Electronic Supplementray Information for Mechanistic and Stereoselective Study on the Reaction of Trifluoropyuvates with Arylpropenes Catalyzed by the Cationic Lewis Acid Rhodium Complex

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Content

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Part 1: The relative free energies of the C-C bond formation step

Table S1 Single-point energies for the C-C bond formation step calculated by all electronic basis set def2-DZVP using B3LYP, B3LYP-D3, and M06L (unit: kcal/mol)

	Methods			
	B3LYP 6-311++G(2d,2p)//SDD	B3LYP def2-DZVP	B3LYP-D3 def2-DZVP	M06L def2-DZVP
TS2*S*$_{exo}$	0	0	0	0
TS2*R*$_{exo}$	0.97	0.77	0.73	0.27
TS2*R*$_{endo}$	4.09	0.24	0.94	1.42
TS2*S*$_{endo}$	6.85	4.21	4.28	2.73

Part 2: The energy profile of the *endo* addition pathway

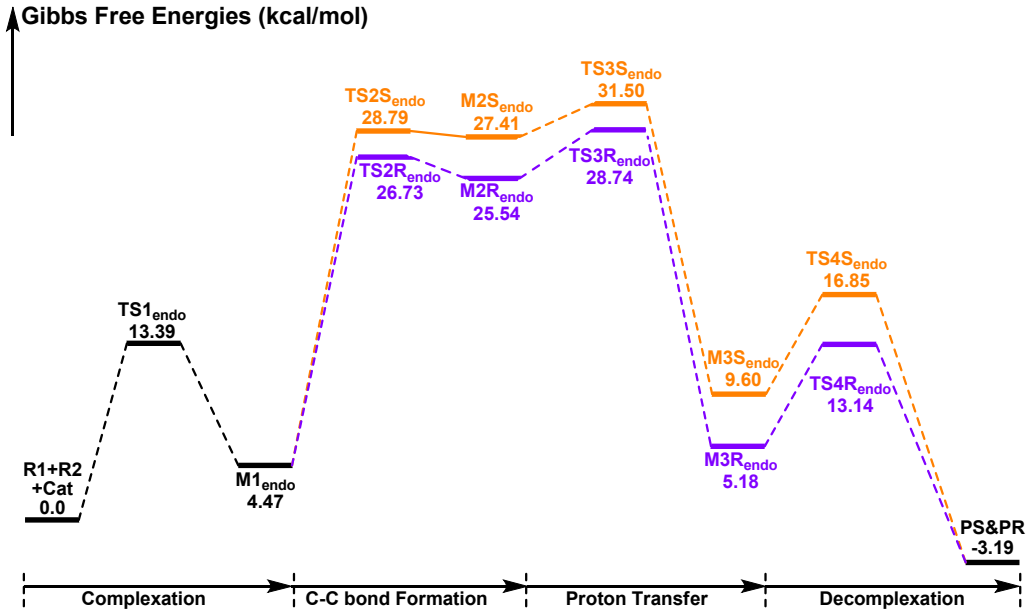

Figure S1 The Gibbs free energy profile of the endo addition pathways

Part 3: List of the energies and Cartesian coordinates of all the structures involved in the reaction

Cat

Total energy= -1649.65220471
Sum of electronic and zero-point Energies= -1648.964090
Sum of electronic and thermal Energies= -1648.927325
Sum of electronic and thermal Enthalpies= -1648.926381
Sum of electronic and thermal Free Energies= -1649.034082

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.000179	-1.617459	-0.006947
2	6	0	-3.163625	-2.167678	-0.113961
3	1	0	-3.113597	-2.759036	-1.035487
4	7	0	-3.623777	0.163568	-0.220500
5	6	0	-2.317303	0.003226	-0.128518
6	6	0	-4.346848	1.403133	-0.334914
7	7	0	-1.947822	-1.323981	-0.070958
8	6	0	-4.320247	-1.141458	-0.217748
9	1	0	-5.015835	-1.161242	0.624856
10	7	0	1.946983	-1.322557	0.067405
11	6	0	4.318478	-1.139533	0.227591
12	1	0	5.017161	-1.158539	-0.612610
13	7	0	3.621699	0.165212	0.228386
14	6	0	3.162466	-2.166003	0.117141
15	1	0	3.107803	-2.757598	1.038241
16	6	0	4.520151	1.990391	1.596695
17	1	0	4.094233	1.522377	2.479221
18	6	0	1.223823	0.972396	0.073475
19	6	0	-0.002237	3.058602	0.011064
20	1	0	-0.002533	4.143432	0.016291
21	6	0	4.344177	1.405476	0.338759
22	6	0	-4.904052	1.980718	0.806394
23	1	0	-4.769214	1.512491	1.776883
24	6	0	4.894109	1.983403	-0.805898
25	1	0	4.753995	1.515118	-1.775434
26	6	0	-4.515546	1.988037	-1.593825
27	1	0	-4.084639	1.520400	-2.473952
28	6	0	-0.000885	0.297228	-0.002527
29	6	0	1.220013	2.379269	0.077578
30	1	0	2.142742	2.945394	0.129177
31	6	0	-1.223889	2.378874	-0.061449
32	1	0	-2.147181	2.944530	-0.106602

33	6	0	-1.226159	0.971757	-0.071626
34	6	0	5.617970	3.170446	-0.685136
35	1	0	6.043025	3.624444	-1.576048
36	6	0	2.315680	0.004525	0.130128
37	6	0	-5.241406	3.172379	-1.697917
38	1	0	-5.372777	3.630461	-2.674890
39	6	0	-5.627841	3.167311	0.681508
40	1	0	-6.058378	3.621054	1.569876
41	6	0	5.806382	3.784383	0.561064
42	6	0	-5.809271	3.781292	-0.565895
43	6	0	5.245799	3.175159	1.696362
44	1	0	5.382713	3.633530	2.672529
45	6	0	6.593306	5.065162	0.690795
46	1	0	6.947233	5.418337	-0.282527
47	1	0	7.467180	4.926303	1.339302
48	1	0	5.984606	5.859495	1.140214
49	6	0	-6.597994	5.060403	-0.700442
50	1	0	-6.938980	5.424948	0.273107
51	1	0	-7.480891	4.913185	-1.334788
52	1	0	-5.996208	5.849165	-1.168099
53	1	0	4.887658	-1.236866	1.155559
54	1	0	-4.892874	-1.237732	-1.143812
55	6	0	-3.262641	-3.184869	1.071347
56	6	0	3.269151	-3.181598	-1.068554
57	6	0	4.575778	-3.978740	-0.884509
58	1	0	4.646494	-4.755814	-1.653884
59	1	0	5.464760	-3.344861	-0.976868
60	1	0	4.608622	-4.472739	0.094228
61	6	0	2.085109	-4.163029	-0.999795
62	1	0	2.047560	-4.681642	-0.033936
63	1	0	1.121699	-3.656221	-1.158816
64	1	0	2.178736	-4.921779	-1.785283
65	6	0	3.271663	-2.472380	-2.433740
66	1	0	2.341957	-1.915934	-2.601591
67	1	0	4.112160	-1.776610	-2.538586
68	1	0	3.362736	-3.214589	-3.235045
69	6	0	-2.078377	-4.165199	0.993570
70	1	0	-2.047347	-4.682667	0.026667
71	1	0	-1.114196	-3.658545	1.146429
72	1	0	-2.166471	-4.925000	1.778726
73	6	0	-4.569513	-3.983114	0.894185
74	1	0	-5.458563	-3.350135	0.992203
75	1	0	-4.607575	-4.476536	-0.084756
76	1	0	-4.634692	-4.760787	1.663417

77	6	0	-3.258115	-2.477545	2.437397
78	1	0	-4.099412	-1.783424	2.547844
79	1	0	-3.343485	-3.220933	3.238142
80	1	0	-2.328405	-1.920001	2.600782

R1

Total energy= -679.40825743
Sum of electronic and zero-point Energies= -679.331634
Sum of electronic and thermal Energies= -679.321763
Sum of electronic and thermal Enthalpies= -679.320819
Sum of electronic and thermal Free Energies= -679.369497

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.785308	1.987948	-0.053918
2	6	0	0.361691	0.862573	-0.021303
3	6	0	-1.158948	0.597240	0.003799
4	6	0	1.336190	-0.343323	0.006481
5	9	0	1.131578	-1.084589	1.110549
6	9	0	2.602866	0.085989	0.014490
7	9	0	1.157861	-1.122224	-1.074098
8	8	0	-1.956382	1.503530	0.052511
9	8	0	-1.428190	-0.703272	-0.034076
10	6	0	-2.831495	-1.068260	-0.013526
11	1	0	-2.845340	-2.157200	-0.032112
12	1	0	-3.301141	-0.690736	0.897585
13	1	0	-3.334773	-0.659673	-0.892789

R2

Total energy= -348.97458633
Sum of electronic and zero-point Energies= -348.812438
Sum of electronic and thermal Energies= -348.804394
Sum of electronic and thermal Enthalpies= -348.803450
Sum of electronic and thermal Free Energies= -348.845468

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.694989	0.123720	-0.024703
2	6	0	2.351624	1.245243	-0.364942

3	1	0	3.438140	1.282911	-0.354965
4	1	0	1.841134	2.150379	-0.682214
5	6	0	0.206085	0.056876	-0.009248
6	6	0	-0.466558	-1.165738	-0.190400
7	6	0	-0.576661	1.209751	0.197320
8	6	0	-1.861360	-1.229316	-0.193581
9	1	0	0.100791	-2.078486	-0.343503
10	6	0	-1.968697	1.147314	0.195140
11	1	0	-0.088316	2.161698	0.383737
12	6	0	-2.620264	-0.073474	-0.003842
13	1	0	-2.354041	-2.186724	-0.343509
14	1	0	-2.546417	2.053208	0.361015
15	1	0	-3.705962	-0.122980	-0.001092
16	6	0	2.461783	-1.127930	0.340755
17	1	0	3.533654	-0.919122	0.409513
18	1	0	2.127357	-1.540743	1.300859
19	1	0	2.328007	-1.918817	-0.408827

TS1*endo*

Imaginary frequency= -148.49

Total energy=-2329.04861152

Sum of electronic and zero-point Energies= -2328.283898

Sum of electronic and thermal Energies= -2328.236306

Sum of electronic and thermal Enthalpies= -2328.235362

Sum of electronic and thermal Free Energies= -2328.367483

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.089163	-0.842431	-0.620782
2	6	0	2.984027	-0.354069	-1.589770
3	1	0	3.364346	-1.296124	-1.183472
4	7	0	3.036711	1.811169	-0.587211
5	6	0	1.825720	1.269956	-0.417734
6	6	0	3.527793	3.063543	-0.089283
7	7	0	1.744424	0.004972	-0.854559
8	6	0	3.936545	0.813105	-1.202050
9	1	0	4.452859	1.267493	-2.050718
10	7	0	-2.046949	-0.817687	-0.908791
11	6	0	-4.394308	-1.058823	-1.192911
12	1	0	-5.015465	-1.632356	-0.499735
13	7	0	-4.006622	0.205000	-0.525060
14	6	0	-3.036887	-1.732014	-1.517337

15	1	0	-2.871569	-1.714692	-2.602558
16	6	0	-5.863220	1.748105	-0.911676
17	1	0	-5.746629	1.597343	-1.983315
18	6	0	-1.822277	1.344382	0.095815
19	6	0	-1.043577	3.543737	0.733371
20	1	0	-1.259741	4.557623	1.056586
21	6	0	-5.003667	1.104538	-0.015104
22	6	0	3.829259	3.213232	1.268424
23	1	0	3.672012	2.383658	1.952674
24	6	0	-5.145846	1.281764	1.362948
25	1	0	-4.486915	0.759824	2.050823
26	6	0	3.747344	4.120719	-0.980657
27	1	0	3.513775	3.998178	-2.033540
28	6	0	-0.482580	0.962886	-0.050943
29	6	0	-2.102328	2.661095	0.510622
30	1	0	-3.122702	3.002827	0.638911
31	6	0	0.288467	3.175495	0.497810
32	1	0	1.075983	3.907292	0.629651
33	6	0	0.576100	1.866858	0.076515
34	6	0	-6.144048	2.132415	1.840815
35	1	0	-6.253898	2.269548	2.912205
36	6	0	-2.691648	0.286369	-0.401567
37	6	0	4.255452	5.325820	-0.504868
38	1	0	4.420813	6.145630	-1.200287
39	6	0	4.335419	4.429399	1.730985
40	1	0	4.567347	4.540389	2.786352
41	6	0	-7.012551	2.798128	0.962691
42	6	0	4.556735	5.504543	0.858373
43	6	0	-6.853966	2.592139	-0.418418
44	1	0	-7.516787	3.096856	-1.114896
45	6	0	-8.099486	3.706799	1.483156
46	1	0	-8.016099	4.713836	1.047053
47	1	0	-8.055148	3.799402	2.575349
48	1	0	-9.094816	3.323522	1.214158
49	6	0	5.095017	6.821070	1.359278
50	1	0	5.994492	7.117427	0.806226
51	1	0	5.350749	6.769741	2.422033
52	1	0	4.360120	7.625779	1.228596
53	1	0	-4.983662	-0.830967	-2.085529
54	1	0	4.683014	0.503308	-0.464626
55	6	0	2.782579	-0.575010	-3.122876
56	6	0	-2.892171	-3.217554	-1.052661
57	6	0	-4.032221	-4.018357	-1.714252
58	1	0	-3.920667	-5.084780	-1.482760

59	1	0	-5.018882	-3.706207	-1.353925
60	1	0	-4.013763	-3.909443	-2.806201
61	6	0	-1.551877	-3.784582	-1.557440
62	1	0	-1.469420	-3.699771	-2.648227
63	1	0	-0.672173	-3.291655	-1.113113
64	1	0	-1.474585	-4.848341	-1.297511
65	6	0	-2.970371	-3.353052	0.478487
66	1	0	-2.122725	-2.870331	0.976397
67	1	0	-3.896056	-2.931836	0.888164
68	1	0	-2.947593	-4.416626	0.751268
69	6	0	1.857209	-1.784919	-3.345688
70	1	0	2.269719	-2.696598	-2.897139
71	1	0	0.856486	-1.615683	-2.925249
72	1	0	1.733933	-1.972267	-4.420098
73	6	0	4.153158	-0.904264	-3.746960
74	1	0	4.857162	-0.066904	-3.689813
75	1	0	4.615265	-1.771242	-3.258688
76	1	0	4.028916	-1.150337	-4.808766
77	6	0	2.179592	0.665052	-3.808904
78	1	0	2.816477	1.549317	-3.691997
79	1	0	2.072561	0.482885	-4.881830
80	1	0	1.187109	0.904564	-3.410310
81	8	0	0.628279	-1.375076	1.701814
82	8	0	1.911858	-3.154362	0.067789
83	6	0	1.311429	-2.270188	2.180506
84	6	0	2.033212	-3.271176	1.259783
85	8	0	1.507667	-2.499493	3.452526
86	6	0	0.875577	-1.603042	4.413506
87	1	0	1.147428	-2.002267	5.387949
88	1	0	1.270821	-0.593567	4.278691
89	1	0	-0.207906	-1.618796	4.266506
90	6	0	2.893622	-4.393576	1.890116
91	9	0	3.877465	-3.856611	2.632201
92	9	0	3.437471	-5.147438	0.931858
93	9	0	2.127887	-5.167301	2.674784

TS1*exo*

Imaginary frequency= -167.24

Total energy= -2329.04586156

Sum of electronic and zero-point Energies= -2328.282347

Sum of electronic and thermal Energies= -2328.234345

Sum of electronic and thermal Enthalpies= -2328.233401

Sum of electronic and thermal Free Energies= -2328.367632

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.081245	-0.914085	-0.890765
2	6	0	3.096893	-0.723005	-1.651171
3	1	0	3.337160	-1.709898	-1.239927
4	7	0	3.301571	1.396137	-0.572038
5	6	0	2.031872	0.974892	-0.501998
6	6	0	3.863296	2.595110	-0.020396
7	7	0	1.848509	-0.253224	-1.005652
8	6	0	4.137341	0.330685	-1.167982
9	1	0	4.746866	0.753004	-1.966880
10	7	0	-2.101344	-0.794575	-0.938712
11	6	0	-4.481139	-0.782640	-1.085326
12	1	0	-5.142699	-1.248840	-0.350958
13	7	0	-3.913124	0.451413	-0.497842
14	6	0	-3.226806	-1.624715	-1.428720
15	1	0	-3.124409	-1.693586	-2.518856
16	6	0	-4.957122	2.595978	-1.046392
17	1	0	-4.451443	2.582940	-2.007531
18	6	0	-1.604413	1.331640	0.057664
19	6	0	-0.627180	3.379236	0.894655
20	1	0	-0.744493	4.358753	1.344838
21	6	0	-4.756948	1.558655	-0.132341
22	6	0	4.044293	3.711494	-0.840116
23	1	0	3.740903	3.674350	-1.882817
24	6	0	-5.404260	1.557223	1.104630
25	1	0	-5.238442	0.742637	1.803734
26	6	0	4.253449	2.632573	1.321986
27	1	0	4.113366	1.758885	1.952752
28	6	0	-0.308206	0.875796	-0.205932
29	6	0	-1.762127	2.607635	0.632735
30	1	0	-2.743029	3.005406	0.855609
31	6	0	0.664048	2.933612	0.569250
32	1	0	1.514503	3.573206	0.766400
33	6	0	0.829656	1.661705	-0.007929
34	6	0	-6.250872	2.615173	1.431285
35	1	0	-6.748365	2.618996	2.396445
36	6	0	-2.593102	0.368291	-0.424388
37	6	0	4.810348	3.800437	1.841694
38	1	0	5.106909	3.829300	2.887603
39	6	0	4.605272	4.872017	-0.305736
40	1	0	4.738212	5.741237	-0.943508

41	6	0	-6.471393	3.673026	0.534136
42	6	0	4.997045	4.936831	1.039513
43	6	0	-5.808637	3.647712	-0.704004
44	1	0	-5.962804	4.458375	-1.411622
45	6	0	-7.422009	4.790856	0.880096
46	1	0	-7.154375	5.721290	0.362597
47	1	0	-7.437171	4.986569	1.958429
48	1	0	-8.449140	4.537228	0.579867
49	6	0	5.622278	6.188096	1.607220
50	1	0	5.287470	6.371496	2.633865
51	1	0	5.376360	7.067269	1.002431
52	1	0	6.716959	6.103597	1.632972
53	1	0	-5.070836	-0.519126	-1.968015
54	1	0	4.804083	-0.076123	-0.398428
55	6	0	2.982882	-0.899568	-3.197116
56	6	0	-3.221461	-3.089585	-0.890165
57	6	0	-4.475038	-3.797201	-1.445372
58	1	0	-4.455897	-4.857406	-1.163271
59	1	0	-5.405342	-3.368926	-1.052440
60	1	0	-4.511388	-3.743470	-2.540785
61	6	0	-1.976739	-3.810106	-1.431724
62	1	0	-1.947159	-3.784641	-2.528211
63	1	0	-1.044479	-3.363141	-1.053751
64	1	0	-1.981203	-4.860150	-1.119046
65	6	0	-3.228921	-3.138481	0.647932
66	1	0	-2.329012	-2.682692	1.074928
67	1	0	-4.100300	-2.626640	1.075135
68	1	0	-3.267396	-4.179919	0.984357
69	6	0	1.936506	-1.988356	-3.503478
70	1	0	2.204843	-2.942462	-3.035657
71	1	0	0.932303	-1.705045	-3.149732
72	1	0	1.868428	-2.154144	-4.585832
73	6	0	4.348418	-1.389177	-3.727482
74	1	0	5.139701	-0.643639	-3.592969
75	1	0	4.661425	-2.314733	-3.226234
76	1	0	4.275236	-1.598719	-4.802932
77	6	0	2.587743	0.410155	-3.902623
78	1	0	3.306963	1.216445	-3.715040
79	1	0	2.551736	0.255252	-4.986564
80	1	0	1.594474	0.754952	-3.585010
81	8	0	1.534708	-3.464951	-0.031517
82	8	0	0.457470	-1.444826	1.513245
83	6	0	1.640238	-3.498383	1.176365
84	6	0	0.981026	-2.407065	2.032903

85	8	0	2.272111	-4.388541	1.913322
86	6	0	2.925946	-5.483555	1.209406
87	1	0	3.394579	-6.079441	1.991736
88	1	0	2.178474	-6.064697	0.670906
89	1	0	3.673322	-5.083103	0.519684
90	6	0	0.948537	-2.550808	3.576099
91	9	0	0.322934	-3.692533	3.903058
92	9	0	0.286352	-1.524363	4.115882
93	9	0	2.196629	-2.570396	4.062440

M1$_{endo}$

Total energy= -2329.06563526

Sum of electronic and zero-point Energies= -2328.299154

Sum of electronic and thermal Energies= -2328.251258

Sum of electronic and thermal Enthalpies= -2328.250314

Sum of electronic and thermal Free Energies= -2328.382283

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.007071	-0.889219	-0.722386
2	6	0	3.276055	-0.878357	-1.076789
3	1	0	3.440265	-1.837932	-0.577109
4	7	0	3.429827	1.327540	-0.180840
5	6	0	2.147709	0.938475	-0.213205
6	6	0	3.965513	2.615242	0.151791
7	7	0	1.982671	-0.315791	-0.622031
8	6	0	4.290555	0.176889	-0.543846
9	1	0	5.026394	0.491274	-1.285880
10	7	0	-2.112488	-0.754284	-0.779270
11	6	0	-4.470102	-0.661302	-1.025619
12	1	0	-5.055376	-1.045671	-0.182397
13	7	0	-3.867460	0.633903	-0.641350
14	6	0	-3.233930	-1.539229	-1.359717
15	1	0	-3.089996	-1.552004	-2.449300
16	6	0	-5.160885	2.621478	-1.233109
17	1	0	-4.872791	2.476756	-2.270484
18	6	0	-1.530872	1.455186	-0.060351
19	6	0	-0.537674	3.550802	0.641318
20	1	0	-0.661152	4.578157	0.968448
21	6	0	-4.685955	1.745197	-0.254545
22	6	0	4.366545	2.889215	1.463878
23	1	0	4.249665	2.131606	2.233666

24	6	0	-5.059456	1.918939	1.083737
25	1	0	-4.696691	1.227785	1.839512
26	6	0	4.117326	3.583000	-0.844909
27	1	0	3.808817	3.363089	-1.862687
28	6	0	-0.231483	0.961980	-0.178677
29	6	0	-1.676703	2.790384	0.354502
30	1	0	-2.657063	3.239083	0.457265
31	6	0	0.755174	3.032747	0.509311
32	1	0	1.610282	3.659376	0.732194
33	6	0	0.922182	1.705158	0.081429
34	6	0	-5.890165	2.980940	1.435095
35	1	0	-6.172353	3.114277	2.476683
36	6	0	-2.544907	0.460121	-0.465356
37	6	0	4.655566	4.828873	-0.520472
38	1	0	4.763228	5.581201	-1.297543
39	6	0	4.902663	4.138078	1.773917
40	1	0	5.204547	4.348030	2.797119
41	6	0	-6.374522	3.876866	0.467139
42	6	0	5.057281	5.127836	0.789247
43	6	0	-5.996589	3.678420	-0.868094
44	1	0	-6.359772	4.359168	-1.633576
45	6	0	-7.283029	5.015221	0.862854
46	1	0	-6.816192	5.648387	1.627328
47	1	0	-8.222915	4.640959	1.287977
48	1	0	-7.530652	5.646836	0.004067
49	6	0	5.653757	6.471095	1.132106
50	1	0	5.508935	7.190282	0.319967
51	1	0	6.733339	6.388208	1.314362
52	1	0	5.206793	6.886392	2.042798
53	1	0	-5.135265	-0.529973	-1.881043
54	1	0	4.823165	-0.172166	0.347202
55	6	0	3.331044	-1.143199	-2.618112
56	6	0	-3.326302	-3.018931	-0.897007
57	6	0	-4.617216	-3.628140	-1.482567
58	1	0	-4.660417	-4.700121	-1.258063
59	1	0	-5.518487	-3.167480	-1.062077
60	1	0	-4.652886	-3.514805	-2.573188
61	6	0	-2.124088	-3.792018	-1.468832
62	1	0	-2.125375	-3.770187	-2.566106
63	1	0	-1.171124	-3.373415	-1.124585
64	1	0	-2.155850	-4.842344	-1.155607
65	6	0	-3.348443	-3.141556	0.635863
66	1	0	-2.436234	-2.736143	1.088080
67	1	0	-4.201736	-2.614707	1.078352

68	1	0	-3.428694	-4.195582	0.926584
69	6	0	2.207906	-2.117259	-3.024257
70	1	0	2.272319	-3.062823	-2.474162
71	1	0	1.204817	-1.692354	-2.850400
72	1	0	2.275644	-2.344973	-4.094397
73	6	0	4.683906	-1.815048	-2.932784
74	1	0	5.534438	-1.164830	-2.698012
75	1	0	4.804349	-2.748058	-2.368096
76	1	0	4.743112	-2.059130	-3.999512
77	6	0	3.189577	0.151984	-3.438018
78	1	0	3.998519	0.863115	-3.236671
79	1	0	3.223360	-0.081028	-4.508671
80	1	0	2.234437	0.655386	-3.244157
81	8	0	-0.064158	-1.274028	1.261598
82	8	0	0.995491	-3.425490	-0.101846
83	6	0	0.416091	-2.251977	1.862494
84	6	0	1.033530	-3.424178	1.103564
85	8	0	0.414111	-2.372364	3.147072
86	6	0	-0.154453	-1.295885	3.970205
87	1	0	-0.049027	-1.653266	4.991625
88	1	0	0.421857	-0.384766	3.802319
89	1	0	-1.202355	-1.159173	3.700271
90	6	0	1.690504	-4.571978	1.907036
91	9	0	2.666982	-4.072752	2.679085
92	9	0	2.205271	-5.469497	1.071499
93	9	0	0.773772	-5.162915	2.684947

M1*exo*

Total energy= -2329.06131129

Sum of electronic and zero-point Energies=	-2328.295059
Sum of electronic and thermal Energies=	-2328.247290
Sum of electronic and thermal Enthalpies=	-2328.246346
Sum of electronic and thermal Free Energies=	-2328.376556

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.004109	-0.957973	-0.816834
2	6	0	3.268623	-0.900175	-1.216885
3	1	0	3.451923	-1.899762	-0.807169
4	7	0	3.421455	1.224114	-0.146779
5	6	0	2.144012	0.829364	-0.183437
6	6	0	3.943136	2.509599	0.224713

7	7	0	1.977986	-0.392258	-0.688370
8	6	0	4.284089	0.114697	-0.612827
9	1	0	5.008005	0.493581	-1.339935
10	7	0	-2.107577	-0.831824	-0.838071
11	6	0	-4.435590	-0.641753	-1.258502
12	1	0	-5.315497	-1.000424	-0.722114
13	7	0	-3.866686	0.524857	-0.553859
14	6	0	-3.258360	-1.661701	-1.289298
15	1	0	-3.067910	-1.975880	-2.320716
16	6	0	-4.801306	2.662466	-1.308349
17	1	0	-4.302075	2.533876	-2.262643
18	6	0	-1.530155	1.305130	0.076224
19	6	0	-0.540318	3.337684	0.941487
20	1	0	-0.662936	4.333107	1.361828
21	6	0	-4.649877	1.701628	-0.305275
22	6	0	4.050877	3.514547	-0.743390
23	1	0	3.726204	3.321540	-1.763505
24	6	0	-5.305214	1.852103	0.920364
25	1	0	-5.194324	1.095378	1.688672
26	6	0	4.369743	2.747225	1.532840
27	1	0	4.291766	1.959220	2.278945
28	6	0	-0.230175	0.827104	-0.082747
29	6	0	-1.677734	2.598676	0.609013
30	1	0	-2.661024	3.026507	0.763143
31	6	0	0.753710	2.845356	0.737608
32	1	0	1.607473	3.462066	0.986065
33	6	0	0.921372	1.558600	0.202327
34	6	0	-6.101186	2.979729	1.139104
35	1	0	-6.609142	3.093206	2.095912
36	6	0	-2.543938	0.351082	-0.418502
37	6	0	4.886734	3.997326	1.872636
38	1	0	5.210369	4.178740	2.895741
39	6	0	4.567035	4.758824	-0.390605
40	1	0	4.643824	5.537462	-1.145574
41	6	0	-6.261198	3.960678	0.152506
42	6	0	4.990369	5.024857	0.922362
43	6	0	-5.600697	3.782177	-1.073917
44	1	0	-5.715613	4.527127	-1.857794
45	6	0	-7.099866	5.187853	0.401160
46	1	0	-6.466473	6.069664	0.584399
47	1	0	-7.750039	5.060204	1.275093
48	1	0	-7.733338	5.422173	-0.466575
49	6	0	5.528529	6.384935	1.293354
50	1	0	5.944069	6.390628	2.306024

51	1	0	4.737212	7.143831	1.251371
52	1	0	6.313528	6.705839	0.598988
53	1	0	-4.744443	-0.337610	-2.264394
54	1	0	4.830823	-0.300607	0.239994
55	6	0	3.287726	-1.025713	-2.776931
56	6	0	-3.502809	-2.959290	-0.453351
57	6	0	-4.731709	-3.687184	-1.035945
58	1	0	-4.871661	-4.647136	-0.525720
59	1	0	-5.658191	-3.113164	-0.915523
60	1	0	-4.601985	-3.894797	-2.105618
61	6	0	-2.288814	-3.894763	-0.599687
62	1	0	-2.090789	-4.137114	-1.651752
63	1	0	-1.384385	-3.446085	-0.179602
64	1	0	-2.467592	-4.837513	-0.068310
65	6	0	-3.735499	-2.650694	1.035861
66	1	0	-2.867610	-2.154908	1.486263
67	1	0	-4.611745	-2.011791	1.194935
68	1	0	-3.908761	-3.581272	1.589179
69	6	0	2.194310	-2.012654	-3.224147
70	1	0	2.293218	-2.981543	-2.724584
71	1	0	1.181563	-1.630992	-3.024027
72	1	0	2.260682	-2.181866	-4.305693
73	6	0	4.656053	-1.606291	-3.197736
74	1	0	5.487368	-0.941370	-2.940330
75	1	0	4.840774	-2.578450	-2.722410
76	1	0	4.680282	-1.757377	-4.282582
77	6	0	3.066575	0.334629	-3.461441
78	1	0	3.872151	1.044419	-3.243864
79	1	0	3.035242	0.202993	-4.551500
80	1	0	2.115414	0.790366	-3.156530
81	8	0	1.169221	-3.628968	-0.495226
82	8	0	0.084475	-1.575122	1.073911
83	6	0	1.361040	-3.594428	0.705116
84	6	0	0.678245	-2.535744	1.566078
85	8	0	2.095727	-4.397263	1.436849
86	6	0	2.776570	-5.490276	0.745425
87	1	0	3.287655	-6.040807	1.532376
88	1	0	2.037841	-6.112236	0.240874
89	1	0	3.490693	-5.075442	0.029773
90	6	0	0.643729	-2.652301	3.105967
91	9	0	0.125404	-3.836387	3.451052
92	9	0	-0.097789	-1.676494	3.625940
93	9	0	1.892666	-2.556922	3.574637

TS2R_{endo}

Imaginary frequency= -154.12

Total energy= -2678.03130451

Sum of electronic and zero-point Energies= -2677.102401

Sum of electronic and thermal Energies= -2677.045510

Sum of electronic and thermal Enthalpies= -2677.044566

Sum of electronic and thermal Free Energies= -2677.198901

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.318363	-0.322203	0.979839
2	6	0	-1.288521	2.461447	1.606862
3	1	0	-2.263348	2.028376	1.378974
4	7	0	0.240454	3.747342	0.322333
5	6	0	0.621501	2.458505	0.326219
6	6	0	0.922183	4.892421	-0.201089
7	7	0	-0.241247	1.657073	0.938983
8	6	0	-1.121216	3.836302	0.907827
9	1	0	-1.172615	4.686348	1.589857
10	7	0	1.589250	-2.007763	0.940860
11	6	0	2.964461	-3.944504	0.991440
12	1	0	2.773162	-4.670919	0.192615
13	7	0	3.640397	-2.759887	0.421788
14	6	0	1.665770	-3.343463	1.591460
15	1	0	1.821025	-3.170103	2.666094
16	6	0	6.077791	-2.564002	0.538028
17	1	0	5.985702	-2.240551	1.570922
18	6	0	2.967458	-0.376199	-0.145284
19	6	0	4.025185	1.535051	-1.194142
20	1	0	4.868442	1.956762	-1.731720
21	6	0	4.928590	-2.855243	-0.200363
22	6	0	0.537157	5.427217	-1.435729
23	1	0	-0.246577	4.943759	-2.011989
24	6	0	5.040842	-3.282272	-1.529703
25	1	0	4.146388	-3.516511	-2.100308
26	6	0	1.928041	5.512599	0.546221
27	1	0	2.215602	5.102224	1.509708
28	6	0	1.892958	0.461398	0.155173
29	6	0	4.057626	0.183206	-0.834621
30	1	0	4.921739	-0.415824	-1.093580
31	6	0	2.942224	2.361450	-0.874076
32	1	0	2.960017	3.406690	-1.159867

33	6	0	1.850517	1.820674	-0.177180
34	6	0	6.300344	-3.399109	-2.113826
35	1	0	6.379547	-3.726613	-3.147729
36	6	0	2.759099	-1.741516	0.374011
37	6	0	2.554478	6.655812	0.047574
38	1	0	3.339843	7.129316	0.631180
39	6	0	1.164695	6.574804	-1.917164
40	1	0	0.861330	6.983344	-2.877985
41	6	0	7.467882	-3.101496	-1.391107
42	6	0	2.181273	7.209771	-1.185146
43	6	0	7.334052	-2.683093	-0.059926
44	1	0	8.223634	-2.448203	0.518831
45	6	0	8.825775	-3.241046	-2.035279
46	1	0	8.891143	-2.653168	-2.959046
47	1	0	9.029126	-4.284861	-2.306345
48	1	0	9.622722	-2.907478	-1.363592
49	6	0	2.832916	8.468955	-1.702037
50	1	0	3.772405	8.676231	-1.179930
51	1	0	2.176696	9.337592	-1.557690
52	1	0	3.043183	8.400547	-2.775382
53	1	0	3.598123	-4.413312	1.746571
54	1	0	-1.853556	3.983383	0.106548
55	6	0	-1.133521	2.484435	3.166408
56	6	0	0.395385	-4.222417	1.456976
57	6	0	0.689239	-5.596461	2.093781
58	1	0	-0.215477	-6.215816	2.089823
59	1	0	1.464916	-6.145673	1.547130
60	1	0	1.017417	-5.492734	3.135600
61	6	0	-0.746127	-3.551687	2.242732
62	1	0	-0.482654	-3.443827	3.302932
63	1	0	-0.982015	-2.555955	1.848597
64	1	0	-1.658565	-4.157339	2.189084
65	6	0	-0.018673	-4.412041	-0.012452
66	1	0	-0.224276	-3.452114	-0.498826
67	1	0	0.757288	-4.921235	-0.595696
68	1	0	-0.924536	-5.027113	-0.071372
69	6	0	-1.081057	1.042268	3.703356
70	1	0	-1.934010	0.446425	3.359386
71	1	0	-0.153436	0.534250	3.391911
72	1	0	-1.085126	1.043556	4.799899
73	6	0	-2.378898	3.182004	3.750076
74	1	0	-2.472763	4.216294	3.398813
75	1	0	-3.297288	2.648165	3.475516
76	1	0	-2.320803	3.210071	4.844364

77	6	0	0.138082	3.221570	3.625645
78	1	0	0.135800	4.279421	3.341295
79	1	0	0.213092	3.182337	4.718983
80	1	0	1.045461	2.757073	3.221103
81	8	0	-0.250927	-0.697289	-0.919896
82	8	0	-2.390740	-0.596778	0.783943
83	6	0	-1.414828	-0.695529	-1.374051
84	6	0	-2.654920	-0.616118	-0.456995
85	8	0	-1.626816	-0.760530	-2.654376
86	6	0	-0.481154	-0.783644	-3.564995
87	1	0	-0.922391	-0.786464	-4.559393
88	1	0	0.126402	0.108120	-3.405436
89	1	0	0.100262	-1.690252	-3.390134
90	6	0	-3.630383	0.494404	-0.947560
91	9	0	-2.937430	1.659490	-1.053549
92	9	0	-4.606210	0.679698	-0.049382
93	9	0	-4.193245	0.266306	-2.145616
94	6	0	-8.308168	-1.259547	-0.523348
95	6	0	-7.073332	-1.592270	0.018381
96	6	0	-6.014475	-2.035001	-0.812811
97	6	0	-6.258269	-2.153697	-2.204301
98	6	0	-7.504240	-1.844664	-2.735318
99	6	0	-8.529570	-1.389700	-1.899127
100	1	0	-9.101817	-0.900233	0.124723
101	1	0	-6.915208	-1.471481	1.083822
102	1	0	-5.484164	-2.532841	-2.862045
103	1	0	-7.680769	-1.961213	-3.800207
104	1	0	-9.500961	-1.142796	-2.317874
105	6	0	-4.713764	-2.359633	-0.252193
106	6	0	-4.541145	-2.682973	1.186855
107	1	0	-3.923488	-1.876946	1.629531
108	1	0	-5.470101	-2.795204	1.744245
109	1	0	-3.944023	-3.595539	1.294832
110	6	0	-3.520787	-2.274601	-1.015961
111	1	0	-2.716996	-2.936073	-0.693650
112	1	0	-3.606840	-2.177003	-2.093493

TS2*S*$_{endo}$

Imaginary frequency= -185.17

Total energy= -2678.02909483

Sum of electronic and zero-point Energies= -2677.100250

Sum of electronic and thermal Energies= -2677.043659

Sum of electronic and thermal Enthalpies= -2677.042715

Sum of electronic and thermal Free Energies= -2677.193478

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.258911	-0.309595	0.774092
2	6	0	-1.394648	2.362865	1.694471
3	1	0	-2.388581	1.957296	1.497421
4	7	0	0.046217	3.802127	0.474372
5	6	0	0.441580	2.524595	0.329345
6	6	0	0.578551	4.967631	-0.164909
7	7	0	-0.400953	1.645347	0.864561
8	6	0	-1.279547	3.807248	1.136707
9	1	0	-1.310171	4.580838	1.905869
10	7	0	1.638908	-1.954162	0.601339
11	6	0	3.231559	-3.718128	0.758474
12	1	0	3.200608	-4.422345	-0.080856
13	7	0	3.815813	-2.445396	0.303096
14	6	0	1.822263	-3.295589	1.244105
15	1	0	1.861614	-3.121512	2.329368
16	6	0	6.162392	-1.908986	0.753711
17	1	0	5.876836	-1.580452	1.749026
18	6	0	2.962293	-0.129469	-0.237906
19	6	0	3.938507	1.902459	-1.122968
20	1	0	4.773150	2.408061	-1.597986
21	6	0	5.179765	-2.367065	-0.131063
22	6	0	0.449957	5.137075	-1.546956
23	1	0	-0.038675	4.371746	-2.143675
24	6	0	5.538692	-2.804993	-1.408575
25	1	0	4.775035	-3.167563	-2.091049
26	6	0	1.187690	5.962731	0.608001
27	1	0	1.280145	5.829045	1.681824
28	6	0	1.825381	0.614758	0.073044
29	6	0	4.039086	0.534443	-0.850824
30	1	0	4.943640	0.003189	-1.119902
31	6	0	2.794205	2.637792	-0.796941
32	1	0	2.758704	3.698566	-1.014527
33	6	0	1.708866	1.985317	-0.191244
34	6	0	6.878495	-2.770355	-1.800154
35	1	0	7.151454	-3.109049	-2.796305
36	6	0	2.830606	-1.534949	0.186713
37	6	0	1.679445	7.111566	-0.007871
38	1	0	2.155492	7.878137	0.598514
39	6	0	0.954096	6.289622	-2.151957

40	1	0	0.855486	6.412882	-3.227420
41	6	0	7.877143	-2.307570	-0.931652
42	6	0	1.577320	7.293278	-1.397036
43	6	0	7.495401	-1.876165	0.349428
44	1	0	8.252874	-1.514660	1.040755
45	6	0	9.326447	-2.275810	-1.351904
46	1	0	9.740410	-1.262748	-1.275858
47	1	0	9.450511	-2.615592	-2.384723
48	1	0	9.939744	-2.919865	-0.709050
49	6	0	2.138555	8.530192	-2.054711
50	1	0	1.838380	9.438294	-1.519077
51	1	0	1.802763	8.617785	-3.092675
52	1	0	3.236509	8.509636	-2.059725
53	1	0	3.840020	-4.150536	1.554902
54	1	0	-2.052977	4.024045	0.390004
55	6	0	-1.125278	2.217068	3.231470
56	6	0	0.724391	-4.365222	0.994056
57	6	0	1.229252	-5.710771	1.562175
58	1	0	0.430665	-6.459540	1.504032
59	1	0	2.087958	-6.105267	1.007490
60	1	0	1.517820	-5.617331	2.616846
61	6	0	-0.548664	-3.983054	1.770515
62	1	0	-0.341808	-3.934734	2.848037
63	1	0	-0.954791	-3.018188	1.459540
64	1	0	-1.330634	-4.736306	1.618146
65	6	0	0.423637	-4.524945	-0.506172
66	1	0	0.045134	-3.596444	-0.945023
67	1	0	1.316466	-4.822768	-1.069223
68	1	0	-0.332735	-5.302781	-0.659890
69	6	0	-1.099906	0.726292	3.622483
70	1	0	-1.988809	0.193761	3.268418
71	1	0	-0.210336	0.199142	3.233409
72	1	0	-1.058200	0.627526	4.713989
73	6	0	-2.295989	2.888466	3.979609
74	1	0	-2.372955	3.957638	3.750890
75	1	0	-3.254042	2.417567	3.726989
76	1	0	-2.153777	2.795758	5.062270
77	6	0	0.201407	2.868533	3.662523
78	1	0	0.209070	3.949947	3.487786
79	1	0	0.358493	2.712001	4.736404
80	1	0	1.060029	2.429500	3.140729
81	8	0	-0.318450	-0.518913	-1.144005
82	8	0	-2.048456	-1.156551	0.815759
83	6	0	-1.460776	-0.926459	-1.454061

84	6	0	-2.496902	-1.240894	-0.370685
85	8	0	-1.796666	-1.115059	-2.691430
86	6	0	-0.801285	-0.879410	-3.740969
87	1	0	-1.310577	-1.149155	-4.663691
88	1	0	-0.519274	0.174636	-3.738719
89	1	0	0.064923	-1.519035	-3.566059
90	6	0	-3.362437	-2.491664	-0.672582
91	9	0	-4.069396	-2.410760	-1.810610
92	9	0	-4.211816	-2.713268	0.341670
93	9	0	-2.554170	-3.569616	-0.778022
94	6	0	-8.276686	-1.636715	-0.405733
95	6	0	-7.108041	-1.146532	0.162773
96	6	0	-6.152007	-0.458709	-0.625874
97	6	0	-6.431371	-0.272542	-2.004035
98	6	0	-7.612384	-0.744791	-2.560517
99	6	0	-8.536251	-1.432305	-1.765401
100	1	0	-8.988610	-2.178239	0.209621
101	1	0	-6.916635	-1.337046	1.212021
102	1	0	-5.740844	0.282957	-2.628246
103	1	0	-7.819124	-0.574223	-3.612621
104	1	0	-9.457758	-1.804665	-2.203649
105	6	0	-4.923979	0.051354	-0.040037
106	6	0	-4.805829	0.310307	1.424274
107	1	0	-4.622498	1.381798	1.577986
108	1	0	-5.684182	0.033619	2.005248
109	1	0	-3.917130	-0.211640	1.812000
110	6	0	-3.762560	0.284033	-0.812765
111	1	0	-3.079725	1.039451	-0.433268
112	1	0	-3.837640	0.243007	-1.894204

TS2R_{exo}

Imaginary frequency= -142.18
Total energy= -2678.03379329
Sum of electronic and zero-point Energies= -2677.104056
Sum of electronic and thermal Energies= -2677.047165
Sum of electronic and thermal Enthalpies= -2677.046221
Sum of electronic and thermal Free Energies= -2677.197701

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.454309	-0.385183	1.213781
2	6	0	-1.917537	1.495027	2.515482

3	1	0	-2.657715	0.688982	2.544334
4	7	0	-1.563779	3.206494	0.895728
5	6	0	-0.690256	2.205423	0.696101
6	6	0	-1.725006	4.428349	0.165351
7	7	0	-0.881858	1.166998	1.507548
8	6	0	-2.550129	2.782409	1.917001
9	1	0	-2.690655	3.578865	2.649524
10	7	0	2.330604	-1.309256	0.746746
11	6	0	4.627130	-1.960443	0.842255
12	1	0	5.173179	-2.762768	0.343386
13	7	0	4.360301	-0.874871	-0.117765
14	6	0	3.205176	-2.378176	1.323544
15	1	0	3.145724	-2.301231	2.414561
16	6	0	6.191498	0.757874	-0.187184
17	1	0	5.955864	1.049207	0.832578
18	6	0	2.434427	0.688559	-0.591182
19	6	0	2.179550	2.776812	-1.789281
20	1	0	2.557427	3.489642	-2.515224
21	6	0	5.425703	-0.226332	-0.823588
22	6	0	-1.410491	5.645589	0.781493
23	1	0	-1.002446	5.650944	1.787922
24	6	0	5.731187	-0.614681	-2.130191
25	1	0	5.141594	-1.388084	-2.614053
26	6	0	-2.256849	4.417042	-1.127111
27	1	0	-2.515935	3.473302	-1.598208
28	6	0	1.208508	0.950833	0.018202
29	6	0	2.921016	1.621085	-1.523473
30	1	0	3.858288	1.458473	-2.041299
31	6	0	0.977933	3.052107	-1.128294
32	1	0	0.451792	3.975503	-1.338411
33	6	0	0.476081	2.125081	-0.200778
34	6	0	6.788169	0.000148	-2.804702
35	1	0	7.017863	-0.302090	-3.823180
36	6	0	3.065218	-0.524263	-0.035858
37	6	0	-2.451889	5.621835	-1.805253
38	1	0	-2.860500	5.604933	-2.812262
39	6	0	-1.619424	6.840552	0.097004
40	1	0	-1.370610	7.781448	0.581890
41	6	0	7.559080	0.996905	-2.190656
42	6	0	-2.141565	6.850787	-1.207173
43	6	0	7.244722	1.361537	-0.870763
44	1	0	7.831199	2.130390	-0.373505
45	6	0	8.694208	1.669356	-2.923591
46	1	0	8.486668	2.735545	-3.081403

47	1	0	8.862548	1.212549	-3.903691
48	1	0	9.629163	1.606763	-2.353760
49	6	0	-2.359543	8.153210	-1.937953
50	1	0	-2.803402	7.988522	-2.924606
51	1	0	-1.414277	8.692504	-2.078538
52	1	0	-3.024789	8.818403	-1.373717
53	1	0	5.248788	-1.578285	1.659479
54	1	0	-3.511365	2.589880	1.427325
55	6	0	-1.343996	1.652063	3.963821
56	6	0	2.836572	-3.849763	0.955187
57	6	0	3.864069	-4.780447	1.635343
58	1	0	3.584152	-5.826580	1.466175
59	1	0	4.879610	-4.650410	1.246300
60	1	0	3.893600	-4.614780	2.719911
61	6	0	1.451651	-4.196791	1.521648
62	1	0	1.390923	-3.985948	2.596723
63	1	0	0.671322	-3.629794	1.016420
64	1	0	1.236309	-5.261598	1.373486
65	6	0	2.839066	-4.083267	-0.565888
66	1	0	2.099836	-3.451249	-1.069960
67	1	0	3.819850	-3.888448	-1.014966
68	1	0	2.584645	-5.127165	-0.784736
69	6	0	-0.654803	0.345682	4.398219
70	1	0	-1.328345	-0.514351	4.319133
71	1	0	0.240930	0.127292	3.796712
72	1	0	-0.326214	0.423982	5.441373
73	6	0	-2.530293	1.906537	4.916112
74	1	0	-3.053900	2.842712	4.689929
75	1	0	-3.261556	1.089779	4.867643
76	1	0	-2.174008	1.974072	5.950369
77	6	0	-0.334882	2.809877	4.068410
78	1	0	-0.785149	3.778691	3.824627
79	1	0	0.046369	2.879094	5.093977
80	1	0	0.527547	2.657091	3.408510
81	8	0	-1.026483	-2.047520	2.121653
82	8	0	-0.480041	-1.195626	-0.366832
83	6	0	-1.641940	-2.567040	1.195431
84	6	0	-1.425992	-2.037573	-0.211791
85	8	0	-2.471267	-3.575145	1.290358
86	6	0	-2.663722	-4.165631	2.610979
87	1	0	-3.365093	-4.982003	2.449496
88	1	0	-1.709318	-4.539130	2.985850
89	1	0	-3.081754	-3.419613	3.289543
90	6	0	-1.613328	-2.975782	-1.419318

91	9	0	-0.619406	-3.889779	-1.388865
92	9	0	-1.509259	-2.290132	-2.565632
93	9	0	-2.775486	-3.630035	-1.407042
94	6	0	-5.897060	-2.507292	-4.035979
95	6	0	-4.879888	-1.743377	-3.474109
96	6	0	-4.835960	-1.511069	-2.079257
97	6	0	-5.866419	-2.061710	-1.278089
98	6	0	-6.889911	-2.809025	-1.847506
99	6	0	-6.906287	-3.039680	-3.227361
100	1	0	-5.903060	-2.690816	-5.106196
101	1	0	-4.097096	-1.360462	-4.118361
102	1	0	-5.890191	-1.861831	-0.212356
103	1	0	-7.681068	-3.206245	-1.218590
104	1	0	-7.704728	-3.627797	-3.670722
105	6	0	-3.771462	-0.712290	-1.472561
106	6	0	-3.069048	0.340745	-2.277121
107	1	0	-2.889474	0.046267	-3.313192
108	1	0	-3.709723	1.234121	-2.313625
109	1	0	-2.118394	0.623417	-1.819948
110	6	0	-3.404701	-0.878559	-0.139995
111	1	0	-2.837710	-0.089815	0.343091
112	1	0	-3.979302	-1.531768	0.507259

TS2S_{exo}

Imaginary frequency= -155.39
Total energy= -2678.03431640
Sum of electronic and zero-point Energies= -2677.105664
Sum of electronic and thermal Energies= -2677.048750
Sum of electronic and thermal Enthalpies= -2677.047806
Sum of electronic and thermal Free Energies= -2677.200280

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.379472	-0.023017	1.432233
2	6	0	-2.160289	1.838766	2.386903
3	1	0	-2.808038	0.969921	2.539156
4	7	0	-1.929817	3.255417	0.483797
5	6	0	-0.944935	2.339875	0.496333
6	6	0	-2.254036	4.187574	-0.554665
7	7	0	-1.045187	1.465727	1.490451
8	6	0	-2.906198	2.913684	1.545539
9	1	0	-3.167721	3.808610	2.113170

10	7	0	2.268968	-0.953612	1.038861
11	6	0	4.584183	-1.562345	1.147623
12	1	0	5.041210	-2.430956	0.667371
13	7	0	4.285800	-0.538308	0.130986
14	6	0	3.191443	-1.868843	1.778099
15	1	0	3.189166	-1.558726	2.829918
16	6	0	5.985446	1.204109	-0.170854
17	1	0	5.695642	1.637132	0.782438
18	6	0	2.296505	0.867506	-0.533472
19	6	0	1.913682	2.723994	-2.039405
20	1	0	2.247951	3.338642	-2.869107
21	6	0	5.322409	0.070209	-0.649028
22	6	0	-2.110288	5.559291	-0.326148
23	1	0	-1.712699	5.909761	0.621661
24	6	0	5.696108	-0.496498	-1.872115
25	1	0	5.179938	-1.380744	-2.235402
26	6	0	-2.763281	3.730755	-1.775661
27	1	0	-2.886152	2.664540	-1.945403
28	6	0	1.061741	1.154933	0.043712
29	6	0	2.724526	1.669820	-1.605755
30	1	0	3.668825	1.482771	-2.103017
31	6	0	0.690050	3.018206	-1.426591
32	1	0	0.102949	3.858423	-1.778333
33	6	0	0.247021	2.218673	-0.361674
34	6	0	6.719549	0.085930	-2.618682
35	1	0	6.999953	-0.353747	-3.572582
36	6	0	2.977530	-0.235995	0.171377
37	6	0	-3.109112	4.649181	-2.766222
38	1	0	-3.496873	4.286987	-3.715026
39	6	0	-2.467418	6.467008	-1.322984
40	1	0	-2.347119	7.531852	-1.140077
41	6	0	7.391968	1.230421	-2.161305
42	6	0	-2.972727	6.030402	-2.557078
43	6	0	7.007631	1.777458	-0.928181
44	1	0	7.512944	2.664917	-0.555793
45	6	0	8.514528	1.837557	-2.967140
46	1	0	8.690820	2.880913	-2.686435
47	1	0	8.300685	1.801217	-4.041115
48	1	0	9.453367	1.290555	-2.806738
49	6	0	-3.387487	7.018953	-3.619498
50	1	0	-3.245601	6.609251	-4.625252
51	1	0	-2.819523	7.952010	-3.542906
52	1	0	-4.451050	7.275465	-3.520674
53	1	0	5.294575	-1.160569	1.876398

54	1	0	-3.815397	2.518205	1.079696
55	6	0	-1.669073	2.308852	3.795382
56	6	0	2.817593	-3.381410	1.754254
57	6	0	3.919710	-4.159710	2.503895
58	1	0	3.651787	-5.220968	2.563410
59	1	0	4.892847	-4.096679	2.004646
60	1	0	4.040539	-3.788667	3.529621
61	6	0	1.494698	-3.595951	2.506739
62	1	0	1.562834	-3.233932	3.540890
63	1	0	0.666591	-3.072787	2.025227
64	1	0	1.246002	-4.663649	2.542631
65	6	0	2.688373	-3.907443	0.314891
66	1	0	1.907216	-3.371337	-0.234273
67	1	0	3.623411	-3.805366	-0.248704
68	1	0	2.428183	-4.972599	0.322796
69	6	0	-0.838544	1.187309	4.446421
70	1	0	-1.410355	0.256647	4.530563
71	1	0	0.074551	0.968675	3.870621
72	1	0	-0.524710	1.484889	5.454061
73	6	0	-2.910032	2.568742	4.671940
74	1	0	-3.537406	3.374801	4.274063
75	1	0	-3.531546	1.668356	4.757292
76	1	0	-2.604582	2.860607	5.683425
77	6	0	-0.808812	3.582172	3.714192
78	1	0	-1.363886	4.435503	3.309207
79	1	0	-0.467643	3.864425	4.717173
80	1	0	0.083559	3.427147	3.095813
81	8	0	-1.128731	-1.567087	2.564974
82	8	0	-0.723699	-0.883659	-0.015897
83	6	0	-1.963689	-1.926598	1.741639
84	6	0	-1.753292	-1.592831	0.269418
85	8	0	-3.069401	-2.579489	2.004087
86	6	0	-3.337478	-2.914088	3.398467
87	1	0	-4.268579	-3.476897	3.374683
88	1	0	-2.521577	-3.522034	3.793344
89	1	0	-3.451936	-1.997224	3.979068
90	6	0	-2.993391	-1.238574	-0.575545
91	9	0	-3.922330	-2.194511	-0.612991
92	9	0	-2.632097	-0.926278	-1.826773
93	9	0	-3.558640	-0.137729	-0.020364
94	6	0	-3.829980	-3.834143	-4.605180
95	6	0	-2.732984	-3.452857	-3.841790
96	6	0	-2.486741	-4.049283	-2.581599
97	6	0	-3.374277	-5.058501	-2.132289

98	6	0	-4.453616	-5.453440	-2.912688
99	6	0	-4.689496	-4.838530	-4.147379
100	1	0	-4.016277	-3.349543	-5.558887
101	1	0	-2.089413	-2.659417	-4.204203
102	1	0	-3.188464	-5.565734	-1.191550
103	1	0	-5.110367	-6.244417	-2.563433
104	1	0	-5.538189	-5.144050	-4.752700
105	6	0	-1.349129	-3.639251	-1.764531
106	6	0	-0.107333	-3.093367	-2.398794
107	1	0	0.696795	-3.830923	-2.269604
108	1	0	-0.208057	-2.897416	-3.466040
109	1	0	0.225361	-2.180776	-1.888389
110	6	0	-1.373331	-3.747397	-0.368431
111	1	0	-0.424467	-3.751266	0.162195
112	1	0	-2.198733	-4.257955	0.118921

M2R_{endo}

Total energy= -2678.03991725
Sum of electronic and zero-point Energies= -2677.108466
Sum of electronic and thermal Energies= -2677.052225
Sum of electronic and thermal Enthalpies= -2677.051281
Sum of electronic and thermal Free Energies= -2677.200522

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.113526	-0.205940	0.696998
2	6	0	-0.763822	2.892884	1.386352
3	1	0	-1.800464	2.745512	1.082325
4	7	0	1.116949	3.782610	0.239631
5	6	0	1.155978	2.437854	0.206569
6	6	0	2.093907	4.722666	-0.221803
7	7	0	0.081773	1.867028	0.738802
8	6	0	-0.202051	4.202988	0.769855
9	1	0	-0.069240	5.007825	1.494912
10	7	0	0.973806	-2.187599	0.649746
11	6	0	1.988889	-4.327436	0.900364
12	1	0	1.750247	-5.023781	0.088007
13	7	0	2.917463	-3.299161	0.403798
14	6	0	0.767547	-3.490032	1.357578
15	1	0	0.867075	-3.285185	2.433353
16	6	0	5.298775	-3.514233	0.911865
17	1	0	5.102160	-3.129518	1.907906

18	6	0	2.774246	-0.863090	-0.250569
19	6	0	4.297480	0.752452	-1.215898
20	1	0	5.234218	0.968747	-1.719662
21	6	0	4.249488	-3.634489	-0.002145
22	6	0	1.911166	5.366542	-1.451235
23	1	0	1.045271	5.126211	-2.062009
24	6	0	4.492726	-4.140851	-1.284979
25	1	0	3.672661	-4.239797	-1.990909
26	6	0	3.205060	5.030755	0.567824
27	1	0	3.341277	4.538921	1.526315
28	6	0	1.911358	0.193094	0.041246
29	6	0	3.990770	-0.573332	-0.893545
30	1	0	4.690735	-1.359331	-1.151525
31	6	0	3.432904	1.807344	-0.901615
32	1	0	3.712002	2.822964	-1.157373
33	6	0	2.217263	1.528369	-0.259446
34	6	0	5.787918	-4.508358	-1.647953
35	1	0	5.971336	-4.897590	-2.646243
36	6	0	2.236430	-2.148690	0.231027
37	6	0	4.137715	5.966314	0.115529
38	1	0	5.003818	6.194293	0.731740
39	6	0	2.845716	6.303486	-1.887809
40	1	0	2.698848	6.795334	-2.846682
41	6	0	6.857599	-4.388676	-0.744894
42	6	0	3.975037	6.619452	-1.114528
43	6	0	6.590555	-3.886540	0.536206
44	1	0	7.403130	-3.786132	1.251180
45	6	0	8.252549	-4.804965	-1.144301
46	1	0	8.568501	-4.308335	-2.069813
47	1	0	8.305368	-5.885637	-1.328284
48	1	0	8.978924	-4.562613	-0.363675
49	6	0	4.971970	7.647971	-1.589694
50	1	0	5.896766	7.608789	-1.005911
51	1	0	4.564005	8.663384	-1.498576
52	1	0	5.226692	7.498904	-2.645604
53	1	0	2.445003	-4.887975	1.718754
54	1	0	-0.824927	4.572693	-0.053505
55	6	0	-0.721512	2.820534	2.949496
56	6	0	-0.596263	-4.204084	1.156030
57	6	0	-0.491063	-5.622665	1.759041
58	1	0	-1.469086	-6.116278	1.718839
59	1	0	0.217929	-6.257871	1.215261
60	1	0	-0.180716	-5.587782	2.811061
61	6	0	-1.690180	-3.447736	1.931784

62	1	0	-1.452780	-3.413488	3.003689
63	1	0	-1.816331	-2.420557	1.578874
64	1	0	-2.650962	-3.965750	1.826788
65	6	0	-0.970988	-4.305851	-0.332469
66	1	0	-1.070808	-3.314726	-0.789477
67	1	0	-0.222959	-4.861908	-0.909680
68	1	0	-1.925288	-4.832828	-0.446202
69	6	0	-1.128358	1.410362	3.414159
70	1	0	-2.088257	1.103967	2.987980
71	1	0	-0.378527	0.655483	3.130045
72	1	0	-1.206453	1.383407	4.507875
73	6	0	-1.753261	3.830448	3.491171
74	1	0	-1.519010	4.858986	3.192193
75	1	0	-2.764076	3.597111	3.133699
76	1	0	-1.771026	3.803530	4.586975
77	6	0	0.671073	3.147073	3.519268
78	1	0	0.993637	4.165813	3.277351
79	1	0	0.653089	3.065639	4.612709
80	1	0	1.432102	2.447625	3.153580
81	8	0	-0.409429	-0.436191	-1.231743
82	8	0	-2.203107	-0.286653	0.741017
83	6	0	-1.617783	-0.526977	-1.544596
84	6	0	-2.730062	-0.329208	-0.480775
85	8	0	-1.973687	-0.756238	-2.771398
86	6	0	-0.937946	-0.895000	-3.797946
87	1	0	-1.488907	-1.068374	-4.720118
88	1	0	-0.359656	0.028927	-3.853049
89	1	0	-0.299138	-1.744565	-3.554936
90	6	0	-3.428029	1.022982	-0.857115
91	9	0	-2.507651	1.995095	-1.067336
92	9	0	-4.230235	1.425036	0.143275
93	9	0	-4.173448	0.946630	-1.980034
94	6	0	-8.656074	-0.410882	-0.234209
95	6	0	-7.425574	-0.700744	0.330063
96	6	0	-6.311737	-1.064834	-0.485910
97	6	0	-6.518398	-1.138132	-1.897758
98	6	0	-7.756673	-0.859662	-2.450156
99	6	0	-8.826181	-0.490952	-1.623244
100	1	0	-9.486861	-0.121849	0.400316
101	1	0	-7.314470	-0.620894	1.403153
102	1	0	-5.717947	-1.446218	-2.557375
103	1	0	-7.899409	-0.933325	-3.522922
104	1	0	-9.795421	-0.270032	-2.061561
105	6	0	-5.041282	-1.360810	0.098207

106	6	0	-4.833982	-1.513187	1.552753
107	1	0	-3.919889	-0.958724	1.822327
108	1	0	-5.673214	-1.231515	2.184888
109	1	0	-4.583312	-2.566653	1.751662
110	6	0	-3.813309	-1.529981	-0.710825
111	1	0	-3.268238	-2.411278	-0.362777
112	1	0	-4.001774	-1.617644	-1.776605

M2*S*$_{endo}$

Total energy= -2678.03603749

Sum of electronic and zero-point Energies= -2677.104920

Sum of electronic and thermal Energies= -2677.048521

Sum of electronic and thermal Enthalpies= -2677.047577

Sum of electronic and thermal Free Energies= -2677.197388

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.178389	-0.301468	0.659362
2	6	0	-1.450242	2.376713	1.619371
3	1	0	-2.448216	1.981376	1.418927
4	7	0	0.030323	3.825131	0.469099
5	6	0	0.418223	2.545231	0.304943
6	6	0	0.581111	4.997814	-0.139732
7	7	0	-0.456318	1.663847	0.784894
8	6	0	-1.320352	3.824517	1.078964
9	1	0	-1.383309	4.592360	1.851776
10	7	0	1.589153	-1.942624	0.593282
11	6	0	3.211712	-3.655339	0.970247
12	1	0	3.282185	-4.414238	0.182800
13	7	0	3.796588	-2.397167	0.479382
14	6	0	1.748841	-3.258504	1.296840
15	1	0	1.670667	-3.049075	2.373398
16	6	0	6.190309	-2.178566	0.926558
17	1	0	5.958632	-2.015472	1.975223
18	6	0	2.952871	-0.109148	-0.173065
19	6	0	3.978818	1.931832	-0.978703
20	1	0	4.838761	2.441032	-1.402369
21	6	0	5.149879	-2.363998	0.009443
22	6	0	0.509555	5.176772	-1.524647
23	1	0	0.053583	4.411282	-2.146649
24	6	0	5.440728	-2.585854	-1.340127
25	1	0	4.633623	-2.746939	-2.049222

26	6	0	1.150601	5.992098	0.664491
27	1	0	1.202526	5.849828	1.739896
28	6	0	1.799937	0.629927	0.092280
29	6	0	4.063466	0.560729	-0.715234
30	1	0	4.983054	0.034977	-0.939775
31	6	0	2.818604	2.664481	-0.708575
32	1	0	2.795165	3.727167	-0.919374
33	6	0	1.705061	2.005681	-0.164581
34	6	0	6.769577	-2.596220	-1.768860
35	1	0	6.988243	-2.762851	-2.820545
36	6	0	2.801014	-1.515079	0.250076
37	6	0	1.656630	7.149665	0.078015
38	1	0	2.102368	7.914646	0.709092
39	6	0	1.027896	6.338433	-2.100177
40	1	0	0.974203	6.468441	-3.178028
41	6	0	7.825443	-2.406396	-0.866278
42	6	0	1.608223	7.342479	-1.312758
43	6	0	7.512285	-2.200614	0.487348
44	1	0	8.314915	-2.053627	1.206034
45	6	0	9.262128	-2.420357	-1.328752
46	1	0	9.742998	-1.448138	-1.161065
47	1	0	9.335778	-2.651450	-2.395912
48	1	0	9.849758	-3.166057	-0.779369
49	6	0	2.167155	8.599590	-1.933184
50	1	0	1.680416	9.493763	-1.524445
51	1	0	2.028166	8.605418	-3.018582
52	1	0	3.240651	8.699094	-1.728862
53	1	0	3.757569	-4.012772	1.845823
54	1	0	-2.065281	4.043581	0.303801
55	6	0	-1.183274	2.217767	3.157426
56	6	0	0.719804	-4.377095	0.972748
57	6	0	1.210230	-5.688278	1.627260
58	1	0	0.444760	-6.465116	1.514856
59	1	0	2.130713	-6.070067	1.171200
60	1	0	1.390511	-5.556364	2.701867
61	6	0	-0.638131	-4.027737	1.608737
62	1	0	-0.542159	-3.970806	2.701849
63	1	0	-1.041488	-3.077298	1.253924
64	1	0	-1.373577	-4.810123	1.384945
65	6	0	0.585283	-4.584569	-0.545481
66	1	0	0.267538	-3.667951	-1.050028
67	1	0	1.532682	-4.904252	-0.995975
68	1	0	-0.155882	-5.363545	-0.757900
69	6	0	-1.141759	0.725788	3.539490

70	1	0	-2.037072	0.188449	3.212763
71	1	0	-0.264956	0.205579	3.115614
72	1	0	-1.061942	0.622401	4.628462
73	6	0	-2.360132	2.874149	3.909239
74	1	0	-2.438360	3.946646	3.697114
75	1	0	-3.315937	2.405735	3.643034
76	1	0	-2.224887	2.764229	4.991204
77	6	0	0.137268	2.875216	3.599633
78	1	0	0.141427	3.956877	3.427664
79	1	0	0.285759	2.716171	4.674383
80	1	0	1.002074	2.440720	3.084560
81	8	0	-0.298562	-0.414938	-1.289178
82	8	0	-1.947033	-1.164858	0.660531
83	6	0	-1.465571	-0.728931	-1.616570
84	6	0	-2.516984	-1.103390	-0.542322
85	8	0	-1.822059	-0.771526	-2.862752
86	6	0	-0.823731	-0.491503	-3.898464
87	1	0	-1.362632	-0.609609	-4.836190
88	1	0	-0.454815	0.528654	-3.781738
89	1	0	-0.011635	-1.215825	-3.817938
90	6	0	-3.135308	-2.483962	-0.936123
91	9	0	-3.902178	-2.437441	-2.046646
92	9	0	-3.906191	-2.935816	0.069547
93	9	0	-2.169156	-3.396180	-1.161735
94	6	0	-8.477922	-1.338910	-0.114617
95	6	0	-7.249941	-0.989368	0.419111
96	6	0	-6.153014	-0.640855	-0.426735
97	6	0	-6.372464	-0.659293	-1.838462
98	6	0	-7.605177	-1.007849	-2.361165
99	6	0	-8.660074	-1.349017	-1.503855
100	1	0	-9.298058	-1.605157	0.544076
101	1	0	-7.132133	-0.994304	1.494502
102	1	0	-5.579913	-0.391459	-2.524156
103	1	0	-7.755474	-1.011997	-3.435709
104	1	0	-9.626240	-1.620156	-1.919514
105	6	0	-4.892341	-0.267782	0.130933
106	6	0	-4.645854	-0.153127	1.584569
107	1	0	-4.468977	0.906407	1.820743
108	1	0	-5.432805	-0.529381	2.233864
109	1	0	-3.685497	-0.654724	1.793439
110	6	0	-3.700031	0.028529	-0.694730
111	1	0	-3.217344	0.929091	-0.307643
112	1	0	-3.919043	0.168070	-1.750161

M2R_{exo}

Total energy= -2678.05731128

Sum of electronic and zero-point Energies= -2677.126362

Sum of electronic and thermal Energies= -2677.069798

Sum of electronic and thermal Enthalpies= -2677.068854

Sum of electronic and thermal Free Energies= -2677.219134

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.469230	-0.408113	-1.290063
2	6	0	2.364001	0.888426	-2.451582
3	1	0	2.904630	-0.061703	-2.393393
4	7	0	2.221796	2.723860	-0.951349
5	6	0	1.135336	1.938262	-0.816643
6	6	0	2.500651	3.995306	-0.353400
7	7	0	1.185536	0.831739	-1.551328
8	6	0	3.205811	2.024615	-1.808133
9	1	0	3.624358	2.722791	-2.534387
10	7	0	-2.487852	-0.991590	-0.770213
11	6	0	-4.858895	-1.344809	-0.718348
12	1	0	-5.283578	-2.052877	-0.000236
13	7	0	-4.427803	-0.132236	-0.004808
14	6	0	-3.545858	-1.860883	-1.374666
15	1	0	-3.567171	-1.634519	-2.449587
16	6	0	-6.104032	1.632128	0.258756
17	1	0	-5.974848	1.887528	-0.789311
18	6	0	-2.263751	1.101009	0.399151
19	6	0	-1.669792	3.185546	1.480103
20	1	0	-1.931571	3.998689	2.149785
21	6	0	-5.341426	0.602887	0.818088
22	6	0	1.962350	5.165853	-0.901888
23	1	0	1.308068	5.105423	-1.766400
24	6	0	-5.515921	0.256285	2.162950
25	1	0	-4.934097	-0.555717	2.590309
26	6	0	3.358795	4.073952	0.747117
27	1	0	3.787098	3.167562	1.165783
28	6	0	-1.003493	1.104493	-0.202664
29	6	0	-2.598220	2.163660	1.255310
30	1	0	-3.560500	2.204103	1.750108
31	6	0	-0.419823	3.194729	0.853096
32	1	0	0.265741	4.013161	1.038035
33	6	0	-0.078485	2.141975	-0.010212

34	6	0	-6.433396	0.957731	2.944417
35	1	0	-6.560916	0.685284	3.989296
36	6	0	-3.084202	-0.032129	-0.072760
37	6	0	3.662976	5.318068	1.302586
38	1	0	4.330277	5.370002	2.159035
39	6	0	2.267728	6.400660	-0.333142
40	1	0	1.841176	7.303568	-0.763345
41	6	0	-7.196302	2.005736	2.405398
42	6	0	3.123494	6.499876	0.776155
43	6	0	-7.020088	2.325228	1.050876
44	1	0	-7.606644	3.127110	0.609528
45	6	0	-8.162158	2.780855	3.268229
46	1	0	-7.645247	3.581798	3.814297
47	1	0	-8.637882	2.136082	4.015061
48	1	0	-8.948139	3.249711	2.667334
49	6	0	3.447940	7.845481	1.377872
50	1	0	4.175352	7.755543	2.190593
51	1	0	2.548033	8.326116	1.782278
52	1	0	3.862602	8.527367	0.625336
53	1	0	-5.629877	-1.096873	-1.452233
54	1	0	4.024127	1.639309	-1.188604
55	6	0	1.996419	1.126029	-3.956784
56	6	0	-3.365169	-3.401873	-1.243417
57	6	0	-4.615501	-4.073658	-1.852367
58	1	0	-4.492267	-5.162924	-1.849176
59	1	0	-5.528460	-3.847607	-1.289894
60	1	0	-4.771322	-3.759812	-2.892539
61	6	0	-2.143212	-3.858489	-2.056646
62	1	0	-2.220933	-3.538899	-3.104336
63	1	0	-1.214621	-3.460055	-1.649721
64	1	0	-2.070676	-4.953026	-2.048128
65	6	0	-3.206381	-3.837743	0.223963
66	1	0	-2.351451	-3.346267	0.696787
67	1	0	-4.099125	-3.616355	0.820984
68	1	0	-3.043220	-4.920849	0.277078
69	6	0	1.064070	0.006365	-4.452440
70	1	0	1.525469	-0.981266	-4.350772
71	1	0	0.117845	-0.009524	-3.895047
72	1	0	0.822317	0.159949	-5.510877
73	6	0	3.300487	1.070925	-4.779343
74	1	0	3.996855	1.873764	-4.510912
75	1	0	3.818945	0.113432	-4.641959
76	1	0	3.076081	1.177943	-5.846941
77	6	0	1.303618	2.483177	-4.177979

78	1	0	1.941527	3.327890	-3.894248
79	1	0	1.059659	2.605841	-5.239807
80	1	0	0.364574	2.554937	-3.616517
81	8	0	0.737163	-2.236779	-2.154257
82	8	0	0.266499	-1.305998	0.331924
83	6	0	1.511570	-2.611711	-1.280239
84	6	0	1.354099	-2.134100	0.188185
85	8	0	2.509764	-3.442839	-1.476460
86	6	0	2.677343	-3.991887	-2.816918
87	1	0	3.507121	-4.691345	-2.730697
88	1	0	1.764380	-4.506758	-3.120499
89	1	0	2.916563	-3.188685	-3.516071
90	6	0	1.060422	-3.390906	1.059917
91	9	0	0.039940	-4.100574	0.543695
92	9	0	0.721644	-3.020505	2.309247
93	9	0	2.120535	-4.216234	1.155397
94	6	0	5.058647	-2.059276	5.028630
95	6	0	4.077955	-1.462500	4.259026
96	6	0	3.865952	-1.862516	2.900807
97	6	0	4.698100	-2.900496	2.372965
98	6	0	5.664768	-3.500190	3.158332
99	6	0	5.849774	-3.081245	4.483716
100	1	0	5.213642	-1.739979	6.053869
101	1	0	3.482059	-0.670633	4.694529
102	1	0	4.570021	-3.246725	1.356454
103	1	0	6.280957	-4.293292	2.748103
104	1	0	6.614496	-3.552685	5.094194
105	6	0	2.870797	-1.223822	2.112350
106	6	0	1.937777	-0.216033	2.676355
107	1	0	1.745318	-0.332085	3.742074
108	1	0	2.376884	0.781597	2.514660
109	1	0	0.997209	-0.229770	2.116749
110	6	0	2.731844	-1.469990	0.645883
111	1	0	2.716228	-0.490628	0.153831
112	1	0	3.560322	-2.042227	0.237580

M2S_{exo}

Total energy= -2678.06049848

Sum of electronic and zero-point Energies= -2677.128914

Sum of electronic and thermal Energies= -2677.072454

Sum of electronic and thermal Enthalpies= -2677.071510

Sum of electronic and thermal Free Energies= -2677.220386

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.313985	-0.023787	-1.478776
2	6	0	-2.545357	-1.356502	-2.419526
3	1	0	-3.008181	-0.378977	-2.582129
4	7	0	-2.593322	-2.788231	-0.513890
5	6	0	-1.445765	-2.077463	-0.535363
6	6	0	-3.121251	-3.544398	0.581264
7	7	0	-1.381087	-1.198293	-1.523880
8	6	0	-3.485433	-2.265297	-1.576534
9	1	0	-3.912489	-3.093801	-2.144818
10	7	0	2.394875	0.468852	-1.140969
11	6	0	4.772057	0.723174	-1.119021
12	1	0	5.174723	1.541323	-0.511328
13	7	0	4.289781	-0.348621	-0.233691
14	6	0	3.497384	1.125240	-1.909764
15	1	0	3.524725	0.645266	-2.898592
16	6	0	5.806224	-2.206484	0.249198
17	1	0	5.584449	-2.617330	-0.731717
18	6	0	2.055105	-1.334994	0.417976
19	6	0	1.330131	-3.107283	1.902753
20	1	0	1.552657	-3.802430	2.706261
21	6	0	5.180505	-1.027180	0.660361
22	6	0	-3.381061	-4.909603	0.420008
23	1	0	-3.138092	-5.396447	-0.520091
24	6	0	5.468560	-0.486077	1.919596
25	1	0	4.985908	0.435418	2.233712
26	6	0	-3.431851	-2.912029	1.790101
27	1	0	-3.244070	-1.847816	1.905691
28	6	0	0.771352	-1.336140	-0.129590
29	6	0	2.333522	-2.240488	1.457382
30	1	0	3.311653	-2.279636	1.920593
31	6	0	0.052213	-3.112577	1.331525
32	1	0	-0.692586	-3.814586	1.688465
33	6	0	-0.238553	-2.210274	0.297917
34	6	0	6.363799	-1.139445	2.764563
35	1	0	6.577368	-0.717964	3.743903
36	6	0	2.941058	-0.381233	-0.277907
37	6	0	-3.981318	-3.653706	2.836857
38	1	0	-4.213642	-3.157094	3.775565
39	6	0	-3.939141	-5.635857	1.470340
40	1	0	-4.134519	-6.697302	1.338731
41	6	0	6.995212	-2.331693	2.372809

42	6	0	-4.247854	-5.023126	2.695735
43	6	0	6.701584	-2.851236	1.104444
44	1	0	7.178694	-3.772775	0.780989
45	6	0	7.972162	-3.022254	3.293344
46	1	0	8.262285	-4.003444	2.904850
47	1	0	7.545818	-3.163807	4.293669
48	1	0	8.886881	-2.427953	3.416869
49	6	0	-4.870407	-5.817968	3.817870
50	1	0	-4.837326	-5.268244	4.763767
51	1	0	-4.359174	-6.777136	3.960201
52	1	0	-5.922919	-6.045027	3.602171
53	1	0	5.569796	0.350664	-1.765636
54	1	0	-4.303162	-1.702145	-1.113974
55	6	0	-2.155717	-1.924829	-3.824217
56	6	0	3.374379	2.656571	-2.155473
57	6	0	4.687029	3.147872	-2.804605
58	1	0	4.595694	4.206449	-3.074848
59	1	0	5.547418	3.056631	-2.132208
60	1	0	4.912744	2.589986	-3.722362
61	6	0	2.230022	2.933814	-3.144742
62	1	0	2.396113	2.412566	-4.096574
63	1	0	1.262160	2.613745	-2.753948
64	1	0	2.166693	4.007141	-3.362436
65	6	0	3.126312	3.421419	-0.844563
66	1	0	2.212507	3.071367	-0.353310
67	1	0	3.952514	3.305086	-0.132662
68	1	0	3.018792	4.493876	-1.046629
69	6	0	-1.147527	-0.975770	-4.497848
70	1	0	-1.551779	0.037179	-4.601185
71	1	0	-0.210740	-0.906051	-3.925617
72	1	0	-0.892803	-1.342885	-5.499353
73	6	0	-3.429453	-1.975970	-4.691876
74	1	0	-4.176168	-2.671977	-4.292504
75	1	0	-3.897197	-0.986621	-4.771460
76	1	0	-3.181228	-2.309752	-5.706049
77	6	0	-1.533694	-3.329636	-3.730842
78	1	0	-2.217733	-4.060143	-3.284610
79	1	0	-1.281564	-3.692328	-4.734376
80	1	0	-0.607800	-3.324904	-3.142928
81	8	0	-0.875403	1.773458	-2.565258
82	8	0	-0.347226	1.123680	0.020423
83	6	0	-1.492148	2.390125	-1.704513
84	6	0	-1.273628	2.112138	-0.194382
85	8	0	-2.373321	3.334585	-1.951636

86	6	0	-2.626547	3.671949	-3.346461
87	1	0	-3.378158	4.458976	-3.312298
88	1	0	-1.706332	4.031607	-3.810674
89	1	0	-3.006352	2.795990	-3.875036
90	6	0	-2.633684	1.689471	0.441965
91	9	0	-3.501514	2.714301	0.555476
92	9	0	-2.431696	1.187847	1.675628
93	9	0	-3.242324	0.735242	-0.293239
94	6	0	-2.189850	4.478121	5.154008
95	6	0	-1.329547	3.873066	4.257142
96	6	0	-1.458686	4.096806	2.849017
97	6	0	-2.495382	4.980709	2.408439
98	6	0	-3.336896	5.594415	3.317548
99	6	0	-3.191389	5.342435	4.689071
100	1	0	-2.089091	4.283459	6.216652
101	1	0	-0.574745	3.196789	4.636137
102	1	0	-2.617332	5.210754	1.358250
103	1	0	-4.107500	6.273500	2.968300
104	1	0	-3.858872	5.823500	5.398171
105	6	0	-0.580646	3.458072	1.931288
106	6	0	0.635396	2.726566	2.347173
107	1	0	1.500193	3.231585	1.890823
108	1	0	0.799006	2.648036	3.418916
109	1	0	0.617825	1.732610	1.875370
110	6	0	-0.800501	3.497539	0.451887
111	1	0	0.158030	3.708226	-0.032127
112	1	0	-1.511074	4.261055	0.150175

TS3R_{endo}

Imaginary frequency= -1017.95

Total energy= -2678.03018869

Sum of electronic and zero-point Energies= -2677.102359

Sum of electronic and thermal Energies= -2677.046852

Sum of electronic and thermal Enthalpies= -2677.045907

Sum of electronic and thermal Free Energies= -2677.193121

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.175456	-0.280015	0.854915
2	6	0	-1.365433	2.574510	1.319957
3	1	0	-2.321839	2.199758	0.955335
4	7	0	0.375161	3.794660	0.257480

5	6	0	0.692513	2.489985	0.298224
6	6	0	1.190693	4.908854	-0.122044
7	7	0	-0.277969	1.724571	0.783460
8	6	0	-1.039980	3.948667	0.675393
9	1	0	-1.129714	4.789004	1.365315
10	7	0	1.388525	-2.036433	0.950124
11	6	0	2.660463	-4.028641	1.066690
12	1	0	2.448384	-4.677160	0.206863
13	7	0	3.453469	-2.866525	0.614917
14	6	0	1.393869	-3.356929	1.642325
15	1	0	1.573795	-3.149527	2.708398
16	6	0	5.887236	-3.073117	0.742997
17	1	0	5.824120	-2.914229	1.815743
18	6	0	2.939514	-0.446739	0.042577
19	6	0	4.212694	1.433127	-0.805063
20	1	0	5.136376	1.824647	-1.219004
21	6	0	4.722441	-3.052516	-0.027828
22	6	0	0.997275	5.519437	-1.366915
23	1	0	0.256387	5.120718	-2.054176
24	6	0	4.794769	-3.268597	-1.409643
25	1	0	3.886084	-3.268784	-2.005372
26	6	0	2.141640	5.419250	0.766194
27	1	0	2.282144	4.951248	1.735857
28	6	0	1.877736	0.435832	0.244578
29	6	0	4.133705	0.073578	-0.487686
30	1	0	4.994440	-0.561980	-0.655081
31	6	0	3.136782	2.303462	-0.599376
32	1	0	3.236733	3.352368	-0.852819
33	6	0	1.943383	1.801471	-0.058586
34	6	0	6.033111	-3.482225	-2.012083
35	1	0	6.081504	-3.647135	-3.085756
36	6	0	2.615325	-1.811517	0.496609
37	6	0	2.907432	6.526651	0.397829
38	1	0	3.649673	6.914362	1.090823
39	6	0	1.762694	6.629831	-1.717733
40	1	0	1.609489	7.097212	-2.687454
41	6	0	7.216995	-3.494156	-1.256338
42	6	0	2.730171	7.152362	-0.843733
43	6	0	7.121101	-3.291748	0.127975
44	1	0	8.023596	-3.303638	0.733666
45	6	0	8.554444	-3.703853	-1.923587
46	1	0	9.329746	-3.959826	-1.194666
47	1	0	8.880166	-2.794899	-2.446954
48	1	0	8.507788	-4.504048	-2.671024

49	6	0	3.541780	8.365156	-1.228861
50	1	0	2.924086	9.272891	-1.217656
51	1	0	3.949170	8.268133	-2.241967
52	1	0	4.375974	8.522673	-0.538019
53	1	0	3.211068	-4.600372	1.815004
54	1	0	-1.659965	4.148911	-0.205153
55	6	0	-1.427104	2.574077	2.884706
56	6	0	0.093819	-4.193919	1.563673
57	6	0	0.379657	-5.583442	2.171971
58	1	0	-0.549461	-6.161428	2.238473
59	1	0	1.084106	-6.162923	1.564089
60	1	0	0.791705	-5.499868	3.185473
61	6	0	-0.982258	-3.502430	2.419761
62	1	0	-0.646472	-3.396462	3.459183
63	1	0	-1.223784	-2.504677	2.036385
64	1	0	-1.904553	-4.094827	2.431243
65	6	0	-0.404171	-4.359218	0.117498
66	1	0	-0.670247	-3.394506	-0.328750
67	1	0	0.348513	-4.830462	-0.525525
68	1	0	-1.294425	-4.999345	0.097178
69	6	0	-1.591647	1.131605	3.398330
70	1	0	-2.452568	0.634015	2.938502
71	1	0	-0.698669	0.518564	3.199842
72	1	0	-1.737865	1.131246	4.485180
73	6	0	-2.672881	3.382687	3.303152
74	1	0	-2.615109	4.427166	2.975136
75	1	0	-3.588325	2.947327	2.883490
76	1	0	-2.773413	3.387055	4.394592
77	6	0	-0.169920	3.191127	3.524825
78	1	0	-0.037259	4.244221	3.252625
79	1	0	-0.248809	3.147863	4.617649
80	1	0	0.739477	2.646724	3.242486
81	8	0	-0.152324	-0.712983	-1.091851
82	8	0	-2.360535	-0.594924	0.448051
83	6	0	-1.265834	-0.874232	-1.632312
84	6	0	-2.597448	-0.713328	-0.878648
85	8	0	-1.359847	-1.156736	-2.896311
86	6	0	-0.141249	-1.237384	-3.703167
87	1	0	-0.494188	-1.442920	-4.711634
88	1	0	0.385410	-0.283181	-3.656779
89	1	0	0.485813	-2.049482	-3.332493
90	6	0	-3.249934	0.596100	-1.433931
91	9	0	-2.347480	1.607040	-1.450175
92	9	0	-4.275393	0.973296	-0.656682

93	9	0	-3.703032	0.469066	-2.698417
94	6	0	-8.412872	-1.683573	-0.032536
95	6	0	-7.091155	-1.965411	0.287204
96	6	0	-6.048722	-1.730284	-0.644931
97	6	0	-6.402021	-1.218896	-1.918178
98	6	0	-7.726124	-0.937928	-2.232052
99	6	0	-8.735609	-1.166628	-1.291817
100	1	0	-9.195566	-1.876469	0.694740
101	1	0	-6.870860	-2.398193	1.255679
102	1	0	-5.641923	-1.018226	-2.662067
103	1	0	-7.973234	-0.540800	-3.211867
104	1	0	-9.770583	-0.952281	-1.542533
105	6	0	-4.676354	-2.067718	-0.298359
106	6	0	-4.231818	-2.310869	1.021912
107	1	0	-3.383197	-1.356796	1.015510
108	1	0	-4.935082	-2.266118	1.849143
109	1	0	-3.477697	-3.091590	1.131839
110	6	0	-3.541983	-1.985613	-1.262307
111	1	0	-2.892446	-2.854025	-1.122726
112	1	0	-3.823892	-1.931794	-2.310619

TS3S_{endo}

Imaginary frequency= -1225.51

Total energy= -2678.02493145

Sum of electronic and zero-point Energies= -2677.097110

Sum of electronic and thermal Energies= -2677.041477

Sum of electronic and thermal Enthalpies= -2677.040533

Sum of electronic and thermal Free Energies= -2677.188552

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.088796	-0.294423	0.542409
2	6	0	-0.929218	2.653692	1.580786
3	1	0	-1.987339	2.484824	1.367966
4	7	0	0.790362	3.778434	0.391142
5	6	0	0.900062	2.450901	0.208605
6	6	0	1.593122	4.830051	-0.159171
7	7	0	-0.107995	1.759473	0.733382
8	6	0	-0.500349	4.053123	1.063209
9	1	0	-0.359559	4.790867	1.854835
10	7	0	1.104617	-2.213261	0.356024
11	6	0	2.421131	-4.157897	0.830466

12	1	0	2.387621	-4.960099	0.085733
13	7	0	3.205926	-3.033183	0.299549
14	6	0	1.030158	-3.520034	1.095347
15	1	0	0.948569	-3.274071	2.163753
16	6	0	5.491322	-2.605576	1.074344
17	1	0	5.085322	-2.099945	1.945918
18	6	0	2.781018	-0.667338	-0.432929
19	6	0	4.149647	1.114913	-1.333465
20	1	0	5.061582	1.435500	-1.826991
21	6	0	4.622919	-3.129746	0.109781
22	6	0	1.493068	5.162029	-1.513372
23	1	0	0.825742	4.600765	-2.161368
24	6	0	5.137415	-3.797664	-1.004441
25	1	0	4.460357	-4.207523	-1.748609
26	6	0	2.437061	5.566022	0.680769
27	1	0	2.508007	5.307297	1.733078
28	6	0	1.826195	0.294051	-0.114170
29	6	0	3.963915	-0.244571	-1.063818
30	1	0	4.729195	-0.955934	-1.349752
31	6	0	3.197964	2.074865	-0.972345
32	1	0	3.388182	3.121600	-1.177930
33	6	0	2.009499	1.662645	-0.349921
34	6	0	6.519495	-3.926768	-1.155466
35	1	0	6.913453	-4.444011	-2.026472
36	6	0	2.379103	-2.007654	0.030481
37	6	0	3.183450	6.619973	0.158764
38	1	0	3.838773	7.185626	0.816625
39	6	0	2.252403	6.216041	-2.024942
40	1	0	2.172720	6.465926	-3.079773
41	6	0	7.406768	-3.400609	-0.205664
42	6	0	3.107090	6.962110	-1.201561
43	6	0	6.868508	-2.736551	0.908633
44	1	0	7.537359	-2.322029	1.659066
45	6	0	8.900257	-3.556190	-0.358477
46	1	0	9.417936	-2.599892	-0.217928
47	1	0	9.163569	-3.944584	-1.347198
48	1	0	9.302128	-4.250864	0.390751
49	6	0	3.929304	8.100847	-1.753714
50	1	0	3.767385	9.022250	-1.181516
51	1	0	3.681325	8.302878	-2.800256
52	1	0	5.002421	7.876383	-1.700487
53	1	0	2.888252	-4.545812	1.738298
54	1	0	-1.208648	4.458386	0.330744
55	6	0	-0.707456	2.414923	3.114152

56	6	0	-0.154472	-4.466341	0.755665
57	6	0	0.066792	-5.800350	1.503758
58	1	0	-0.803124	-6.452283	1.362257
59	1	0	0.944802	-6.345677	1.140424
60	1	0	0.188109	-5.639018	2.582614
61	6	0	-1.465656	-3.855073	1.280422
62	1	0	-1.431333	-3.754791	2.373973
63	1	0	-1.668226	-2.869278	0.860456
64	1	0	-2.314391	-4.505491	1.037016
65	6	0	-0.239110	-4.736625	-0.757086
66	1	0	-0.321503	-3.807530	-1.328134
67	1	0	0.641156	-5.278772	-1.122345
68	1	0	-1.116622	-5.353311	-0.982751
69	6	0	-1.012284	0.947770	3.471598
70	1	0	-2.017895	0.646909	3.162648
71	1	0	-0.291908	0.249244	3.015439
72	1	0	-0.938875	0.805166	4.556284
73	6	0	-1.696577	3.315465	3.881895
74	1	0	-1.519097	4.379928	3.690033
75	1	0	-2.736006	3.092689	3.610246
76	1	0	-1.592786	3.155889	4.961301
77	6	0	0.732451	2.737514	3.553568
78	1	0	0.988507	3.791714	3.402652
79	1	0	0.848173	2.526428	4.623256
80	1	0	1.467051	2.123495	3.018909
81	8	0	-0.480061	-0.137674	-1.381852
82	8	0	-2.342943	-0.721053	0.472553
83	6	0	-1.675810	-0.170054	-1.741273
84	6	0	-2.826789	-0.519871	-0.788133
85	8	0	-2.010863	0.047177	-2.975036
86	6	0	-0.959069	0.306196	-3.962117
87	1	0	-1.493596	0.444455	-4.899382
88	1	0	-0.413163	1.208204	-3.681478
89	1	0	-0.293648	-0.556951	-4.011361
90	6	0	-3.452746	-1.847589	-1.327370
91	9	0	-4.151074	-1.682993	-2.468446
92	9	0	-4.271290	-2.380886	-0.409782
93	9	0	-2.478230	-2.745692	-1.591923
94	6	0	-8.543192	-0.441007	0.756888
95	6	0	-7.228192	-0.069506	1.002521
96	6	0	-6.290593	0.038901	-0.055533
97	6	0	-6.745494	-0.218744	-1.372096
98	6	0	-8.063465	-0.588571	-1.612208
99	6	0	-8.965914	-0.704096	-0.550913

100	1	0	-9.244980	-0.515954	1.581962
101	1	0	-6.930399	0.158199	2.019102
102	1	0	-6.070889	-0.150113	-2.215214
103	1	0	-8.388128	-0.786469	-2.629191
104	1	0	-9.996584	-0.988911	-0.742124
105	6	0	-4.927206	0.467321	0.220672
106	6	0	-4.363586	0.540515	1.510936
107	1	0	-3.699803	1.387835	1.691518
108	1	0	-4.952729	0.258577	2.379432
109	1	0	-3.358413	-0.255426	1.241649
110	6	0	-3.909336	0.676825	-0.855071
111	1	0	-3.331543	1.579853	-0.636358
112	1	0	-4.308054	0.761602	-1.862409

TS3R_{exo}

Imaginary frequency= -1385.67

Total energy= -2678.03305821

Sum of electronic and zero-point Energies= -2677.106575

Sum of electronic and thermal Energies= -2677.050305

Sum of electronic and thermal Enthalpies= -2677.049361

Sum of electronic and thermal Free Energies= -2677.201229

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.129634	-0.224545	-1.420630
2	6	0	3.085949	-0.277285	-2.166407
3	1	0	3.154573	-1.367730	-2.149632
4	7	0	3.578753	1.378453	-0.535911
5	6	0	2.255127	1.146787	-0.564751
6	6	0	4.307683	2.370524	0.198783
7	7	0	1.908869	0.149460	-1.372084
8	6	0	4.256901	0.353509	-1.366383
9	1	0	5.008305	0.830396	-1.998649
10	7	0	-2.238560	0.205322	-1.275552
11	6	0	-4.473094	0.991919	-1.576398
12	1	0	-5.238101	0.454114	-1.006266
13	7	0	-3.680358	1.826146	-0.655654
14	6	0	-3.408873	0.050798	-2.196993
15	1	0	-3.092248	0.463425	-3.166825
16	6	0	-4.636576	4.045565	-0.284789
17	1	0	-4.353364	4.313882	-1.298649
18	6	0	-1.302876	1.874786	0.185982

19	6	0	-0.010973	3.445147	1.505153
20	1	0	0.017738	4.271760	2.207176
21	6	0	-4.323574	2.773314	0.206862
22	6	0	4.502997	3.642154	-0.345269
23	1	0	4.070875	3.889228	-1.310503
24	6	0	-4.691935	2.417290	1.507945
25	1	0	-4.464416	1.423118	1.882469
26	6	0	4.872890	2.043210	1.437151
27	1	0	4.727068	1.050888	1.853430
28	6	0	-0.094833	1.332540	-0.252369
29	6	0	-1.252016	2.952895	1.087768
30	1	0	-2.157070	3.411761	1.464303
31	6	0	1.191286	2.915412	1.026368
32	1	0	2.133791	3.341104	1.352300
33	6	0	1.155848	1.842999	0.122619
34	6	0	-5.347793	3.344945	2.319891
35	1	0	-5.625774	3.063109	3.332581
36	6	0	-2.454515	1.276701	-0.520006
37	6	0	5.620052	2.995506	2.128373
38	1	0	6.053716	2.735614	3.090972
39	6	0	5.250299	4.588304	0.359511
40	1	0	5.395036	5.577276	-0.066932
41	6	0	-5.661863	4.627516	1.849168
42	6	0	5.821702	4.282328	1.602826
43	6	0	-5.298271	4.958871	0.533116
44	1	0	-5.533572	5.947227	0.145646
45	6	0	-6.369122	5.632336	2.726073
46	1	0	-6.650296	5.195528	3.688326
47	1	0	-7.280401	6.006072	2.243572
48	1	0	-5.731768	6.503661	2.924449
49	6	0	6.641119	5.299975	2.358882
50	1	0	6.669315	6.258923	1.833864
51	1	0	7.675287	4.955253	2.489373
52	1	0	6.232806	5.472769	3.362602
53	1	0	-4.969162	1.616826	-2.321686
54	1	0	4.759496	-0.369947	-0.714479
55	6	0	3.012085	0.170584	-3.667595
56	6	0	-3.922364	-1.387577	-2.468376
57	6	0	-5.126501	-1.279935	-3.429906
58	1	0	-5.480891	-2.281729	-3.699418
59	1	0	-5.969269	-0.744161	-2.979341
60	1	0	-4.852591	-0.762635	-4.358354
61	6	0	-2.818787	-2.195535	-3.172892
62	1	0	-2.512103	-1.705710	-4.107555

63	1	0	-1.933070	-2.310806	-2.545316
64	1	0	-3.180716	-3.198662	-3.427394
65	6	0	-4.367229	-2.093669	-1.173604
66	1	0	-3.592563	-2.059880	-0.404094
67	1	0	-5.276908	-1.646129	-0.757403
68	1	0	-4.593071	-3.146689	-1.378976
69	6	0	1.702727	-0.326116	-4.306178
70	1	0	1.595539	-1.412414	-4.228739
71	1	0	0.821260	0.136288	-3.833266
72	1	0	1.676475	-0.055114	-5.368211
73	6	0	4.195270	-0.484055	-4.409612
74	1	0	5.163461	-0.163534	-4.007211
75	1	0	4.148766	-1.578428	-4.345020
76	1	0	4.173517	-0.210816	-5.471060
77	6	0	3.085432	1.700436	-3.825091
78	1	0	4.031998	2.113738	-3.460493
79	1	0	3.005557	1.965974	-4.885879
80	1	0	2.264419	2.204085	-3.301351
81	8	0	0.574123	-2.478117	-2.153578
82	8	0	-0.151114	-1.424327	0.243225
83	6	0	0.757291	-3.183217	-1.173157
84	6	0	0.297210	-2.765245	0.236441
85	8	0	1.318633	-4.370747	-1.186095
86	6	0	1.725729	-4.906623	-2.479961
87	1	0	2.107205	-5.902296	-2.261425
88	1	0	0.861192	-4.957133	-3.144580
89	1	0	2.506958	-4.277331	-2.909969
90	6	0	-0.937655	-3.645566	0.589698
91	9	0	-1.801593	-3.670683	-0.444318
92	9	0	-1.582399	-3.162120	1.661096
93	9	0	-0.589720	-4.920031	0.844203
94	6	0	0.498853	-2.795649	6.216239
95	6	0	0.804627	-2.177245	5.011068
96	6	0	0.832290	-2.913397	3.800655
97	6	0	0.557900	-4.300510	3.861269
98	6	0	0.250052	-4.914098	5.069949
99	6	0	0.217095	-4.165784	6.250095
100	1	0	0.490296	-2.214194	7.133165
101	1	0	1.055109	-1.122817	5.009448
102	1	0	0.560667	-4.903861	2.962546
103	1	0	0.034927	-5.978044	5.091700
104	1	0	-0.017194	-4.649813	7.193941
105	6	0	1.201964	-2.240614	2.559765
106	6	0	1.191379	-0.855088	2.392623

107	1	0	0.877943	-0.192495	3.193599
108	1	0	1.936438	-0.436020	1.716583
109	1	0	0.304172	-0.958175	1.324498
110	6	0	1.480605	-2.979023	1.274642
111	1	0	2.367960	-2.541642	0.808803
112	1	0	1.664519	-4.044623	1.393794

TS3S_{exo}

Imaginary frequency= -1335.10

Total energy= -2678.04037841

Sum of electronic and zero-point Energies= -2677.112413

Sum of electronic and thermal Energies= -2677.056811

Sum of electronic and thermal Enthalpies= -2677.055867

Sum of electronic and thermal Free Energies= -2677.204513

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.008110	-0.277951	-1.439778
2	6	0	3.234856	-0.166568	-2.023990
3	1	0	3.360969	-1.250503	-1.962579
4	7	0	3.561033	1.536760	-0.393851
5	6	0	2.255685	1.227670	-0.477932
6	6	0	4.195093	2.484598	0.474488
7	7	0	2.003066	0.219519	-1.303115
8	6	0	4.332352	0.549054	-1.185723
9	1	0	5.080066	1.062462	-1.792583
10	7	0	-2.115751	0.019393	-1.435045
11	6	0	-4.433819	0.453105	-1.654615
12	1	0	-4.998053	-0.209068	-0.985177
13	7	0	-3.731632	1.476502	-0.857255
14	6	0	-3.262020	-0.259181	-2.363567
15	1	0	-3.046281	0.295007	-3.290351
16	6	0	-4.538447	3.782662	-0.688727
17	1	0	-4.047510	4.003515	-1.632275
18	6	0	-1.372387	1.805477	0.002418
19	6	0	-0.258283	3.429621	1.412580
20	1	0	-0.319107	4.255669	2.114081
21	6	0	-4.442860	2.497422	-0.144761
22	6	0	4.548147	3.747272	-0.012219
23	1	0	4.313788	4.013390	-1.038844
24	6	0	-5.078477	2.201912	1.064949
25	1	0	-5.009237	1.201981	1.483842

26	6	0	4.494928	2.135059	1.795290
27	1	0	4.224960	1.151454	2.169246
28	6	0	-0.109253	1.327053	-0.348415
29	6	0	-1.440846	2.880561	0.907223
30	1	0	-2.393738	3.288205	1.221502
31	6	0	1.002223	2.953046	1.032205
32	1	0	1.894959	3.416552	1.435436
33	6	0	1.084285	1.879401	0.133492
34	6	0	-5.794072	3.197800	1.731240
35	1	0	-6.282492	2.962766	2.673515
36	6	0	-2.443939	1.098207	-0.724791
37	6	0	5.133834	3.056161	2.625597
38	1	0	5.357146	2.780875	3.653284
39	6	0	5.186725	4.658324	0.828344
40	1	0	5.449485	5.641481	0.446000
41	6	0	-5.893518	4.495177	1.207844
42	6	0	5.491630	4.329798	2.158516
43	6	0	-5.251657	4.769690	-0.010386
44	1	0	-5.313007	5.768872	-0.434418
45	6	0	-6.686902	5.563489	1.919783
46	1	0	-6.879029	5.290633	2.962292
47	1	0	-7.659235	5.720026	1.433914
48	1	0	-6.162406	6.525575	1.906802
49	6	0	6.206753	5.312606	3.053174
50	1	0	5.910938	6.343661	2.831549
51	1	0	7.294437	5.251478	2.912573
52	1	0	6.002186	5.114179	4.110385
53	1	0	-5.126267	0.925552	-2.352414
54	1	0	4.846648	-0.136803	-0.503601
55	6	0	3.196103	0.210292	-3.543078
56	6	0	-3.535283	-1.730161	-2.775281
57	6	0	-4.903989	-1.782327	-3.489460
58	1	0	-5.075411	-2.787854	-3.890621
59	1	0	-5.734509	-1.553520	-2.812125
60	1	0	-4.945462	-1.078637	-4.330309
61	6	0	-2.463079	-2.191648	-3.781008
62	1	0	-2.455414	-1.546971	-4.669314
63	1	0	-1.460500	-2.188057	-3.346881
64	1	0	-2.673907	-3.214537	-4.116470
65	6	0	-3.554963	-2.670120	-1.560440
66	1	0	-2.589187	-2.660401	-1.045076
67	1	0	-4.330380	-2.391634	-0.836983
68	1	0	-3.759893	-3.699090	-1.879358
69	6	0	1.950265	-0.413513	-4.202908

70	1	0	1.886008	-1.490955	-4.016147
71	1	0	1.014566	0.051187	-3.850139
72	1	0	1.985103	-0.259771	-5.288264
73	6	0	4.450180	-0.393036	-4.208165
74	1	0	5.376117	0.011626	-3.783142
75	1	0	4.474782	-1.483873	-4.092766
76	1	0	4.455434	-0.168405	-5.280954
77	6	0	3.171761	1.732461	-3.770859
78	1	0	4.087284	2.220989	-3.418363
79	1	0	3.084826	1.946804	-4.842677
80	1	0	2.317762	2.206274	-3.271880
81	8	0	0.388367	-2.537155	-2.058003
82	8	0	0.044820	-1.329601	0.302588
83	6	0	0.605820	-3.229849	-1.070422
84	6	0	0.464461	-2.671985	0.357297
85	8	0	0.963641	-4.489805	-1.096108
86	6	0	1.136553	-5.117038	-2.402874
87	1	0	1.412115	-6.146391	-2.181759
88	1	0	0.197415	-5.074265	-2.957033
89	1	0	1.933158	-4.608414	-2.948547
90	6	0	1.853411	-2.689507	1.057978
91	9	0	2.247140	-3.935757	1.379413
92	9	0	1.819451	-1.956040	2.181705
93	9	0	2.803176	-2.170985	0.252784
94	6	0	-1.554836	-2.882692	6.043536
95	6	0	-1.772157	-2.585343	4.704140
96	6	0	-0.920326	-3.101957	3.697150
97	6	0	0.145133	-3.943673	4.093291
98	6	0	0.362982	-4.230878	5.436215
99	6	0	-0.483871	-3.702424	6.415055
100	1	0	-2.226318	-2.485990	6.798967
101	1	0	-2.628836	-1.979870	4.430918
102	1	0	0.826311	-4.356943	3.360456
103	1	0	1.193736	-4.869602	5.720226
104	1	0	-0.316598	-3.936689	7.462500
105	6	0	-1.204456	-2.801637	2.297817
106	6	0	-1.961536	-1.704108	1.884566
107	1	0	-2.550034	-1.808400	0.972649
108	1	0	-2.352697	-0.997178	2.610474
109	1	0	-0.909424	-1.239361	1.125759
110	6	0	-0.583440	-3.568120	1.157915
111	1	0	-1.374398	-3.824178	0.447535
112	1	0	-0.097926	-4.495646	1.454196

M3R_{endo}

Total energy= -2678.06273274

Sum of electronic and zero-point Energies= -2677.130476

Sum of electronic and thermal Energies= -2677.074151

Sum of electronic and thermal Enthalpies= -2677.073207

Sum of electronic and thermal Free Energies= -2677.222993

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.413578	-0.338714	1.107787
2	6	0	-1.528206	2.252569	1.732622
3	1	0	-2.437113	1.743077	1.405287
4	7	0	-0.108210	3.706644	0.484279
5	6	0	0.404772	2.466245	0.495972
6	6	0	0.431293	4.895790	-0.107261
7	7	0	-0.360820	1.579940	1.121716
8	6	0	-1.456006	3.673118	1.100641
9	1	0	-1.548889	4.481630	1.828357
10	7	0	1.826473	-1.886360	0.979860
11	6	0	3.373754	-3.682389	0.998149
12	1	0	3.244119	-4.420169	0.197918
13	7	0	3.927169	-2.434693	0.423639
14	6	0	2.032531	-3.209600	1.619698
15	1	0	2.187882	-3.029139	2.693412
16	6	0	6.358920	-2.183869	0.463288
17	1	0	6.301517	-1.979521	1.528676
18	6	0	3.018387	-0.109372	-0.085055
19	6	0	3.888382	1.938955	-1.040679
20	1	0	4.690021	2.464755	-1.549224
21	6	0	5.187290	-2.421505	-0.259699
22	6	0	0.161314	5.196469	-1.447507
23	1	0	-0.436372	4.512887	-2.044332
24	6	0	5.254134	-2.698371	-1.630450
25	1	0	4.342835	-2.899125	-2.187078
26	6	0	1.192103	5.775524	0.667437
27	1	0	1.397078	5.539093	1.707689
28	6	0	1.865470	0.609351	0.237957
29	6	0	4.052102	0.582592	-0.739115
30	1	0	4.973547	0.081738	-1.010360
31	6	0	2.728367	2.641317	-0.695793
32	1	0	2.649120	3.695195	-0.934233
33	6	0	1.687638	1.968018	-0.035296

34	6	0	6.491726	-2.716562	-2.271224
35	1	0	6.536666	-2.931345	-3.336165
36	6	0	2.955104	-1.502341	0.399961
37	6	0	1.692447	6.945473	0.094466
38	1	0	2.289825	7.621597	0.700656
39	6	0	0.667230	6.368281	-2.006845
40	1	0	0.459284	6.593396	-3.050209
41	6	0	7.680166	-2.468745	-1.564813
42	6	0	1.439038	7.262658	-1.247347
43	6	0	7.591866	-2.206955	-0.190052
44	1	0	8.499398	-2.018797	0.377861
45	6	0	9.012965	-2.472829	-2.273310
46	1	0	9.842985	-2.526326	-1.561998
47	1	0	9.145311	-1.559920	-2.869099
48	1	0	9.095963	-3.320553	-2.962995
49	6	0	1.964548	8.537970	-1.859897
50	1	0	1.153363	9.261414	-2.019357
51	1	0	2.424605	8.351989	-2.838497
52	1	0	2.711387	9.012654	-1.214648
53	1	0	4.059295	-4.090772	1.742797
54	1	0	-2.211419	3.817444	0.321141
55	6	0	-1.508805	2.210809	3.295030
56	6	0	0.837158	-4.189732	1.501042
57	6	0	1.240580	-5.524589	2.157888
58	1	0	0.387855	-6.213625	2.169671
59	1	0	2.053838	-6.018463	1.613389
60	1	0	1.565722	-5.377344	3.195323
61	6	0	-0.351216	-3.596709	2.282384
62	1	0	-0.096016	-3.453202	3.340183
63	1	0	-0.660820	-2.625122	1.874204
64	1	0	-1.215811	-4.269524	2.237421
65	6	0	0.432160	-4.433316	0.037339
66	1	0	0.159156	-3.498576	-0.464747
67	1	0	1.238115	-4.900416	-0.540460
68	1	0	-0.430162	-5.109029	-0.006592
69	6	0	-1.462250	0.745656	3.770712
70	1	0	-2.284579	0.157111	3.347001
71	1	0	-0.514358	0.253537	3.501031
72	1	0	-1.543546	0.699224	4.863195
73	6	0	-2.822462	2.842632	3.799084
74	1	0	-2.919065	3.891405	3.495058
75	1	0	-3.696115	2.299579	3.417253
76	1	0	-2.861082	2.813653	4.894172
77	6	0	-0.305439	2.966942	3.885234

78	1	0	-0.329707	4.037021	3.650301
79	1	0	-0.307306	2.877134	4.977989
80	1	0	0.646811	2.559063	3.524746
81	8	0	-0.210808	-0.727165	-0.781412
82	8	0	-2.520349	-0.881096	0.667726
83	6	0	-1.302280	-0.878584	-1.360397
84	6	0	-2.689767	-1.001076	-0.715378
85	8	0	-1.351846	-0.977489	-2.656635
86	6	0	-0.115717	-0.872156	-3.431094
87	1	0	-0.437320	-0.947237	-4.467679
88	1	0	0.355548	0.091954	-3.233763
89	1	0	0.548027	-1.695791	-3.164152
90	6	0	-3.537024	0.214899	-1.202192
91	9	0	-2.788614	1.346873	-1.171845
92	9	0	-4.584669	0.406328	-0.388564
93	9	0	-3.987837	0.066059	-2.455583
94	6	0	-8.188468	-1.530288	-0.544567
95	6	0	-6.931117	-1.865472	-0.044775
96	6	0	-5.906601	-2.307247	-0.902516
97	6	0	-6.179800	-2.388534	-2.279136
98	6	0	-7.440945	-2.057832	-2.778275
99	6	0	-8.449676	-1.626724	-1.914478
100	1	0	-8.962073	-1.183870	0.135487
101	1	0	-6.730909	-1.766064	1.018150
102	1	0	-5.415972	-2.736377	-2.968127
103	1	0	-7.633383	-2.138816	-3.844697
104	1	0	-9.428685	-1.362395	-2.304720
105	6	0	-4.580989	-2.710312	-0.351485
106	6	0	-4.475493	-3.359196	0.824358
107	1	0	-3.258835	-1.355722	1.105486
108	1	0	-5.350164	-3.634316	1.406541
109	1	0	-3.512610	-3.685550	1.210416
110	6	0	-3.311000	-2.380211	-1.121508
111	1	0	-2.548837	-3.132303	-0.896147
112	1	0	-3.466373	-2.385569	-2.200610

M3*S*$_{endo}$

Total energy= -2678.05759417

Sum of electronic and zero-point Energies= -2677.124432

Sum of electronic and thermal Energies= -2677.068404

Sum of electronic and thermal Enthalpies= -2677.067460

Sum of electronic and thermal Free Energies= -2677.216096

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.307503	-0.239456	0.941526
2	6	0	-1.305025	2.484660	1.760171
3	1	0	-2.314903	2.104856	1.591126
4	7	0	0.108680	3.845297	0.413014
5	6	0	0.464503	2.556387	0.294161
6	6	0	0.695049	4.989666	-0.220417
7	7	0	-0.354653	1.720489	0.923758
8	6	0	-1.161842	3.918204	1.173380
9	1	0	-1.093934	4.700232	1.931732
10	7	0	1.659086	-1.852982	0.874890
11	6	0	3.208863	-3.635032	1.123520
12	1	0	3.113594	-4.458058	0.406469
13	7	0	3.774574	-2.455485	0.434259
14	6	0	1.842635	-3.114128	1.642716
15	1	0	1.949335	-2.834659	2.701068
16	6	0	6.204156	-2.203423	0.581002
17	1	0	6.089364	-1.876502	1.610603
18	6	0	2.909853	-0.172886	-0.281521
19	6	0	3.839355	1.782235	-1.368884
20	1	0	4.645987	2.243011	-1.929982
21	6	0	5.069939	-2.512604	-0.177451
22	6	0	0.395135	5.285358	-1.552759
23	1	0	-0.272657	4.637781	-2.114031
24	6	0	5.209931	-2.941937	-1.500925
25	1	0	4.329388	-3.194737	-2.084956
26	6	0	1.544100	5.829020	0.509977
27	1	0	1.772386	5.596029	1.545884
28	6	0	1.797625	0.610198	0.032326
29	6	0	3.950708	0.436417	-1.002762
30	1	0	4.838018	-0.120590	-1.278737
31	6	0	2.727803	2.556284	-1.018686
32	1	0	2.690139	3.601513	-1.301775
33	6	0	1.678285	1.963675	-0.297594
34	6	0	6.483143	-3.044063	-2.063080
35	1	0	6.584292	-3.373627	-3.093948
36	6	0	2.809184	-1.526674	0.299016
37	6	0	2.099242	6.950665	-0.101783
38	1	0	2.762822	7.594765	0.470034
39	6	0	0.961184	6.411069	-2.154550
40	1	0	0.728813	6.633402	-3.192763
41	6	0	7.632434	-2.736415	-1.320617

42	6	0	1.820863	7.259938	-1.443640
43	6	0	7.470125	-2.312567	0.008250
44	1	0	8.346631	-2.065539	0.602136
45	6	0	9.009738	-2.882214	-1.920747
46	1	0	9.661066	-2.048570	-1.635114
47	1	0	8.967788	-2.926745	-3.013668
48	1	0	9.494692	-3.803265	-1.570863
49	6	0	2.433812	8.475936	-2.094625
50	1	0	2.146347	9.394614	-1.568276
51	1	0	2.118767	8.572064	-3.138116
52	1	0	3.529789	8.426886	-2.074694
53	1	0	3.871489	-3.952485	1.931031
54	1	0	-1.979458	4.167995	0.487718
55	6	0	-1.024588	2.352779	3.296576
56	6	0	0.668627	-4.123169	1.556152
57	6	0	1.069665	-5.398864	2.324584
58	1	0	0.227350	-6.100013	2.354050
59	1	0	1.911110	-5.916995	1.850010
60	1	0	1.350040	-5.169957	3.360531
61	6	0	-0.558282	-3.502059	2.250535
62	1	0	-0.354404	-3.325088	3.314668
63	1	0	-0.844333	-2.545037	1.798724
64	1	0	-1.423418	-4.171574	2.183221
65	6	0	0.337584	-4.482723	0.097933
66	1	0	0.082249	-3.594583	-0.488235
67	1	0	1.176756	-4.983887	-0.398566
68	1	0	-0.516669	-5.167644	0.063065
69	6	0	-1.079901	0.870756	3.727022
70	1	0	-1.987533	0.371618	3.366876
71	1	0	-0.203696	0.288169	3.388474
72	1	0	-1.076788	0.802073	4.821504
73	6	0	-2.149251	3.104739	4.039191
74	1	0	-2.169078	4.170893	3.786146
75	1	0	-3.134371	2.683043	3.803912
76	1	0	-2.002697	3.028618	5.122483
77	6	0	0.340250	2.940229	3.697241
78	1	0	0.398477	4.017760	3.507589
79	1	0	0.509799	2.790282	4.770087
80	1	0	1.166329	2.453210	3.164885
81	8	0	-0.343158	-0.682489	-0.921683
82	8	0	-2.476630	-0.876593	0.709737
83	6	0	-1.455197	-0.960107	-1.408704
84	6	0	-2.786847	-1.018723	-0.651839
85	8	0	-1.576998	-1.217007	-2.676721

86	6	0	-0.386884	-1.187688	-3.527879
87	1	0	-0.754735	-1.448963	-4.517781
88	1	0	0.037816	-0.182853	-3.517016
89	1	0	0.333621	-1.923623	-3.168775
90	6	0	-3.404311	-2.435546	-0.848084
91	9	0	-3.939860	-2.602865	-2.066067
92	9	0	-4.358078	-2.649893	0.070915
93	9	0	-2.457990	-3.385766	-0.680452
94	6	0	-8.293760	-1.622422	-0.291192
95	6	0	-7.122408	-0.974661	0.097960
96	6	0	-6.226359	-0.463884	-0.859274
97	6	0	-6.534598	-0.639160	-2.219551
98	6	0	-7.710000	-1.284038	-2.608670
99	6	0	-8.594386	-1.777605	-1.647503
100	1	0	-8.968101	-2.014387	0.465474
101	1	0	-6.885797	-0.878945	1.153800
102	1	0	-5.870145	-0.249712	-2.985097
103	1	0	-7.934261	-1.397162	-3.665966
104	1	0	-9.506060	-2.284486	-1.951555
105	6	0	-5.011118	0.286823	-0.429797
106	6	0	-5.048273	1.125749	0.621586
107	1	0	-4.182089	1.715474	0.908432
108	1	0	-5.959520	1.298831	1.186590
109	1	0	-3.260112	-0.509688	1.170121
110	6	0	-3.706446	0.123705	-1.196640
111	1	0	-3.119701	1.044026	-1.115293
112	1	0	-3.879484	-0.059485	-2.258348

M3R_{exo}

Total energy= -2678.05088870
Sum of electronic and zero-point Energies= -2677.117861
Sum of electronic and thermal Energies= -2677.061670
Sum of electronic and thermal Enthalpies= -2677.060726
Sum of electronic and thermal Free Energies= -2677.210046

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.202237	-0.066645	-1.507537
2	6	0	2.980776	0.171036	-2.280936
3	1	0	3.140488	-0.910706	-2.305261
4	7	0	3.357096	1.792414	-0.580435
5	6	0	2.059873	1.449850	-0.603038

6	6	0	4.012108	2.782282	0.224743
7	7	0	1.786780	0.466644	-1.454606
8	6	0	4.105476	0.865431	-1.464008
9	1	0	4.809109	1.427096	-2.080080
10	7	0	-2.322934	0.110293	-1.293540
11	6	0	-4.654181	0.620170	-1.472505
12	1	0	-5.386009	0.010505	-0.934816
13	7	0	-3.935216	1.474731	-0.508105
14	6	0	-3.520567	-0.222448	-2.125484
15	1	0	-3.321734	0.167105	-3.132790
16	6	0	-5.164358	3.525764	0.018992
17	1	0	-4.992813	3.871107	-0.996436
18	6	0	-1.540987	1.803730	0.227145
19	6	0	-0.380754	3.434131	1.595625
20	1	0	-0.419687	4.229999	2.332603
21	6	0	-4.647125	2.291864	0.429243
22	6	0	4.157199	4.085822	-0.256607
23	1	0	3.744853	4.351820	-1.225524
24	6	0	-4.871978	1.836979	1.732006
25	1	0	-4.483911	0.870222	2.040980
26	6	0	4.546065	2.429358	1.469687
27	1	0	4.434775	1.413414	1.838340
28	6	0	-0.292063	1.412624	-0.253431
29	6	0	-1.576279	2.842179	1.174972
30	1	0	-2.514827	3.193137	1.584558
31	6	0	0.860976	3.042171	1.085013
32	1	0	1.762523	3.539417	1.422650
33	6	0	0.913630	2.012601	0.132396
34	6	0	-5.590628	2.631644	2.627004
35	1	0	-5.755978	2.275291	3.640464
36	6	0	-2.641164	1.106561	-0.472492
37	6	0	5.212023	3.388517	2.230401
38	1	0	5.619989	3.110643	3.199098
39	6	0	4.825621	5.036456	0.516440
40	1	0	4.930737	6.050429	0.139602
41	6	0	-6.108938	3.875166	2.239236
42	6	0	5.364903	4.706042	1.767752
43	6	0	-5.886794	4.304823	0.920168
44	1	0	-6.281746	5.264909	0.597040
45	6	0	-6.885607	4.736002	3.205626
46	1	0	-6.993708	4.247819	4.179118
47	1	0	-7.890312	4.954771	2.823244
48	1	0	-6.388055	5.701048	3.364841
49	6	0	6.106280	5.728684	2.593671

50	1	0	5.973671	6.738690	2.193577
51	1	0	7.183097	5.515043	2.609547
52	1	0	5.764111	5.723957	3.635036
53	1	0	-5.186669	1.238939	-2.198395
54	1	0	4.671432	0.158274	-0.847115
55	6	0	2.836896	0.663124	-3.760602
56	6	0	-3.869852	-1.728517	-2.286746
57	6	0	-5.144559	-1.823414	-3.152673
58	1	0	-5.381617	-2.874663	-3.353174
59	1	0	-6.016442	-1.380074	-2.658033
60	1	0	-5.010387	-1.322083	-4.119695
61	6	0	-2.729014	-2.437162	-3.035678
62	1	0	-2.535175	-1.958620	-4.004914
63	1	0	-1.799855	-2.431460	-2.462837
64	1	0	-2.992785	-3.483662	-3.230355
65	6	0	-4.120424	-2.412772	-0.931088
66	1	0	-3.264876	-2.308834	-0.258125
67	1	0	-5.002425	-2.007331	-0.422013
68	1	0	-4.299360	-3.483928	-1.080303
69	6	0	1.585839	0.035022	-4.402110
70	1	0	1.595900	-1.057569	-4.334755
71	1	0	0.658944	0.395896	-3.928672
72	1	0	1.528426	0.310006	-5.461816
73	6	0	4.077490	0.182018	-4.540442
74	1	0	5.006623	0.601788	-4.137507
75	1	0	4.162890	-0.911543	-4.518364
76	1	0	4.006540	0.491105	-5.589572
77	6	0	2.724451	2.195888	-3.856657
78	1	0	3.622769	2.705672	-3.491198
79	1	0	2.590132	2.491525	-4.903774
80	1	0	1.860114	2.574858	-3.297710
81	8	0	0.596128	-2.331891	-2.276290
82	8	0	-0.008663	-1.347123	0.116660
83	6	0	0.907293	-3.038763	-1.331417
84	6	0	0.644062	-2.643474	0.129747
85	8	0	1.481198	-4.216111	-1.410448
86	6	0	1.728951	-4.756060	-2.743330
87	1	0	2.177707	-5.732015	-2.568226
88	1	0	0.783347	-4.851232	-3.279626
89	1	0	2.416548	-4.101953	-3.282128
90	6	0	-0.416335	-3.624679	0.710205
91	9	0	-1.361886	-3.886333	-0.216830
92	9	0	-1.026605	-3.090851	1.778366
93	9	0	0.141737	-4.787010	1.065359

94	6	0	0.466587	-3.561138	5.606206
95	6	0	0.686670	-2.689928	4.540867
96	6	0	1.528073	-3.053237	3.472799
97	6	0	2.131685	-4.322716	3.501902
98	6	0	1.914943	-5.192109	4.572080
99	6	0	1.082234	-4.815992	5.627762
100	1	0	-0.193603	-3.263421	6.416288
101	1	0	0.184916	-1.726808	4.522985
102	1	0	2.794181	-4.633026	2.699532
103	1	0	2.399989	-6.164322	4.578627
104	1	0	0.908285	-5.496625	6.456532
105	6	0	1.804195	-2.091099	2.368104
106	6	0	1.925705	-0.770226	2.602342
107	1	0	1.838318	-0.355358	3.602043
108	1	0	2.184813	-0.073810	1.811178
109	1	0	0.210677	-0.876835	0.958539
110	6	0	1.965246	-2.601264	0.942168
111	1	0	2.646646	-1.949045	0.387394
112	1	0	2.389614	-3.606029	0.913639

M3S_{exo}

Total energy= -2678.05561456

Sum of electronic and zero-point Energies= -2677.123531

Sum of electronic and thermal Energies= -2677.067211

Sum of electronic and thermal Enthalpies= -2677.066267

Sum of electronic and thermal Free Energies= -2677.215867

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.163962	-0.556979	-1.431070
2	6	0	3.043976	-0.506038	-2.203539
3	1	0	3.195688	-1.543717	-1.897451
4	7	0	3.379009	1.508808	-0.978476
5	6	0	2.080928	1.171455	-0.954274
6	6	0	4.021071	2.622336	-0.343063
7	7	0	1.819893	0.015286	-1.555578
8	6	0	4.149487	0.402407	-1.594733
9	1	0	4.839162	0.802697	-2.340152
10	7	0	-2.270059	-0.366144	-1.285909
11	6	0	-4.621480	-0.112436	-1.358731
12	1	0	-5.081477	-0.655104	-0.522822
13	7	0	-3.931784	1.085600	-0.841806

14	6	0	-3.466015	-0.892532	-2.023926
15	1	0	-3.368776	-0.531309	-3.059165
16	6	0	-5.052019	3.257599	-0.978480
17	1	0	-4.781266	3.308539	-2.029191
18	6	0	-1.534763	1.714627	-0.320546
19	6	0	-0.407724	3.650301	0.600923
20	1	0	-0.460742	4.608300	1.108016
21	6	0	-4.656127	2.154240	-0.215630
22	6	0	4.300033	3.779628	-1.074531
23	1	0	4.002800	3.844023	-2.117080
24	6	0	-5.006832	2.074604	1.135338
25	1	0	-4.707667	1.212049	1.724351
26	6	0	4.402770	2.531242	1.000360
27	1	0	4.188251	1.626717	1.562766
28	6	0	-0.276522	1.229400	-0.677234
29	6	0	-1.593278	2.959440	0.333095
30	1	0	-2.540498	3.389723	0.634030
31	6	0	0.845414	3.146505	0.232049
32	1	0	1.739840	3.716701	0.453467
33	6	0	0.920424	1.907048	-0.421189
34	6	0	-5.736669	3.109862	1.721636
35	1	0	-6.000727	3.044984	2.774064
36	6	0	-2.614996	0.817133	-0.773683
37	6	0	5.048903	3.606495	1.607678
38	1	0	5.335872	3.532540	2.653718
39	6	0	4.947635	4.848660	-0.453578
40	1	0	5.155067	5.749911	-1.024820
41	6	0	-6.135058	4.229458	0.977161
42	6	0	5.333967	4.781140	0.893051
43	6	0	-5.780345	4.284502	-0.380680
44	1	0	-6.077451	5.143864	-0.976794
45	6	0	-6.940682	5.339589	1.606522
46	1	0	-6.944884	5.262714	2.698278
47	1	0	-7.984176	5.308821	1.266473
48	1	0	-6.544334	6.324359	1.333355
49	6	0	6.059236	5.927913	1.553852
50	1	0	5.905821	6.865494	1.010130
51	1	0	7.140765	5.739610	1.587693
52	1	0	5.724674	6.069662	2.587516
53	1	0	-5.399618	0.174459	-2.066863
54	1	0	4.730423	-0.106894	-0.818399
55	6	0	2.954661	-0.491304	-3.763902
56	6	0	-3.671749	-2.427846	-2.105634
57	6	0	-5.081763	-2.681695	-2.684036

58	1	0	-5.222725	-3.754002	-2.861270
59	1	0	-5.874828	-2.354639	-2.002354
60	1	0	-5.220875	-2.166498	-3.642672
61	6	0	-2.645094	-3.034372	-3.080748
62	1	0	-2.734245	-2.581517	-4.076474
63	1	0	-1.618243	-2.902545	-2.731139
64	1	0	-2.818391	-4.111874	-3.190523
65	6	0	-3.553425	-3.106635	-0.732206
66	1	0	-2.544999	-2.996189	-0.321662
67	1	0	-4.266496	-2.699251	-0.005990
68	1	0	-3.759903	-4.179533	-0.825725
69	6	0	1.736533	-1.322327	-4.203337
70	1	0	1.786188	-2.348599	-3.822279
71	1	0	0.796910	-0.873817	-3.845177
72	1	0	1.677690	-1.367409	-5.297170
73	6	0	4.230966	-1.155765	-4.317359
74	1	0	5.135823	-0.602878	-4.039152
75	1	0	4.336661	-2.183153	-3.947077
76	1	0	4.193749	-1.195293	-5.412103
77	6	0	2.820809	0.934996	-4.326748
78	1	0	3.687410	1.561443	-4.085818
79	1	0	2.742074	0.898977	-5.419614
80	1	0	1.920862	1.435522	-3.949906
81	8	0	0.306277	-2.941519	-1.490759
82	8	0	0.041606	-1.230267	0.503937
83	6	0	0.612783	-3.382699	-0.391163
84	6	0	0.530220	-2.533652	0.888056
85	8	0	1.032534	-4.598134	-0.144604
86	6	0	1.158774	-5.513619	-1.275568
87	1	0	1.534697	-6.438245	-0.842075
88	1	0	0.179014	-5.665585	-1.731732
89	1	0	1.865748	-5.105458	-1.999699
90	6	0	1.966003	-2.314332	1.448865
91	9	0	2.388438	-3.388569	2.126923
92	9	0	2.010939	-1.245696	2.254790
93	9	0	2.840179	-2.102765	0.438754
94	6	0	0.588279	-0.598074	6.059439
95	6	0	-0.101579	-0.780570	4.862456
96	6	0	-0.147437	-2.042565	4.241023
97	6	0	0.528780	-3.113310	4.851900
98	6	0	1.212851	-2.930345	6.054800
99	6	0	1.246505	-1.673935	6.662698
100	1	0	0.617523	0.386422	6.518304
101	1	0	-0.596121	0.064815	4.391991

102	1	0	0.505855	-4.102811	4.405487
103	1	0	1.718711	-3.773807	6.516553
104	1	0	1.785437	-1.531824	7.595316
105	6	0	-0.935770	-2.237784	2.992574
106	6	0	-2.097911	-1.586250	2.781761
107	1	0	-2.699582	-1.775109	1.895697
108	1	0	-2.515327	-0.909777	3.521594
109	1	0	-0.684655	-0.958065	1.121013
110	6	0	-0.443143	-3.190468	1.912412
111	1	0	-1.300449	-3.550971	1.339753
112	1	0	0.061513	-4.066790	2.321735

TS4*R*$_{endo}$

Imaginary frequency= -154.95

Total energy= -2678.04129539

Sum of electronic and zero-point Energies= -2677.111629

Sum of electronic and thermal Energies= -2677.055133

Sum of electronic and thermal Enthalpies= -2677.054189

Sum of electronic and thermal Free Energies= -2677.208537

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.560508	-0.278648	1.248926
2	6	0	-1.511472	2.076450	1.992541
3	1	0	-2.339325	1.463497	1.622847
4	7	0	-0.341515	3.635115	0.632493
5	6	0	0.322654	2.487986	0.634008
6	6	0	0.002621	4.855348	-0.045803
7	7	0	-0.281287	1.528021	1.391330
8	6	0	-1.591521	3.511731	1.415940
9	1	0	-1.613426	4.296276	2.175477
10	7	0	2.027025	-1.704826	1.034367
11	6	0	3.709531	-3.375204	1.029853
12	1	0	3.571016	-4.167159	0.286202
13	7	0	4.114798	-2.132717	0.337623
14	6	0	2.389706	-2.961652	1.728753
15	1	0	2.611458	-2.696305	2.774131
16	6	0	6.526371	-1.734399	0.299364
17	1	0	6.494424	-1.537899	1.367144
18	6	0	3.036600	0.118479	-0.145489
19	6	0	3.670879	2.206442	-1.205359
20	1	0	4.388885	2.776377	-1.786121

21	6	0	5.349364	-2.040942	-0.387598
22	6	0	-0.415519	5.052489	-1.364976
23	1	0	-0.973411	4.276032	-1.879663
24	6	0	5.381721	-2.304537	-1.761402
25	1	0	4.465758	-2.558784	-2.286652
26	6	0	0.710525	5.846399	0.636015
27	1	0	1.023802	5.683468	1.662890
28	6	0	1.853850	0.745794	0.258469
29	6	0	3.954559	0.868802	-0.901096
30	1	0	4.877283	0.426724	-1.258672
31	6	0	2.500590	2.831515	-0.766955
32	1	0	2.330970	3.878737	-0.993430
33	6	0	1.571680	2.090958	-0.015075
34	6	0	6.595233	-2.240198	-2.443956
35	1	0	6.615732	-2.445387	-3.511432
36	6	0	3.103543	-1.257377	0.368074
37	6	0	1.012323	7.040678	-0.019440
38	1	0	1.568546	7.810849	0.508132
39	6	0	-0.105123	6.251366	-2.003958
40	1	0	-0.424609	6.403788	-3.031611
41	6	0	7.790159	-1.926227	-1.776429
42	6	0	0.610492	7.264064	-1.344067
43	6	0	7.734089	-1.679921	-0.397254
44	1	0	8.647394	-1.440855	0.141938
45	6	0	9.094474	-1.846963	-2.530306
46	1	0	9.950499	-1.834044	-1.848668
47	1	0	9.141704	-0.934158	-3.140392
48	1	0	9.211850	-2.695167	-3.214228
49	6	0	0.918455	8.566588	-2.039890
50	1	0	0.029047	9.209305	-2.080266
51	1	0	1.241161	8.399395	-3.073730
52	1	0	1.705085	9.122294	-1.519070
53	1	0	4.489735	-3.681662	1.728992
54	1	0	-2.442723	3.654184	0.743448
55	6	0	-1.528001	1.974773	3.555926
56	6	0	1.269726	-4.034920	1.758479
57	6	0	1.822483	-5.286009	2.469032
58	1	0	1.037513	-6.045350	2.561992
59	1	0	2.652286	-5.739112	1.912438
60	1	0	2.180571	-5.048502	3.478911
61	6	0	0.086046	-3.487119	2.578545
62	1	0	0.398412	-3.217254	3.595003
63	1	0	-0.361510	-2.597732	2.111771
64	1	0	-0.703138	-4.244341	2.661857

65	6	0	0.793935	-4.406517	0.342403
66	1	0	0.459678	-3.518631	-0.203936
67	1	0	1.583200	-4.888755	-0.245139
68	1	0	-0.043352	-5.112452	0.402472
69	6	0	-1.401105	0.496625	3.964787
70	1	0	-2.196927	-0.113422	3.521345
71	1	0	-0.430363	0.071682	3.665147
72	1	0	-1.469560	0.398689	5.054571
73	6	0	-2.890265	2.508209	4.044777
74	1	0	-3.028371	3.569298	3.804878
75	1	0	-3.720599	1.949100	3.597765
76	1	0	-2.962069	2.405278	5.133569
77	6	0	-0.385071	2.778744	4.198642
78	1	0	-0.445310	3.848159	3.968153
79	1	0	-0.430059	2.678953	5.289500
80	1	0	0.597908	2.415001	3.875775
81	8	0	-0.166179	-1.142562	-1.125384
82	8	0	-2.354804	-1.075508	0.404077
83	6	0	-1.249829	-1.233100	-1.684505
84	6	0	-2.612697	-1.251246	-0.964193
85	8	0	-1.397211	-1.353609	-2.991884
86	6	0	-0.196284	-1.348571	-3.808692
87	1	0	-0.553797	-1.446631	-4.833918
88	1	0	0.340947	-0.408009	-3.675911
89	1	0	0.440256	-2.194933	-3.540782
90	6	0	-3.440155	-0.024635	-1.432575
91	9	0	-2.680848	1.099081	-1.386178
92	9	0	-4.488666	0.176602	-0.613334
93	9	0	-3.906060	-0.144663	-2.685601
94	6	0	-8.132825	-1.724350	-0.358200
95	6	0	-6.845103	-2.060220	0.056991
96	6	0	-5.878823	-2.504730	-0.865686
97	6	0	-6.244694	-2.584954	-2.221022
98	6	0	-7.536509	-2.254127	-2.635671
99	6	0	-8.485794	-1.821319	-1.706619
100	1	0	-8.858471	-1.375508	0.372223
101	1	0	-6.576082	-1.958626	1.104805
102	1	0	-5.530504	-2.933215	-2.960317
103	1	0	-7.799128	-2.335182	-3.686570
104	1	0	-9.488745	-1.557153	-2.031360
105	6	0	-4.519069	-2.908293	-0.405516
106	6	0	-4.331736	-3.528822	0.775942
107	1	0	-3.091270	-1.488071	0.901265
108	1	0	-5.161987	-3.780887	1.429389

109	1	0	-3.345514	-3.854385	1.095659
110	6	0	-3.308664	-2.615607	-1.277494
111	1	0	-2.551933	-3.386561	-1.103842
112	1	0	-3.551331	-2.635558	-2.340670

TS4*S*$_{endo}$

Imaginary frequency= -164.29

Total energy= -2678.03868729

Sum of electronic and zero-point Energies= -2677.108720

Sum of electronic and thermal Energies= -2677.052307

Sum of electronic and thermal Enthalpies= -2677.051363

Sum of electronic and thermal Free Energies= -2677.203080

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.582611	-0.310076	1.108295
2	6	0	-1.308215	2.205554	1.948291
3	1	0	-2.246705	1.699000	1.707235
4	7	0	-0.048803	3.710881	0.595056
5	6	0	0.493825	2.489738	0.538335
6	6	0	0.317735	4.876996	-0.157791
7	7	0	-0.222906	1.554202	1.176733
8	6	0	-1.311552	3.646485	1.363866
9	1	0	-1.323341	4.437831	2.115681
10	7	0	2.034292	-1.688593	1.133783
11	6	0	3.636272	-3.456107	1.179476
12	1	0	3.628193	-4.331951	0.526211
13	7	0	4.068446	-2.285142	0.389792
14	6	0	2.235359	-3.041489	1.702158
15	1	0	2.271015	-2.931832	2.791005
16	6	0	6.503274	-2.044013	0.467609
17	1	0	6.439368	-1.866234	1.537558
18	6	0	3.144879	0.014057	-0.146293
19	6	0	3.929802	2.075523	-1.137591
20	1	0	4.697354	2.627117	-1.665513
21	6	0	5.340393	-2.257585	-0.279046
22	6	0	0.052851	4.932989	-1.528722
23	1	0	-0.410563	4.086529	-2.024664
24	6	0	5.404755	-2.485099	-1.655028
25	1	0	4.492356	-2.662817	-2.221178
26	6	0	0.893865	5.971654	0.496796
27	1	0	1.094403	5.921868	1.562959

28	6	0	1.965495	0.679954	0.200947
29	6	0	4.146413	0.729044	-0.830798
30	1	0	5.084466	0.262055	-1.109674
31	6	0	2.757702	2.741085	-0.751783
32	1	0	2.637912	3.791056	-0.996702
33	6	0	1.757604	2.039320	-0.059039
34	6	0	6.645709	-2.478981	-2.286945
35	1	0	6.696601	-2.654358	-3.358163
36	6	0	3.144029	-1.335186	0.412826
37	6	0	1.209681	7.115555	-0.234425
38	1	0	1.660808	7.962386	0.276769
39	6	0	0.381341	6.083870	-2.245326
40	1	0	0.175758	6.123106	-3.311883
41	6	0	7.831024	-2.258141	-1.568690
42	6	0	0.964278	7.190367	-1.615688
43	6	0	7.735784	-2.038808	-0.184424
44	1	0	8.639388	-1.861894	0.393361
45	6	0	9.172769	-2.274949	-2.252296
46	1	0	9.789221	-1.423719	-1.941072
47	1	0	9.068283	-2.243553	-3.341139
48	1	0	9.733692	-3.185546	-2.000585
49	6	0	1.323279	8.433833	-2.390312
50	1	0	0.865044	9.325399	-1.945429
51	1	0	0.992602	8.365773	-3.431265
52	1	0	2.408211	8.599501	-2.391873
53	1	0	4.354182	-3.628675	1.987322
54	1	0	-2.151092	3.804547	0.678581
55	6	0	-1.125565	2.111617	3.497200
56	6	0	1.072410	-4.032952	1.389400
57	6	0	1.416146	-5.379585	2.062284
58	1	0	0.596158	-6.089305	1.911839
59	1	0	2.326490	-5.829422	1.646444
60	1	0	1.562675	-5.258841	3.144689
61	6	0	-0.230030	-3.495050	2.015850
62	1	0	-0.091092	-3.263741	3.082548
63	1	0	-0.601618	-2.591046	1.506713
64	1	0	-1.021229	-4.251259	1.939566
65	6	0	0.869447	-4.237084	-0.123002
66	1	0	0.581201	-3.305832	-0.624694
67	1	0	1.768615	-4.629025	-0.613557
68	1	0	0.063950	-4.957117	-0.292499
69	6	0	-1.160195	0.628373	3.916207
70	1	0	-2.066529	0.129450	3.550101
71	1	0	-0.289228	0.080724	3.532612

72	1	0	-1.149635	0.539074	5.008977
73	6	0	-2.314864	2.827627	4.167692
74	1	0	-2.342293	3.897893	3.935770
75	1	0	-3.272087	2.388845	3.859460
76	1	0	-2.240314	2.731359	5.257117
77	6	0	0.194908	2.749061	3.960876
78	1	0	0.243372	3.816969	3.717970
79	1	0	0.292098	2.658958	5.049171
80	1	0	1.063647	2.254561	3.512218
81	8	0	-0.516810	-0.450137	-1.244065
82	8	0	-2.485591	-0.801478	0.516161
83	6	0	-1.628797	-0.705133	-1.685161
84	6	0	-2.877650	-0.955520	-0.824681
85	8	0	-1.904663	-0.809097	-2.970921
86	6	0	-0.818418	-0.613667	-3.915986
87	1	0	-1.265372	-0.766657	-4.895931
88	1	0	-0.426022	0.400971	-3.825497
89	1	0	-0.029203	-1.346257	-3.731010
90	6	0	-3.308488	-2.437438	-1.020973
91	9	0	-3.940454	-2.644426	-2.191424
92	9	0	-4.133892	-2.820713	-0.030138
93	9	0	-2.235591	-3.262059	-0.989587
94	6	0	-8.221188	-2.313717	-0.093261
95	6	0	-7.111361	-1.541536	0.253902
96	6	0	-6.378070	-0.848487	-0.725055
97	6	0	-6.786850	-0.960447	-2.065613
98	6	0	-7.901586	-1.729237	-2.412093
99	6	0	-8.622920	-2.406602	-1.428717
100	1	0	-8.766754	-2.848933	0.682220
101	1	0	-6.793408	-1.495946	1.291476
102	1	0	-6.255514	-0.426371	-2.848630
103	1	0	-8.206369	-1.791027	-3.453729
104	1	0	-9.486263	-3.010754	-1.697155
105	6	0	-5.225142	0.014135	-0.341890
106	6	0	-5.246773	0.752509	0.783582
107	1	0	-4.422317	1.413486	1.044861
108	1	0	-6.109493	0.770651	1.444103
109	1	0	-3.295348	-0.678859	1.049055
110	6	0	-3.993859	0.058804	-1.234025
111	1	0	-3.531107	1.048300	-1.165136
112	1	0	-4.239951	-0.109966	-2.282330

TS4R_{exo}

Imaginary frequency= -159.93
Total energy= -2678.03228089
Sum of electronic and zero-point Energies= -2677.102941
Sum of electronic and thermal Energies= -2677.046227
Sum of electronic and thermal Enthalpies= -2677.045283
Sum of electronic and thermal Free Energies= -2677.199219

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.432017	-0.221195	-1.577515
2	6	0	-2.403062	-1.471538	-2.580414
3	1	0	-2.827784	-0.513855	-2.887953
4	7	0	-2.673834	-2.734408	-0.579444
5	6	0	-1.510630	-2.064841	-0.544201
6	6	0	-3.237372	-3.590299	0.427098
7	7	0	-1.354010	-1.224165	-1.565246
8	6	0	-3.449545	-2.276109	-1.754411
9	1	0	-3.866478	-3.139571	-2.277808
10	7	0	2.456050	0.078178	-1.215838
11	6	0	4.838585	0.185712	-1.124586
12	1	0	5.357169	1.056504	-0.716954
13	7	0	4.236333	-0.569903	-0.008683
14	6	0	3.621890	0.537557	-2.016887
15	1	0	3.638681	-0.085975	-2.918975
16	6	0	5.898366	-2.140694	0.853767
17	1	0	5.897510	-2.645525	-0.109478
18	6	0	1.907780	-1.318042	0.656089
19	6	0	0.973088	-2.862279	2.272088
20	1	0	1.086225	-3.450530	3.175950
21	6	0	5.048340	-1.051090	1.070341
22	6	0	-2.999428	-4.965796	0.392350
23	1	0	-2.364293	-5.386369	-0.382408
24	6	0	5.044611	-0.391295	2.303064
25	1	0	4.396527	0.469384	2.454985
26	6	0	-4.065541	-3.047678	1.419244
27	1	0	-4.257720	-1.978842	1.436784
28	6	0	0.678674	-1.347217	-0.007186
29	6	0	2.050871	-2.095087	1.819843
30	1	0	2.985770	-2.119075	2.364422
31	6	0	-0.240388	-2.909880	1.577052
32	1	0	-1.050539	-3.525454	1.947773
33	6	0	-0.392807	-2.149910	0.402690
34	6	0	5.879241	-0.844949	3.324888

35	1	0	5.875107	-0.329067	4.278681
36	6	0	2.905313	-0.569136	-0.123820
37	6	0	-4.632833	-3.882815	2.378077
38	1	0	-5.269371	-3.452986	3.148543
39	6	0	-3.572972	-5.791990	1.360506
40	1	0	-3.378022	-6.860720	1.333000
41	6	0	6.732675	-1.940466	3.134515
42	6	0	-4.396650	-5.267610	2.366099
43	6	0	6.726953	-2.580945	1.881957
44	1	0	7.380280	-3.432361	1.712639
45	6	0	7.643763	-2.426550	4.234759
46	1	0	7.552605	-1.807779	5.133579
47	1	0	8.693132	-2.408888	3.915651
48	1	0	7.410091	-3.461083	4.513931
49	6	0	-5.035517	-6.161684	3.400634
50	1	0	-4.620211	-7.173481	3.368260
51	1	0	-6.118043	-6.239212	3.235084
52	1	0	-4.895088	-5.764214	4.413344
53	1	0	5.571986	-0.442707	-1.642922
54	1	0	-4.273588	-1.637114	-1.416340
55	6	0	-1.869751	-2.184036	-3.864597
56	6	0	3.570602	2.015877	-2.500103
57	6	0	4.866210	2.298328	-3.287740
58	1	0	4.833661	3.312053	-3.707403
59	1	0	5.759989	2.238908	-2.654092
60	1	0	4.993213	1.595341	-4.119459
61	6	0	2.377162	2.188015	-3.454938
62	1	0	2.446697	1.496748	-4.305182
63	1	0	1.421856	2.019357	-2.949681
64	1	0	2.359395	3.207883	-3.856979
65	6	0	3.440864	2.995158	-1.320380
66	1	0	2.563188	2.771726	-0.707165
67	1	0	4.324149	2.981301	-0.670599
68	1	0	3.336211	4.021824	-1.696608
69	6	0	-0.753681	-1.332618	-4.499764
70	1	0	-1.067679	-0.298151	-4.663761
71	1	0	0.154099	-1.319623	-3.873399
72	1	0	-0.468897	-1.752874	-5.471261
73	6	0	-3.036710	-2.282652	-4.871880
74	1	0	-3.867635	-2.884686	-4.486961
75	1	0	-3.425630	-1.288876	-5.127375
76	1	0	-2.691043	-2.756328	-5.799918
77	6	0	-1.318530	-3.589389	-3.567025
78	1	0	-2.085348	-4.263521	-3.167773

79	1	0	-0.938391	-4.043368	-4.490178
80	1	0	-0.486210	-3.554270	-2.850981
81	8	0	-0.978089	1.861713	-2.467317
82	8	0	-0.489163	1.513450	0.072764
83	6	0	-1.593729	2.599108	-1.717146
84	6	0	-1.413816	2.563277	-0.194575
85	8	0	-2.443459	3.532792	-2.090853
86	6	0	-2.656431	3.711077	-3.520563
87	1	0	-3.371010	4.531746	-3.597638
88	1	0	-1.711764	3.970368	-4.005300
89	1	0	-3.071632	2.795833	-3.947867
90	6	0	-0.714990	3.894411	0.213920
91	9	0	0.242815	4.217609	-0.687261
92	9	0	-0.118949	3.775763	1.410510
93	9	0	-1.576160	4.922180	0.266893
94	6	0	-1.981702	4.376031	4.984228
95	6	0	-1.903080	3.315794	4.084241
96	6	0	-2.728660	3.267817	2.944588
97	6	0	-3.633694	4.323849	2.734842
98	6	0	-3.717225	5.383368	3.640800
99	6	0	-2.893633	5.415525	4.765207
100	1	0	-1.326702	4.398396	5.849909
101	1	0	-1.177885	2.522126	4.249965
102	1	0	-4.295905	4.313628	1.875279
103	1	0	-4.431072	6.183855	3.462324
104	1	0	-2.952871	6.244159	5.466052
105	6	0	-2.663974	2.106109	2.012181
106	6	0	-2.491527	0.849364	2.463084
107	1	0	-2.412786	0.626908	3.522812
108	1	0	-2.486901	-0.001246	1.786219
109	1	0	-0.630900	1.221840	1.000189
110	6	0	-2.780826	2.341840	0.511914
111	1	0	-3.227652	1.458547	0.043219
112	1	0	-3.422441	3.191822	0.279372

TS4*S*$_{exo}$

Imaginary frequency= -119.04
Total energy= -2678.03827686
Sum of electronic and zero-point Energies= -2677.108629
Sum of electronic and thermal Energies= -2677.052404
Sum of electronic and thermal Enthalpies= -2677.051460
Sum of electronic and thermal Free Energies= -2677.201300

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.002234	-0.329018	-1.419985
2	6	0	-3.137128	-0.532055	-2.125389
3	1	0	-3.217807	0.555974	-2.215999
4	7	0	-3.578461	-1.724062	-0.115412
5	6	0	-2.274623	-1.546224	-0.219862
6	6	0	-4.286446	-2.396500	0.942082
7	7	0	-1.925498	-0.811062	-1.327311
8	6	0	-4.288896	-1.079247	-1.242296
9	1	0	-4.918823	-1.824259	-1.732963
10	7	0	2.019392	-0.696245	-1.351969
11	6	0	4.321565	-1.235771	-1.494246
12	1	0	4.937795	-0.413377	-1.113534
13	7	0	3.645066	-1.895973	-0.362520
14	6	0	3.129739	-0.748497	-2.351131
15	1	0	2.865963	-1.554141	-3.054463
16	6	0	4.567662	-4.014838	0.441563
17	1	0	4.148024	-4.507740	-0.430565
18	6	0	1.287417	-1.991682	0.538980
19	6	0	0.106865	-3.210673	2.269205
20	1	0	0.134336	-3.844216	3.149493
21	6	0	4.370499	-2.642621	0.626818
22	6	0	-4.678394	-3.725530	0.774050
23	1	0	-4.431470	-4.253552	-0.142555
24	6	0	4.909410	-1.993873	1.739961
25	1	0	4.759735	-0.926597	1.874694
26	6	0	-4.594337	-1.699287	2.114355
27	1	0	-4.288325	-0.663644	2.227305
28	6	0	0.048087	-1.574806	0.045511
29	6	0	1.314264	-2.812478	1.680435
30	1	0	2.250920	-3.142255	2.114118
31	6	0	-1.130954	-2.836441	1.738379
32	1	0	-2.043386	-3.198431	2.197468
33	6	0	-1.163004	-2.006610	0.602750
34	6	0	5.637001	-2.730524	2.677217
35	1	0	6.051130	-2.224214	3.545018
36	6	0	2.363015	-1.529029	-0.340304
37	6	0	-5.293390	-2.352297	3.127296
38	1	0	-5.530971	-1.812270	4.040038
39	6	0	-5.375099	-4.362945	1.799875
40	1	0	-5.673791	-5.400509	1.673737
41	6	0	5.842906	-4.108153	2.517780

42	6	0	-5.694093	-3.690980	2.989013
43	6	0	5.295252	-4.735577	1.385837
44	1	0	5.442279	-5.803006	1.241980
45	6	0	6.641297	-4.900449	3.523987
46	1	0	6.863203	-4.306227	4.415729
47	1	0	7.596580	-5.230772	3.095906
48	1	0	6.102626	-5.802187	3.838169
49	6	0	-6.470000	-4.375825	4.088041
50	1	0	-6.494746	-5.463769	3.943470
51	1	0	-7.511548	-4.017814	4.111011
52	1	0	-6.034461	-4.164602	5.075012
53	1	0	4.963157	-1.950229	-2.011400
54	1	0	-4.930788	-0.286412	-0.847715
55	6	0	-3.069570	-1.109783	-3.581558
56	6	0	3.404178	0.521119	-3.199213
57	6	0	4.700986	0.273574	-4.001098
58	1	0	4.871383	1.103166	-4.696581
59	1	0	5.582419	0.201917	-3.353909
60	1	0	4.635594	-0.648238	-4.592392
61	6	0	2.253945	0.723654	-4.202627
62	1	0	2.147308	-0.147232	-4.861649
63	1	0	1.301672	0.891223	-3.694602
64	1	0	2.452628	1.598385	-4.833142
65	6	0	3.570866	1.778831	-2.329771
66	1	0	2.666622	1.990156	-1.750647
67	1	0	4.410643	1.690905	-1.629984
68	1	0	3.770717	2.647175	-2.968645
69	6	0	-1.872914	-0.480560	-4.314986
70	1	0	-1.936257	0.612992	-4.325461
71	1	0	-0.916983	-0.760153	-3.851006
72	1	0	-1.846718	-0.830563	-5.353657
73	6	0	-4.365631	-0.699553	-4.307034
74	1	0	-5.256734	-1.141223	-3.846384
75	1	0	-4.491717	0.390000	-4.315648
76	1	0	-4.331516	-1.041489	-5.347641
77	6	0	-2.924799	-2.642061	-3.585742
78	1	0	-3.767080	-3.143682	-3.095148
79	1	0	-2.889944	-3.005079	-4.619211
80	1	0	-1.999998	-2.964115	-3.092580
81	8	0	-0.276972	1.963397	-2.360895
82	8	0	0.403303	1.695751	0.200553
83	6	0	-0.368267	2.963357	-1.663036
84	6	0	-0.077777	2.976837	-0.145084
85	8	0	-0.730947	4.151103	-2.100659

86	6	0	-1.067248	4.277610	-3.510195
87	1	0	-1.311376	5.329845	-3.646983
88	1	0	-0.209066	3.997122	-4.123843
89	1	0	-1.928324	3.647793	-3.742005
90	6	0	-1.441059	3.147815	0.579481
91	9	0	-1.907465	4.403705	0.502982
92	9	0	-1.354391	2.802197	1.871498
93	9	0	-2.371520	2.337711	0.007002
94	6	0	0.279132	4.721654	5.086755
95	6	0	0.869392	4.077563	4.000503
96	6	0	0.881776	4.673590	2.725732
97	6	0	0.273216	5.932158	2.574245
98	6	0	-0.313194	6.578676	3.663694
99	6	0	-0.314338	5.976789	4.923465
100	1	0	0.274136	4.238402	6.060107
101	1	0	1.305598	3.091833	4.134555
102	1	0	0.277326	6.428912	1.608785
103	1	0	-0.768632	7.555571	3.525186
104	1	0	-0.777665	6.477535	5.769124
105	6	0	1.550640	3.997720	1.577850
106	6	0	2.681858	3.284432	1.741774
107	1	0	3.191217	2.824268	0.897619
108	1	0	3.163860	3.185994	2.710128
109	1	0	1.153496	1.794500	0.825441
110	6	0	0.948623	4.103663	0.185093
111	1	0	1.748723	4.011297	-0.555018
112	1	0	0.461744	5.064669	0.016766

TS1S_A

Imaginary frequency= -402.31
Total energy= -1028.35771827
Sum of electronic and zero-point Energies= -1028.118639
Sum of electronic and thermal Energies= -1028.101359
Sum of electronic and thermal Enthalpies= -1028.100415
Sum of electronic and thermal Free Energies= -1028.164584

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.292952	1.452527	1.311193
2	1	0	-0.032310	2.182904	1.025397
3	6	0	1.348096	0.510470	0.408499
4	6	0	2.713578	0.491270	-0.345462

5	6	0	0.254781	0.757049	-0.936056
6	1	0	0.232074	-0.149672	-1.535087
7	1	0	0.791274	1.550365	-1.459218
8	6	0	-1.010949	1.244617	-0.426188
9	6	0	-0.887079	2.506440	0.252477
10	1	0	-1.761977	2.903234	0.763801
11	1	0	-0.342779	3.275290	-0.303295
12	6	0	0.996765	-0.866724	1.037773
13	9	0	0.818699	-1.887330	0.163063
14	9	0	-0.144548	-0.769129	1.753870
15	9	0	1.974718	-1.250405	1.890421
16	8	0	3.437225	1.458334	-0.412710
17	8	0	2.967685	-0.688017	-0.931260
18	6	0	-2.235957	0.449716	-0.399128
19	6	0	-2.244011	-0.932998	-0.698167
20	6	0	-3.474627	1.075003	-0.123884
21	6	0	-3.430807	-1.656151	-0.694750
22	1	0	-1.316547	-1.453212	-0.902144
23	6	0	-4.661209	0.349493	-0.133534
24	1	0	-3.512517	2.141113	0.068833
25	6	0	-4.644068	-1.019294	-0.413855
26	1	0	-3.411360	-2.719942	-0.913024
27	1	0	-5.601105	0.853662	0.071829
28	1	0	-5.570942	-1.586074	-0.420411
29	6	0	4.207157	-0.773798	-1.668813
30	1	0	4.241974	-1.790064	-2.061841
31	1	0	4.213822	-0.047057	-2.485106
32	1	0	5.057660	-0.592089	-1.007169

TS1R_B

Imaginary frequency= -401.96
Total energy= -1028.35771808
Sum of electronic and zero-point Energies= -1028.118639
Sum of electronic and thermal Energies= -1028.101358
Sum of electronic and thermal Enthalpies= -1028.100413
Sum of electronic and thermal Free Energies= -1028.164590

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.292432	1.448862	1.314509
2	1	0	0.032468	2.180271	1.029544
3	6	0	-1.348064	0.508881	0.409691

4	6	0	-2.713269	0.492770	-0.344726
5	6	0	-0.254559	0.757929	-0.934586
6	1	0	-0.231705	-0.147872	-1.535034
7	1	0	-0.791274	1.551972	-1.456394
8	6	0	1.011044	1.244939	-0.423988
9	6	0	0.886758	2.505537	0.256886
10	1	0	0.341899	3.275035	-0.297441
11	1	0	1.761601	2.901897	0.768622
12	6	0	-0.997185	-0.869836	1.035818
13	9	0	-1.973882	-1.253887	1.889680
14	9	0	0.145636	-0.774874	1.749935
15	9	0	-0.821944	-1.889033	0.158918
16	8	0	-3.433640	1.462188	-0.413589
17	8	0	-2.970960	-0.686322	-0.929276
18	6	0	2.236366	0.450447	-0.398433
19	6	0	2.244943	-0.931733	-0.699921
20	6	0	3.474803	1.075665	-0.121956
21	6	0	3.431997	-1.654470	-0.697696
22	1	0	1.317708	-1.451983	-0.904904
23	6	0	4.661642	0.350589	-0.132789
24	1	0	3.512329	2.141442	0.072687
25	6	0	4.645010	-1.017702	-0.415535
26	1	0	3.412936	-2.717880	-0.917852
27	1	0	5.601337	0.854733	0.073557
28	1	0	5.572079	-1.584154	-0.422976
29	6	0	-4.209636	-0.768250	-1.668608
30	1	0	-4.247234	-1.784462	-2.061519
31	1	0	-5.060514	-0.583717	-1.008232
32	1	0	-4.212771	-0.041550	-2.484946

P*R*

Total energy= -1028.40085728
Sum of electronic and zero-point Energies= -1028.157582
Sum of electronic and thermal Energies= -1028.139650
Sum of electronic and thermal Enthalpies= -1028.138706
Sum of electronic and thermal Free Energies= -1028.204319

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.500880	1.572106	1.191118
2	1	0	-0.606135	1.786479	1.519027
3	6	0	-1.357079	0.517104	0.276775

4	6	0	-2.709446	0.409466	-0.467670
5	6	0	-0.232016	0.769795	-0.785241
6	1	0	-0.098034	-0.136968	-1.377254
7	1	0	-0.639643	1.529484	-1.460603
8	6	0	1.097176	1.294531	-0.245863
9	6	0	1.153725	2.557624	0.221973
10	1	0	0.297308	3.223992	0.166191
11	1	0	2.057352	2.975753	0.655052
12	6	0	-1.138109	-0.768104	1.110213
13	9	0	-2.223783	-1.034516	1.866032
14	9	0	-0.089968	-0.610837	1.950507
15	9	0	-0.891868	-1.867426	0.365903
16	8	0	-3.616621	1.197694	-0.344105
17	8	0	-2.717221	-0.649479	-1.285848
18	6	0	2.319075	0.439569	-0.305982
19	6	0	2.265759	-0.966115	-0.269290
20	6	0	3.589294	1.039711	-0.426507
21	6	0	3.430670	-1.733898	-0.319364
22	1	0	1.315654	-1.479209	-0.189042
23	6	0	4.751816	0.273726	-0.475575
24	1	0	3.665788	2.119235	-0.510327
25	6	0	4.679975	-1.120480	-0.417866
26	1	0	3.356145	-2.817560	-0.280901
27	1	0	5.714860	0.768001	-0.574181
28	1	0	5.585424	-1.719700	-0.462385
29	6	0	-3.929773	-0.854043	-2.046684
30	1	0	-3.747097	-1.745484	-2.646373
31	1	0	-4.775937	-1.012117	-1.373723
32	1	0	-4.123741	0.007231	-2.690300

P*S*

Total energy= -1028.40085728
Sum of electronic and zero-point Energies= -1028.157582
Sum of electronic and thermal Energies= -1028.139650
Sum of electronic and thermal Enthalpies= -1028.138706
Sum of electronic and thermal Free Energies= -1028.204319

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.500880	1.572106	1.191118
2	1	0	0.606135	1.786479	1.519027
3	6	0	1.357079	0.517104	0.276775

4	6	0	2.709446	0.409466	-0.467670
5	6	0	0.232016	0.769795	-0.785241
6	1	0	0.098034	-0.136969	-1.377254
7	1	0	0.639643	1.529484	-1.460603
8	6	0	-1.097176	1.294531	-0.245863
9	6	0	-1.153725	2.557624	0.221973
10	1	0	-2.057352	2.975753	0.655052
11	1	0	-0.297308	3.223992	0.166191
12	6	0	1.138109	-0.768104	1.110213
13	9	0	0.891868	-1.867426	0.365903
14	9	0	0.089968	-0.610836	1.950508
15	9	0	2.223783	-1.034516	1.866032
16	8	0	3.616621	1.197694	-0.344106
17	8	0	2.717221	-0.649480	-1.285848
18	6	0	-2.319075	0.439569	-0.305981
19	6	0	-2.265759	-0.966115	-0.269290
20	6	0	-3.589294	1.039711	-0.426507
21	6	0	-3.430670	-1.733898	-0.319364
22	1	0	-1.315654	-1.479209	-0.189042
23	6	0	-4.751816	0.273726	-0.475575
24	1	0	-3.665788	2.119235	-0.510328
25	6	0	-4.679975	-1.120480	-0.417866
26	1	0	-3.356145	-2.817560	-0.280900
27	1	0	-5.714860	0.768001	-0.574182
28	1	0	-5.585424	-1.719700	-0.462385
29	6	0	3.929773	-0.854044	-2.046684
30	1	0	3.747096	-1.745484	-2.646373
31	1	0	4.123740	0.007230	-2.690301
32	1	0	4.775937	-1.012117	-1.373724

M1$_{endo}$-Cl

Total energy= -2789.49735783

Sum of electronic and zero-point Energies= -2788.731521

Sum of electronic and thermal Energies= -2788.681128

Sum of electronic and thermal Enthalpies= -2788.680184

Sum of electronic and thermal Free Energies= -2788.817765

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.075661	-0.890221	-0.803306
2	6	0	3.266212	-0.595727	-0.795352
3	1	0	3.377302	-1.294128	0.044316

4	7	0	3.114233	1.683700	-0.126965
5	6	0	1.879613	1.176702	-0.355831
6	6	0	3.487662	3.054239	0.054802
7	7	0	1.873511	-0.082389	-0.759629
8	6	0	4.120794	0.673379	-0.512285
9	1	0	4.663173	1.026287	-1.395509
10	7	0	-2.154367	-1.033552	-0.633792
11	6	0	-4.507596	-1.269132	-0.757553
12	1	0	-4.971012	-1.687743	0.143958
13	7	0	-4.073014	0.118765	-0.484673
14	6	0	-3.179005	-1.976449	-1.135261
15	1	0	-3.087180	-1.998132	-2.230675
16	6	0	-5.637947	1.929492	-0.978668
17	1	0	-5.394226	1.823032	-2.031876
18	6	0	-1.827731	1.263446	-0.086842
19	6	0	-1.071026	3.480359	0.518899
20	1	0	-1.300781	4.491533	0.839974
21	6	0	-5.003273	1.113140	-0.039021
22	6	0	4.001180	3.465759	1.289862
23	1	0	4.076536	2.750252	2.103957
24	6	0	-5.314678	1.242030	1.320375
25	1	0	-4.827771	0.600963	2.050129
26	6	0	3.391315	3.969711	-0.998477
27	1	0	3.003282	3.646785	-1.960534
28	6	0	-0.486664	0.922903	-0.298724
29	6	0	-2.118744	2.574179	0.322883
30	1	0	-3.140262	2.893403	0.491956
31	6	0	0.264731	3.119050	0.315406
32	1	0	1.045206	3.849754	0.488535
33	6	0	0.572472	1.816125	-0.111932
34	6	0	-6.242152	2.198604	1.730133
35	1	0	-6.472569	2.298674	2.788211
36	6	0	-2.725256	0.128590	-0.367164
37	6	0	3.784379	5.294716	-0.802349
38	1	0	3.696146	6.002930	-1.622409
39	6	0	4.397900	4.789487	1.470516
40	1	0	4.786761	5.102102	2.436624
41	6	0	-6.884451	3.033496	0.801202
42	6	0	4.294010	5.727257	0.430549
43	6	0	-6.566919	2.881741	-0.556064
44	1	0	-7.049140	3.518909	-1.293103
45	6	0	-7.902709	4.050727	1.256658
46	1	0	-7.564037	4.580533	2.154355
47	1	0	-8.856154	3.567866	1.509456

48	1	0	-8.105350	4.791965	0.477091
49	6	0	4.741100	7.154584	0.633769
50	1	0	4.346895	7.813057	-0.146733
51	1	0	5.836315	7.231898	0.609558
52	1	0	4.414325	7.540966	1.606019
53	1	0	-5.241506	-1.283740	-1.565783
54	1	0	4.840134	0.524517	0.296586
55	6	0	3.670939	-1.374766	-2.080430
56	6	0	-3.020347	-3.436084	-0.634236
57	6	0	-4.203249	-4.263855	-1.175269
58	1	0	-4.081916	-5.320033	-0.907025
59	1	0	-5.162241	-3.928129	-0.762632
60	1	0	-4.264784	-4.202881	-2.269144
61	6	0	-1.710794	-4.008274	-1.208886
62	1	0	-1.718634	-3.991199	-2.305952
63	1	0	-0.838303	-3.438848	-0.864736
64	1	0	-1.569851	-5.047916	-0.889185
65	6	0	-2.985779	-3.517729	0.902118
66	1	0	-2.156578	-2.931489	1.313964
67	1	0	-3.914058	-3.154375	1.358949
68	1	0	-2.853528	-4.559145	1.219178
69	6	0	2.824875	-2.657313	-2.182291
70	1	0	2.990678	-3.312889	-1.319622
71	1	0	1.754833	-2.428624	-2.244356
72	1	0	3.093280	-3.221505	-3.083845
73	6	0	5.152281	-1.782124	-1.935650
74	1	0	5.821762	-0.913985	-1.915208
75	1	0	5.319250	-2.361220	-1.018096
76	1	0	5.454908	-2.408147	-2.783332
77	6	0	3.481358	-0.532214	-3.353248
78	1	0	4.083477	0.384160	-3.340919
79	1	0	3.792991	-1.110856	-4.231360
80	1	0	2.432641	-0.250751	-3.490065
81	8	0	0.092910	-1.299426	1.341639
82	8	0	1.254387	-3.833365	0.585543
83	6	0	0.767110	-2.025322	2.066750
84	6	0	1.614929	-3.188089	1.533553
85	8	0	0.822209	-1.936500	3.367795
86	6	0	0.024736	-0.900589	4.022711
87	1	0	0.237873	-1.017279	5.083185
88	1	0	0.339937	0.079874	3.661454
89	1	0	-1.032025	-1.073415	3.811972
90	6	0	2.966927	-3.468859	2.237151
91	9	0	3.612941	-2.302264	2.436646

92	9	0	3.722684	-4.255565	1.470946
93	9	0	2.776014	-4.060666	3.422494
94	17	0	-0.351861	-0.387476	-3.071444

M1$_{exo}$-Cl

Total energy= -2789.49547150

Sum of electronic and zero-point Energies= -2788.730673

Sum of electronic and thermal Energies= -2788.681627

Sum of electronic and thermal Enthalpies= -2788.680683

Sum of electronic and thermal Free Energies= -2788.814574

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.057440	-0.903119	-0.859900
2	6	0	3.301437	-0.942502	-0.934463
3	1	0	3.324607	-1.774813	-0.219863
4	7	0	3.389343	1.276433	-0.055446
5	6	0	2.109337	0.922578	-0.314317
6	6	0	3.916446	2.582316	0.195405
7	7	0	1.970695	-0.292322	-0.817859
8	6	0	4.283252	0.172182	-0.462561
9	1	0	4.943496	0.523516	-1.260516
10	7	0	-2.136286	-0.837966	-0.677312
11	6	0	-4.498433	-0.787080	-0.886552
12	1	0	-5.059122	-1.191843	-0.036060
13	7	0	-3.913119	0.518138	-0.514636
14	6	0	-3.247316	-1.637157	-1.243981
15	1	0	-3.116674	-1.642615	-2.335071
16	6	0	-4.962689	2.646253	-1.113964
17	1	0	-4.505811	2.573271	-2.096754
18	6	0	-1.569954	1.378205	-0.004670
19	6	0	-0.581169	3.434418	0.797034
20	1	0	-0.700053	4.427959	1.217762
21	6	0	-4.727854	1.643425	-0.167417
22	6	0	3.826324	3.590865	-0.773371
23	1	0	3.320200	3.391280	-1.713763
24	6	0	-5.325437	1.720768	1.094855
25	1	0	-5.147734	0.936046	1.825034
26	6	0	4.586364	2.831139	1.396261
27	1	0	4.658489	2.046683	2.144388
28	6	0	-0.273463	0.915665	-0.251754
29	6	0	-1.720342	2.668444	0.527818

30	1	0	-2.701897	3.074360	0.741686
31	6	0	0.707792	2.955148	0.542398
32	1	0	1.562267	3.578682	0.775045
33	6	0	0.875585	1.671945	-0.005667
34	6	0	-6.141963	2.807806	1.408364
35	1	0	-6.602081	2.862231	2.391795
36	6	0	-2.580448	0.370140	-0.369641
37	6	0	5.151360	4.086145	1.629773
38	1	0	5.668975	4.270363	2.567772
39	6	0	4.381520	4.843789	-0.521464
40	1	0	4.300513	5.622485	-1.276252
41	6	0	-6.378599	3.830879	0.477648
42	6	0	5.055071	5.113693	0.681384
43	6	0	-5.777936	3.729343	-0.786823
44	1	0	-5.953301	4.506273	-1.526883
45	6	0	-7.236344	5.021226	0.833401
46	1	0	-6.618382	5.861422	1.178460
47	1	0	-7.939731	4.781511	1.637561
48	1	0	-7.808505	5.375195	-0.031139
49	6	0	5.653622	6.475668	0.937326
50	1	0	6.185027	6.506065	1.893607
51	1	0	4.878331	7.252247	0.957318
52	1	0	6.362252	6.753314	0.147199
53	1	0	-5.182862	-0.665807	-1.728783
54	1	0	4.902568	-0.142673	0.381661
55	6	0	3.642370	-1.546291	-2.331199
56	6	0	-3.289376	-3.118228	-0.779351
57	6	0	-4.547409	-3.778147	-1.379370
58	1	0	-4.557857	-4.850182	-1.149737
59	1	0	-5.470393	-3.346229	-0.974659
60	1	0	-4.572141	-3.671090	-2.471134
61	6	0	-2.045114	-3.841176	-1.327889
62	1	0	-2.015217	-3.802520	-2.424147
63	1	0	-1.117242	-3.394583	-0.948404
64	1	0	-2.049366	-4.896633	-1.029390
65	6	0	-3.322677	-3.238303	0.753853
66	1	0	-2.441714	-2.774436	1.210918
67	1	0	-4.211372	-2.764113	1.186467
68	1	0	-3.340101	-4.294459	1.048375
69	6	0	2.663407	-2.690602	-2.651854
70	1	0	2.689789	-3.466930	-1.879053
71	1	0	1.635048	-2.325014	-2.738072
72	1	0	2.929106	-3.157336	-3.608445
73	6	0	5.065751	-2.137173	-2.250480

74	1	0	5.826918	-1.369727	-2.066844
75	1	0	5.142544	-2.887151	-1.452556
76	1	0	5.321859	-2.630984	-3.195196
77	6	0	3.578627	-0.489649	-3.447645
78	1	0	4.287594	0.331305	-3.285996
79	1	0	3.831719	-0.949703	-4.410534
80	1	0	2.573563	-0.064566	-3.533185
81	8	0	1.214457	-3.845972	0.254763
82	8	0	0.106714	-1.437167	1.211539
83	6	0	1.284893	-3.533061	1.422735
84	6	0	0.594083	-2.271040	1.951579
85	8	0	1.917272	-4.166414	2.392522
86	6	0	2.609888	-5.394206	2.030795
87	1	0	3.098548	-5.723308	2.946001
88	1	0	1.883575	-6.134227	1.687952
89	1	0	3.342320	-5.186690	1.248454
90	6	0	0.474011	-2.036195	3.476223
91	9	0	-0.119356	-3.089002	4.055298
92	9	0	-0.253437	-0.942924	3.717984
93	9	0	1.693645	-1.869896	4.007448
94	17	0	-0.302957	-0.275926	-3.085555

TS2R_{endo}-Cl

Imaginary frequency= -156.91
Total energy= -3138.45209039
Sum of electronic and zero-point Energies= -3137.523241
Sum of electronic and thermal Energies= -3137.464354
Sum of electronic and thermal Enthalpies= -3137.463410
Sum of electronic and thermal Free Energies= -3137.619644

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.513716	-0.281577	1.187340
2	6	0	-1.354146	2.492313	1.541948
3	1	0	-2.215030	1.971248	1.118383
4	7	0	0.197650	3.747735	0.233945
5	6	0	0.666067	2.496801	0.442370
6	6	0	0.832868	4.858635	-0.401832
7	7	0	-0.137382	1.728112	1.155994
8	6	0	-1.155029	3.859824	0.817085
9	1	0	-1.189711	4.716560	1.494510
10	7	0	1.692033	-1.975670	0.861448

11	6	0	3.069307	-3.900714	0.860557
12	1	0	2.848263	-4.613381	0.055137
13	7	0	3.733543	-2.708270	0.292267
14	6	0	1.791361	-3.302669	1.504796
15	1	0	1.981569	-3.125357	2.574626
16	6	0	6.172957	-2.582342	0.179871
17	1	0	6.184999	-2.294013	1.229040
18	6	0	3.023533	-0.307447	-0.197247
19	6	0	3.995254	1.629426	-1.273434
20	1	0	4.793125	2.069984	-1.865428
21	6	0	4.953010	-2.814963	-0.454959
22	6	0	0.446141	5.235885	-1.694384
23	1	0	-0.313987	4.660252	-2.216229
24	6	0	4.928407	-3.190234	-1.804246
25	1	0	3.976816	-3.374861	-2.296790
26	6	0	1.808814	5.601105	0.272383
27	1	0	2.100894	5.316277	1.279644
28	6	0	1.974679	0.520208	0.224053
29	6	0	4.054937	0.268880	-0.957470
30	1	0	4.890892	-0.326017	-1.305769
31	6	0	2.933755	2.438704	-0.854225
32	1	0	2.924602	3.487509	-1.128519
33	6	0	1.900851	1.882414	-0.081488
34	6	0	6.123504	-3.310747	-2.510636
35	1	0	6.096744	-3.595759	-3.559780
36	6	0	2.841126	-1.689979	0.276021
37	6	0	2.407845	6.694275	-0.354947
38	1	0	3.172823	7.257951	0.174160
39	6	0	1.045312	6.334209	-2.306834
40	1	0	0.741431	6.613863	-3.314098
41	6	0	7.361446	-3.072439	-1.889353
42	6	0	2.036914	7.081459	-1.651525
43	6	0	7.365645	-2.705808	-0.536477
44	1	0	8.309971	-2.515720	-0.037159
45	6	0	8.648911	-3.220691	-2.663103
46	1	0	8.604271	-2.682939	-3.618769
47	1	0	8.851275	-4.274347	-2.896264
48	1	0	9.502327	-2.835834	-2.096140
49	6	0	2.671237	8.276239	-2.320421
50	1	0	3.583182	8.586542	-1.802555
51	1	0	1.985565	9.136029	-2.327690
52	1	0	2.925804	8.062569	-3.364505
53	1	0	3.723938	-4.389075	1.586408
54	1	0	-1.892501	4.019107	0.023389

55	6	0	-1.612619	2.611592	3.076230
56	6	0	0.507502	-4.168408	1.411346
57	6	0	0.793567	-5.527497	2.081521
58	1	0	-0.111665	-6.145229	2.095651
59	1	0	1.567471	-6.093021	1.545508
60	1	0	1.127565	-5.398631	3.118818
61	6	0	-0.619918	-3.462093	2.187846
62	1	0	-0.336483	-3.292823	3.233702
63	1	0	-0.876210	-2.488740	1.747227
64	1	0	-1.530181	-4.074674	2.184433
65	6	0	0.070047	-4.390499	-0.046535
66	1	0	-0.108439	-3.437670	-0.557051
67	1	0	0.818621	-4.944509	-0.625177
68	1	0	-0.857714	-4.974778	-0.077429
69	6	0	-1.883237	1.214076	3.666948
70	1	0	-2.716836	0.722247	3.151416
71	1	0	-1.003654	0.570055	3.594108
72	1	0	-2.143432	1.300468	4.730987
73	6	0	-2.885805	3.461954	3.278856
74	1	0	-2.761882	4.495251	2.939720
75	1	0	-3.742609	3.029095	2.744243
76	1	0	-3.144448	3.498125	4.345077
77	6	0	-0.423489	3.263556	3.805368
78	1	0	-0.227706	4.281528	3.444301
79	1	0	-0.632845	3.335536	4.879112
80	1	0	0.488863	2.671871	3.677328
81	8	0	-0.391023	-0.613343	-0.745206
82	8	0	-2.707004	-0.540205	0.793677
83	6	0	-1.507632	-0.620911	-1.268288
84	6	0	-2.832443	-0.582210	-0.458263
85	8	0	-1.660163	-0.648639	-2.574294
86	6	0	-0.465336	-0.637398	-3.403917
87	1	0	-0.837046	-0.622616	-4.427903
88	1	0	0.124582	0.256334	-3.192598
89	1	0	0.121402	-1.537322	-3.217693
90	6	0	-3.829738	0.457904	-1.056075
91	9	0	-3.201330	1.663447	-1.128371
92	9	0	-4.887035	0.599598	-0.243755
93	9	0	-4.287261	0.185110	-2.290930
94	6	0	-8.418430	-1.621634	-0.919509
95	6	0	-7.199785	-1.854913	-0.292300
96	6	0	-6.059148	-2.227146	-1.043423
97	6	0	-6.197580	-2.374267	-2.444145
98	6	0	-7.423857	-2.160386	-3.063066

99	6	0	-8.535490	-1.777417	-2.304639
100	1	0	-9.278568	-1.320425	-0.328949
101	1	0	-7.123449	-1.712753	0.779940
102	1	0	-5.352969	-2.697754	-3.042548
103	1	0	-7.516414	-2.296409	-4.136526
104	1	0	-9.492366	-1.608451	-2.790532
105	6	0	-4.773066	-2.459963	-0.392476
106	6	0	-4.668858	-2.745851	1.060251
107	1	0	-4.140780	-1.877584	1.508886
108	1	0	-5.617909	-2.913802	1.567389
109	1	0	-4.007219	-3.601440	1.234574
110	6	0	-3.548194	-2.293522	-1.070392
111	1	0	-2.717451	-2.879686	-0.682511
112	1	0	-3.557118	-2.191001	-2.149396
113	17	0	1.631794	-0.027879	3.241615

TS2S_{endo}-Cl

Imaginary frequency= -157.58
Total energy= -3138.44969544
Sum of electronic and zero-point Energies= -3137.521487
Sum of electronic and thermal Energies= -3137.462239
Sum of electronic and thermal Enthalpies= -3137.461295
Sum of electronic and thermal Free Energies= -3137.618482

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.550004	-0.208461	1.199317
2	6	0	-1.553330	2.387947	1.628109
3	1	0	-2.360037	1.808149	1.163252
4	7	0	-0.144242	3.792190	0.311795
5	6	0	0.446289	2.594146	0.517196
6	6	0	0.324362	4.918526	-0.435831
7	7	0	-0.267055	1.752712	1.244171
8	6	0	-1.467933	3.796146	0.960933
9	1	0	-1.516546	4.616338	1.682076
10	7	0	1.882610	-1.789982	0.809904
11	6	0	3.487721	-3.542649	0.813424
12	1	0	3.380093	-4.285515	0.014559
13	7	0	4.000228	-2.280928	0.241992
14	6	0	2.128107	-3.115430	1.429870
15	1	0	2.265145	-2.941204	2.506216
16	6	0	6.425339	-1.966151	0.194365

17	1	0	6.395694	-1.749564	1.258410
18	6	0	3.050359	0.038699	-0.187371
19	6	0	3.864862	2.098708	-1.161704
20	1	0	4.632676	2.633812	-1.711749
21	6	0	5.233587	-2.242972	-0.485593
22	6	0	-0.026793	5.055460	-1.782246
23	1	0	-0.626371	4.286746	-2.262167
24	6	0	5.264135	-2.527862	-1.854268
25	1	0	4.341108	-2.752596	-2.381741
26	6	0	1.084605	5.914506	0.189149
27	1	0	1.345365	5.811472	1.238726
28	6	0	1.924335	0.746886	0.247245
29	6	0	4.038737	0.735710	-0.901042
30	1	0	4.932353	0.234761	-1.253474
31	6	0	2.726339	2.789872	-0.734587
32	1	0	2.628064	3.844822	-0.960418
33	6	0	1.731802	2.107558	-0.014800
34	6	0	6.481552	-2.516665	-2.538044
35	1	0	6.495818	-2.733771	-3.603199
36	6	0	3.001733	-1.368322	0.243636
37	6	0	1.504632	7.025763	-0.540222
38	1	0	2.098487	7.792560	-0.048581
39	6	0	0.396470	6.174428	-2.501172
40	1	0	0.120749	6.270721	-3.548363
41	6	0	7.684319	-2.234799	-1.875243
42	6	0	1.170826	7.174533	-1.896337
43	6	0	7.634357	-1.961026	-0.498421
44	1	0	8.554354	-1.739648	0.037500
45	6	0	9.001834	-2.230055	-2.612488
46	1	0	9.509943	-1.262678	-2.513590
47	1	0	8.864136	-2.432138	-3.679323
48	1	0	9.683747	-2.990291	-2.210836
49	6	0	1.646036	8.375050	-2.678483
50	1	0	1.474416	9.305461	-2.124757
51	1	0	1.134568	8.452517	-3.643084
52	1	0	2.724257	8.315752	-2.877605
53	1	0	4.185865	-3.932430	1.557238
54	1	0	-2.250028	3.954651	0.211233
55	6	0	-1.850902	2.426489	3.160691
56	6	0	0.981225	-4.149304	1.277426
57	6	0	1.447160	-5.474464	1.914254
58	1	0	0.628719	-6.204173	1.908022
59	1	0	2.288196	-5.920657	1.369951
60	1	0	1.756519	-5.328819	2.956966

61	6	0	-0.251160	-3.644963	2.050699
62	1	0	-0.013965	-3.492718	3.111545
63	1	0	-0.631507	-2.698521	1.650054
64	1	0	-1.065970	-4.376727	1.991949
65	6	0	0.614874	-4.388109	-0.197799
66	1	0	0.282909	-3.464685	-0.683447
67	1	0	1.459906	-4.786623	-0.771634
68	1	0	-0.199986	-5.116822	-0.270122
69	6	0	-2.012469	0.991423	3.696664
70	1	0	-2.806445	0.453518	3.166214
71	1	0	-1.086203	0.418637	3.599856
72	1	0	-2.276975	1.016979	4.761317
73	6	0	-3.189465	3.166274	3.369091
74	1	0	-3.137390	4.222188	3.079610
75	1	0	-3.999124	2.697898	2.794451
76	1	0	-3.472966	3.133155	4.427640
77	6	0	-0.733631	3.142423	3.938738
78	1	0	-0.605548	4.183435	3.616887
79	1	0	-0.974625	3.161352	5.008565
80	1	0	0.223352	2.624001	3.819863
81	8	0	-0.388040	-0.538576	-0.720125
82	8	0	-2.533813	-1.232651	0.896173
83	6	0	-1.421402	-1.008763	-1.197018
84	6	0	-2.664254	-1.371813	-0.342204
85	8	0	-1.551720	-1.250476	-2.482243
86	6	0	-0.427741	-0.955995	-3.357915
87	1	0	-0.756211	-1.268209	-4.347987
88	1	0	-0.217419	0.115381	-3.338947
89	1	0	0.449812	-1.523314	-3.043032
90	6	0	-3.351575	-2.698394	-0.786955
91	9	0	-3.829057	-2.709370	-2.043691
92	9	0	-4.366023	-2.982254	0.045321
93	9	0	-2.450078	-3.706292	-0.693185
94	6	0	-8.297701	-2.090401	-1.076819
95	6	0	-7.239102	-1.462503	-0.429242
96	6	0	-6.231355	-0.799255	-1.166883
97	6	0	-6.341161	-0.775505	-2.576754
98	6	0	-7.412925	-1.386733	-3.218197
99	6	0	-8.391792	-2.050402	-2.471681
100	1	0	-9.052124	-2.610711	-0.494081
101	1	0	-7.175965	-1.519027	0.651782
102	1	0	-5.604319	-0.243077	-3.168365
103	1	0	-7.489069	-1.342648	-4.300664
104	1	0	-9.227042	-2.529959	-2.974177

105	6	0	-5.107477	-0.152371	-0.491232
106	6	0	-5.187812	0.236170	0.944806
107	1	0	-4.860854	1.273858	1.072933
108	1	0	-6.174857	0.121052	1.391085
109	1	0	-4.451339	-0.379653	1.495682
110	6	0	-3.862918	0.030318	-1.111465
111	1	0	-3.247894	0.837488	-0.719739
112	1	0	-3.775286	-0.136813	-2.180149
113	17	0	1.653392	0.065951	3.252425

TS2R_{exo}-Cl

Imaginary frequency= -101.01
Total energy= -3138.45284327
Sum of electronic and zero-point Energies= -3137.523796
Sum of electronic and thermal Energies= -3137.464644
Sum of electronic and thermal Enthalpies= -3137.463700
Sum of electronic and thermal Free Energies= -3137.619759

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.393317	-0.257260	1.223486
2	6	0	-2.164207	1.795213	2.073380
3	1	0	-2.885767	0.982325	1.942167
4	7	0	-1.506343	3.346796	0.380698
5	6	0	-0.601479	2.343592	0.473556
6	6	0	-1.363823	4.627824	-0.235811
7	7	0	-0.909575	1.411826	1.361422
8	6	0	-2.639978	3.049227	1.277832
9	1	0	-2.830144	3.914322	1.915207
10	7	0	2.097385	-1.457854	0.670669
11	6	0	4.334105	-2.327983	0.771338
12	1	0	4.660667	-3.210784	0.214446
13	7	0	4.179549	-1.195542	-0.152975
14	6	0	2.911255	-2.486669	1.388313
15	1	0	2.933928	-2.188628	2.443145
16	6	0	6.138951	0.256831	-0.394321
17	1	0	5.943313	0.661766	0.594518
18	6	0	2.392673	0.491294	-0.702788
19	6	0	2.275635	2.487658	-2.062483
20	1	0	2.676565	3.099458	-2.864581
21	6	0	5.280679	-0.710471	-0.928321
22	6	0	-0.388242	5.531413	0.207601

23	1	0	0.285196	5.246467	1.010636
24	6	0	5.537482	-1.246983	-2.194433
25	1	0	4.876410	-2.008203	-2.599374
26	6	0	-2.246533	5.007205	-1.251583
27	1	0	-3.007772	4.311828	-1.593427
28	6	0	1.235597	0.919286	-0.048195
29	6	0	2.919281	1.291828	-1.728779
30	1	0	3.807520	0.993384	-2.272524
31	6	0	1.130656	2.918185	-1.384985
32	1	0	0.663766	3.852100	-1.672871
33	6	0	0.602125	2.131908	-0.348043
34	6	0	6.637533	-0.800050	-2.927132
35	1	0	6.828794	-1.220765	-3.911205
36	6	0	2.905658	-0.756346	-0.113934
37	6	0	-2.142531	6.274693	-1.827176
38	1	0	-2.833354	6.557955	-2.617300
39	6	0	-0.286533	6.788412	-0.385147
40	1	0	0.477986	7.478739	-0.036572
41	6	0	7.502540	0.177924	-2.413413
42	6	0	-1.160284	7.183970	-1.411111
43	6	0	7.236386	0.693793	-1.135769
44	1	0	7.898050	1.446889	-0.714997
45	6	0	8.674862	0.679749	-3.221205
46	1	0	8.398947	1.569042	-3.804329
47	1	0	9.027082	-0.077518	-3.929467
48	1	0	9.513448	0.963240	-2.576043
49	6	0	-1.035301	8.548325	-2.045478
50	1	0	-1.857244	8.743262	-2.741425
51	1	0	-0.094691	8.641854	-2.603672
52	1	0	-1.036216	9.341062	-1.287578
53	1	0	5.097748	-2.095557	1.519676
54	1	0	-3.543425	2.852174	0.691074
55	6	0	-2.053797	2.041888	3.615683
56	6	0	2.397390	-3.957853	1.340963
57	6	0	3.416909	-4.834357	2.101816
58	1	0	3.053820	-5.867498	2.155855
59	1	0	4.398398	-4.860186	1.615346
60	1	0	3.557848	-4.476767	3.129941
61	6	0	1.050340	-4.071806	2.071017
62	1	0	1.102937	-3.645696	3.080708
63	1	0	0.262132	-3.557337	1.524170
64	1	0	0.756167	-5.124645	2.163050
65	6	0	2.241894	-4.467792	-0.102508
66	1	0	1.528015	-3.858692	-0.665437

67	1	0	3.192637	-4.466109	-0.648077
68	1	0	1.871631	-5.500154	-0.099256
69	6	0	-1.682001	0.739044	4.345629
70	1	0	-2.412772	-0.052239	4.141935
71	1	0	-0.694218	0.377306	4.055756
72	1	0	-1.672538	0.912072	5.429323
73	6	0	-3.449661	2.470277	4.121306
74	1	0	-3.773330	3.435458	3.716832
75	1	0	-4.213407	1.723924	3.865928
76	1	0	-3.433356	2.566324	5.213181
77	6	0	-1.021733	3.132559	3.950653
78	1	0	-1.257452	4.090272	3.470290
79	1	0	-1.004483	3.311036	5.032849
80	1	0	-0.014707	2.830395	3.646199
81	8	0	-1.279592	-1.693755	2.255233
82	8	0	-0.742328	-1.196394	-0.331849
83	6	0	-1.977490	-2.236904	1.408394
84	6	0	-1.702557	-1.968679	-0.075225
85	8	0	-2.946134	-3.091647	1.648945
86	6	0	-3.184638	-3.451175	3.040161
87	1	0	-3.956959	-4.217685	3.002988
88	1	0	-2.266642	-3.842068	3.482359
89	1	0	-3.532825	-2.575108	3.590809
90	6	0	-1.901087	-3.131476	-1.071977
91	9	0	-0.997030	-4.093445	-0.771431
92	9	0	-1.658077	-2.721060	-2.324535
93	9	0	-3.111821	-3.696094	-1.026755
94	6	0	-5.187670	-2.700769	-4.677930
95	6	0	-4.350516	-1.874034	-3.934663
96	6	0	-4.636304	-1.584507	-2.581958
97	6	0	-5.805407	-2.139213	-2.012676
98	6	0	-6.649947	-2.948434	-2.765233
99	6	0	-6.341757	-3.236994	-4.098700
100	1	0	-4.940689	-2.926639	-5.711205
101	1	0	-3.452233	-1.481111	-4.397605
102	1	0	-6.072103	-1.903060	-0.987883
103	1	0	-7.552502	-3.351008	-2.314619
104	1	0	-7.000505	-3.871737	-4.684730
105	6	0	-3.746937	-0.731880	-1.784458
106	6	0	-2.880122	0.297290	-2.453317
107	1	0	-3.036888	0.366302	-3.529599
108	1	0	-3.080241	1.283036	-2.018199
109	1	0	-1.819871	0.079621	-2.261918
110	6	0	-3.656333	-0.864109	-0.408324

111	1	0	-3.229798	-0.047209	0.162571
112	1	0	-4.321108	-1.532277	0.127263
113	17	0	1.737890	0.559503	2.970151

TS2S_{exo}-Cl

Imaginary frequency= -96.39
Total energy= -3138.45480900
Sum of electronic and zero-point Energies= -3137.525838
Sum of electronic and thermal Energies= -3137.466560
Sum of electronic and thermal Enthalpies= -3137.465616
Sum of electronic and thermal Free Energies= -3137.623811

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.373030	0.052593	-1.389718
2	6	0	2.430649	1.803468	-2.040726
3	1	0	2.993138	0.865318	-1.990902
4	7	0	1.952595	3.271021	-0.223960
5	6	0	0.908811	2.439518	-0.437817
6	6	0	2.159434	4.179160	0.863734
7	7	0	1.092655	1.579029	-1.426247
8	6	0	3.075849	2.849356	-1.081538
9	1	0	3.486828	3.716797	-1.601235
10	7	0	-2.183066	-1.010046	-0.908965
11	6	0	-4.464806	-1.733552	-1.016284
12	1	0	-4.746072	-2.610898	-0.424103
13	7	0	-4.253958	-0.585735	-0.121909
14	6	0	-3.085465	-1.890345	-1.714963
15	1	0	-3.136658	-1.441281	-2.715163
16	6	0	-6.120531	0.961325	0.218994
17	1	0	-5.913595	1.397789	-0.753964
18	6	0	-2.335127	0.914823	0.524956
19	6	0	-2.074791	2.860484	1.939770
20	1	0	-2.453844	3.500488	2.730457
21	6	0	-5.312824	-0.075435	0.695957
22	6	0	1.931702	5.545664	0.682473
23	1	0	1.563497	5.904894	-0.274228
24	6	0	-5.575024	-0.644208	1.947615
25	1	0	-4.948619	-1.452673	2.314368
26	6	0	2.637623	3.708205	2.092927
27	1	0	2.820007	2.645321	2.227925
28	6	0	-1.112782	1.238530	-0.067610

29	6	0	-2.820350	1.743417	1.550315
30	1	0	-3.759706	1.530562	2.046404
31	6	0	-0.851749	3.174240	1.337501
32	1	0	-0.305309	4.050324	1.665312
33	6	0	-0.352870	2.349903	0.316554
34	6	0	-6.632001	-0.162878	2.719607
35	1	0	-6.824046	-0.604741	3.694362
36	6	0	-2.944811	-0.261230	-0.117673
37	6	0	2.868450	4.604836	3.134778
38	1	0	3.232213	4.231266	4.089048
39	6	0	2.165288	6.433534	1.734245
40	1	0	1.976340	7.494043	1.588119
41	6	0	-7.450544	0.881032	2.260353
42	6	0	2.638674	5.981068	2.974021
43	6	0	-7.174946	1.434001	1.000986
44	1	0	-7.792262	2.246878	0.626914
45	6	0	-8.610926	1.376206	3.089205
46	1	0	-8.873309	2.408081	2.833506
47	1	0	-8.385277	1.333811	4.160374
48	1	0	-9.504885	0.760221	2.922040
49	6	0	2.916046	6.945300	4.102087
50	1	0	2.565073	6.550345	5.062389
51	1	0	2.430169	7.911287	3.931179
52	1	0	3.993485	7.131372	4.205940
53	1	0	-5.274271	-1.518873	-1.718241
54	1	0	3.865613	2.413015	-0.460349
55	6	0	2.427086	2.243582	-3.541964
56	6	0	-2.660231	-3.374582	-1.904559
57	6	0	-3.763379	-4.077557	-2.725180
58	1	0	-3.468822	-5.111566	-2.941003
59	1	0	-4.719699	-4.115564	-2.190582
60	1	0	-3.929742	-3.571829	-3.684775
61	6	0	-1.352948	-3.442288	-2.708589
62	1	0	-1.440921	-2.903616	-3.660561
63	1	0	-0.518648	-3.004967	-2.158731
64	1	0	-1.099683	-4.485282	-2.936107
65	6	0	-2.475694	-4.102223	-0.561636
66	1	0	-1.772168	-3.568897	0.085670
67	1	0	-3.417654	-4.210664	-0.011181
68	1	0	-2.081928	-5.112026	-0.728824
69	6	0	1.842697	1.125332	-4.423127
70	1	0	2.394995	0.186818	-4.295593
71	1	0	0.791593	0.935787	-4.195168
72	1	0	1.911675	1.411057	-5.480540

73	6	0	3.894341	2.459292	-3.973321
74	1	0	4.374323	3.293878	-3.450502
75	1	0	4.497367	1.559140	-3.795524
76	1	0	3.936817	2.680475	-5.046193
77	6	0	1.623139	3.537789	-3.758275
78	1	0	2.008739	4.371754	-3.159309
79	1	0	1.677739	3.841371	-4.810886
80	1	0	0.566298	3.395218	-3.509487
81	8	0	1.243972	-1.496118	-2.443445
82	8	0	0.860511	-0.805029	0.130806
83	6	0	2.074735	-1.853013	-1.618881
84	6	0	1.858577	-1.516917	-0.139995
85	8	0	3.192082	-2.494677	-1.880552
86	6	0	3.463852	-2.819078	-3.274741
87	1	0	4.395444	-3.381885	-3.254193
88	1	0	2.649819	-3.424071	-3.678309
89	1	0	3.578457	-1.898496	-3.850310
90	6	0	3.102706	-1.276661	0.741921
91	9	0	3.985945	-2.278738	0.747242
92	9	0	2.742506	-1.007255	2.003516
93	9	0	3.735708	-0.180278	0.252455
94	6	0	3.524741	-4.281979	4.828749
95	6	0	2.505773	-3.792434	4.017011
96	6	0	2.424257	-4.157064	2.654427
97	6	0	3.395410	-5.050459	2.146604
98	6	0	4.408160	-5.543293	2.961926
99	6	0	4.480021	-5.157978	4.304796
100	1	0	3.574299	-3.980489	5.870973
101	1	0	1.777734	-3.110146	4.440847
102	1	0	3.340387	-5.383985	1.116342
103	1	0	5.138772	-6.235616	2.553828
104	1	0	5.271993	-5.544157	4.940382
105	6	0	1.343987	-3.639462	1.804908
106	6	0	0.144363	-3.015446	2.459941
107	1	0	-0.322544	-3.716686	3.162202
108	1	0	0.434079	-2.130402	3.039652
109	1	0	-0.600360	-2.710135	1.724129
110	6	0	1.401841	-3.677426	0.423014
111	1	0	0.476904	-3.571402	-0.133631
112	1	0	2.214122	-4.178965	-0.090962
113	17	0	-1.619268	1.068301	-3.102664

M1$_{endo}$-BF$_4$

Total energy= -2753.71060145

Sum of electronic and zero-point Energies= -2752.930516
Sum of electronic and thermal Energies= -2752.877441
Sum of electronic and thermal Enthalpies= -2752.876497
Sum of electronic and thermal Free Energies= -2753.018706

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.038414	-0.946398	0.423702
2	6	0	-3.228337	-0.594179	1.115948
3	1	0	-3.538827	-1.423251	0.469851
4	7	0	-3.191163	1.653544	0.308774
5	6	0	-1.957301	1.119795	0.247170
6	6	0	-3.613012	2.983595	-0.013986
7	7	0	-1.886914	-0.133969	0.671853
8	6	0	-4.134265	0.643324	0.830104
9	1	0	-4.627495	1.032877	1.724370
10	7	0	2.071677	-1.105068	-0.025035
11	6	0	4.419875	-1.345829	-0.226202
12	1	0	4.784534	-1.788943	-1.159518
13	7	0	3.944987	0.034130	-0.482402
14	6	0	3.154041	-2.053724	0.332120
15	1	0	3.211612	-2.077807	1.425890
16	6	0	4.989459	2.009405	0.515082
17	1	0	4.412933	1.833020	1.418362
18	6	0	1.671736	1.182840	-0.568809
19	6	0	0.831131	3.379689	-1.135613
20	1	0	1.011921	4.380001	-1.516110
21	6	0	4.837979	1.147547	-0.575904
22	6	0	-4.120871	3.262662	-1.287978
23	1	0	-4.169764	2.472711	-2.032494
24	6	0	5.592662	1.348180	-1.737381
25	1	0	5.475259	0.673173	-2.580481
26	6	0	-3.551753	3.993543	0.950343
27	1	0	-3.161503	3.770931	1.939374
28	6	0	0.370112	0.854439	-0.184999
29	6	0	1.898562	2.478035	-1.060621
30	1	0	2.885889	2.787433	-1.383048
31	6	0	-0.461810	3.032994	-0.728728
32	1	0	-1.257261	3.765152	-0.797383
33	6	0	-0.708150	1.738990	-0.238968
34	6	0	6.484129	2.417283	-1.804558
35	1	0	7.064910	2.570046	-2.711139
36	6	0	2.601850	0.054238	-0.376709

37	6	0	-3.978142	5.283078	0.628764
38	1	0	-3.916678	6.067044	1.379351
39	6	0	-4.545355	4.554119	-1.595762
40	1	0	-4.930139	4.766564	-2.590308
41	6	0	6.638378	3.305648	-0.727194
42	6	0	-4.478383	5.586179	-0.645689
43	6	0	5.878432	3.082041	0.429377
44	1	0	5.986074	3.752321	1.278469
45	6	0	7.611181	4.456893	-0.813934
46	1	0	7.414277	5.080250	-1.694690
47	1	0	8.644149	4.096288	-0.901794
48	1	0	7.554362	5.095490	0.073016
49	6	0	-4.954803	6.977239	-0.986101
50	1	0	-4.597125	7.711401	-0.257391
51	1	0	-6.051876	7.026055	-0.994633
52	1	0	-4.612035	7.284867	-1.980767
53	1	0	5.237896	-1.327358	0.496554
54	1	0	-4.901305	0.432490	0.078779
55	6	0	-3.291386	-1.135268	2.576734
56	6	0	2.917897	-3.511543	-0.142068
57	6	0	4.167282	-4.341994	0.215156
58	1	0	3.998243	-5.400272	-0.016464
59	1	0	5.049818	-4.018340	-0.349398
60	1	0	4.402112	-4.268095	1.284336
61	6	0	1.711916	-4.082274	0.630544
62	1	0	1.902086	-4.087162	1.710513
63	1	0	0.798156	-3.500097	0.450634
64	1	0	1.507319	-5.114347	0.320655
65	6	0	2.652687	-3.596366	-1.654636
66	1	0	1.752014	-3.038854	-1.934382
67	1	0	3.488286	-3.201183	-2.244571
68	1	0	2.508203	-4.641602	-1.953284
69	6	0	-2.390277	-2.378844	2.694954
70	1	0	-2.673484	-3.146753	1.964613
71	1	0	-1.333698	-2.132395	2.547746
72	1	0	-2.484113	-2.821535	3.694095
73	6	0	-4.746438	-1.571262	2.849160
74	1	0	-5.446432	-0.727501	2.830524
75	1	0	-5.086848	-2.308548	2.110705
76	1	0	-4.819927	-2.033886	3.840114
77	6	0	-2.856543	-0.085722	3.614649
78	1	0	-3.454606	0.831796	3.555150
79	1	0	-2.985181	-0.489978	4.625992
80	1	0	-1.801878	0.183142	3.500599

81	8	0	-0.349568	-1.375486	-1.586687
82	8	0	-1.692226	-3.774908	-0.550715
83	6	0	-1.164054	-2.094437	-2.172481
84	6	0	-2.080672	-3.107387	-1.471737
85	8	0	-1.315823	-2.115782	-3.462905
86	6	0	-0.488468	-1.229378	-4.286479
87	1	0	-0.775991	-1.460333	-5.309732
88	1	0	-0.718764	-0.193341	-4.033122
89	1	0	0.564381	-1.453009	-4.110372
90	6	0	-3.531271	-3.216321	-2.008153
91	9	0	-3.997936	-1.981205	-2.275599
92	9	0	-4.310785	-3.784976	-1.089317
93	9	0	-3.567129	-3.942931	-3.131372
94	5	0	1.646871	-0.321873	3.263792
95	9	0	2.046222	-1.637513	3.391622
96	9	0	1.176504	0.221137	4.432288
97	9	0	2.584875	0.468602	2.632855
98	9	0	0.416050	-0.349292	2.353242

M1$_{exo}$-BF$_4$

Total energy= -2753.70795681

Sum of electronic and zero-point Energies= -2752.928149

Sum of electronic and thermal Energies= -2752.874324

Sum of electronic and thermal Enthalpies= -2752.873380

Sum of electronic and thermal Free Energies= -2753.018014

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.008818	-0.872278	0.564768
2	6	0	-3.289661	-0.858020	1.062756
3	1	0	-3.439145	-1.786030	0.499481
4	7	0	-3.494605	1.267002	-0.019116
5	6	0	-2.198561	0.903832	0.054545
6	6	0	-4.046792	2.552821	-0.316033
7	7	0	-1.995866	-0.268929	0.635979
8	6	0	-4.327060	0.207122	0.593016
9	1	0	-4.902865	0.638975	1.415080
10	7	0	2.083488	-0.820692	0.236849
11	6	0	4.450853	-0.647907	0.419609
12	1	0	5.193236	-1.054337	-0.271943
13	7	0	3.814842	0.542004	-0.185439
14	6	0	3.255552	-1.614790	0.684835

15	1	0	3.152576	-1.782215	1.760104
16	6	0	4.552043	2.697065	0.719527
17	1	0	4.003441	2.481072	1.632322
18	6	0	1.434926	1.316155	-0.612201
19	6	0	0.374054	3.291014	-1.520436
20	1	0	0.456329	4.244791	-2.031753
21	6	0	4.531461	1.774275	-0.334068
22	6	0	-3.748781	3.662056	0.486137
23	1	0	-3.066316	3.556405	1.324469
24	6	0	5.246352	2.032763	-1.505171
25	1	0	5.230819	1.310193	-2.316248
26	6	0	-4.943246	2.684840	-1.380309
27	1	0	-5.176103	1.823525	-1.999913
28	6	0	0.160901	0.871083	-0.263330
29	6	0	1.536835	2.558792	-1.258178
30	1	0	2.499829	2.951917	-1.562117
31	6	0	-0.890458	2.837987	-1.130429
32	1	0	-1.762750	3.444689	-1.340114
33	6	0	-1.009231	1.602526	-0.470792
34	6	0	5.966317	3.223716	-1.626238
35	1	0	6.516419	3.423149	-2.542319
36	6	0	2.481466	0.361387	-0.204518
37	6	0	-5.527671	3.924308	-1.644968
38	1	0	-6.221463	4.017468	-2.476608
39	6	0	-4.325408	4.897718	0.198870
40	1	0	-4.079301	5.755474	0.820158
41	6	0	5.993772	4.164291	-0.587389
42	6	0	-5.226639	5.051176	-0.866986
43	6	0	5.273978	3.880673	0.585489
44	1	0	5.281235	4.595538	1.404928
45	6	0	6.775742	5.449071	-0.715138
46	1	0	6.134299	6.322977	-0.547423
47	1	0	7.227571	5.545728	-1.707312
48	1	0	7.581505	5.497722	0.028298
49	6	0	-5.863127	6.390786	-1.148895
50	1	0	-6.373147	6.396313	-2.117223
51	1	0	-5.116941	7.193888	-1.150241
52	1	0	-6.605292	6.644841	-0.380618
53	1	0	4.959869	-0.358062	1.343521
54	1	0	-5.027679	-0.192487	-0.145246
55	6	0	-3.370295	-1.230588	2.574156
56	6	0	3.380492	-3.013253	0.010187
57	6	0	4.672837	-3.683338	0.522348
58	1	0	4.740839	-4.708791	0.140440

59	1	0	5.575718	-3.154381	0.197114
60	1	0	4.686362	-3.733379	1.618440
61	6	0	2.191959	-3.890981	0.444817
62	1	0	2.157984	-4.000666	1.535624
63	1	0	1.232099	-3.477713	0.118324
64	1	0	2.280149	-4.894953	0.011882
65	6	0	3.417223	-2.909031	-1.524323
66	1	0	2.496491	-2.466510	-1.921793
67	1	0	4.259787	-2.301711	-1.876425
68	1	0	3.528236	-3.905539	-1.968748
69	6	0	-2.347801	-2.341021	2.874283
70	1	0	-2.545040	-3.238795	2.278312
71	1	0	-1.324701	-2.011305	2.667101
72	1	0	-2.392815	-2.621135	3.933742
73	6	0	-4.783351	-1.784181	2.851443
74	1	0	-5.561514	-1.020907	2.734308
75	1	0	-5.023973	-2.619549	2.181092
76	1	0	-4.843689	-2.155760	3.880911
77	6	0	-3.094448	-0.021653	3.485208
78	1	0	-3.768676	0.818725	3.280665
79	1	0	-3.242224	-0.306844	4.533688
80	1	0	-2.063908	0.332069	3.383111
81	8	0	-1.505337	-3.759139	-0.071564
82	8	0	-0.218220	-1.599477	-1.339341
83	6	0	-1.611091	-3.571414	-1.263025
84	6	0	-0.800723	-2.476962	-1.955686
85	8	0	-2.366985	-4.217080	-2.127175
86	6	0	-3.182762	-5.304649	-1.603049
87	1	0	-3.702508	-5.708302	-2.469891
88	1	0	-2.536295	-6.057104	-1.147009
89	1	0	-3.890787	-4.911447	-0.870636
90	6	0	-0.655218	-2.463785	-3.495013
91	9	0	-0.240131	-3.662077	-3.922333
92	9	0	0.231324	-1.537915	-3.864998
93	9	0	-1.841429	-2.180682	-4.050036
94	5	0	1.202510	-0.379585	3.488091
95	9	0	2.434184	0.186499	3.245114
96	9	0	1.215865	-1.761063	3.386325
97	9	0	0.286973	0.106220	2.356215
98	9	0	0.602736	0.076734	4.632589

TS2R_{endo}-BF_4

Imaginary frequency= -142.34

Total energy= -3102.66904613
Sum of electronic and zero-point Energies= -3101.725698
Sum of electronic and thermal Energies= -3101.663518
Sum of electronic and thermal Enthalpies= -3101.662573
Sum of electronic and thermal Free Energies= -3101.825245

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.308047	-0.327313	0.673165
2	6	0	-1.391052	2.461624	1.397060
3	1	0	-2.328265	2.001833	1.082428
4	7	0	0.076961	3.762291	0.032082
5	6	0	0.506696	2.483631	0.089715
6	6	0	0.753718	4.926282	-0.444536
7	7	0	-0.277310	1.683819	0.793780
8	6	0	-1.228555	3.855602	0.721869
9	1	0	-1.199306	4.680982	1.435425
10	7	0	1.449087	-2.043997	0.231587
11	6	0	2.818042	-3.980464	0.047774
12	1	0	2.586930	-4.694998	-0.749317
13	7	0	3.432316	-2.767398	-0.533124
14	6	0	1.548823	-3.429399	0.757725
15	1	0	1.743421	-3.348751	1.832420
16	6	0	5.730713	-2.068214	-0.058881
17	1	0	5.379696	-1.597845	0.854757
18	6	0	2.746138	-0.338690	-0.827796
19	6	0	3.666710	1.612541	-1.922448
20	1	0	4.422389	2.055853	-2.563338
21	6	0	4.814462	-2.714678	-0.894739
22	6	0	0.209995	5.647167	-1.515499
23	1	0	-0.691950	5.288099	-2.002939
24	6	0	5.258404	-3.351296	-2.059557
25	1	0	4.543724	-3.856194	-2.703457
26	6	0	1.913700	5.389020	0.185271
27	1	0	2.326556	4.840510	1.026901
28	6	0	1.742551	0.490177	-0.323874
29	6	0	3.725540	0.241725	-1.649718
30	1	0	4.520016	-0.356065	-2.080867
31	6	0	2.663619	2.429855	-1.390178
32	1	0	2.657117	3.487178	-1.625701
33	6	0	1.677300	1.865443	-0.563984
34	6	0	6.612575	-3.324707	-2.388251
35	1	0	6.950367	-3.819489	-3.295881

36	6	0	2.571368	-1.737197	-0.395816
37	6	0	2.534407	6.552800	-0.273355
38	1	0	3.438938	6.900860	0.219049
39	6	0	0.831060	6.814740	-1.952857
40	1	0	0.401532	7.365741	-2.786152
41	6	0	7.546343	-2.663072	-1.573460
42	6	0	2.004535	7.287887	-1.342575
43	6	0	7.081883	-2.038295	-0.407704
44	1	0	7.787562	-1.528200	0.243146
45	6	0	9.007970	-2.630325	-1.950240
46	1	0	9.159492	-2.119788	-2.909891
47	1	0	9.413939	-3.643612	-2.060310
48	1	0	9.602899	-2.108335	-1.194353
49	6	0	2.660611	8.560797	-1.819850
50	1	0	3.624239	8.722693	-1.326792
51	1	0	2.027768	9.433483	-1.612317
52	1	0	2.831683	8.540708	-2.903020
53	1	0	3.513598	-4.450501	0.746409
54	1	0	-2.020947	4.053379	-0.007445
55	6	0	-1.408335	2.493450	2.959922
56	6	0	0.268255	-4.289450	0.591489
57	6	0	0.569916	-5.708144	1.116272
58	1	0	-0.339323	-6.320810	1.096069
59	1	0	1.324898	-6.220538	0.508435
60	1	0	0.930099	-5.680391	2.152296
61	6	0	-0.848283	-3.678103	1.458954
62	1	0	-0.548087	-3.632211	2.513169
63	1	0	-1.107120	-2.661981	1.138837
64	1	0	-1.756470	-4.290476	1.398849
65	6	0	-0.192492	-4.365946	-0.873906
66	1	0	-0.399752	-3.369654	-1.279453
67	1	0	0.557784	-4.838808	-1.518797
68	1	0	-1.107867	-4.965264	-0.950873
69	6	0	-1.634784	1.070860	3.507624
70	1	0	-2.555858	0.634168	3.106700
71	1	0	-0.804502	0.404606	3.259730
72	1	0	-1.718644	1.099673	4.601301
73	6	0	-2.607921	3.361364	3.398799
74	1	0	-2.503626	4.410822	3.100421
75	1	0	-3.548046	2.983045	2.977015
76	1	0	-2.702201	3.342620	4.490899
77	6	0	-0.106628	3.070163	3.543311
78	1	0	0.088056	4.091771	3.194156
79	1	0	-0.171672	3.109307	4.637570

80	1	0	0.757386	2.447796	3.288349
81	8	0	-0.610001	-0.592886	-1.164102
82	8	0	-2.647622	-0.465038	0.673196
83	6	0	-1.792618	-0.608166	-1.534193
84	6	0	-2.979038	-0.515960	-0.545465
85	8	0	-2.105556	-0.682965	-2.800963
86	6	0	-1.028692	-0.704069	-3.785978
87	1	0	-1.534998	-0.766013	-4.747348
88	1	0	-0.446101	0.215599	-3.708757
89	1	0	-0.396989	-1.577990	-3.619592
90	6	0	-3.992151	0.577662	-1.001545
91	9	0	-3.314507	1.744717	-1.180253
92	9	0	-4.909277	0.782055	-0.046278
93	9	0	-4.635630	0.322427	-2.153810
94	6	0	-8.632258	-1.277691	-0.156099
95	6	0	-7.347314	-1.560354	0.291123
96	6	0	-6.342228	-1.982099	-0.612829
97	6	0	-6.689404	-2.127070	-1.978798
98	6	0	-7.982656	-1.866131	-2.415346
99	6	0	-8.956158	-1.435042	-1.508040
100	1	0	-9.384527	-0.936510	0.548660
101	1	0	-7.113388	-1.419240	1.340045
102	1	0	-5.956414	-2.487503	-2.691959
103	1	0	-8.235528	-2.002426	-3.462563
104	1	0	-9.965776	-1.228307	-1.851754
105	6	0	-4.990776	-2.267540	-0.151204
106	6	0	-4.688067	-2.538971	1.275414
107	1	0	-4.031626	-1.712531	1.619600
108	1	0	-5.558228	-2.627869	1.924146
109	1	0	-4.075850	-3.443348	1.367084
110	6	0	-3.866927	-2.183261	-1.006666
111	1	0	-3.028219	-2.820563	-0.733846
112	1	0	-4.032702	-2.104989	-2.075295
113	5	0	2.354993	-0.773636	3.249432
114	9	0	1.694069	-1.919356	3.654581
115	9	0	2.686228	0.055521	4.293619
116	9	0	3.422532	-1.038843	2.412265
117	9	0	1.347797	0.025826	2.440055

TS2S_{endo}-BF_4

Imaginary frequency= -113.67

Total energy= -3102.66634521

Sum of electronic and zero-point Energies= -3101.722990

Sum of electronic and thermal Energies= -3101.659973
Sum of electronic and thermal Enthalpies= -3101.659029
Sum of electronic and thermal Free Energies= -3101.824972

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.320454	-0.368316	0.727059
2	6	0	-1.524535	2.318624	1.476576
3	1	0	-2.433452	1.780486	1.191983
4	7	0	-0.247818	3.665519	-0.029863
5	6	0	0.292566	2.432329	0.068810
6	6	0	0.309712	4.848071	-0.609558
7	7	0	-0.374268	1.610143	0.862068
8	6	0	-1.484731	3.713407	0.778094
9	1	0	-1.419422	4.545029	1.483292
10	7	0	1.565628	-2.007353	0.276076
11	6	0	3.167919	-3.765528	0.287095
12	1	0	3.026117	-4.568805	-0.443635
13	7	0	3.639498	-2.545029	-0.398293
14	6	0	1.836761	-3.304897	0.946592
15	1	0	2.022184	-3.086596	2.007513
16	6	0	5.869401	-1.566537	-0.119417
17	1	0	5.506636	-1.030959	0.752394
18	6	0	2.695890	-0.238626	-0.869972
19	6	0	3.410634	1.734886	-2.070696
20	1	0	4.098329	2.212025	-2.761789
21	6	0	4.992129	-2.390445	-0.835671
22	6	0	-0.294614	5.413645	-1.739469
23	1	0	-1.156544	4.928174	-2.188932
24	6	0	5.451440	-3.100336	-1.948770
25	1	0	4.768312	-3.739244	-2.501423
26	6	0	1.415242	5.475191	-0.026540
27	1	0	1.876144	5.047084	0.858729
28	6	0	1.658433	0.527960	-0.339385
29	6	0	3.588006	0.383309	-1.758191
30	1	0	4.403318	-0.170167	-2.209381
31	6	0	2.372258	2.491056	-1.515311
32	1	0	2.272949	3.535816	-1.783467
33	6	0	1.472362	1.883186	-0.624735
34	6	0	6.783053	-2.974981	-2.348364
35	1	0	7.131751	-3.526459	-3.218038
36	6	0	2.659089	-1.622145	-0.365696
37	6	0	1.925367	6.646278	-0.590487

38	1	0	2.790236	7.121398	-0.134464
39	6	0	0.216972	6.589296	-2.284699
40	1	0	-0.257409	7.018712	-3.164068
41	6	0	7.674892	-2.145452	-1.653235
42	6	0	1.337472	7.224283	-1.723736
43	6	0	7.193133	-1.442282	-0.537460
44	1	0	7.866520	-0.793704	0.017851
45	6	0	9.120366	-2.028653	-2.072515
46	1	0	9.476622	-0.994866	-1.999785
47	1	0	9.267813	-2.370725	-3.102024
48	1	0	9.767405	-2.638024	-1.427110
49	6	0	1.883626	8.495652	-2.327411
50	1	0	2.769095	8.845298	-1.787547
51	1	0	1.135934	9.298545	-2.305978
52	1	0	2.163820	8.348619	-3.377976
53	1	0	3.908817	-4.089192	1.020945
54	1	0	-2.348939	3.884368	0.127806
55	6	0	-1.501730	2.381936	3.038703
56	6	0	0.683509	-4.341491	0.889490
57	6	0	1.183041	-5.648341	1.539101
58	1	0	0.365778	-6.377158	1.594326
59	1	0	1.996330	-6.110688	0.967222
60	1	0	1.544057	-5.472505	2.560277
61	6	0	-0.502149	-3.813903	1.718611
62	1	0	-0.201212	-3.627362	2.757828
63	1	0	-0.912523	-2.883727	1.311910
64	1	0	-1.315529	-4.549079	1.733647
65	6	0	0.231647	-4.620986	-0.554500
66	1	0	-0.127325	-3.710807	-1.045806
67	1	0	1.041056	-5.037325	-1.166128
68	1	0	-0.586612	-5.350126	-0.557880
69	6	0	-1.594520	0.959143	3.622187
70	1	0	-2.477516	0.429803	3.247042
71	1	0	-0.710809	0.363550	3.381207
72	1	0	-1.669663	1.008382	4.715682
73	6	0	-2.749301	3.165204	3.500283
74	1	0	-2.745237	4.206322	3.157362
75	1	0	-3.673344	2.694319	3.140653
76	1	0	-2.793130	3.184503	4.595515
77	6	0	-0.230553	3.071293	3.565987
78	1	0	-0.148591	4.109743	3.222278
79	1	0	-0.247284	3.095380	4.662402
80	1	0	0.676432	2.540684	3.260144
81	8	0	-0.647205	-0.634248	-1.080581

82	8	0	-2.588046	-1.027132	0.833751
83	6	0	-1.793771	-0.974847	-1.404651
84	6	0	-2.936043	-1.187374	-0.377228
85	8	0	-2.103477	-1.185727	-2.657793
86	6	0	-1.067640	-1.020178	-3.671511
87	1	0	-1.554328	-1.281113	-4.609471
88	1	0	-0.729412	0.017577	-3.681894
89	1	0	-0.235298	-1.694324	-3.463208
90	6	0	-3.706519	-2.514021	-0.655536
91	9	0	-4.351393	-2.563942	-1.836865
92	9	0	-4.610512	-2.726054	0.315183
93	9	0	-2.831763	-3.548085	-0.636805
94	6	0	-8.670130	-1.581673	-0.349427
95	6	0	-7.498986	-1.026891	0.150316
96	6	0	-6.523134	-0.486714	-0.723945
97	6	0	-6.786362	-0.508561	-2.116803
98	6	0	-7.970474	-1.043088	-2.607823
99	6	0	-8.912524	-1.586795	-1.727630
100	1	0	-9.397495	-2.009633	0.333642
101	1	0	-7.320893	-1.047381	1.219120
102	1	0	-6.079984	-0.065760	-2.809666
103	1	0	-8.164620	-1.033572	-3.676045
104	1	0	-9.835699	-2.008810	-2.114461
105	6	0	-5.290453	0.081455	-0.207811
106	6	0	-5.150646	0.511482	1.204762
107	1	0	-4.802665	1.550771	1.239713
108	1	0	-6.051664	0.418751	1.808915
109	1	0	-4.323708	-0.084057	1.640047
110	6	0	-4.105015	0.164102	-0.990450
111	1	0	-3.452914	0.998633	-0.735775
112	1	0	-4.191342	-0.011086	-2.057558
113	5	0	2.742941	0.236780	2.924743
114	9	0	2.880414	1.536803	2.481577
115	9	0	2.754363	0.121949	4.293274
116	9	0	3.618623	-0.634032	2.302070
117	9	0	1.339799	-0.206500	2.527335

TS2R_{exo}-BF_4

Imaginary frequency= -86.75

Total energy= -3102.67292268

Sum of electronic and zero-point Energies= -3101.729367

Sum of electronic and thermal Energies= -3101.665925

Sum of electronic and thermal Enthalpies= -3101.664981

Sum of electronic and thermal Free Energies= -3101.830824

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.475944	-0.321304	1.044762
2	6	0	-2.025065	1.487848	2.359875
3	1	0	-2.685806	0.615793	2.398108
4	7	0	-1.898969	3.045013	0.545802
5	6	0	-0.910959	2.129573	0.445182
6	6	0	-2.019841	4.316958	-0.095664
7	7	0	-0.937385	1.197575	1.385839
8	6	0	-2.767376	2.683466	1.688037
9	1	0	-2.870068	3.548353	2.345192
10	7	0	2.150805	-1.353868	0.236813
11	6	0	4.393161	-2.100344	-0.099286
12	1	0	4.750560	-2.961537	-0.668307
13	7	0	3.982562	-1.028819	-1.029141
14	6	0	3.102760	-2.394066	0.722932
15	1	0	3.289052	-2.198661	1.781100
16	6	0	5.633269	0.778362	-1.156053
17	1	0	5.382550	1.057854	-0.136401
18	6	0	2.007560	0.544507	-1.215685
19	6	0	1.466513	2.483657	-2.555906
20	1	0	1.674365	3.115161	-3.413916
21	6	0	4.966620	-0.289445	-1.764832
22	6	0	-1.039881	5.304306	0.075480
23	1	0	-0.155403	5.092626	0.668925
24	6	0	5.299230	-0.670153	-3.068911
25	1	0	4.782834	-1.505716	-3.532861
26	6	0	-3.167589	4.602814	-0.840838
27	1	0	-3.931401	3.841292	-0.969433
28	6	0	0.912722	0.863979	-0.413489
29	6	0	2.282997	1.373956	-2.314639
30	1	0	3.112848	1.162898	-2.978853
31	6	0	0.402364	2.814435	-1.710480
32	1	0	-0.188947	3.697244	-1.920528
33	6	0	0.121640	2.000259	-0.600131
34	6	0	6.284095	0.031376	-3.763487
35	1	0	6.534482	-0.265588	-4.779241
36	6	0	2.733892	-0.632056	-0.706372
37	6	0	-3.325820	5.863909	-1.418064
38	1	0	-4.222467	6.075261	-1.995075
39	6	0	-1.204077	6.553755	-0.518810

40	1	0	-0.434114	7.309678	-0.383680
41	6	0	6.958183	1.113361	-3.174004
42	6	0	-2.350318	6.859433	-1.270441
43	6	0	6.616324	1.472502	-1.862593
44	1	0	7.126659	2.305189	-1.385177
45	6	0	8.029115	1.858235	-3.933996
46	1	0	8.377297	2.734059	-3.377562
47	1	0	7.661929	2.199266	-4.909609
48	1	0	8.897972	1.215641	-4.126449
49	6	0	-2.521712	8.225112	-1.890233
50	1	0	-3.460684	8.296504	-2.448083
51	1	0	-1.700003	8.455894	-2.579675
52	1	0	-2.524075	9.010223	-1.123568
53	1	0	5.210179	-1.737964	0.532551
54	1	0	-3.762668	2.406293	1.326639
55	6	0	-1.565110	1.767287	3.829425
56	6	0	2.596116	-3.863539	0.612162
57	6	0	3.721033	-4.799959	1.102943
58	1	0	3.355493	-5.833069	1.140641
59	1	0	4.596678	-4.789651	0.444213
60	1	0	4.054052	-4.527003	2.112345
61	6	0	1.390133	-4.050116	1.548235
62	1	0	1.662529	-3.840461	2.590136
63	1	0	0.568518	-3.385046	1.280166
64	1	0	1.019399	-5.081127	1.498163
65	6	0	2.207182	-4.229556	-0.830320
66	1	0	1.381651	-3.610309	-1.193951
67	1	0	3.049726	-4.114384	-1.523171
68	1	0	1.884747	-5.276433	-0.881102
69	6	0	-0.949666	0.499907	4.449303
70	1	0	-1.652943	-0.339477	4.425206
71	1	0	-0.035558	0.188453	3.941705
72	1	0	-0.690786	0.691002	5.498091
73	6	0	-2.821839	2.124065	4.654411
74	1	0	-3.280474	3.068596	4.342133
75	1	0	-3.584189	1.337080	4.583686
76	1	0	-2.552428	2.229175	5.711634
77	6	0	-0.548065	2.919357	3.905489
78	1	0	-0.931850	3.843737	3.457026
79	1	0	-0.315191	3.140414	4.954105
80	1	0	0.391222	2.657008	3.409081
81	8	0	-1.328155	-1.971008	2.380311
82	8	0	-0.744143	-1.385005	-0.233392
83	6	0	-2.006289	-2.465718	1.498100

84	6	0	-1.720286	-2.134647	0.028170
85	8	0	-2.983717	-3.335000	1.665054
86	6	0	-3.256670	-3.756012	3.031245
87	1	0	-4.056884	-4.489317	2.945065
88	1	0	-2.361369	-4.206310	3.463912
89	1	0	-3.578016	-2.897564	3.624751
90	6	0	-1.968008	-3.238350	-1.026234
91	9	0	-1.101513	-4.243861	-0.763837
92	9	0	-1.707832	-2.779377	-2.257535
93	9	0	-3.199201	-3.753860	-1.008042
94	6	0	-5.404532	-2.372239	-4.613805
95	6	0	-4.543918	-1.621057	-3.819218
96	6	0	-4.731761	-1.542353	-2.421207
97	6	0	-5.829471	-2.230232	-1.855996
98	6	0	-6.695076	-2.969439	-2.654893
99	6	0	-6.483716	-3.047556	-4.035530
100	1	0	-5.234900	-2.430291	-5.685035
101	1	0	-3.708837	-1.109044	-4.284347
102	1	0	-6.025498	-2.157834	-0.791440
103	1	0	-7.540655	-3.479866	-2.203097
104	1	0	-7.160847	-3.625816	-4.657937
105	6	0	-3.818661	-0.746203	-1.591981
106	6	0	-2.970634	0.298557	-2.259993
107	1	0	-2.171352	-0.173586	-2.847265
108	1	0	-3.561523	0.905397	-2.954420
109	1	0	-2.504976	0.957241	-1.527293
110	6	0	-3.690388	-0.944669	-0.229570
111	1	0	-3.220348	-0.169023	0.364852
112	1	0	-4.341045	-1.633715	0.296709
113	5	0	2.764470	0.248343	3.218947
114	9	0	3.972882	0.087709	2.572755
115	9	0	2.219215	-0.957945	3.639252
116	9	0	1.804662	0.803201	2.176025
117	9	0	2.798528	1.196090	4.211536

TS2S_{exo}-BF_4

Imaginary frequency= -62.78
Total energy= -3102.67398015
Sum of electronic and zero-point Energies= -3101.730538
Sum of electronic and thermal Energies= -3101.667121
Sum of electronic and thermal Enthalpies= -3101.666177
Sum of electronic and thermal Free Energies= -3101.833361

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.573766	-0.188803	-1.233501
2	6	0	-2.026139	-2.080505	-2.121244
3	1	0	-2.646506	-1.182340	-2.235251
4	7	0	-2.020624	-3.150425	0.012595
5	6	0	-0.950012	-2.344836	-0.105007
6	6	0	-2.476817	-3.872109	1.160589
7	7	0	-0.860261	-1.726452	-1.272922
8	6	0	-2.791940	-3.120598	-1.245461
9	1	0	-2.804998	-4.121135	-1.686595
10	7	0	2.226045	0.999521	-0.610346
11	6	0	4.481483	1.771941	-0.383128
12	1	0	4.753715	2.749419	0.024752
13	7	0	4.043988	0.883058	0.709438
14	6	0	3.244324	1.821814	-1.329664
15	1	0	3.480694	1.298466	-2.259742
16	6	0	5.663530	-0.762394	1.533579
17	1	0	5.497804	-1.353204	0.637101
18	6	0	2.023423	-0.553432	1.208004
19	6	0	1.427639	-2.171009	2.907512
20	1	0	1.621380	-2.626760	3.873380
21	6	0	4.954685	0.430554	1.717553
22	6	0	-2.300378	-5.258898	1.229737
23	1	0	-1.783278	-5.776268	0.426660
24	6	0	5.169241	1.201387	2.863281
25	1	0	4.618990	2.128147	3.000085
26	6	0	-3.144095	-3.198618	2.187741
27	1	0	-3.292160	-2.124612	2.117219
28	6	0	0.932231	-1.014563	0.472663
29	6	0	2.265246	-1.144179	2.459878
30	1	0	3.090198	-0.817473	3.081763
31	6	0	0.354002	-2.636736	2.140431
32	1	0	-0.258849	-3.447565	2.515373
33	6	0	0.092079	-2.046954	0.893560
34	6	0	6.080404	0.767799	3.827854
35	1	0	6.237454	1.367809	4.720636
36	6	0	2.783732	0.474979	0.473481
37	6	0	-3.614054	-3.914331	3.290760
38	1	0	-4.127202	-3.385355	4.089786
39	6	0	-2.781813	-5.961557	2.332172
40	1	0	-2.637883	-7.038212	2.381462
41	6	0	6.793554	-0.429182	3.667070

42	6	0	-3.443763	-5.302940	3.381808
43	6	0	6.567905	-1.185788	2.506045
44	1	0	7.107854	-2.118213	2.360420
45	6	0	7.794956	-0.882728	4.701500
46	1	0	7.754287	-1.967621	4.849888
47	1	0	7.620854	-0.397039	5.667144
48	1	0	8.819809	-0.638457	4.390971
49	6	0	-3.958796	-6.080494	4.568946
50	1	0	-4.444862	-5.423833	5.297128
51	1	0	-3.145113	-6.609669	5.080623
52	1	0	-4.687888	-6.839706	4.259113
53	1	0	5.362598	1.345629	-0.871088
54	1	0	-3.822605	-2.819612	-1.039830
55	6	0	-1.680772	-2.578607	-3.557987
56	6	0	2.799790	3.260757	-1.721453
57	6	0	3.983034	3.941185	-2.441148
58	1	0	3.681687	4.930464	-2.805797
59	1	0	4.845879	4.085391	-1.780619
60	1	0	4.312966	3.352734	-3.306548
61	6	0	1.620007	3.176374	-2.704108
62	1	0	1.887941	2.600159	-3.598056
63	1	0	0.747321	2.700096	-2.249373
64	1	0	1.320967	4.180528	-3.030109
65	6	0	2.386517	4.092453	-0.496920
66	1	0	1.547021	3.626959	0.029257
67	1	0	3.206056	4.217767	0.220659
68	1	0	2.071364	5.095644	-0.808555
69	6	0	-1.061141	-1.429485	-4.374596
70	1	0	-1.716060	-0.550152	-4.389556
71	1	0	-0.085658	-1.122233	-3.988957
72	1	0	-0.908289	-1.747902	-5.413173
73	6	0	-3.001545	-2.987360	-4.244469
74	1	0	-3.474469	-3.853166	-3.766721
75	1	0	-3.725791	-2.162125	-4.240119
76	1	0	-2.810606	-3.256296	-5.289733
77	6	0	-0.708137	-3.770796	-3.537131
78	1	0	-1.099546	-4.617728	-2.960541
79	1	0	-0.534803	-4.127075	-4.559624
80	1	0	0.262144	-3.487967	-3.117225
81	8	0	-1.419686	1.752778	-2.822372
82	8	0	-0.875387	0.885081	-0.210888
83	6	0	-2.282068	1.767507	-1.968689
84	6	0	-1.965050	1.424700	-0.507555
85	8	0	-3.562344	2.051257	-2.153302

86	6	0	-3.961091	2.398224	-3.507048
87	1	0	-5.030589	2.593604	-3.445852
88	1	0	-3.421511	3.289905	-3.833439
89	1	0	-3.757187	1.563810	-4.180815
90	6	0	-3.130643	1.047423	0.438111
91	9	0	-4.151769	1.903624	0.452482
92	9	0	-2.687756	0.882531	1.693218
93	9	0	-3.602188	-0.153984	0.013601
94	6	0	-4.425402	4.393742	4.074421
95	6	0	-3.276237	3.954040	3.423378
96	6	0	-3.064423	4.231966	2.054403
97	6	0	-4.045297	4.989687	1.373274
98	6	0	-5.189126	5.432595	2.028179
99	6	0	-5.387049	5.132971	3.380197
100	1	0	-4.570891	4.158961	5.124880
101	1	0	-2.547690	3.377626	3.981728
102	1	0	-3.901406	5.260256	0.332916
103	1	0	-5.924955	6.020243	1.486935
104	1	0	-6.281070	5.480419	3.890326
105	6	0	-1.847099	3.765042	1.373854
106	6	0	-0.675370	3.326960	2.208159
107	1	0	-0.319857	4.154365	2.835136
108	1	0	-0.950407	2.510605	2.885159
109	1	0	0.151482	2.986057	1.584149
110	6	0	-1.743355	3.703504	-0.001697
111	1	0	-0.759039	3.610898	-0.448597
112	1	0	-2.529351	4.087675	-0.642170
113	5	0	2.741343	-1.247659	-3.325064
114	9	0	2.168850	-0.119400	-3.897761
115	9	0	2.589662	-2.374616	-4.094105
116	9	0	1.944501	-1.514378	-2.055968
117	9	0	4.037827	-1.030155	-2.914530

M1$_{endo}$-OTf

Total energy= -3290.69019920
Sum of electronic and zero-point Energies= -3289.897785
Sum of electronic and thermal Energies= -3289.840193
Sum of electronic and thermal Enthalpies= -3289.839249
Sum of electronic and thermal Free Energies= -3289.993616

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	45	0	0.037227	0.891472	0.562376
2	6	0	3.384792	0.719893	0.669391
3	1	0	3.484740	1.678152	0.145110
4	7	0	3.357388	-1.296366	-0.614182
5	6	0	2.097279	-0.913156	-0.315277
6	6	0	3.809077	-2.557469	-1.119546
7	7	0	2.020307	0.197596	0.399342
8	6	0	4.307180	-0.338106	-0.010935
9	1	0	4.945915	-0.867975	0.701005
10	7	0	-2.033562	1.020561	0.331292
11	6	0	-4.401514	1.157500	0.364183
12	1	0	-4.873003	1.782643	-0.402601
13	7	0	-3.891808	-0.081644	-0.259866
14	6	0	-3.120272	1.799928	0.967053
15	1	0	-3.088943	1.581334	2.042103
16	6	0	-5.272285	-2.101309	-0.223014
17	1	0	-4.974815	-2.262444	0.809050
18	6	0	-1.591872	-1.047258	-0.773810
19	6	0	-0.715188	-3.001308	-1.899923
20	1	0	-0.888678	-3.897886	-2.486734
21	6	0	-4.764275	-1.003961	-0.922583
22	6	0	4.382261	-2.621825	-2.394997
23	1	0	4.435811	-1.724652	-3.005404
24	6	0	-5.148469	-0.783016	-2.251188
25	1	0	-4.756669	0.076063	-2.789019
26	6	0	3.739469	-3.709005	-0.329051
27	1	0	3.307446	-3.657085	0.666226
28	6	0	-0.277615	-0.745863	-0.407456
29	6	0	-1.808394	-2.209179	-1.531235
30	1	0	-2.806182	-2.498618	-1.837977
31	6	0	0.595002	-2.668848	-1.540097
32	1	0	1.412168	-3.305071	-1.858280
33	6	0	0.829175	-1.514771	-0.772955
34	6	0	-6.023379	-1.670319	-2.874859
35	1	0	-6.312710	-1.496036	-3.908513
36	6	0	-2.545610	-0.043230	-0.266079
37	6	0	4.223608	-4.920436	-0.825976
38	1	0	4.158388	-5.812258	-0.207866
39	6	0	4.870348	-3.835396	-2.875437
40	1	0	5.309463	-3.876691	-3.869381
41	6	0	-6.536572	-2.785432	-2.191642
42	6	0	4.801448	-5.004907	-2.100608
43	6	0	-6.147380	-2.983704	-0.859711
44	1	0	-6.533855	-3.838926	-0.311233

45	6	0	-7.484745	-3.737480	-2.879557
46	1	0	-7.041125	-4.149596	-3.794464
47	1	0	-8.411682	-3.229905	-3.175230
48	1	0	-7.752718	-4.574528	-2.227572
49	6	0	5.352013	-6.308812	-2.625784
50	1	0	5.055096	-7.152563	-1.994909
51	1	0	6.449405	-6.287785	-2.658264
52	1	0	5.005340	-6.506210	-3.646943
53	1	0	-5.147818	0.915916	1.123861
54	1	0	4.945265	0.097176	-0.784938
55	6	0	3.719681	0.993585	2.168878
56	6	0	-3.004886	3.340141	0.810190
57	6	0	-4.239217	3.982721	1.475162
58	1	0	-4.150685	5.075470	1.462149
59	1	0	-5.168347	3.722515	0.953872
60	1	0	-4.337646	3.667791	2.521517
61	6	0	-1.740924	3.816399	1.550236
62	1	0	-1.769306	3.534066	2.610290
63	1	0	-0.831811	3.388161	1.109161
64	1	0	-1.649439	4.908097	1.497133
65	6	0	-2.927028	3.771171	-0.664739
66	1	0	-2.049610	3.341589	-1.160594
67	1	0	-3.814532	3.470473	-1.233676
68	1	0	-2.851931	4.863109	-0.733543
69	6	0	2.802570	2.101892	2.719877
70	1	0	2.895043	3.024664	2.136118
71	1	0	1.751770	1.796822	2.724137
72	1	0	3.077846	2.334548	3.755922
73	6	0	5.174985	1.503268	2.235379
74	1	0	5.898186	0.747247	1.908418
75	1	0	5.313370	2.396569	1.612571
76	1	0	5.429899	1.774132	3.266505
77	6	0	3.567273	-0.269619	3.033415
78	1	0	4.227488	-1.081968	2.705890
79	1	0	3.828607	-0.041940	4.073927
80	1	0	2.537812	-0.637925	3.021760
81	8	0	0.187984	1.756319	-1.361753
82	8	0	1.550537	3.758614	0.042958
83	6	0	0.770115	2.682479	-1.925129
84	6	0	1.565020	3.746276	-1.159183
85	8	0	0.759831	2.877625	-3.212469
86	6	0	0.037192	1.928770	-4.057976
87	1	0	0.179364	2.299635	-5.070767
88	1	0	0.472641	0.935526	-3.935019

89	1	0	-1.018339	1.930472	-3.782103
90	6	0	2.369461	4.793947	-1.969531
91	9	0	3.220320	4.174518	-2.802398
92	9	0	3.063343	5.571495	-1.139185
93	9	0	1.533294	5.558131	-2.688083
94	8	0	-2.361880	-0.961389	2.577791
95	8	0	-0.013081	-0.017025	2.414176
96	8	0	-1.079509	-0.242324	4.625811
97	16	0	-1.076034	-0.749797	3.250572
98	6	0	-0.305319	-2.442378	3.353098
99	9	0	0.887045	-2.383555	3.954946
100	9	0	-1.107325	-3.248483	4.055327
101	9	0	-0.143927	-2.954806	2.125230

M1$_{exo}$-OTf

Total energy= -3290.68891480

Sum of electronic and zero-point Energies= -3289.895170

Sum of electronic and thermal Energies= -3289.838037

Sum of electronic and thermal Enthalpies= -3289.837093

Sum of electronic and thermal Free Energies= -3289.990194

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.004922	-0.971242	0.575110
2	6	0	-3.346949	-1.097112	0.608118
3	1	0	-3.348426	-2.029734	0.028936
4	7	0	-3.481890	0.956915	-0.607648
5	6	0	-2.197033	0.677660	-0.299783
6	6	0	-4.029144	2.197360	-1.067968
7	7	0	-2.034539	-0.439582	0.389555
8	6	0	-4.352583	-0.091982	-0.032412
9	1	0	-5.023773	0.363638	0.700928
10	7	0	2.071537	-0.924428	0.366687
11	6	0	4.435463	-0.890626	0.396858
12	1	0	4.908023	-1.485430	-0.393787
13	7	0	3.839572	0.326771	-0.196647
14	6	0	3.209131	-1.595508	1.036354
15	1	0	3.164032	-1.319084	2.098433
16	6	0	5.109007	2.410500	-0.070389
17	1	0	4.829919	2.492384	0.976025
18	6	0	1.474283	1.118432	-0.713136
19	6	0	0.454404	3.027167	-1.795017

20	1	0	0.560806	3.948928	-2.358157
21	6	0	4.642367	1.332087	-0.826153
22	6	0	-4.628473	2.258263	-2.331358
23	1	0	-4.639069	1.375014	-2.963894
24	6	0	5.002280	1.214588	-2.174437
25	1	0	4.643317	0.370142	-2.756530
26	6	0	-4.014261	3.330317	-0.248498
27	1	0	-3.561721	3.279113	0.737780
28	6	0	0.185309	0.706163	-0.367062
29	6	0	1.603799	2.313104	-1.438535
30	1	0	2.578039	2.686571	-1.730109
31	6	0	-0.827866	2.583952	-1.455544
32	1	0	-1.690756	3.160256	-1.766120
33	6	0	-0.976809	1.395174	-0.720559
34	6	0	5.812436	2.185570	-2.760330
35	1	0	6.083544	2.092190	-3.809347
36	6	0	2.501482	0.185694	-0.214407
37	6	0	-4.573665	4.524107	-0.707739
38	1	0	-4.548453	5.403262	-0.068845
39	6	0	-5.192087	3.453293	-2.773656
40	1	0	-5.648274	3.493805	-3.759865
41	6	0	6.285744	3.281079	-2.019177
42	6	0	-5.172998	4.606956	-1.972357
43	6	0	5.920911	3.375452	-0.669102
44	1	0	6.275166	4.215312	-0.076899
45	6	0	7.170154	4.320689	-2.664111
46	1	0	6.708365	4.729322	-3.571227
47	1	0	8.134599	3.890240	-2.962934
48	1	0	7.371524	5.152306	-1.981648
49	6	0	-5.790947	5.893725	-2.463497
50	1	0	-5.546225	6.732403	-1.804222
51	1	0	-6.884970	5.814695	-2.510625
52	1	0	-5.444548	6.140981	-3.474025
53	1	0	5.194650	-0.617439	1.131935
54	1	0	-4.960293	-0.549082	-0.817659
55	6	0	-3.665732	-1.480438	2.085450
56	6	0	3.195579	-3.144527	0.967552
57	6	0	4.477210	-3.665197	1.649149
58	1	0	4.461611	-4.760225	1.701365
59	1	0	5.379045	-3.375258	1.096679
60	1	0	4.568854	-3.282648	2.673376
61	6	0	1.973637	-3.654656	1.756699
62	1	0	2.014957	-3.327973	2.803501
63	1	0	1.030073	-3.292874	1.325929

64	1	0	1.937433	-4.750722	1.748058
65	6	0	3.134573	-3.663753	-0.479419
66	1	0	2.245180	-3.295070	-1.001048
67	1	0	4.012046	-3.363959	-1.064236
68	1	0	3.098716	-4.759679	-0.484768
69	6	0	-2.648336	-2.524071	2.584047
70	1	0	-2.632765	-3.411434	1.941101
71	1	0	-1.635395	-2.109971	2.628500
72	1	0	-2.911386	-2.849170	3.598135
73	6	0	-5.069394	-2.121525	2.110436
74	1	0	-5.854680	-1.416787	1.812582
75	1	0	-5.124751	-2.991431	1.442840
76	1	0	-5.306668	-2.465389	3.123874
77	6	0	-3.631903	-0.257091	3.017156
78	1	0	-4.351384	0.515449	2.719981
79	1	0	-3.888250	-0.560599	4.039322
80	1	0	-2.636234	0.193883	3.044067
81	8	0	-1.141327	-4.177701	-0.077552
82	8	0	-0.080285	-1.831066	-1.328776
83	6	0	-1.324291	-3.913742	-1.244354
84	6	0	-0.580966	-2.762913	-1.933613
85	8	0	-2.122176	-4.522897	-2.100046
86	6	0	-2.876479	-5.663999	-1.599050
87	1	0	-3.424101	-6.039100	-2.461605
88	1	0	-2.185765	-6.416854	-1.214263
89	1	0	-3.560891	-5.335610	-0.814393
90	6	0	-0.408810	-2.776344	-3.471969
91	9	0	0.070022	-3.962629	-3.866700
92	9	0	0.436797	-1.816113	-3.850032
93	9	0	-1.596718	-2.561697	-4.054312
94	8	0	2.165273	1.124363	2.600074
95	8	0	-0.053437	-0.094496	2.435191
96	8	0	1.010480	0.195218	4.640609
97	16	0	0.926186	0.739993	3.282773
98	6	0	-0.046960	2.320890	3.445557
99	9	0	-1.204173	2.099456	4.077067
100	9	0	0.670071	3.204241	4.145880
101	9	0	-0.306231	2.834980	2.235483

TS2R_{endo}-OTf

Imaginary frequency= -149.48

Total energy= -3639.64902855

Sum of electronic and zero-point Energies= -3638.692148

Sum of electronic and thermal Energies= -3638.626260
Sum of electronic and thermal Enthalpies= -3638.625316
Sum of electronic and thermal Free Energies= -3638.799930

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.225240	-0.281247	0.572195
2	6	0	-1.511346	2.565884	0.983481
3	1	0	-2.441564	2.056157	0.730131
4	7	0	-0.047956	3.717308	-0.507118
5	6	0	0.392073	2.455452	-0.306831
6	6	0	0.588793	4.810127	-1.168883
7	7	0	-0.386608	1.731730	0.479390
8	6	0	-1.369326	3.865670	0.137948
9	1	0	-1.379927	4.778892	0.736148
10	7	0	1.363048	-2.022630	0.275899
11	6	0	2.637564	-4.023842	0.101256
12	1	0	2.308436	-4.768240	-0.633698
13	7	0	3.244022	-2.874651	-0.600754
14	6	0	1.463069	-3.374033	0.885003
15	1	0	1.767245	-3.232869	1.928202
16	6	0	5.678390	-2.797043	-0.818807
17	1	0	5.741695	-2.494744	0.222230
18	6	0	2.609947	-0.444548	-1.012770
19	6	0	3.542776	1.416882	-2.246305
20	1	0	4.300770	1.807375	-2.917830
21	6	0	4.425110	-3.014849	-1.397569
22	6	0	0.039738	5.319989	-2.352536
23	1	0	-0.839869	4.850550	-2.784574
24	6	0	4.332494	-3.407753	-2.738059
25	1	0	3.357102	-3.581812	-3.183088
26	6	0	1.721050	5.417065	-0.614046
27	1	0	2.140647	5.034566	0.311457
28	6	0	1.629114	0.432596	-0.540803
29	6	0	3.588652	0.067979	-1.879767
30	1	0	4.375858	-0.564914	-2.271137
31	6	0	2.544743	2.276685	-1.774758
32	1	0	2.541006	3.311897	-2.091777
33	6	0	1.564060	1.783211	-0.898324
34	6	0	5.493037	-3.562234	-3.494508
35	1	0	5.414571	-3.859436	-4.537125
36	6	0	2.430504	-1.804688	-0.476244
37	6	0	2.309576	6.508695	-1.256057

38	1	0	3.194528	6.965788	-0.820098
39	6	0	0.628529	6.419204	-2.974923
40	1	0	0.195414	6.803915	-3.894881
41	6	0	6.762211	-3.339040	-2.934389
42	6	0	1.772913	7.032747	-2.440364
43	6	0	6.833196	-2.956348	-1.587044
44	1	0	7.803763	-2.776712	-1.132560
45	6	0	8.011563	-3.519602	-3.762613
46	1	0	7.930572	-3.000376	-4.723941
47	1	0	8.188607	-4.580280	-3.985019
48	1	0	8.894920	-3.138162	-3.240613
49	6	0	2.386233	8.239431	-3.109312
50	1	0	3.426038	8.384938	-2.797648
51	1	0	1.834917	9.153656	-2.852303
52	1	0	2.363196	8.146114	-4.201082
53	1	0	3.371388	-4.491031	0.761274
54	1	0	-2.149560	3.944814	-0.627055
55	6	0	-1.539156	2.799944	2.529067
56	6	0	0.143462	-4.188226	0.915980
57	6	0	0.443014	-5.558978	1.555448
58	1	0	-0.484880	-6.130749	1.676552
59	1	0	1.121334	-6.160704	0.938339
60	1	0	0.897571	-5.444347	2.547446
61	6	0	-0.866354	-3.440029	1.806065
62	1	0	-0.472537	-3.302782	2.820191
63	1	0	-1.102710	-2.448155	1.400086
64	1	0	-1.803473	-4.004556	1.884282
65	6	0	-0.452063	-4.393583	-0.487876
66	1	0	-0.669296	-3.438050	-0.975089
67	1	0	0.221852	-4.958289	-1.144483
68	1	0	-1.386704	-4.963058	-0.420394
69	6	0	-1.735456	1.456896	3.257648
70	1	0	-2.639666	0.947396	2.906340
71	1	0	-0.884140	0.790172	3.110248
72	1	0	-1.840759	1.630115	4.337047
73	6	0	-2.762360	3.687591	2.848244
74	1	0	-2.680083	4.694393	2.423848
75	1	0	-3.689710	3.237449	2.472207
76	1	0	-2.864830	3.801826	3.933759
77	6	0	-0.256951	3.484956	3.033725
78	1	0	-0.112923	4.473871	2.581107
79	1	0	-0.309849	3.632738	4.119392
80	1	0	0.630154	2.880587	2.824559
81	8	0	-0.733419	-0.738966	-1.243476

82	8	0	-2.755241	-0.414513	0.578456
83	6	0	-1.913895	-0.765499	-1.609356
84	6	0	-3.094263	-0.582658	-0.624997
85	8	0	-2.240862	-0.938100	-2.865140
86	6	0	-1.173224	-1.059991	-3.849903
87	1	0	-1.686255	-1.186859	-4.801415
88	1	0	-0.570633	-0.149218	-3.851604
89	1	0	-0.556715	-1.929894	-3.619725
90	6	0	-4.129062	0.445706	-1.174349
91	9	0	-3.471969	1.599964	-1.473028
92	9	0	-5.041577	0.728984	-0.234736
93	9	0	-4.778250	0.071626	-2.291619
94	6	0	-8.715211	-1.383101	-0.017712
95	6	0	-7.415910	-1.627371	0.412472
96	6	0	-6.428647	-2.092155	-0.490274
97	6	0	-6.807675	-2.317670	-1.836112
98	6	0	-8.113820	-2.092053	-2.255221
99	6	0	-9.069975	-1.620115	-1.349972
100	1	0	-9.453649	-1.010886	0.684979
101	1	0	-7.159951	-1.424260	1.445707
102	1	0	-6.087829	-2.710091	-2.545116
103	1	0	-8.389320	-2.289445	-3.286915
104	1	0	-10.089376	-1.442698	-1.680479
105	6	0	-5.062685	-2.336843	-0.045273
106	6	0	-4.722432	-2.497257	1.389477
107	1	0	-4.084988	-1.628842	1.657683
108	1	0	-5.575140	-2.561555	2.063469
109	1	0	-4.082654	-3.374881	1.533947
110	6	0	-3.960929	-2.304126	-0.929934
111	1	0	-3.101759	-2.898851	-0.624116
112	1	0	-4.147588	-2.308980	-1.998159
113	8	0	3.621427	-0.501788	2.302884
114	8	0	1.214556	0.259436	2.300992
115	8	0	1.932180	-1.648456	3.776138
116	16	0	2.357771	-0.442011	3.049861
117	6	0	2.603833	0.866413	4.352387
118	9	0	1.473753	1.062966	5.039194
119	9	0	3.561704	0.466534	5.194967
120	9	0	2.977509	2.020665	3.787460

TS2S_{endo}-OTf

Imaginary frequency= -167.63

Total energy= -3639.64442889

Sum of electronic and zero-point Energies= -3638.688481
Sum of electronic and thermal Energies= -3638.622291
Sum of electronic and thermal Enthalpies= -3638.621347
Sum of electronic and thermal Free Energies= -3638.795563

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.272655	-0.266417	0.766378
2	6	0	-1.708264	2.397997	1.303731
3	1	0	-2.580839	1.777871	1.076563
4	7	0	-0.458238	3.681982	-0.271473
5	6	0	0.129760	2.482321	-0.075111
6	6	0	-0.119664	4.698392	-1.222097
7	7	0	-0.505927	1.698642	0.779062
8	6	0	-1.743411	3.705761	0.453869
9	1	0	-1.807209	4.612332	1.058872
10	7	0	1.510029	-1.915665	0.310973
11	6	0	3.089920	-3.697440	0.208799
12	1	0	2.910762	-4.521424	-0.490369
13	7	0	3.503611	-2.499686	-0.544616
14	6	0	1.800493	-3.229732	0.943211
15	1	0	2.046519	-3.033900	1.993667
16	6	0	5.905745	-2.197883	-0.910778
17	1	0	6.005883	-1.892027	0.126432
18	6	0	2.569994	-0.178227	-0.946660
19	6	0	3.297413	1.800812	-2.136082
20	1	0	3.998108	2.279858	-2.812718
21	6	0	4.641105	-2.524846	-1.414082
22	6	0	-0.575785	4.608402	-2.540891
23	1	0	-1.166387	3.750660	-2.850948
24	6	0	4.503945	-2.926564	-2.746024
25	1	0	3.523907	-3.194225	-3.131192
26	6	0	0.627627	5.810973	-0.818487
27	1	0	0.971911	5.880980	0.209408
28	6	0	1.541174	0.594553	-0.404019
29	6	0	3.467228	0.446911	-1.827758
30	1	0	4.288504	-0.102947	-2.271061
31	6	0	2.244450	2.551630	-1.603556
32	1	0	2.141585	3.595326	-1.874911
33	6	0	1.336823	1.939709	-0.723348
34	6	0	5.626845	-2.978969	-3.574179
35	1	0	5.510937	-3.286913	-4.610222
36	6	0	2.543693	-1.560702	-0.437472

37	6	0	0.929763	6.813723	-1.738565
38	1	0	1.515782	7.671888	-1.418336
39	6	0	-0.266426	5.618575	-3.452996
40	1	0	-0.620069	5.537860	-4.477748
41	6	0	6.899901	-2.645864	-3.091307
42	6	0	0.492225	6.733928	-3.070943
43	6	0	7.019129	-2.256744	-1.746797
44	1	0	7.997452	-1.994434	-1.351192
45	6	0	8.115965	-2.704328	-3.983761
46	1	0	8.631336	-1.736474	-4.017277
47	1	0	7.847503	-2.979608	-5.008498
48	1	0	8.842909	-3.440078	-3.616936
49	6	0	0.841804	7.817855	-4.061700
50	1	0	0.577280	8.810228	-3.677369
51	1	0	0.321851	7.672552	-5.013892
52	1	0	1.920026	7.831641	-4.267587
53	1	0	3.880690	-3.997719	0.900255
54	1	0	-2.569891	3.717336	-0.266227
55	6	0	-1.716686	2.640098	2.847684
56	6	0	0.639909	-4.261079	0.931833
57	6	0	1.161811	-5.570275	1.560295
58	1	0	0.345915	-6.297866	1.644259
59	1	0	1.953251	-6.033645	0.959612
60	1	0	1.559732	-5.396621	2.568067
61	6	0	-0.507929	-3.732078	1.810047
62	1	0	-0.163731	-3.548870	2.836306
63	1	0	-0.927422	-2.798935	1.422020
64	1	0	-1.324563	-4.462248	1.857167
65	6	0	0.130691	-4.539438	-0.492939
66	1	0	-0.253558	-3.630729	-0.967661
67	1	0	0.916481	-4.949138	-1.138861
68	1	0	-0.682112	-5.273705	-0.466390
69	6	0	-1.734684	1.289412	3.588375
70	1	0	-2.598734	0.682514	3.291929
71	1	0	-0.826042	0.712166	3.400854
72	1	0	-1.802449	1.457812	4.670540
73	6	0	-3.013208	3.395401	3.208712
74	1	0	-3.059292	4.396171	2.764059
75	1	0	-3.903072	2.839627	2.886047
76	1	0	-3.078192	3.520458	4.295853
77	6	0	-0.497044	3.459534	3.301006
78	1	0	-0.455627	4.444066	2.818752
79	1	0	-0.541009	3.630654	4.383477
80	1	0	0.436965	2.933619	3.087373

81	8	0	-0.795074	-0.644557	-1.008112
82	8	0	-2.688027	-1.187426	0.926578
83	6	0	-1.898613	-1.113337	-1.309449
84	6	0	-3.003120	-1.396487	-0.266205
85	8	0	-2.203013	-1.412277	-2.547379
86	6	0	-1.194438	-1.206015	-3.578768
87	1	0	-1.668512	-1.538625	-4.500410
88	1	0	-0.937464	-0.146587	-3.632716
89	1	0	-0.311093	-1.806658	-3.356453
90	6	0	-3.801052	-2.705353	-0.536327
91	9	0	-4.452255	-2.752586	-1.711108
92	9	0	-4.695411	-2.901412	0.444532
93	9	0	-2.935499	-3.747371	-0.518492
94	6	0	-8.710756	-1.946125	-0.186068
95	6	0	-7.549495	-1.334557	0.273489
96	6	0	-6.647128	-0.726470	-0.629585
97	6	0	-6.967941	-0.739506	-2.007111
98	6	0	-8.140973	-1.333747	-2.459091
99	6	0	-9.013282	-1.943584	-1.551716
100	1	0	-9.382769	-2.424151	0.520488
101	1	0	-7.323759	-1.360558	1.333642
102	1	0	-6.315270	-0.246315	-2.719250
103	1	0	-8.379699	-1.317740	-3.518408
104	1	0	-9.928032	-2.409844	-1.906705
105	6	0	-5.419413	-0.091912	-0.153886
106	6	0	-5.286380	0.377014	1.254484
107	1	0	-4.929650	1.412715	1.270139
108	1	0	-6.203222	0.310877	1.839337
109	1	0	-4.489459	-0.221936	1.732997
110	6	0	-4.278615	0.023125	-0.959419
111	1	0	-3.590840	0.827490	-0.710111
112	1	0	-4.347823	-0.211621	-2.015770
113	8	0	1.266714	0.174752	2.521841
114	8	0	2.508586	-0.571810	4.515246
115	8	0	3.567237	-0.856145	2.245692
116	16	0	2.647020	-0.126852	3.124923
117	6	0	3.363706	1.589446	3.232844
118	9	0	4.623878	1.510566	3.672512
119	9	0	3.363568	2.174839	2.026833
120	9	0	2.655958	2.345317	4.079011

TS2R_{exo}-OTf

Imaginary frequency= -122.81

Total energy= -3639.64827207
Sum of electronic and zero-point Energies= -3638.691804
Sum of electronic and thermal Energies= -3638.625564
Sum of electronic and thermal Enthalpies= -3638.624620
Sum of electronic and thermal Free Energies= -3638.797560

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.083093	-0.436463	-0.952256
2	6	0	1.840841	2.196464	-1.854965
3	1	0	2.724347	1.557847	-1.948077
4	7	0	1.161303	3.389992	0.104617
5	6	0	0.496845	2.213059	0.019069
6	6	0	0.760501	4.569808	0.799682
7	7	0	0.840693	1.467424	-1.018642
8	6	0	2.180521	3.432801	-0.968065
9	1	0	2.101025	4.380551	-1.501793
10	7	0	-1.374118	-2.034595	-0.346753
11	6	0	-3.318312	-3.421311	-0.173752
12	1	0	-3.392379	-4.425237	0.249759
13	7	0	-3.197871	-2.433364	0.913027
14	6	0	-2.025304	-3.202813	-1.015633
15	1	0	-2.299343	-2.883404	-2.024915
16	6	0	-5.209818	-1.159025	1.515355
17	1	0	-5.068443	-0.541443	0.633816
18	6	0	-1.769050	-0.404133	1.367869
19	6	0	-1.756095	1.369267	3.011518
20	1	0	-2.085646	1.760032	3.969164
21	6	0	-4.292252	-2.177712	1.800115
22	6	0	-0.538704	5.078304	0.658872
23	1	0	-1.257087	4.559230	0.030614
24	6	0	-4.475765	-2.987870	2.923782
25	1	0	-3.766149	-3.783168	3.133990
26	6	0	1.692169	5.257235	1.583861
27	1	0	2.700090	4.866879	1.692760
28	6	0	-0.887977	0.363519	0.606485
29	6	0	-2.206537	0.110650	2.597877
30	1	0	-2.876129	-0.455553	3.234722
31	6	0	-0.896525	2.139739	2.222017
32	1	0	-0.573900	3.110495	2.579070
33	6	0	-0.454577	1.637809	0.986198
34	6	0	-5.565882	-2.767062	3.767286
35	1	0	-5.701635	-3.401248	4.639852

36	6	0	-2.120564	-1.658706	0.681547
37	6	0	1.320300	6.436845	2.230361
38	1	0	2.051971	6.961551	2.839496
39	6	0	-0.900374	6.246840	1.325793
40	1	0	-1.912976	6.627962	1.216562
41	6	0	-6.486306	-1.740547	3.509754
42	6	0	0.020624	6.950033	2.119161
43	6	0	-6.289681	-0.944283	2.370118
44	1	0	-6.995784	-0.148367	2.145627
45	6	0	-7.645593	-1.480315	4.441435
46	1	0	-7.424149	-0.646852	5.121874
47	1	0	-7.869160	-2.356794	5.058122
48	1	0	-8.551226	-1.210241	3.886822
49	6	0	-0.379889	8.227680	2.816028
50	1	0	0.396210	8.564255	3.510656
51	1	0	-1.310746	8.098869	3.381161
52	1	0	-0.554337	9.036276	2.094116
53	1	0	-4.226331	-3.217768	-0.748519
54	1	0	3.182962	3.365724	-0.533562
55	6	0	1.419583	2.564818	-3.317603
56	6	0	-1.162099	-4.493260	-1.161065
57	6	0	-2.034225	-5.579830	-1.827915
58	1	0	-1.424685	-6.466785	-2.037955
59	1	0	-2.868755	-5.903424	-1.195860
60	1	0	-2.448314	-5.227593	-2.781290
61	6	0	0.022133	-4.217299	-2.099062
62	1	0	-0.321317	-3.859554	-3.078147
63	1	0	0.689684	-3.464480	-1.684476
64	1	0	0.605700	-5.132025	-2.259695
65	6	0	-0.648691	-5.000730	0.197200
66	1	0	-0.016038	-4.256877	0.690325
67	1	0	-1.469929	-5.254257	0.878183
68	1	0	-0.049805	-5.909034	0.058461
69	6	0	1.150323	1.294294	-4.143503
70	1	0	2.022595	0.631300	-4.154084
71	1	0	0.295452	0.734308	-3.760531
72	1	0	0.929273	1.570878	-5.182111
73	6	0	2.616435	3.297915	-3.965085
74	1	0	2.834853	4.259909	-3.488048
75	1	0	3.528607	2.687776	-3.928038
76	1	0	2.397336	3.501942	-5.019551
77	6	0	0.177925	3.470349	-3.358601
78	1	0	0.321429	4.403167	-2.799842
79	1	0	-0.044831	3.746867	-4.396276

80	1	0	-0.700725	2.959317	-2.958715
81	8	0	1.723573	-1.327729	-2.382787
82	8	0	1.381556	-1.258498	0.281376
83	6	0	2.629284	-1.755030	-1.678480
84	6	0	2.480888	-1.700989	-0.157925
85	8	0	3.736567	-2.316773	-2.105231
86	6	0	3.887822	-2.477328	-3.545939
87	1	0	4.820411	-3.025279	-3.668626
88	1	0	3.044919	-3.045261	-3.943149
89	1	0	3.948072	-1.495678	-4.019422
90	6	0	3.107086	-2.835051	0.680155
91	9	0	2.479862	-3.988113	0.353793
92	9	0	2.909072	-2.613547	1.987183
93	9	0	4.413295	-3.014483	0.463862
94	6	0	6.761054	-1.708715	3.876439
95	6	0	5.589451	-1.162398	3.361632
96	6	0	5.544773	-0.664273	2.039800
97	6	0	6.726990	-0.719863	1.264446
98	6	0	7.900220	-1.248870	1.790424
99	6	0	7.920564	-1.749779	3.096317
100	1	0	6.770830	-2.102399	4.888492
101	1	0	4.698209	-1.157129	3.978650
102	1	0	6.735773	-0.309879	0.260160
103	1	0	8.802219	-1.265326	1.185751
104	1	0	8.836985	-2.165611	3.505435
105	6	0	4.317029	-0.091144	1.480087
106	6	0	3.290809	0.539596	2.374781
107	1	0	3.406584	0.281292	3.427296
108	1	0	3.377879	1.632233	2.295144
109	1	0	2.278036	0.277074	2.047985
110	6	0	4.065400	-0.100058	0.115267
111	1	0	3.324855	0.590067	-0.271302
112	1	0	4.815260	-0.451638	-0.584182
113	8	0	-3.683975	-0.805552	-1.961057
114	8	0	-1.463034	0.377407	-2.276033
115	8	0	-3.188880	0.592220	-3.998305
116	16	0	-2.963013	0.315072	-2.576476
117	6	0	-3.634107	1.818960	-1.694869
118	9	0	-2.909222	2.911240	-1.971887
119	9	0	-4.893615	2.025445	-2.091280
120	9	0	-3.629202	1.632329	-0.367205

TS2S_{exo}-OTf

Imaginary frequency= -205.63
Total energy= -3639.65288296
Sum of electronic and zero-point Energies= -3638.695998
Sum of electronic and thermal Energies= -3638.629934
Sum of electronic and thermal Enthalpies= -3638.628990
Sum of electronic and thermal Free Energies= -3638.801323

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.243213	-0.043918	-0.984909
2	6	0	1.525091	2.738727	-1.636419
3	1	0	2.337082	2.080984	-1.960911
4	7	0	1.111787	3.538259	0.567727
5	6	0	0.368771	2.435801	0.329335
6	6	0	1.285241	4.249053	1.799082
7	7	0	0.539789	1.918494	-0.878165
8	6	0	2.050341	3.728535	-0.554730
9	1	0	2.031763	4.770707	-0.878475
10	7	0	-1.392815	-1.793566	-0.492093
11	6	0	-3.285567	-3.266312	-0.366351
12	1	0	-3.224877	-4.320428	-0.083207
13	7	0	-3.110057	-2.423179	0.825395
14	6	0	-2.128538	-2.813246	-1.307038
15	1	0	-2.550316	-2.288165	-2.171994
16	6	0	-5.173296	-1.552555	1.829635
17	1	0	-5.255083	-0.844716	1.010609
18	6	0	-1.730415	-0.411071	1.447728
19	6	0	-1.720082	1.162462	3.285452
20	1	0	-2.026408	1.426764	4.292800
21	6	0	-4.080288	-2.424638	1.878266
22	6	0	0.517337	5.385212	2.065357
23	1	0	-0.234839	5.704103	1.349555
24	6	0	-3.962783	-3.341821	2.927073
25	1	0	-3.112454	-4.017677	2.956507
26	6	0	2.261691	3.835850	2.713947
27	1	0	2.860099	2.954029	2.500804
28	6	0	-0.949117	0.494789	0.728735
29	6	0	-2.117099	-0.068887	2.753060
30	1	0	-2.715182	-0.742496	3.355208
31	6	0	-0.934188	2.059970	2.555563
32	1	0	-0.645533	3.002614	3.004342
33	6	0	-0.525744	1.720256	1.255234
34	6	0	-4.933451	-3.377228	3.928771

35	1	0	-4.833163	-4.089597	4.744040
36	6	0	-2.074402	-1.587565	0.631444
37	6	0	2.452929	4.553290	3.893084
38	1	0	3.208499	4.221980	4.601503
39	6	0	0.715883	6.093326	3.252414
40	1	0	0.108486	6.971476	3.456727
41	6	0	-6.036048	-2.509804	3.900213
42	6	0	1.685488	5.693576	4.182774
43	6	0	-6.135100	-1.597114	2.838679
44	1	0	-6.978052	-0.911313	2.800137
45	6	0	-7.104955	-2.578899	4.963978
46	1	0	-7.571613	-1.601486	5.127223
47	1	0	-6.699635	-2.931671	5.918341
48	1	0	-7.903262	-3.274787	4.671955
49	6	0	1.919146	6.476940	5.451914
50	1	0	2.034413	5.813191	6.316520
51	1	0	1.092678	7.165053	5.655781
52	1	0	2.838230	7.073993	5.381248
53	1	0	-4.272808	-3.084749	-0.801372
54	1	0	3.066723	3.488664	-0.224085
55	6	0	0.979871	3.445317	-2.920053
56	6	0	-1.302737	-4.004140	-1.879839
57	6	0	-2.272875	-4.917080	-2.661637
58	1	0	-1.717246	-5.734602	-3.136299
59	1	0	-3.033874	-5.371884	-2.017691
60	1	0	-2.788826	-4.360924	-3.454535
61	6	0	-0.255178	-3.480599	-2.874113
62	1	0	-0.722002	-2.873066	-3.659437
63	1	0	0.496858	-2.863587	-2.382087
64	1	0	0.260988	-4.318120	-3.359586
65	6	0	-0.611507	-4.814664	-0.769937
66	1	0	-0.003778	-4.171934	-0.124281
67	1	0	-1.329715	-5.341166	-0.130463
68	1	0	0.046984	-5.574112	-1.208252
69	6	0	0.471741	2.397908	-3.926689
70	1	0	1.248870	1.659058	-4.156348
71	1	0	-0.404385	1.865045	-3.552223
72	1	0	0.191279	2.889494	-4.866773
73	6	0	2.159190	4.199478	-3.572842
74	1	0	2.553626	5.001028	-2.937791
75	1	0	2.987419	3.517543	-3.806420
76	1	0	1.832941	4.660611	-4.512493
77	6	0	-0.150702	4.437705	-2.596036
78	1	0	0.182862	5.242746	-1.930623

79	1	0	-0.510036	4.909465	-3.518688
80	1	0	-1.003592	3.940119	-2.127370
81	8	0	1.358725	-0.663647	-2.662882
82	8	0	1.481039	-0.611839	0.028082
83	6	0	2.443925	-0.879989	-2.135783
84	6	0	2.547957	-0.924011	-0.604134
85	8	0	3.574160	-1.079758	-2.774354
86	6	0	3.542814	-1.027181	-4.230270
87	1	0	4.562312	-1.252731	-4.538362
88	1	0	2.844540	-1.774238	-4.611764
89	1	0	3.250908	-0.027236	-4.555968
90	6	0	3.832390	-0.323319	0.007364
91	9	0	4.963244	-0.911369	-0.399370
92	9	0	3.783117	-0.367872	1.347290
93	9	0	3.904412	0.980970	-0.355146
94	6	0	6.358338	-3.500904	3.065319
95	6	0	5.047339	-3.277270	2.664070
96	6	0	4.664727	-3.440086	1.309704
97	6	0	5.651075	-3.862193	0.383731
98	6	0	6.957327	-4.097276	0.793404
99	6	0	7.317232	-3.911940	2.132693
100	1	0	6.636061	-3.356568	4.105086
101	1	0	4.320421	-2.952933	3.399546
102	1	0	5.386680	-4.041600	-0.652249
103	1	0	7.695929	-4.433271	0.071976
104	1	0	8.340287	-4.093724	2.449702
105	6	0	3.287611	-3.206610	0.896557
106	6	0	2.207360	-3.161534	1.934107
107	1	0	2.213605	-4.078718	2.535274
108	1	0	2.370782	-2.326284	2.626665
109	1	0	1.223161	-3.042299	1.482877
110	6	0	2.930228	-2.985875	-0.443509
111	1	0	1.908688	-3.225919	-0.721822
112	1	0	3.669764	-3.121357	-1.224665
113	8	0	-1.787652	0.631345	-2.200528
114	8	0	-3.853941	-0.043757	-3.382913
115	8	0	-3.890858	0.184337	-0.874337
116	16	0	-3.316328	0.579040	-2.166989
117	6	0	-3.714863	2.388532	-2.333804
118	9	0	-5.041768	2.549186	-2.375728
119	9	0	-3.233877	3.068219	-1.281275
120	9	0	-3.180219	2.888127	-3.452776

M1$_{endo}$-DCE

Total energy= -3328.09224160

Sum of electronic and zero-point Energies= -3327.265500

Sum of electronic and thermal Energies= -3327.211087

Sum of electronic and thermal Enthalpies= -3327.210143

Sum of electronic and thermal Free Energies= -3327.358229

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.150245	-0.870755	0.738427
2	6	0	-3.475327	-0.561219	0.901172
3	1	0	-3.567192	-1.393214	0.192271
4	7	0	-3.334768	1.646520	0.003482
5	6	0	-2.103870	1.180120	0.269813
6	6	0	-3.725721	2.914729	-0.538668
7	7	0	-2.083993	-0.037625	0.800177
8	6	0	-4.337512	0.639744	0.405619
9	1	0	-4.975249	1.060531	1.187788
10	7	0	1.912785	-1.058716	0.459842
11	6	0	4.231343	-1.414887	0.193187
12	1	0	4.481697	-1.913389	-0.750575
13	7	0	3.820663	-0.017481	-0.087689
14	6	0	2.972580	-2.010743	0.875080
15	1	0	3.086822	-1.909730	1.964837
16	6	0	5.487633	1.776773	-0.116582
17	1	0	5.436493	1.818974	0.967619
18	6	0	1.582580	1.204673	-0.219800
19	6	0	0.821617	3.420109	-0.830804
20	1	0	1.046438	4.417058	-1.195892
21	6	0	4.683199	0.872786	-0.812816
22	6	0	-3.910349	3.048137	-1.919753
23	1	0	-3.720207	2.200546	-2.572362
24	6	0	4.749092	0.806056	-2.210205
25	1	0	4.131512	0.092176	-2.748265
26	6	0	-3.976764	3.996593	0.309117
27	1	0	-3.840477	3.885998	1.381262
28	6	0	0.259192	0.921841	0.129078
29	6	0	1.863261	2.494770	-0.701031
30	1	0	2.872283	2.782344	-0.971766
31	6	0	-0.503609	3.094034	-0.522729
32	1	0	-1.282744	3.833708	-0.661505
33	6	0	-0.803909	1.808420	-0.039090
34	6	0	5.606595	1.658495	-2.901953

35	1	0	5.649122	1.606553	-3.987243
36	6	0	2.476387	0.053139	0.011301
37	6	0	-4.396572	5.213569	-0.230978
38	1	0	-4.584830	6.053504	0.432601
39	6	0	-4.331116	4.267921	-2.445530
40	1	0	-4.469149	4.367236	-3.519395
41	6	0	6.416373	2.583157	-2.221644
42	6	0	-4.582170	5.370158	-1.611928
43	6	0	6.342589	2.625933	-0.822371
44	1	0	6.960844	3.333528	-0.276113
45	6	0	7.347432	3.493700	-2.984630
46	1	0	6.822609	4.009712	-3.797479
47	1	0	8.166557	2.924994	-3.443457
48	1	0	7.791444	4.250504	-2.330697
49	6	0	-5.056060	6.679615	-2.193333
50	1	0	-5.030522	7.480818	-1.448349
51	1	0	-6.088063	6.597231	-2.558796
52	1	0	-4.438930	6.984393	-3.046742
53	1	0	5.108505	-1.426666	0.841777
54	1	0	-4.967693	0.382813	-0.449966
55	6	0	-3.890639	-1.111360	2.300698
56	6	0	2.671846	-3.505782	0.598906
57	6	0	3.892541	-4.327781	1.060575
58	1	0	3.687861	-5.399354	0.955697
59	1	0	4.784653	-4.101961	0.464503
60	1	0	4.129597	-4.133982	2.114222
61	6	0	1.448831	-3.921295	1.440796
62	1	0	1.635057	-3.769385	2.511270
63	1	0	0.550383	-3.347803	1.171422
64	1	0	1.218230	-4.981947	1.287086
65	6	0	2.397087	-3.781632	-0.888805
66	1	0	1.540261	-3.204358	-1.252638
67	1	0	3.258072	-3.537855	-1.521941
68	1	0	2.174373	-4.844736	-1.037120
69	6	0	-3.045644	-2.350783	2.647008
70	1	0	-3.188739	-3.151751	1.913752
71	1	0	-1.975279	-2.121888	2.686032
72	1	0	-3.332744	-2.740074	3.630817
73	6	0	-5.366596	-1.556259	2.213815
74	1	0	-6.045055	-0.714028	2.037716
75	1	0	-5.516748	-2.287239	1.409236
76	1	0	-5.670324	-2.029978	3.154394
77	6	0	-3.735280	-0.052822	3.406839
78	1	0	-4.355423	0.832362	3.224278

79	1	0	-4.045308	-0.472595	4.370736
80	1	0	-2.696632	0.279618	3.508315
81	8	0	-0.424109	-1.259962	-1.300446
82	8	0	-1.702606	-3.489610	-0.206100
83	6	0	-0.981012	-2.113372	-1.997831
84	6	0	-1.670875	-3.346236	-1.399136
85	8	0	-1.034977	-2.063920	-3.292765
86	6	0	-0.410319	-0.934019	-3.984443
87	1	0	-0.582797	-1.131574	-5.040025
88	1	0	-0.897418	-0.009943	-3.668369
89	1	0	0.655440	-0.918194	-3.751574
90	6	0	-2.306123	-4.382617	-2.360348
91	9	0	-3.260331	-3.796990	-3.098928
92	9	0	-2.846269	-5.375005	-1.656152
93	9	0	-1.366205	-4.882150	-3.175962
94	6	0	1.551669	1.944158	3.601805
95	17	0	0.107343	-0.345216	3.085856
96	17	0	3.140240	2.654608	4.125214
97	1	0	1.903081	0.014322	4.572631
98	1	0	2.461333	0.092064	2.867855
99	1	0	0.801382	2.267666	4.323253
100	1	0	1.331054	2.344620	2.612835
101	6	0	1.721708	0.438678	3.584910

M1$_{exo}$-DCE

Total energy= -3328.09014911

Sum of electronic and zero-point Energies= -3327.263070

Sum of electronic and thermal Energies= -3327.208678

Sum of electronic and thermal Enthalpies= -3327.207733

Sum of electronic and thermal Free Energies= -3327.354267

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.115035	-0.960889	0.707897
2	6	0	-3.466076	-0.932449	0.777483
3	1	0	-3.489373	-1.773553	0.073192
4	7	0	-3.496868	1.270283	-0.145441
5	6	0	-2.233447	0.903448	0.126240
6	6	0	-3.990079	2.560913	-0.529707
7	7	0	-2.121085	-0.300504	0.677409
8	6	0	-4.418217	0.192505	0.271040

9	1	0	-5.082231	0.571344	1.052539
10	7	0	1.962151	-0.970097	0.488760
11	6	0	4.315644	-1.108874	0.335976
12	1	0	4.668857	-1.638905	-0.555848
13	7	0	3.780247	0.214570	-0.067142
14	6	0	3.088985	-1.790185	0.998136
15	1	0	3.140764	-1.624760	2.084757
16	6	0	5.332831	2.105546	-0.062175
17	1	0	5.259221	2.136375	1.021133
18	6	0	1.447119	1.209022	-0.338689
19	6	0	0.506268	3.304649	-1.100689
20	1	0	0.647939	4.289207	-1.534576
21	6	0	4.594007	1.158770	-0.779075
22	6	0	-4.111043	3.580479	0.422103
23	1	0	-3.805616	3.400514	1.448967
24	6	0	4.693142	1.101284	-2.172550
25	1	0	4.134043	0.353381	-2.727718
26	6	0	-4.401039	2.779378	-1.846728
27	1	0	-4.312683	1.981635	-2.578831
28	6	0	0.147264	0.830173	0.006300
29	6	0	1.621961	2.485557	-0.898907
30	1	0	2.606028	2.840722	-1.180232
31	6	0	-0.788659	2.887533	-0.776531
32	1	0	-1.626192	3.545394	-0.972068
33	6	0	-0.984442	1.616236	-0.208839
34	6	0	5.516785	2.006361	-2.843372
35	1	0	5.588324	1.958386	-3.926914
36	6	0	2.434735	0.160728	-0.018326
37	6	0	-4.914631	4.024828	-2.212210
38	1	0	-5.228430	4.190689	-3.239510
39	6	0	-4.622611	4.819835	0.042827
40	1	0	-4.709782	5.609736	0.784982
41	6	0	6.257404	2.970805	-2.144832
42	6	0	-5.031282	5.064458	-1.278697
43	6	0	6.153559	3.001741	-0.744679
44	1	0	6.723026	3.737215	-0.181966
45	6	0	7.133206	3.960557	-2.873850
46	1	0	6.663110	4.952382	-2.908112
47	1	0	7.317746	3.646858	-3.906101
48	1	0	8.100577	4.081312	-2.373255
49	6	0	-5.566972	6.417633	-1.678191
50	1	0	-5.991921	6.397887	-2.686364
51	1	0	-4.772153	7.175034	-1.665398
52	1	0	-6.344696	6.759412	-0.985189

53	1	0	5.151583	-0.983283	1.025675
54	1	0	-5.030292	-0.121508	-0.578317
55	6	0	-3.845329	-1.509097	2.174813
56	6	0	2.947191	-3.318794	0.786136
57	6	0	4.220933	-3.992888	1.333793
58	1	0	4.126709	-5.083229	1.275037
59	1	0	5.111490	-3.707915	0.761041
60	1	0	4.394267	-3.729119	2.384581
61	6	0	1.734454	-3.810783	1.599867
62	1	0	1.847582	-3.571530	2.664865
63	1	0	0.796205	-3.361919	1.246044
64	1	0	1.626105	-4.898018	1.510414
65	6	0	2.764686	-3.692879	-0.694343
66	1	0	1.872191	-3.224517	-1.121693
67	1	0	3.624646	-3.399356	-1.307042
68	1	0	2.651150	-4.778842	-0.791876
69	6	0	-2.874929	-2.643234	2.548974
70	1	0	-2.843091	-3.418081	1.775384
71	1	0	-1.854732	-2.273927	2.701840
72	1	0	-3.189237	-3.115100	3.487420
73	6	0	-5.262723	-2.108646	2.058442
74	1	0	-6.015040	-1.350003	1.813523
75	1	0	-5.304103	-2.888630	1.287798
76	1	0	-5.555896	-2.566006	3.010271
77	6	0	-3.830986	-0.434773	3.276539
78	1	0	-4.564488	0.359533	3.096547
79	1	0	-4.078890	-0.890351	4.242250
80	1	0	-2.846804	0.035526	3.376225
81	8	0	-1.294790	-3.955239	-0.249770
82	8	0	-0.268904	-1.518960	-1.285782
83	6	0	-1.488741	-3.611315	-1.394222
84	6	0	-0.793833	-2.375327	-1.977456
85	8	0	-2.255253	-4.179143	-2.300281
86	6	0	-2.976569	-5.380812	-1.897490
87	1	0	-3.522073	-5.691468	-2.786289
88	1	0	-2.261769	-6.145073	-1.587227
89	1	0	-3.659897	-5.138177	-1.081464
90	6	0	-0.700908	-2.186204	-3.512170
91	9	0	-0.209336	-3.294406	-4.075481
92	9	0	0.095314	-1.156119	-3.800746
93	9	0	-1.924644	-1.941943	-3.997565
94	6	0	1.297918	1.972844	4.004771
95	17	0	-0.017450	-0.207311	2.998003
96	17	0	2.870067	2.685354	4.568008

97	1	0	1.950964	-0.092192	4.331182
98	1	0	2.250016	0.527831	2.669644
99	1	0	0.612992	1.991980	4.852687
100	1	0	0.925058	2.604929	3.199041
101	6	0	1.595977	0.562751	3.536466

TS2R_{endo}-DCE

Imaginary frequency= -151.28
Total energy= -3677.05279038
Sum of electronic and zero-point Energies= -3676.063902
Sum of electronic and thermal Energies= -3676.000545
Sum of electronic and thermal Enthalpies= -3675.999601
Sum of electronic and thermal Free Energies= -3676.164774

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.198267	-0.279090	0.813565
2	6	0	-1.556438	2.552121	1.308439
3	1	0	-2.444252	2.044689	0.932659
4	7	0	-0.033285	3.757657	-0.079491
5	6	0	0.416641	2.505375	0.117926
6	6	0	0.601904	4.850618	-0.752498
7	7	0	-0.369653	1.756055	0.879047
8	6	0	-1.358979	3.901637	0.554361
9	1	0	-1.349150	4.769814	1.216466
10	7	0	1.338075	-2.002758	0.447993
11	6	0	2.631682	-3.982488	0.275932
12	1	0	2.311858	-4.671328	-0.514146
13	7	0	3.281124	-2.802287	-0.336264
14	6	0	1.444134	-3.354960	1.052740
15	1	0	1.745004	-3.216258	2.101839
16	6	0	5.719850	-2.722825	-0.509217
17	1	0	5.767164	-2.447776	0.540622
18	6	0	2.642399	-0.363270	-0.696629
19	6	0	3.628050	1.564786	-1.774997
20	1	0	4.407427	1.990340	-2.398990
21	6	0	4.478000	-2.922949	-1.117128
22	6	0	0.205084	5.194418	-2.050140
23	1	0	-0.561557	4.610647	-2.551997
24	6	0	4.409445	-3.285445	-2.467769
25	1	0	3.442478	-3.448484	-2.935702
26	6	0	1.582200	5.603627	-0.099798

27	1	0	1.877269	5.342417	0.912492
28	6	0	1.663321	0.496336	-0.189617
29	6	0	3.648725	0.193236	-1.503487
30	1	0	4.435290	-0.423838	-1.920938
31	6	0	2.626543	2.403233	-1.274099
32	1	0	2.641217	3.457375	-1.521359
33	6	0	1.612883	1.864352	-0.463088
34	6	0	5.584341	-3.428924	-3.203630
35	1	0	5.524760	-3.704908	-4.253585
36	6	0	2.439865	-1.752160	-0.245379
37	6	0	2.180763	6.679447	-0.757571
38	1	0	2.950324	7.253583	-0.247838
39	6	0	0.805724	6.275390	-2.693017
40	1	0	0.499025	6.531692	-3.704222
41	6	0	6.842398	-3.222885	-2.613376
42	6	0	1.804532	7.034038	-2.060948
43	6	0	6.888813	-2.868510	-1.257840
44	1	0	7.851245	-2.704299	-0.780217
45	6	0	8.107290	-3.396570	-3.418067
46	1	0	8.042088	-2.876430	-4.380856
47	1	0	8.292114	-4.456207	-3.638203
48	1	0	8.979282	-3.012380	-2.879652
49	6	0	2.438682	8.210380	-2.762534
50	1	0	3.359297	8.525295	-2.261202
51	1	0	1.758482	9.072266	-2.779299
52	1	0	2.679200	7.971956	-3.804936
53	1	0	3.335181	-4.502028	0.928980
54	1	0	-2.120679	4.062846	-0.215270
55	6	0	-1.754562	2.706924	2.849404
56	6	0	0.131709	-4.178030	1.069159
57	6	0	0.439537	-5.560141	1.679182
58	1	0	-0.485468	-6.138197	1.788997
59	1	0	1.119786	-6.144722	1.048655
60	1	0	0.893720	-5.465694	2.673622
61	6	0	-0.883719	-3.452741	1.971685
62	1	0	-0.491052	-3.331545	2.989521
63	1	0	-1.133714	-2.456576	1.584492
64	1	0	-1.814896	-4.027393	2.042991
65	6	0	-0.455571	-4.355069	-0.341673
66	1	0	-0.676039	-3.388779	-0.808061
67	1	0	0.223461	-4.900811	-1.007097
68	1	0	-1.387768	-4.929642	-0.290289
69	6	0	-2.036787	1.332124	3.481932
70	1	0	-2.898778	0.849716	3.010355

71	1	0	-1.187623	0.648608	3.392554
72	1	0	-2.247902	1.446425	4.552155
73	6	0	-3.011289	3.577583	3.071892
74	1	0	-2.883929	4.602377	2.705874
75	1	0	-3.887300	3.146067	2.571039
76	1	0	-3.236698	3.639722	4.142970
77	6	0	-0.543631	3.366744	3.531458
78	1	0	-0.349846	4.373891	3.143069
79	1	0	-0.726160	3.465423	4.608153
80	1	0	0.368405	2.773821	3.403319
81	8	0	-0.674481	-0.568217	-1.040363
82	8	0	-2.742895	-0.490567	0.765349
83	6	0	-1.852634	-0.638472	-1.427056
84	6	0	-3.055471	-0.571167	-0.457986
85	8	0	-2.138971	-0.747332	-2.695014
86	6	0	-1.046103	-0.757368	-3.663950
87	1	0	-1.536027	-0.851193	-4.631072
88	1	0	-0.489574	0.178841	-3.595311
89	1	0	-0.395837	-1.611788	-3.469703
90	6	0	-4.098591	0.476887	-0.954969
91	9	0	-3.456791	1.658377	-1.171295
92	9	0	-5.026238	0.683623	-0.011770
93	9	0	-4.723656	0.163497	-2.102044
94	6	0	-8.685068	-1.459273	-0.155537
95	6	0	-7.403467	-1.710736	0.318157
96	6	0	-6.375517	-2.129573	-0.561995
97	6	0	-6.696344	-2.303819	-1.931471
98	6	0	-7.986432	-2.075051	-2.393597
99	6	0	-8.982661	-1.646327	-1.509907
100	1	0	-9.455482	-1.119366	0.529904
101	1	0	-7.189340	-1.545595	1.367822
102	1	0	-5.944496	-2.662620	-2.625661
103	1	0	-8.219634	-2.234509	-3.442039
104	1	0	-9.989877	-1.464642	-1.874112
105	6	0	-5.027486	-2.377074	-0.073359
106	6	0	-4.745538	-2.627646	1.362250
107	1	0	-4.120344	-1.782299	1.715592
108	1	0	-5.626883	-2.736490	1.992590
109	1	0	-4.113697	-3.516451	1.470285
110	6	0	-3.890112	-2.278279	-0.910461
111	1	0	-3.038115	-2.886218	-0.613139
112	1	0	-4.039039	-2.219281	-1.982703
113	6	0	3.963802	0.636565	3.320050
114	17	0	1.319732	0.014454	2.978057

115	17	0	5.675961	0.037012	3.428630
116	1	0	3.087406	-1.285659	3.885065
117	1	0	3.291592	-1.056863	2.115201
118	1	0	3.733884	1.122646	4.268500
119	1	0	3.925490	1.357683	2.503426
120	6	0	3.082580	-0.569895	3.063466

TS2S_{endo}-DCE

Imaginary frequency= -163.92

Total energy= -3677.04899556

Sum of electronic and zero-point Energies= -3676.059780

Sum of electronic and thermal Energies= -3675.996591

Sum of electronic and thermal Enthalpies= -3675.995647

Sum of electronic and thermal Free Energies= -3676.159670

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.270552	-0.210171	0.923801
2	6	0	-1.773389	2.419490	1.415666
3	1	0	-2.616037	1.808296	1.078715
4	7	0	-0.446016	3.745862	-0.062648
5	6	0	0.149583	2.560460	0.152055
6	6	0	0.004765	4.854821	-0.850781
7	7	0	-0.519795	1.750566	0.962206
8	6	0	-1.746745	3.769275	0.634076
9	1	0	-1.789647	4.643264	1.287125
10	7	0	1.586591	-1.825680	0.540517
11	6	0	3.176741	-3.596937	0.447917
12	1	0	3.011962	-4.382903	-0.295965
13	7	0	3.625424	-2.367943	-0.239031
14	6	0	1.869056	-3.152072	1.159684
15	1	0	2.085744	-2.971459	2.222325
16	6	0	6.037807	-2.240824	-0.632305
17	1	0	6.182777	-2.053870	0.427911
18	6	0	2.665595	-0.055824	-0.656741
19	6	0	3.424897	1.958588	-1.764216
20	1	0	4.150830	2.460845	-2.395510
21	6	0	4.742813	-2.400844	-1.137588
22	6	0	-0.375684	4.956055	-2.191570
23	1	0	-0.988913	4.178777	-2.638950
24	6	0	4.549389	-2.650441	-2.499320
25	1	0	3.544032	-2.790584	-2.886660

26	6	0	0.782623	5.861138	-0.265805
27	1	0	1.063794	5.784599	0.780798
28	6	0	1.601803	0.695749	-0.153112
29	6	0	3.600428	0.602238	-1.474521
30	1	0	4.452294	0.074190	-1.885035
31	6	0	2.335795	2.684182	-1.271425
32	1	0	2.231653	3.730371	-1.530848
33	6	0	1.394313	2.044280	-0.447505
34	6	0	5.651480	-2.714813	-3.353612
35	1	0	5.494186	-2.904089	-4.412314
36	6	0	2.640203	-1.448636	-0.172022
37	6	0	1.193999	6.949327	-1.033168
38	1	0	1.802492	7.725046	-0.574768
39	6	0	0.039931	6.053144	-2.947885
40	1	0	-0.256703	6.124327	-3.991182
41	6	0	6.956425	-2.547608	-2.869081
42	6	0	0.833585	7.063181	-2.386062
43	6	0	7.129656	-2.314169	-1.494869
44	1	0	8.133111	-2.185206	-1.096718
45	6	0	8.147695	-2.609594	-3.793492
46	1	0	8.650837	-1.636080	-3.855893
47	1	0	7.852875	-2.899673	-4.806738
48	1	0	8.891977	-3.331038	-3.435443
49	6	0	1.299667	8.239098	-3.209212
50	1	0	1.113143	9.187003	-2.691019
51	1	0	0.793105	8.274266	-4.178638
52	1	0	2.379780	8.185456	-3.398585
53	1	0	3.942375	-3.938517	1.147491
54	1	0	-2.554787	3.850059	-0.100264
55	6	0	-1.929348	2.586662	2.962648
56	6	0	0.717012	-4.190701	1.106979
57	6	0	1.232207	-5.500625	1.738988
58	1	0	0.420760	-6.235925	1.787139
59	1	0	2.046456	-5.948973	1.157877
60	1	0	1.595180	-5.335672	2.761238
61	6	0	-0.459232	-3.676007	1.954773
62	1	0	-0.147725	-3.498598	2.992513
63	1	0	-0.876473	-2.744307	1.559001
64	1	0	-1.270403	-4.412774	1.972104
65	6	0	0.253852	-4.462969	-0.334465
66	1	0	-0.103798	-3.550714	-0.822700
67	1	0	1.055534	-4.883788	-0.952399
68	1	0	-0.567548	-5.187158	-0.333156
69	6	0	-2.057526	1.202304	3.625093

70	1	0	-2.936801	0.663706	3.256021
71	1	0	-1.185253	0.569109	3.438426
72	1	0	-2.158223	1.310326	4.711551
73	6	0	-3.242519	3.354571	3.233995
74	1	0	-3.206635	4.389332	2.875926
75	1	0	-4.102061	2.861778	2.763409
76	1	0	-3.432392	3.390457	4.312974
77	6	0	-0.755774	3.363767	3.584955
78	1	0	-0.663271	4.374704	3.170279
79	1	0	-0.912075	3.472101	4.664716
80	1	0	0.199508	2.849860	3.439509
81	8	0	-0.672386	-0.580940	-0.880459
82	8	0	-2.653060	-1.136706	0.982537
83	6	0	-1.759455	-1.078024	-1.219648
84	6	0	-2.907221	-1.364024	-0.225660
85	8	0	-1.993008	-1.393711	-2.463803
86	6	0	-0.945605	-1.172592	-3.456724
87	1	0	-1.366525	-1.545830	-4.388209
88	1	0	-0.731126	-0.104605	-3.524873
89	1	0	-0.050585	-1.731311	-3.178804
90	6	0	-3.664204	-2.692560	-0.516209
91	9	0	-4.250887	-2.767715	-1.722347
92	9	0	-4.604897	-2.888323	0.420086
93	9	0	-2.783171	-3.718064	-0.436552
94	6	0	-8.609371	-2.006621	-0.479490
95	6	0	-7.487811	-1.372984	0.042829
96	6	0	-6.538240	-0.765277	-0.812109
97	6	0	-6.772601	-0.799963	-2.207567
98	6	0	-7.908176	-1.414097	-2.722428
99	6	0	-8.826247	-2.024811	-1.861515
100	1	0	-9.317970	-2.485300	0.189700
101	1	0	-7.326320	-1.381600	1.114811
102	1	0	-6.085011	-0.304727	-2.884364
103	1	0	-8.083103	-1.413379	-3.794122
104	1	0	-9.711216	-2.507783	-2.266047
105	6	0	-5.352088	-0.111373	-0.271249
106	6	0	-5.304939	0.376883	1.134559
107	1	0	-4.977575	1.422230	1.150257
108	1	0	-6.247777	0.292864	1.673950
109	1	0	-4.515057	-0.190159	1.660378
110	6	0	-4.163922	0.013256	-1.010963
111	1	0	-3.516076	0.843622	-0.739387
112	1	0	-4.171963	-0.231164	-2.067387
113	6	0	4.070252	1.035357	2.979107

114	17	0	1.426009	0.284647	3.030859
115	17	0	5.799641	0.525844	3.208952
116	1	0	3.283740	-0.615560	4.175271
117	1	0	3.388774	-0.967700	2.420262
118	1	0	3.859126	1.801862	3.724705
119	1	0	3.985479	1.448390	1.974297
120	6	0	3.215428	-0.200915	3.169547

TS2R_{exo}-DCE

Imaginary frequency= -148.38
Total energy= -3677.05276312
Sum of electronic and zero-point Energies= -3676.062965
Sum of electronic and thermal Energies= -3675.999832
Sum of electronic and thermal Enthalpies= -3675.998888
Sum of electronic and thermal Free Energies= -3676.163263

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.198317	-0.229705	-1.157834
2	6	0	2.226517	2.024455	-1.863263
3	1	0	2.967476	1.220177	-1.891554
4	7	0	1.600562	3.314145	0.048165
5	6	0	0.728721	2.301234	-0.127344
6	6	0	1.454591	4.504980	0.825939
7	7	0	1.013498	1.508838	-1.154505
8	6	0	2.716716	3.152609	-0.908012
9	1	0	2.891529	4.100747	-1.417176
10	7	0	-1.790482	-1.591022	-0.654692
11	6	0	-3.909834	-2.706127	-0.551511
12	1	0	-4.003516	-3.681468	-0.066787
13	7	0	-3.737655	-1.667581	0.479777
14	6	0	-2.619585	-2.582675	-1.414671
15	1	0	-2.869800	-2.113342	-2.375205
16	6	0	-5.850831	-0.829670	1.385760
17	1	0	-6.038513	-0.328808	0.440448
18	6	0	-2.035190	0.102714	1.036232
19	6	0	-1.927214	1.929406	2.618488
20	1	0	-2.291822	2.406305	3.522606
21	6	0	-4.665315	-1.549012	1.567061
22	6	0	0.391451	5.387241	0.590748
23	1	0	-0.348392	5.153669	-0.169035
24	6	0	-4.423350	-2.204682	2.778694

25	1	0	-3.510822	-2.779308	2.910679
26	6	0	2.424944	4.827234	1.779844
27	1	0	3.256591	4.151398	1.957103
28	6	0	-0.993335	0.713889	0.338491
29	6	0	-2.511852	0.730958	2.198752
30	1	0	-3.316683	0.296655	2.778622
31	6	0	-0.883855	2.528997	1.906790
32	1	0	-0.452973	3.452858	2.271688
33	6	0	-0.403629	1.918333	0.735706
34	6	0	-5.359244	-2.117060	3.810016
35	1	0	-5.164460	-2.628185	4.749565
36	6	0	-2.521842	-1.104414	0.343804
37	6	0	2.320771	6.017078	2.501428
38	1	0	3.081591	6.258441	3.239267
39	6	0	0.292530	6.564709	1.329067
40	1	0	-0.537534	7.241167	1.140242
41	6	0	-6.551426	-1.395096	3.650600
42	6	0	1.253283	6.902399	2.295655
43	6	0	-6.780503	-0.756230	2.421734
44	1	0	-7.699887	-0.195484	2.272687
45	6	0	-7.554281	-1.289459	4.773557
46	1	0	-7.440974	-0.340154	5.314410
47	1	0	-7.428553	-2.098069	5.500677
48	1	0	-8.582013	-1.323578	4.395689
49	6	0	1.128318	8.178552	3.091082
50	1	0	2.056002	8.411250	3.623220
51	1	0	0.327255	8.102434	3.838413
52	1	0	0.882254	9.028778	2.444289
53	1	0	-4.822822	-2.517535	-1.122030
54	1	0	3.629065	2.876504	-0.369860
55	6	0	2.026816	2.501381	-3.340622
56	6	0	-1.982181	-3.963529	-1.749848
57	6	0	-3.032207	-4.763671	-2.552184
58	1	0	-2.619509	-5.738491	-2.836487
59	1	0	-3.946020	-4.950403	-1.976370
60	1	0	-3.313934	-4.238963	-3.474001
61	6	0	-0.745179	-3.775594	-2.640972
62	1	0	-0.949679	-3.104434	-3.484969
63	1	0	0.091834	-3.369726	-2.073702
64	1	0	-0.425634	-4.740992	-3.051442
65	6	0	-1.586787	-4.748573	-0.486033
66	1	0	-0.921307	-4.165670	0.157283
67	1	0	-2.457284	-5.048816	0.107820
68	1	0	-1.058175	-5.666809	-0.767909

69	6	0	1.636105	1.319193	-4.244549
70	1	0	2.404639	0.539098	-4.234123
71	1	0	0.692810	0.853760	-3.950217
72	1	0	1.521738	1.664294	-5.278877
73	6	0	3.389225	3.027087	-3.848950
74	1	0	3.711661	3.937813	-3.333573
75	1	0	4.177536	2.272423	-3.731164
76	1	0	3.317483	3.266861	-4.916009
77	6	0	0.974134	3.618482	-3.451770
78	1	0	1.251458	4.506425	-2.871678
79	1	0	0.873462	3.933844	-4.496939
80	1	0	-0.011455	3.284325	-3.110843
81	8	0	1.511109	-1.336543	-2.470455
82	8	0	1.002167	-1.259566	0.165631
83	6	0	2.301329	-1.903052	-1.721791
84	6	0	2.033942	-1.888189	-0.219392
85	8	0	3.357617	-2.582375	-2.091733
86	6	0	3.604343	-2.723346	-3.522833
87	1	0	4.511465	-3.320853	-3.589730
88	1	0	2.761781	-3.237770	-3.988380
89	1	0	3.752080	-1.738994	-3.970007
90	6	0	2.360670	-3.158726	0.591394
91	9	0	1.550450	-4.143864	0.140736
92	9	0	2.097356	-2.970306	1.890885
93	9	0	3.619442	-3.579138	0.454298
94	6	0	5.752876	-3.089746	4.108504
95	6	0	4.810534	-2.229472	3.554949
96	6	0	5.018278	-1.655479	2.279317
97	6	0	6.218883	-1.961579	1.594933
98	6	0	7.167626	-2.803234	2.163249
99	6	0	6.935535	-3.375510	3.418626
100	1	0	5.567273	-3.538237	5.079972
101	1	0	3.892621	-2.033922	4.097822
102	1	0	6.425638	-1.503257	0.633654
103	1	0	8.091735	-3.010284	1.631712
104	1	0	7.675624	-4.037160	3.859637
105	6	0	4.021502	-0.768465	1.678914
106	6	0	3.090872	0.028859	2.548138
107	1	0	3.249880	-0.126728	3.614923
108	1	0	3.229970	1.096695	2.339833
109	1	0	2.046301	-0.205116	2.305707
110	6	0	3.901009	-0.635319	0.299843
111	1	0	3.373216	0.228538	-0.088068
112	1	0	4.612924	-1.111305	-0.365207

113	6	0	-3.848615	2.356401	-2.141385
114	17	0	-1.636040	0.891106	-2.822134
115	17	0	-5.645408	2.377883	-1.873036
116	1	0	-3.911347	0.576189	-3.407249
117	1	0	-3.642091	0.231518	-1.667090
118	1	0	-3.638072	3.044371	-2.960092
119	1	0	-3.379446	2.704977	-1.221605
120	6	0	-3.463125	0.930589	-2.479224

TS2S_{exo}-DCE

Imaginary frequency= -139.10

Total energy= -3677.05573989

Sum of electronic and zero-point Energies= -3676.065844

Sum of electronic and thermal Energies= -3676.002668

Sum of electronic and thermal Enthalpies= -3676.001723

Sum of electronic and thermal Free Energies= -3676.165945

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.174385	0.054489	-1.183967
2	6	0	1.975931	2.589029	-1.707208
3	1	0	2.768708	1.843782	-1.820652
4	7	0	1.344750	3.552716	0.383367
5	6	0	0.523776	2.532836	0.086213
6	6	0	1.347560	4.408053	1.533497
7	7	0	0.799061	1.927349	-1.065335
8	6	0	2.405826	3.637350	-0.636757
9	1	0	2.450465	4.656093	-1.025203
10	7	0	-1.588390	-1.529603	-0.780531
11	6	0	-3.606524	-2.830372	-0.798894
12	1	0	-3.598936	-3.851182	-0.406760
13	7	0	-3.526840	-1.880190	0.321776
14	6	0	-2.345075	-2.497323	-1.646404
15	1	0	-2.647023	-1.941876	-2.543774
16	6	0	-5.699130	-1.310076	1.298054
17	1	0	-5.935415	-0.735194	0.407230
18	6	0	-2.008827	-0.008470	1.041801
19	6	0	-2.088855	1.686434	2.766905
20	1	0	-2.503658	2.052050	3.700842
21	6	0	-4.460181	-1.945558	1.408244
22	6	0	0.655719	5.621459	1.503590
23	1	0	0.090830	5.897853	0.617978

24	6	0	-4.157796	-2.696684	2.550956
25	1	0	-3.200380	-3.204673	2.625558
26	6	0	2.089264	4.051055	2.666129
27	1	0	2.633608	3.110921	2.678408
28	6	0	-1.043097	0.766515	0.398747
29	6	0	-2.541908	0.468609	2.252343
30	1	0	-3.292168	-0.093237	2.794632
31	6	0	-1.108763	2.443560	2.116630
32	1	0	-0.779204	3.377189	2.554973
33	6	0	-0.563382	1.975360	0.910148
34	6	0	-5.088274	-2.788052	3.583841
35	1	0	-4.844635	-3.369084	4.470079
36	6	0	-2.368239	-1.197287	0.247039
37	6	0	2.117296	4.901755	3.768313
38	1	0	2.690074	4.617277	4.647917
39	6	0	0.689710	6.463355	2.617130
40	1	0	0.144831	7.403355	2.590936
41	6	0	-6.336877	-2.149995	3.495998
42	6	0	1.417635	6.120685	3.764170
43	6	0	-6.625129	-1.415263	2.337700
44	1	0	-7.586138	-0.915881	2.246687
45	6	0	-7.334689	-2.259371	4.622940
46	1	0	-8.268526	-1.742552	4.381366
47	1	0	-6.936804	-1.823259	5.548007
48	1	0	-7.573109	-3.307731	4.840928
49	6	0	1.462635	7.034689	4.964486
50	1	0	1.145478	6.509191	5.877279
51	1	0	0.808332	7.903989	4.827175
52	1	0	2.483869	7.401622	5.145017
53	1	0	-4.539386	-2.682819	-1.349009
54	1	0	3.371334	3.398722	-0.179473
55	6	0	1.725595	3.202670	-3.123761
56	6	0	-1.603543	-3.771692	-2.147737
57	6	0	-2.603435	-4.580275	-3.003844
58	1	0	-2.107342	-5.466501	-3.416221
59	1	0	-3.466128	-4.929682	-2.425238
60	1	0	-2.977657	-3.985952	-3.847013
61	6	0	-0.423669	-3.376819	-3.047367
62	1	0	-0.740861	-2.708879	-3.858177
63	1	0	0.358103	-2.870304	-2.481667
64	1	0	0.018261	-4.270805	-3.503873
65	6	0	-1.092808	-4.645082	-0.988585
66	1	0	-0.470886	-4.067232	-0.297657
67	1	0	-1.907164	-5.095179	-0.409988

68	1	0	-0.484160	-5.468272	-1.380909
69	6	0	1.453273	2.086722	-4.147884
70	1	0	2.295809	1.387856	-4.201049
71	1	0	0.555576	1.508381	-3.916094
72	1	0	1.314106	2.519783	-5.145604
73	6	0	3.022390	3.913694	-3.570901
74	1	0	3.259899	4.790791	-2.959474
75	1	0	3.882475	3.232871	-3.535011
76	1	0	2.916420	4.260043	-4.605364
77	6	0	0.559825	4.206209	-3.118453
78	1	0	0.742569	5.046789	-2.438235
79	1	0	0.420523	4.625888	-4.121757
80	1	0	-0.380990	3.728956	-2.823727
81	8	0	1.468500	-0.832945	-2.623176
82	8	0	1.332615	-0.619710	0.050488
83	6	0	2.472075	-1.124027	-1.975002
84	6	0	2.418925	-1.043465	-0.451687
85	8	0	3.624371	-1.490888	-2.474257
86	6	0	3.735229	-1.586870	-3.927437
87	1	0	4.778624	-1.836976	-4.109263
88	1	0	3.074772	-2.377598	-4.288247
89	1	0	3.476603	-0.629609	-4.382030
90	6	0	3.699742	-0.627882	0.299742
91	9	0	4.755767	-1.404471	0.050896
92	9	0	3.481191	-0.589880	1.618997
93	9	0	4.016426	0.627287	-0.103666
94	6	0	5.338989	-3.830365	3.872056
95	6	0	4.132604	-3.526596	3.252184
96	6	0	3.947907	-3.762112	1.869080
97	6	0	5.016221	-4.341004	1.142081
98	6	0	6.215837	-4.654853	1.769255
99	6	0	6.384356	-4.395657	3.133805
100	1	0	5.466520	-3.628580	4.931393
101	1	0	3.335414	-3.084777	3.838856
102	1	0	4.895544	-4.580089	0.091289
103	1	0	7.019251	-5.109941	1.197853
104	1	0	7.323595	-4.640130	3.621799
105	6	0	2.674976	-3.440630	1.226506
106	6	0	1.459540	-3.228288	2.081977
107	1	0	1.336459	-4.048438	2.797922
108	1	0	1.560002	-2.305187	2.668422
109	1	0	0.555750	-3.150359	1.477360
110	6	0	2.549845	-3.305046	-0.153244
111	1	0	1.558672	-3.398676	-0.584015

112	1	0	3.384836	-3.523114	-0.810199
113	6	0	-4.102559	2.393255	-2.476092
114	17	0	-1.770377	1.000126	-2.793455
115	17	0	-5.871417	2.345168	-2.060311
116	1	0	-4.028092	0.279162	-3.031500
117	1	0	-3.623985	0.614127	-1.311214
118	1	0	-4.023267	2.764387	-3.497919
119	1	0	-3.626889	3.084754	-1.780631
120	6	0	-3.573437	0.980142	-2.332945