.61538
H	-5.7953	-1.74807	-0.1621
H	-5.60773	-0.89157	-1.70382
H	-0.51923	1.26953	-1.39458
H	-1.53296	-0.09007	-1.82087
C	0.13019	-1.46299	-0.20127
O	0.86786	-2.06883	0.71002
O	-0.16723	-2.08706	-1.3869
C	0.76698	-3.06075	-1.8666
H	0.30613	-3.50217	-2.74993
H	1.71306	-2.58095	-2.14863
H	0.95897	-3.82997	-1.11533
H	-0.71275	-0.05527	1.16905

TS10[6a]

Sum of electronic and thermal Free Energies= -1453.007961

Rh	-1.92657	0.02981	-0.24063
C	-2.85384	1.96245	0.20978
C	-2.90027	1.1404	1.37898
C	-3.67515	-0.03066	1.01222
C	-4.27159	0.19832	-0.32069
C	-3.77375	1.40527	-0.80639
O	2.41843	-0.22481	-2.96325
C	2.95845	-1.58774	-0.29033
O	3.075	-2.8101	-0.27285
C	-4.06807	2.02608	-2.14186
H	-3.75127	3.07008	-2.1771
H	-5.14233	1.99873	-2.3471
H	-3.56782	1.49802	-2.96129
C	-5.22419	-0.7344	-1.00189
H	-5.31758	-0.50549	-2.06505
H	-6.22177	-0.65748	-0.55152
H	-4.90717	-1.77692	-0.90741
C	-4.07412	-1.14924	1.91937
H	-3.40027	-1.24878	2.77174
H	-4.11811	-2.1045	1.39019
H	-5.07945	-0.95071	2.31503
C	-2.31399	1.43987	2.72447
H	-3.05068	1.96267	3.34732
H	-1.43242	2.07906	2.64696
H	-2.02069	0.52973	3.25178
C	-2.16817	3.28627	0.08131
H	-1.37151	3.40512	0.81785
H	-2.8914	4.09672	0.24143
H	-1.74197	3.4271	-0.91609
C	2.9889	0.75006	-3.83399
H	3.92827	1.14732	-3.43497
H	2.23094	1.54373	-3.83833
H	3.09896	0.35846	-4.84964
C	1.4915	1.14658	0.17804
C	0.94845	-0.06048	-0.62614
N	1.98852	-0.96629	-1.1072
H	1.57615	-1.67962	-1.69533
C	3.94988	0.63923	0.0546
C	2.91116	1.54966	-0.1389
C	5.29745	1.00497	0.0218
C	3.27885	2.86264	-0.46272
C	5.64179	2.31576	-0.28882
C	4.62151	3.24028	-0.5469
H	2.50249	3.60654	-0.62411
H	6.68287	2.62243	-0.32931
H	4.87441	4.26666	-0.79319
C	6.14979	-0.20628	0.34338
C	5.11542	-1.23277	0.87782
N	3.81366	-0.73603	0.36787
H	6.64917	-0.5806	-0.55905
H	6.92788	0.00381	1.08208
H	5.26958	-2.2522	0.52668
H	5.095	-1.23799	1.97265
H	0.81997	1.99723	0.02863
H	1.45033	0.89239	1.24269
C	-0.09813	-0.83805	0.22232
O	-0.86365	-1.83405	-0.42408
O	0.42951	-1.20594	1.4114
C	-0.15628	-2.28886	2.14622
H	0.35109	-2.29351	3.11007
H	-1.23035	-2.13532	2.28704
H	0.0155	-3.23809	1.6333
H	0.4476	0.30832	-1.53338

TS4[6a']

Sum of electronic and thermal Free Energies= -1452.985504

Rh	0.24955	0.53313	0.02347
C	1.26572	2.5065	0.17782
C	1.62994	1.62504	1.27005
C	0.45521	1.47573	2.14965
C	-0.6252	2.11449	1.52651
C	-0.14024	2.71913	0.27112
O	1.48861	-1.70095	1.52091
C	-0.73824	-2.30292	0.91547

O	-0.78795	-2.92496	1.95281
C	-0.96784	3.60673	-0.60412
H	-1.98475	3.22622	-0.72079
H	-0.52924	3.72556	-1.59653
H	-1.03912	4.60396	-0.15074
C	-2.03513	2.22765	2.01648
H	-2.23826	3.2498	2.35915
H	-2.22945	1.55214	2.85144
H	-2.75384	2.00462	1.2216
C	0.47006	0.76671	3.4676
H	0.90622	-0.23059	3.3754
H	-0.53316	0.66466	3.88511
H	1.0755	1.33177	4.18676
C	3.02194	1.19467	1.60147
H	3.53176	1.99076	2.16054
H	3.59932	0.99668	0.6952
H	3.02001	0.29585	2.21902
C	2.21687	3.09346	-0.81711
H	2.92243	2.3445	-1.18591
H	2.7898	3.8981	-0.33977
H	1.69287	3.52622	-1.67184
C	2.08015	-3.01303	1.65579
H	1.3677	-3.72684	2.0674
H	2.90718	-2.85881	2.35075
H	2.4744	-3.35782	0.69436
C	-0.09071	-0.907	-2.41691
C	1.0257	0.00183	-1.89298
N	0.50145	-1.62176	0.5081
H	0.90904	-2.05096	-0.33339
C	-2.10801	-1.01726	-0.76896
C	-1.41286	-0.41812	-1.83923
C	-3.42456	-0.61847	-0.43774
C	-2.06425	0.66445	-2.48298
C	-4.03257	0.43573	-1.09673
C	-3.33321	1.09188	-2.12379
H	-1.55966	1.13425	-3.32271
H	-5.05073	0.7238	-0.85217
H	-3.80645	1.90093	-2.67134
C	-4.00378	-1.55937	0.59302
C	-3.07591	-2.77807	0.45397
N	-1.7741	-2.18897	0.01123
H	-3.94557	-1.13243	1.60264
H	-5.04922	-1.80915	0.39739
H	-2.92465	-3.34099	1.37129
H	-3.42413	-3.449	-0.33667
H	-0.14782	-0.881	-3.5122
H	0.30332	-0.51393	-0.94316
H	1.06533	0.95069	-2.42776
C	2.40745	-0.52864	-1.79608
O	3.42289	0.14431	-1.78364
O	2.44757	-1.89348	-1.68597
C	3.77211	-2.47287	-1.66517
H	4.31926	-2.15316	-0.7758
H	3.62102	-3.55202	-1.66339
H	4.3269	-2.16634	-2.55319

TS4[6a"]

Sum of electronic and thermal Free Energies= -1453.011989

Rh	1.1414	0.27581	0.38745
C	1.89295	0.61831	-1.85554
C	3.02866	0.27555	-0.9988
C	3.14107	1.28237	-0.00689
C	2.06933	2.25578	-0.23387
C	1.31351	1.83216	-1.38955
O	0.53918	-0.1768	2.29959
C	-1.50942	1.64258	0.80491
O	-1.2083	2.82526	0.63071
C	0.25624	2.63467	-2.08371
H	-0.35159	3.19229	-1.37087
H	-0.40506	2.00195	-2.67986
H	0.73278	3.34714	-2.769
C	1.88168	3.53739	0.50086
H	2.28625	4.3576	-0.10916
H	2.40819	3.54199	1.45617
H	0.82041	3.72836	0.67385
C	4.20156	1.35152	1.04568
H	4.3009	0.39034	1.55731
H	3.97869	2.10899	1.79801
H	5.16841	1.59827	0.59175
C	4.01551	-0.82114	-1.24317
H	4.77849	-0.46484	-1.9483
H	3.54584	-1.70604	-1.67113
H	4.52964	-1.10481	-0.32224
C	1.53432	-0.10137	-3.11063
H	1.58546	-1.18416	-2.97983
H	2.25925	0.17532	-3.88845
H	0.54437	0.1781	-3.47594
C	-0.57151	-0.49771	3.09048
H	-1.29176	0.33593	3.11722

H	-0.2144	-0.69731	4.10797
H	-1.08451	-1.4009	2.7283
C	-1.3968	-1.85501	0.32237
C	-0.12216	-1.42617	-0.40869
N	-0.61684	0.68551	1.23934
H	-1.09635	-0.11992	1.61876
C	-3.34845	-0.01718	0.16
C	-2.76518	-1.29272	-0.06995
C	-4.72132	0.19238	-0.12846
C	-3.61534	-2.25597	-0.65178
C	-5.51965	-0.79115	-0.68692
C	-4.95189	-2.03177	-0.96957
H	-3.20015	-3.23758	-0.86045
H	-6.5646	-0.58968	-0.90216
H	-5.5402	-2.8222	-1.42349
C	-5.14386	1.58341	0.26492
C	-3.80817	2.31174	0.42173
N	-2.82039	1.2222	0.62628
H	-5.79224	2.05815	-0.47588
H	-5.69606	1.55836	1.21298
H	-3.53329	2.87195	-0.47872
H	-3.76379	3.00234	1.26477
H	-1.46951	-2.93281	0.13607
H	-1.25743	-1.84278	1.41256
H	-0.32351	-1.06151	-1.41209
C	0.89722	-2.53806	-0.46081
O	1.57468	-2.80068	-1.43958
O	0.92226	-3.26565	0.66557
C	1.83935	-4.38372	0.68164
H	2.86804	-4.02703	0.59884
H	1.67937	-4.87425	1.64017
H	1.62231	-5.06305	-0.14442

8[6a"]

Sum of electronic and thermal Free Energies= -1453.062849

Rh	0.85868	0.72629	-0.39833
C	2.19812	2.49564	-0.55934
C	2.38474	1.78973	0.69344
C	1.1864	2.00816	1.52543
C	0.24413	2.68772	0.7419
C	0.84873	2.95332	-0.57745
O	1.18124	0.08141	1.35311
C	-0.52246	-1.5482	0.80834
O	-0.76559	-2.02107	1.93961
C	0.20297	3.78361	-1.64161
H	-0.86219	3.56268	-1.73704
H	0.67316	3.63688	-2.61565
H	0.29727	4.84651	-1.38384
C	-1.13346	3.12522	1.1313
H	-1.16271	4.21316	1.26919
H	-1.45661	2.66272	2.06559
H	-1.86562	2.87807	0.35607
C	1.0548	1.57019	2.95049
H	1.31337	0.5151	3.06557
H	0.04178	1.71795	3.32881
H	1.73596	2.15275	3.58271
C	3.67512	1.20443	1.16786
H	4.30497	1.99601	1.59556
H	4.2256	0.74443	0.34369
H	3.50666	0.4525	1.93951
C	3.25409	2.71597	-1.59639
H	3.82586	1.80369	-1.78505
H	3.94902	3.48978	-1.24732
H	2.82822	3.05951	-2.5414
C	1.38539	-1.06339	2.21184
H	0.45472	-1.37181	2.68645
H	2.09371	-0.70716	2.96157
H	1.83579	-1.88906	1.65142
C	0.31792	-1.07426	-2.54559
C	1.56524	-0.28134	-2.14272
N	0.11403	-0.67169	-0.10982
H	0.18974	-1.46022	-0.76628
C	-1.7171	-0.53164	-1.00884
C	-0.90976	-0.27119	-2.13491
C	-2.95046	0.13649	-0.8232
C	-1.35238	0.76238	-2.99891
C	-3.355	1.13249	-1.69475
C	-2.53443	1.4556	-2.78872
H	-0.7592	0.97326	-3.88443
H	-4.31214	1.62731	-1.55882
H	-2.85066	2.21314	-3.49895
C	-3.70207	-0.48145	0.33287
C	-2.99678	-1.84159	0.46741
N	-1.5352	-1.57106	0.04236
H	-3.58888	0.11384	1.24819
H	-4.7713	-0.58614	0.13441
H	-2.96162	-2.23706	1.47914
H	-3.44169	-2.583	-0.20257
H	0.28572	-1.24778	-3.6284

H	0.29271	-2.0658	-2.08828
H	1.77801	0.52846	-2.84046
C	2.83239	-1.00635	-1.88058
O	3.94858	-0.52205	-1.9414
O	2.63373	-2.31263	-1.51907
C	3.83743	-3.08991	-1.32549
H	4.4157	-2.70268	-0.48393
H	3.50186	-4.10851	-1.13253
H	4.45265	-3.05455	-2.22582

TS5[6a"]

Sum of electronic and thermal Free Energies= -1453.059828

Rh	1.1414	0.27581	0.38745
C	1.89295	0.61831	-1.85554
C	3.02866	0.27555	-0.9988
C	3.14107	1.28237	-0.00689
C	2.06933	2.25578	-0.23387
C	1.31351	1.83216	-1.38955
O	1.81558	-0.58769	1.99124
C	-1.50942	1.64258	0.80491
O	-1.2083	2.82526	0.63071
C	0.25624	2.63467	-2.08371
H	-0.35159	3.19229	-1.37087
H	-0.40506	2.00195	-2.67986
H	0.73278	3.34714	-2.769
C	1.88168	3.53739	0.50086
H	2.28625	4.3576	-0.10916
H	2.40819	3.54199	1.45617
H	0.82041	3.72836	0.67385
C	4.20156	1.35152	1.04568
H	4.3009	0.39034	1.55731
H	3.97869	2.10899	1.79801
H	5.16841	1.59827	0.59175
C	4.01551	-0.82114	-1.24317
H	4.77849	-0.46484	-1.9483
H	3.54584	-1.70604	-1.67113
H	4.52964	-1.10481	-0.32224
C	1.53432	-0.10137	-3.11063
H	1.58546	-1.18416	-2.97983
H	2.25925	0.17532	-3.88845
H	0.54437	0.1781	-3.47594
C	1.03659	-1.09097	3.04101
H	0.31483	-0.33686	3.3943
H	1.71107	-1.35659	3.86392
H	0.48892	-1.99813	2.74571
C	-1.3968	-1.85501	0.32237
C	-0.12216	-1.42617	-0.40869
N	-0.61684	0.68551	1.23934
C	-3.34845	-0.01718	0.16
C	-2.76518	-1.29272	-0.06995
C	-4.72132	0.19238	-0.12846
C	-3.61534	-2.25597	-0.65178
C	-5.51965	-0.79115	-0.68692
C	-4.95189	-2.03177	-0.96957
H	-3.20015	-3.23758	-0.86045
H	-6.5646	-0.58968	-0.90216
H	-5.5402	-2.8222	-1.42349
C	-5.14386	1.58341	0.26492
C	-3.80817	2.31174	0.42173
N	-2.82039	1.2222	0.62628
H	-5.79224	2.05815	-0.47588
H	-5.69606	1.55836	1.21298
H	-3.53329	2.87195	-0.47872
H	-3.76379	3.00234	1.26477
H	-1.46951	-2.93281	0.13607
H	-0.98638	-0.72695	1.24272
H	-0.32351	-1.06151	-1.41209
C	0.89722	-2.53806	-0.46081
O	1.57468	-2.80068	-1.43958
O	0.92226	-3.26565	0.66557
C	1.83935	-4.38372	0.68164
H	2.86804	-4.02703	0.59884
H	1.67937	-4.87425	1.64017
H	1.62231	-5.06305	-0.14442
H	-0.16083	0.84641	2.11464

TS6[6a"]

Sum of electronic and thermal Free Energies= -1453.018984

Rh	-0.89527	-0.19204	-0.42014
C	-2.68796	-0.90765	0.55059
C	-1.76987	-2.05095	0.64697
C	-1.45032	-2.41965	-0.67346
C	-2.27881	-1.61576	-1.5965
C	-3.1009	-0.75712	-0.84338
O	2.06078	-0.64576	3.34221
C	1.95201	-1.49206	0.90474
O	1.93015	-2.70316	1.04516
C	-4.18643	0.15127	-1.33341
H	-4.24465	0.14722	-2.42332
H	-4.037	1.18733	-1.01455

H	-5.15784	-0.18348	-0.94998
C	-2.25428	-1.7711	-3.08432
H	-2.74804	-2.70603	-3.37865
H	-1.22949	-1.81886	-3.46551
H	-2.7639	-0.94753	-3.58684
C	-0.55229	-3.53875	-1.10329
H	0.25013	-3.71568	-0.38485
H	-0.1009	-3.3376	-2.07841
H	-1.13103	-4.4665	-1.20403
C	-1.38523	-2.76161	1.91008
H	-0.39769	-3.22724	1.84218
H	-2.10314	-3.56542	2.12047
H	-1.41858	-2.10032	2.78416
C	-3.36885	-0.25035	1.70857
H	-3.79862	0.71059	1.42275
H	-2.69219	-0.08929	2.55146
H	-4.18963	-0.88976	2.06076
C	3.05271	0.36107	3.28474
H	3.83054	0.15228	2.54119
H	3.50741	0.32179	4.28282
H	2.63518	1.3655	3.13509
C	0.4035	1.48395	0.16091
C	-0.74367	1.92774	-0.5753
N	1.19547	-0.68844	1.86793
H	0.92109	0.26064	1.59147
C	2.75247	0.51846	-0.48519
C	1.75506	1.5183	-0.49329
C	3.96719	0.69033	-1.18278
C	2.07942	2.69854	-1.20458
C	4.24527	1.86343	-1.86244
C	3.28773	2.88282	-1.86306
H	1.34268	3.49459	-1.22076
H	5.18427	1.98033	-2.39462
H	3.47947	3.81437	-2.38544
C	4.81779	-0.55316	-1.08582
C	3.80733	-1.61402	-0.63183
N	2.754	-0.81096	0.05278
H	5.2919	-0.81791	-2.03368
H	5.6155	-0.42715	-0.34272
H	3.35735	-2.1402	-1.48089
H	4.19959	-2.35567	0.06307
H	0.37686	1.77575	1.21655
H	0.39542	-1.22	2.20652
H	-0.64461	2.15094	-1.63644
C	-1.86976	2.66624	0.04783
O	-2.82494	3.09918	-0.56987
O	-1.72744	2.81598	1.38866
C	-2.74452	3.61004	2.03283
H	-3.72921	3.15235	1.91342
H	-2.46421	3.64855	3.08481
H	-2.76963	4.61418	1.60456

14[6a]

Sum of electronic and thermal Free Energies= -838.803017

C	-0.65533	-1.09603	-1.86326
O	-0.01886	-1.3447	-2.88017
C	-3.1204	0.37583	0.0707
C	-3.04463	1.54416	0.73342
N	-0.42585	0.16019	-1.20819
H	-0.23942	0.8445	-1.93929
C	-2.17366	-1.97079	-0.00677
C	-2.83988	-0.9368	0.67462
C	-2.11405	-3.27338	0.51598
C	-3.31967	-1.24046	1.96726
C	-2.61368	-3.54828	1.78149
C	-3.19875	-2.51142	2.51899
H	-3.85401	-0.46823	2.51091
H	-2.57103	-4.55584	2.1845
H	-3.60578	-2.70933	3.50531
C	-1.49613	-4.20922	-0.49889
C	-1.54676	-3.37183	-1.79217
N	-1.55541	-1.96373	-1.30413
H	-0.46331	-4.4684	-0.23038
H	-2.04946	-5.1464	-0.59828
H	-0.70663	-3.51451	-2.4679
H	-2.47538	-3.55228	-2.34242
H	-3.40549	0.38813	-0.98084
H	-1.17182	0.52319	-0.6103
H	-2.71973	1.58589	1.76799
C	-3.28989	2.8783	0.13493
O	-3.01768	3.91588	0.7086
O	-3.81516	2.81472	-1.10449
C	-4.07556	4.08614	-1.73294
H	-3.14789	4.65049	-1.85432
H	-4.51308	3.84903	-2.70176
H	-4.77126	4.67221	-1.12882

TS11[6a]

Sum of electronic and thermal Free Energies= -838.728149

C	-0.97581	-0.54439	-1.42364

O	-0.33934	-0.79306	-2.44054
C	-2.82786	0.75816	0.10465
C	-2.74507	2.03475	0.82878
N	-1.48245	0.49383	-0.74465
H	-1.22568	0.90298	-1.64142
C	-2.49414	-1.41915	0.43286
C	-3.16036	-0.38516	1.11424
C	-2.43453	-2.72174	0.95561
C	-3.64015	-0.68882	2.40689
C	-2.93416	-2.99664	2.22111
C	-3.51923	-1.95978	2.95861
H	-4.17449	0.08341	2.95054
H	-2.89151	-4.00419	2.62413
H	-3.92626	-2.15769	3.94494
C	-1.81661	-3.65758	-0.05927
C	-1.86724	-2.82019	-1.35255
N	-1.87589	-1.41209	-0.8645
H	-0.78379	-3.91675	0.20924
H	-2.36994	-4.59476	-0.15865
H	-1.02711	-2.96287	-2.02828
H	-2.79586	-3.00064	-1.9028
H	-3.11295	0.77047	-0.94689
H	-1.57196	1.67172	0.3096
H	-2.42018	2.07649	1.86335
C	-2.99033	3.36889	0.23029
O	-2.71812	4.40647	0.80396
O	-3.5156	3.30531	-1.00913
C	-3.77601	4.57673	-1.63758
H	-2.84833	5.14108	-1.75896
H	-4.21352	4.33962	-2.6064
H	-4.4717	5.1628	-1.03346

15[6a]

Sum of electronic and thermal Free Energies= -1067.311816

C	-0.98069	2.13682	-0.54718
O	-1.25672	3.32053	-0.40056
C	0.97171	-0.57052	0.14872
C	2.1021	-1.14967	-0.30254
N	-0.1589	1.69967	-1.55407
H	1.98866	3.29671	-2.56002
C	-1.51124	-0.25119	0.11933
C	-0.38875	-1.09295	-0.00231
C	-2.81518	-0.77401	0.18816
C	-0.64632	-2.47304	-0.17451
C	-3.03635	-2.1326	0.03025
C	-1.93732	-2.98346	-0.17208
H	0.19512	-3.15383	-0.25363
H	-4.04362	-2.53754	0.07486
H	-2.09343	-4.05167	-0.28623
C	-3.7874	0.35535	0.45434
C	-2.84594	1.4893	0.92024
N	-1.53934	1.15631	0.2983
H	-4.32339	0.63482	-0.46261
H	-4.53654	0.10375	1.21016
H	-3.14169	2.48971	0.61043
H	-2.7356	1.47685	2.01035
H	1.06171	0.36892	0.68892
H	0.21609	0.76615	-1.59
H	2.09215	-2.06792	-0.88132
C	3.45994	-0.61696	-0.07338
O	4.47181	-1.15691	-0.48027
O	3.46761	0.54041	0.63274
C	4.76762	1.09497	0.88054
H	5.28026	1.31467	-0.05961
H	4.59416	2.01115	1.44503
H	5.38058	0.39858	1.45856
C	3.106	5.18088	-3.31496
O	2.48744	6.18699	-2.97043
O	2.64159	3.97951	-2.88782
C	4.36989	5.04323	-4.18399
H	5.14409	4.57183	-3.6154
H	4.14748	4.44863	-5.04532
H	4.69627	6.0136	-4.49507

16[6a]

Sum of electronic and thermal Free Energies= -838.233372

C	1.13526	-0.94056	1.96221
O	1.44669	-1.24197	3.11907
C	-0.71771	1.09476	-0.13831
C	-1.68143	1.96958	-0.49758
N	0.15256	-1.49941	1.23719
H	-0.30951	-2.29879	1.65423
C	1.76761	0.63743	0.02281
C	0.63456	1.08116	-0.70078
C	3.06486	0.84927	-0.49866
C	0.87039	1.59948	-1.99525
C	3.26144	1.38999	-1.75657
C	2.14353	1.74923	-2.52487
H	0.00942	1.87791	-2.59443
H	4.26831	1.52718	-2.14482

H	2.27197	2.15056	-3.5262
C	4.08742	0.40116	0.5231
C	3.24109	0.34169	1.81039
N	1.86542	0.11549	1.32902
H	4.48481	-0.59087	0.26493
H	4.9377	1.08531	0.61098
H	3.50965	-0.45178	2.50571
H	3.29505	1.2998	2.34717
H	-0.93823	0.36247	0.63157
H	-1.51459	2.74859	-1.23488
C	-3.04092	1.98089	0.05716
O	-3.91738	2.75995	-0.28811
O	-3.24336	1.03597	1.01186
C	-4.5615	0.9866	1.5543
H	-5.30033	0.79195	0.77109
H	-4.55272	0.16974	2.27694
H	-4.82077	1.92964	2.04639

TS12[6a]

Sum of electronic and thermal Free Energies= -838.228021

C	0.76646	-0.91965	1.72674
O	1.25037	-1.42284	2.74595
C	-0.79123	0.65753	-0.09867
C	-1.75496	1.53235	-0.45794
N	-0.28924	-0.51943	1.08046
H	-0.76573	-1.31903	1.4805
C	1.39882	0.65834	-0.21266
C	0.26577	1.10207	-0.93625
C	2.69606	0.87018	-0.73414
C	0.5016	1.62039	-2.23072
C	2.89265	1.4109	-1.99204
C	1.77473	1.77014	-2.76034
H	-0.35937	1.89882	-2.8299
H	3.89951	1.54809	-2.38029
H	1.90317	2.17147	-3.76167
C	3.71863	0.42207	0.28762
C	2.8723	0.3626	1.57491
N	1.49662	0.1364	1.09355
H	4.11602	-0.56996	0.02946
H	4.5689	1.10622	0.3755
H	3.14085	-0.43087	2.27023
H	2.92626	1.32071	2.1117
H	-0.22676	1.18702	0.66198
H	-1.58811	2.31136	-1.19524
C	-3.11445	1.54366	0.09679
O	-3.9909	2.32272	-0.24847
O	-3.31688	0.59874	1.0515
C	-4.63502	0.54937	1.59393
H	-5.37386	0.35472	0.81073
H	-4.62625	-0.26749	2.31657
H	-4.89429	1.49241	2.08603

17[6a]

Sum of electronic and thermal Free Energies= -838.241419

C	-0.70534	2.01151	-0.50312
O	-1.04473	3.21112	-0.535
C	0.78729	0.02163	-0.16099
C	1.98777	-0.61438	-0.77291
N	0.32383	1.22482	-0.84593
H	1.02429	1.88055	-1.18225
C	-1.60532	-0.19661	0.13263
C	-0.36181	-0.90098	-0.02403
C	-2.86626	-0.81153	0.21775
C	-0.57741	-2.34471	-0.10219
C	-2.98597	-2.19204	0.13277
C	-1.82855	-2.96513	-0.03536
H	0.3202	-2.94917	-0.19315
H	-3.96384	-2.66749	0.1903
H	-1.89916	-4.04818	-0.09733
C	-3.9272	0.26532	0.34206
C	-3.09747	1.57706	0.47301
N	-1.70567	1.18419	0.22046
H	-4.57862	0.28364	-0.54298
H	-4.58189	0.11534	1.20903
H	-3.3839	2.35842	-0.2345
H	-3.19731	2.0053	1.48008
H	0.95802	0.67429	0.68818
H	1.88212	-1.34334	-1.5698
C	3.34527	-0.25739	-0.4751
O	4.35982	-0.74291	-0.97457
O	3.45739	0.72636	0.50165
C	4.78996	1.08224	0.82825
H	5.33622	1.45314	-0.04644
H	4.71672	1.87068	1.58254
H	5.35129	0.2313	1.23258

18[6a]

Sum of electronic and thermal Free Energies= -1067.324503

C	-1.86627	-1.98408	-0.37566
O	-2.28207	-3.11077	-0.65424
C	0.09389	-0.31617	-0.12959

C	0.98486	-0.37484	1.12658
N	-0.5519	-1.61686	-0.43091
H	0.08265	-2.3636	-0.67307
C	-2.29998	0.36278	0.04861
C	-0.97084	0.75533	-0.01953
C	-3.3759	1.24698	0.12004
C	-0.71508	2.13407	0.0033
C	-3.1136	2.61219	0.14586
C	-1.77774	3.04335	0.0873
H	0.32408	2.46686	-0.03856
H	-3.92352	3.33669	0.20396
H	-1.56065	4.10819	0.10411
C	-4.65204	0.42602	0.19536
C	-4.18143	-1.01251	-0.18061
N	-2.7288	-0.96899	0.0278
H	-5.06793	0.44277	1.21232
H	-5.44135	0.77857	-0.47739
H	-4.63947	-1.79217	0.43242
H	-4.40439	-1.24372	-1.23127
H	0.78025	-0.07029	-0.94851
H	0.40798	-0.67842	2.00963
C	2.21783	-1.25008	1.01928
O	3.13016	-1.23508	1.81754
O	2.19816	-2.08958	-0.05218
C	3.48507	-2.57348	-0.45683
H	4.06698	-1.72099	-0.81693
H	3.999	-3.06546	0.3732
H	3.29741	-3.28339	-1.26505
C	3.24559	1.65022	-0.49514
O	3.04287	0.53577	-1.05243
O	2.43463	2.33244	0.19098
H	1.38018	0.63155	1.29208
C	4.66507	2.25589	-0.64719
H	5.17414	2.23412	0.3239
H	5.2645	1.69803	-1.37327
H	4.59844	3.30605	-0.95385

T3[2a]

Sum of electronic and thermal Free Energies=-1685.958483

Rh	-0.64640100	-0.46338300	-0.58550400
N	-1.48139900	-0.99465600	1.29022300
C	-1.40332500	0.48592500	-2.58362500
C	-0.46844300	-0.56327500	-2.89835700
C	-1.05360400	-1.82340300	-2.49430900
C	-2.29119100	-1.53709300	-1.86901400
C	-2.51296200	-0.09679100	-1.91176700
O	-2.86253700	-0.60974000	1.30820100
C	-0.90709900	-0.71919000	2.51356000
C	1.24885500	-1.54887100	1.56674100
C	1.16885500	-1.25525000	0.19335100
C	2.23381100	-2.40483600	2.09830400
C	2.09608900	-1.92997600	-0.63591900
C	3.12038600	-3.05692600	1.25610300
C	3.03711200	-2.82070100	-0.12750500
H	2.11014200	-1.70835600	-1.69679700
H	3.87170600	-3.73304300	1.65567200
H	3.73242800	-3.31023100	-0.80362800
O	-1.49712700	-0.37150300	3.53718500
C	-3.77906700	0.60329900	-1.51768700
H	-4.16297500	0.21089900	-0.57469800
H	-3.61498300	1.67592300	-1.38767000
H	-4.55280300	0.47445000	-2.28682400
C	-3.28587800	-2.54137200	-1.37373700
H	-3.93512600	-2.10466000	-0.61586200
H	-3.91998800	-2.88799200	-2.20064600
H	-2.79880600	-3.41717900	-0.93806600
C	-0.48632600	-3.18584800	-2.76467600
H	-0.98791500	-3.94873800	-2.16495900
H	-0.61165600	-3.45981500	-3.82050600
H	0.58104400	-3.24103600	-2.53353500
C	0.76413900	-0.40399200	-3.74384900
H	1.36554000	-1.31601200	-3.74970400
H	0.48881800	-0.19543700	-4.78596100
H	1.40469000	0.41493000	-3.40432300
C	-1.25606900	1.93398200	-2.95083200
H	-1.89283000	2.17948800	-3.81041200
H	-1.54285200	2.59453400	-2.12805100
H	-0.22739500	2.17242200	-3.23122900
C	-3.64922800	-1.56167700	2.02618400
H	-3.44549800	-1.50580600	3.09776200
H	-4.69062000	-1.28591000	1.82885100
H	-3.45979100	-2.57809000	1.65992000
C	2.06698600	-2.46671900	3.60326400
C	1.07710300	-1.30891100	3.89240400
N	0.46674900	-1.01405000	2.58077800
H	1.64642200	-3.43443300	3.90729500
H	3.01084300	-2.34177200	4.14260400
H	0.29202800	-1.55333700	4.60742800
H	1.60363000	-0.42064500	4.26194600

C	1.18730300	0.74506900	-0.00869300
C	0.05178000	1.27540800	0.31438400
C	-0.56461400	2.47334000	0.84941400
C	-1.92388100	2.50387100	1.21242600
C	0.21127800	3.64112700	1.02187800
C	-2.48978800	3.67465500	1.71612700
H	-2.51183800	1.59637900	1.13608300
C	-0.36345000	4.80363100	1.52510500
H	1.26302000	3.62663000	0.75410900
C	-1.71857400	4.82768000	1.86978000
H	-3.53778500	3.67982700	2.00232400
H	0.24684900	5.69406100	1.64908600
H	-2.16491600	5.73665000	2.26316000
C	2.51437300	1.16040000	-0.47110900
C	2.60630800	2.18249900	-1.43628200
C	3.70154900	0.64143000	0.07472300
C	3.84816000	2.66536100	-1.84820700
H	1.69317700	2.60035400	-1.84823900
C	4.93955900	1.13244800	-0.33434900
H	3.64548200	-0.13575800	0.82760000
C	5.01918500	2.13964300	-1.29978100
H	3.89920800	3.45224500	-2.59543700
H	5.84721000	0.72831000	0.10468500
H	5.98744900	2.51465600	-1.61869600

T3[6a]

Sum of electronic and thermal Free Energies=-1453.04724

Rh	0.92687300	0.02116500	0.26021700
N	-0.13755100	1.66681500	-0.51083800
C	3.15913600	-0.20698400	0.75727500
C	2.65742600	-1.49363600	0.36183300
C	2.31736900	-1.42744700	-1.05058500
C	2.51048000	-0.09781200	-1.48165700
C	3.01329700	0.67979900	-0.34846300
O	0.35963800	2.88334000	0.05659900
C	-1.47412500	1.77048500	-0.78145700
C	-1.83331800	-0.73460000	-0.72650000
C	-0.86912900	-1.18374700	0.20072600
C	-2.71180100	-1.63490000	-1.37224800
C	-0.84511700	-2.57961700	0.44309600
C	-2.65051400	-2.99115400	-1.11495200
C	-1.69991600	-3.46916500	-0.19547600
H	-0.14840200	-2.96718500	1.18007800
H	-3.33389000	-3.67770500	-1.60778900
H	-1.64784500	-4.52891400	0.03535800
O	-2.13609900	2.80992800	-0.85957400
C	3.50586700	2.09656200	-0.40314800
H	4.60183600	2.12973800	-0.34931600
H	3.20657300	2.58212600	-1.33306300
H	3.10360100	2.69324100	0.41934300
C	2.27992400	0.46295500	-2.85278900
H	1.60114900	1.32040900	-2.81006100
H	3.22176800	0.79784600	-3.30457500
H	1.83571700	-0.27795600	-3.52099300
C	1.86824100	-2.59730000	-1.87479900
H	1.51635700	-2.28375700	-2.85990600
H	2.69418500	-3.30384800	-2.02704500
H	1.05129700	-3.14106900	-1.39124300
C	2.75504600	-2.75448300	1.17338900
H	2.06878600	-3.52135900	0.80739400
H	3.76879300	-3.17447600	1.12170800
H	2.53198700	-2.57950000	2.23049500
C	3.79428700	0.13063600	2.07388600
H	3.37667800	-0.45886900	2.89533100
H	4.87197600	-0.07801100	2.04336300
H	3.67193500	1.18873100	2.31907300
C	0.55513100	3.88797000	-0.93625800
H	-0.40116000	4.24977000	-1.32064900
H	1.08864400	4.69685200	-0.42707700
H	1.16993400	3.51283800	-1.76475700
C	-3.58731600	-0.85732500	-2.33241400
C	-3.36576000	0.60631800	-1.89070400
N	-2.09079400	0.55658600	-1.15334900
H	-3.25197100	-1.00931900	-3.36713300
H	-4.64092400	-1.14775300	-2.28674600
H	-3.29241500	1.31527600	-2.71629900
H	-4.16781400	0.95466000	-1.22802300
C	-0.66141200	-0.35988300	2.03575700
C	0.30527200	0.70170200	2.15422900
H	-0.40703400	-1.29187300	2.52678200
H	1.13580400	0.52564500	2.83362300
H	-0.03860200	1.72771200	2.09542100
C	-2.13191900	-0.07518300	2.23410700
O	-2.89554300	-0.85451700	2.76411800
O	-2.46168400	1.14946000	1.80266700
C	-3.84294900	1.53124500	1.90477100
H	-4.09266200	1.76884500	2.94262300
H	-3.93644800	2.40933400	1.26735300
H	-4.48842500	0.72004800	1.56007600