Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Elecrtonic Supplementray Information for

Quantum mechanical study of mechanism and stereoselectivity on the N-heterocyclic carbene catalyzed [4 + 2] annulation reaction of enals with azodicarboxylates

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Content

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Part 1: The reaction between Cat and R2 (Mechanism A)

As we all know, it is a crucial but usually challenging issue to figure out how the catalyst will first exert its effect on reactants for a catalytic reaction. Since the answers should be different because various factors such as the specific structure of the catalyst, the reactant counterparts, and experimental conditions are important. Thus, we have also studied the possible reaction mechanism on the title reaction in which the **Cat** first reacts with **R2** (Mechanism A). It is interesting to find that the nitrogen atom and carbonyl carbon atom both own the electrophilic ability, i.e. (1) the addition of the catalyst to $N^{A1(A2)}$ atom, (2) the addition of the catalyst to C^{A} atom, and these two possibilities are considered and the detailed parameters are shown in **Fig. S1**.

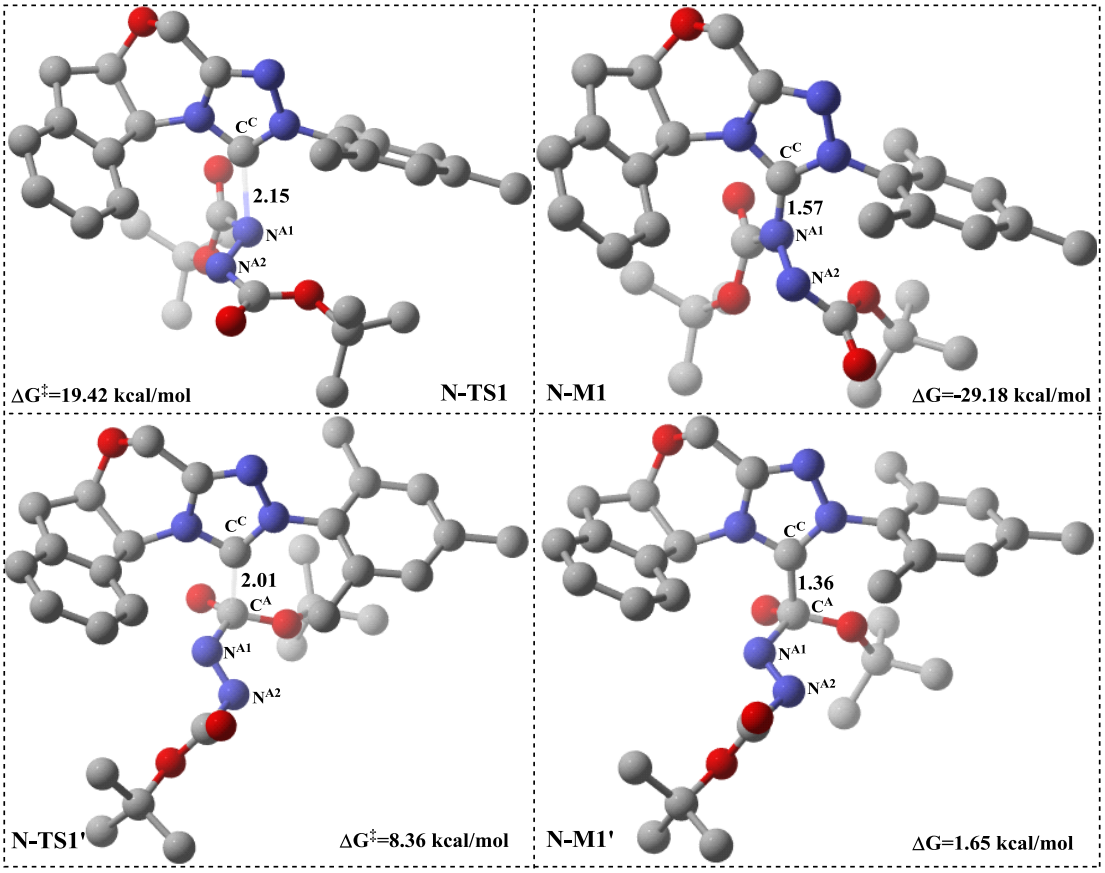

Fig. S1 The optimized structures and Gibbs free energies of the Mechanism A (distance in Å and energy in kcal/mol)

As shown in **Fig. S1**, the energy barrier of **N-TS1** is 19.42 kcal/mol which is higher than that of **Re/Si-TS1**, while the energy barrier of **N-TS1'** is lower than **Re/Si-TS1**. However, the subsequent process would not proceed, because the C^{E4}

atom can not be activated.

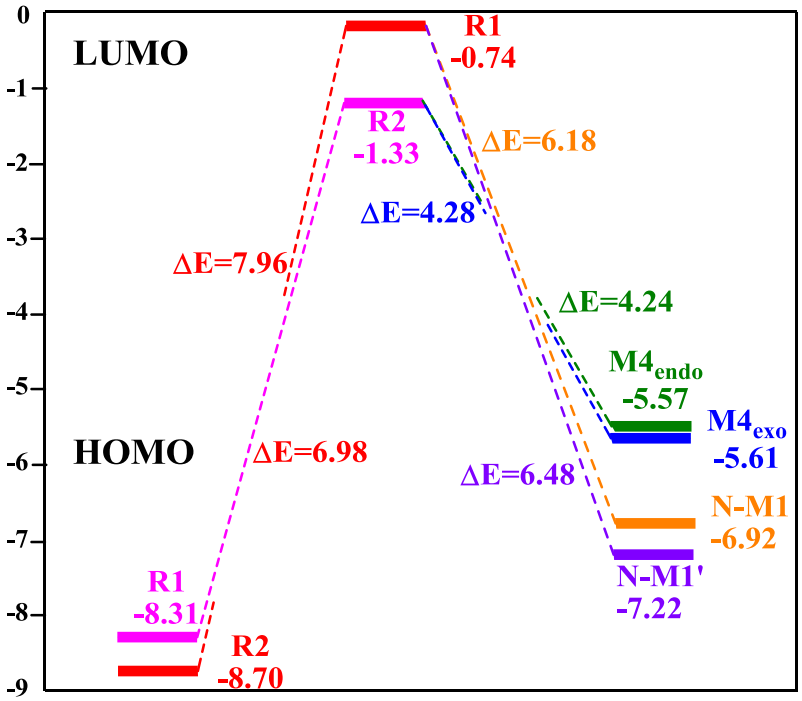

Fig. S2 The FMO energy gap of **R1**, **R2**, **M4$_{endo}$**, **M4$_{exo}$**, **N-M1**, and **N-M1'** optimized at M06-2X/6-31G(d, p)/IEF-PCM$_{(THF)}$ level (units: eV)

On the other hand, the frontier molecular orbital (FMO) analysis show that the Mechanism A and un-catalyzed [4+2] annulation reaction can not occur due to the larger energy gap (>6 eV, **Fig. S2**) and the energy gap between LUMO$_{R2}$ and HOMO$_{M4endo}$/HOMO$_{M4exo}$ is largely lowered by the catalyst. It is interesting to find that the energy gap between LUMO$_{R2}$ and HOMO$_{M4endo}$ is a little lower than that of between LUMO$_{R2}$ and HOMO$_{M4exo}$ (**Fig. S2**), whereas the R-configured **PR** is the predominated product. This phenomenon indicates that the stereoselectivity is unrelated to the energy gap of the FMO.

Part 2: The $2H_2O$-assisted proton transfer mechanism

As discussed in the main text, the H_2O-assisted proton transfer process is presented, and we have also considered the $2H_2O$ cluster-assisted proton transfer mechanism. **Fig. S3** shows the detailed parameters of the $2H_2O$-assisted proton transfer process. The free energy barrier of Re/Si-TS2^{2W} is 9.40/15.43 kcal/mol, which is also higher than that of HCO_3^--assisted proton transfer process.

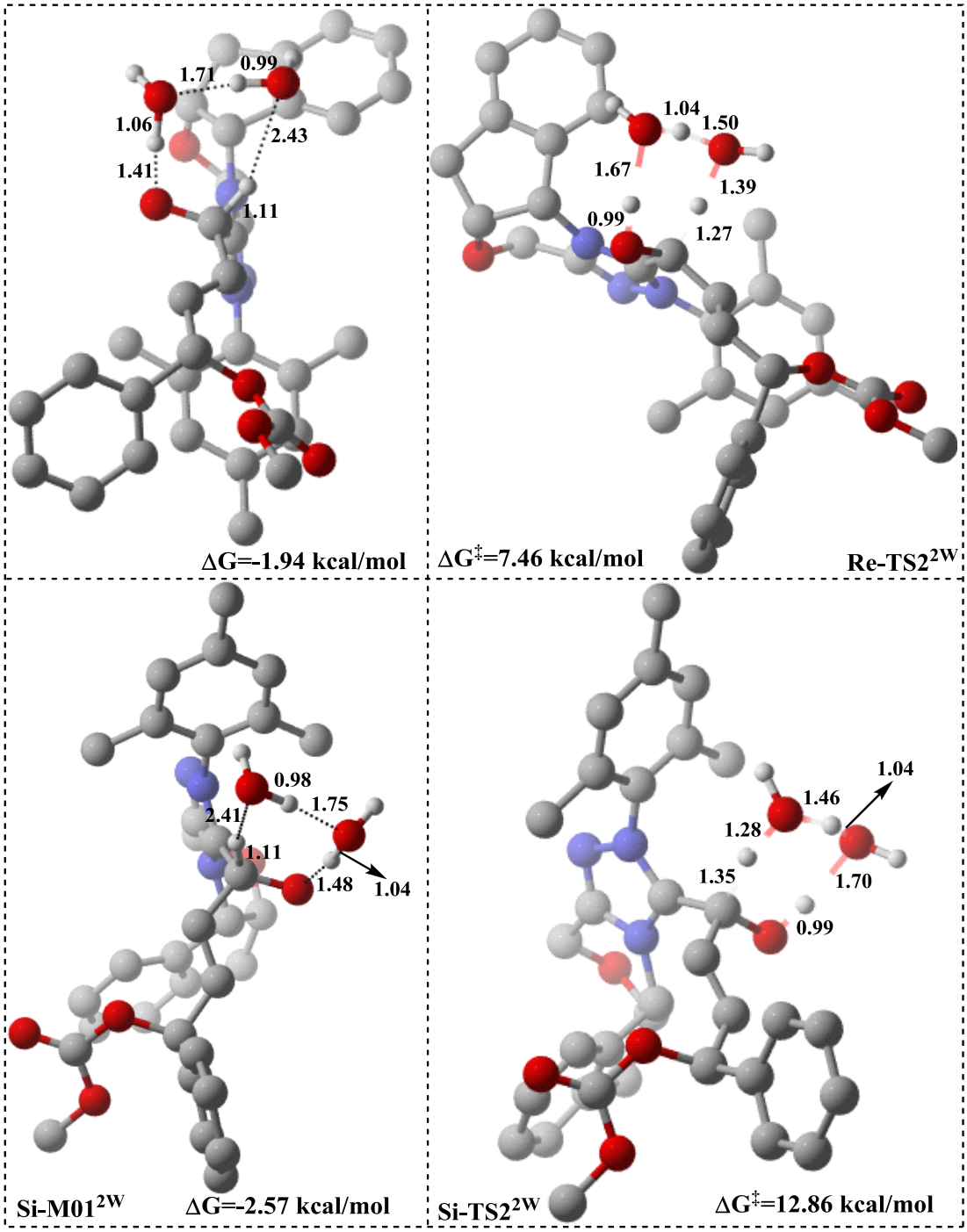

Fig. S3 The optimized structures and Gibbs free energies of the $2H_2O$-assisted proton transfer process (distance in Å and energy in kcal/mol)

Part 3: The energy profile of the other two pathways of Stage 3

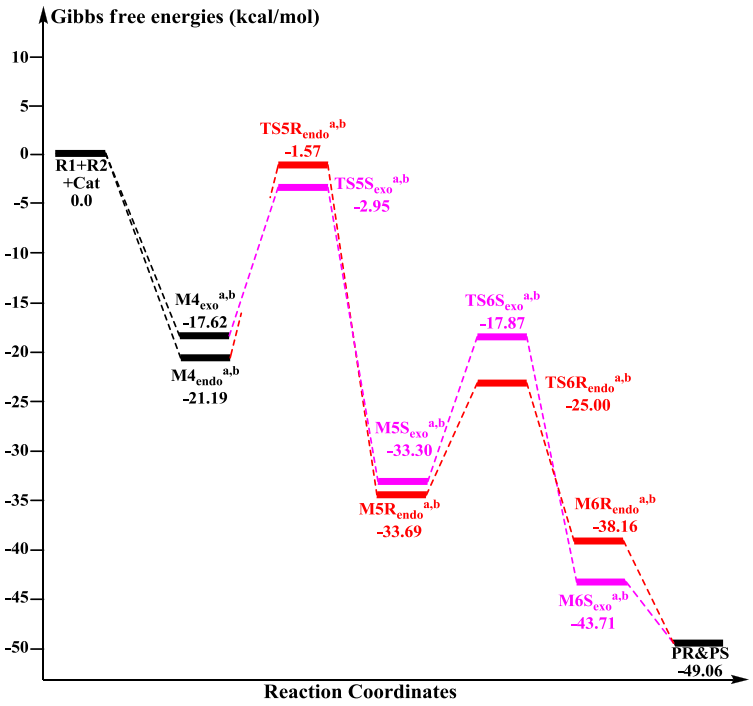

Fig. S3 The energy profile of the other two pathways of **Stage 3**

Part 4: List of the energies and Cartesian coordinates of all the structures involved in the reaction

Cat

Total energy= -1051.91619545
Sum of electronic and zero-point Energies= -1051.532039
Sum of electronic and thermal Energies= -1051.511333
Sum of electronic and thermal Enthalpies= -1051.510389
Sum of electronic and thermal Free Energies= -1051.582214

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.933156	0.626314	0.733794
2	6	0	-3.785056	0.574252	-0.371319
3	6	0	-4.473921	1.713192	-0.776674
4	6	0	-4.289995	2.898385	-0.067351
5	6	0	-3.429775	2.947974	1.033059
6	6	0	-2.741217	1.807740	1.440839
7	6	0	-2.306566	-0.723797	0.983431
8	6	0	-3.230237	-1.668866	0.169427
9	6	0	-3.789967	-0.805608	-0.980023
10	1	0	-5.143905	1.680512	-1.630676
11	1	0	-4.824423	3.794292	-0.367162
12	1	0	-3.302862	3.881455	1.571216
13	1	0	-2.069480	1.833185	2.292908
14	1	0	-4.057730	-1.950990	0.825323
15	1	0	-3.131519	-0.827267	-1.856905
16	1	0	-2.268596	-0.998024	2.040316
17	1	0	-4.776359	-1.143237	-1.305815
18	6	0	-0.536584	-1.742355	-0.464028
19	6	0	0.101643	0.005836	0.815143
20	7	0	0.722507	-1.595111	-0.743609
21	7	0	-0.944014	-0.804352	0.447534
22	7	0	1.079448	-0.520961	0.050989
23	6	0	-1.486443	-2.752397	-1.031710
24	1	0	-1.772762	-2.464949	-2.051543
25	1	0	-1.004578	-3.730251	-1.079060
26	8	0	-2.617519	-2.888397	-0.194028
27	6	0	2.431486	-0.055413	0.000238
28	6	0	2.700640	1.160397	-0.638947
29	6	0	3.435715	-0.836466	0.573889

30	6	0	4.023528	1.592195	-0.684135
31	6	0	4.748709	-0.366114	0.502191
32	6	0	5.059487	0.841292	-0.119734
33	1	0	4.256860	2.531867	-1.179086
34	1	0	5.544312	-0.962637	0.942605
35	6	0	1.590483	1.963897	-1.262469
36	1	0	1.030689	1.360116	-1.983464
37	1	0	0.876455	2.296878	-0.504035
38	1	0	1.990924	2.838861	-1.778015
39	6	0	6.477969	1.348717	-0.176488
40	1	0	6.770528	1.581477	-1.207445
41	1	0	6.583190	2.273377	0.406524
42	1	0	7.178894	0.611046	0.225431
43	6	0	3.103510	-2.136212	1.256291
44	1	0	2.283849	-2.002006	1.969128
45	1	0	2.778085	-2.887966	0.531702
46	1	0	3.971480	-2.523391	1.793326

R1

Total energy= -765.08206647
Sum of electronic and zero-point Energies= -764.859999
Sum of electronic and thermal Energies= -764.844717
Sum of electronic and thermal Enthalpies= -764.843773
Sum of electronic and thermal Free Energies= -764.905502

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.402211	-0.373063	-0.564056
2	6	0	-1.885859	-0.173966	-0.559396
3	1	0	-0.087167	-0.701281	-1.560516
4	6	0	-2.754774	-0.796034	0.240661
5	1	0	-2.257141	0.561527	-1.270837
6	1	0	-2.434030	-1.535167	0.966852
7	6	0	-4.199963	-0.487197	0.142148
8	8	0	-4.670723	0.315589	-0.637651
9	1	0	-4.856791	-1.043952	0.836034
10	6	0	0.314307	0.917601	-0.212243
11	6	0	1.136200	1.549099	-1.142370
12	6	0	0.138743	1.477712	1.054744
13	6	0	1.779107	2.739744	-0.811476
14	1	0	1.280995	1.102082	-2.122142
15	6	0	0.790340	2.660151	1.389095

16	1	0	-0.506388	0.980223	1.774235
17	6	0	1.608776	3.294055	0.454792
18	1	0	2.419628	3.228018	-1.538661
19	1	0	0.656574	3.090872	2.376076
20	1	0	2.114658	4.218136	0.715179
21	8	0	-0.105270	-1.403736	0.392265
22	6	0	1.107290	-1.970779	0.402930
23	8	0	1.422860	-2.774639	1.241040
24	8	0	1.878597	-1.554853	-0.600928
25	6	0	3.190529	-2.131826	-0.628207
26	1	0	3.121402	-3.212153	-0.762151
27	1	0	3.694616	-1.669580	-1.473718
28	1	0	3.715019	-1.910602	0.302087

R2

Total energy= -801.96511442

Sum of electronic and zero-point Energies= -801.680078

Sum of electronic and thermal Energies= -801.661511

Sum of electronic and thermal Enthalpies= -801.660567

Sum of electronic and thermal Free Energies= -801.727862

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.284983	-0.026526	0.054893
2	7	0	-0.435654	-0.781358	-0.604861
3	6	0	1.645149	0.009114	-0.505059
4	8	0	1.874620	0.008820	-1.683666
5	8	0	2.474960	0.094769	0.510523
6	6	0	-1.780020	-0.848445	-0.051888
7	8	0	-2.161194	-1.859496	0.473946
8	8	0	-2.422283	0.271175	-0.294177
9	6	0	-3.836647	0.423748	0.102089
10	6	0	-4.682092	-0.614383	-0.624336
11	6	0	-3.945529	0.316676	1.617525
12	6	0	-4.165053	1.831035	-0.373825
13	1	0	-4.515314	-0.549101	-1.702870
14	1	0	-4.453066	-1.624425	-0.283278
15	1	0	-5.737295	-0.408597	-0.426553
16	1	0	-3.264989	1.027063	2.094461
17	1	0	-4.967523	0.563996	1.916393
18	1	0	-3.714711	-0.691792	1.961801
19	1	0	-5.202401	2.067564	-0.125367

20	1	0	-3.512480	2.560332	0.112391
21	1	0	-4.036912	1.908843	-1.456264
22	6	0	3.929567	0.160896	0.285037
23	6	0	4.392313	-1.109133	-0.417808
24	6	0	4.262749	1.422311	-0.502244
25	6	0	4.483760	0.236915	1.700319
26	1	0	4.083078	-1.989744	0.151571
27	1	0	3.990864	-1.173665	-1.429595
28	1	0	5.483882	-1.102396	-0.474976
29	1	0	3.836033	2.298892	-0.007414
30	1	0	5.349057	1.540374	-0.534252
31	1	0	3.886762	1.365395	-1.523842
32	1	0	5.574531	0.284560	1.662639
33	1	0	4.110759	1.129106	2.209298
34	1	0	4.190422	-0.645763	2.273756

H_2O

Total energy= -76.38997087
Sum of electronic and zero-point Energies= -76.368347
Sum of electronic and thermal Energies= -76.365511
Sum of electronic and thermal Enthalpies= -76.364567
Sum of electronic and thermal Free Energies= -76.385998

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.118970
2	1	0	0.000000	0.757664	-0.475878
3	1	0	0.000000	-0.757664	-0.475878

$2H_2O$

Total energy= -152.79046062
Sum of electronic and zero-point Energies= -152.743138
Sum of electronic and thermal Energies= -152.737750
Sum of electronic and thermal Enthalpies= -152.736805
Sum of electronic and thermal Free Energies= -152.768605

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.482637	0.087355	0.079485
2	1	0	-0.514561	0.041310	0.000430

3	1	0	-1.796529	-0.600664	-0.515415
4	8	0	1.352528	-0.069044	-0.094006
5	1	0	1.702813	0.828683	-0.124251
6	1	0	1.649147	-0.415822	0.755410

HCO_3^-

Total energy= -264.42638437

Sum of electronic and zero-point Energies= -264.399156

Sum of electronic and thermal Energies= -264.395705

Sum of electronic and thermal Enthalpies= -264.394761

Sum of electronic and thermal Free Energies= -264.424875

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.154141	0.000000
2	8	0	1.216593	0.437366	0.000000
3	8	0	-1.005662	0.879870	0.000000
4	8	0	-0.284241	-1.227521	0.000000
5	1	0	0.586482	-1.642573	0.000000

LGH

Total energy= -304.19072405

Sum of electronic and zero-point Energies= -304.122035

Sum of electronic and thermal Energies= -304.116872

Sum of electronic and thermal Enthalpies= -304.115928

Sum of electronic and thermal Free Energies= -304.150263

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.646695	-0.681768	-0.000123
2	6	0	-0.588997	-0.104704	0.000037
3	8	0	-0.446889	1.227715	0.000069
4	8	0	0.573432	-0.746723	0.000210
5	6	0	1.790142	0.012596	-0.000127
6	1	0	1.851279	0.636564	0.892513
7	1	0	2.589576	-0.725380	-0.001154
8	1	0	1.850146	0.637779	-0.891972
9	1	0	-1.336659	1.609882	-0.000101

Re-TS1

Total energy= -1817.00737343
Sum of electronic and zero-point Energies= -1816.398566
Sum of electronic and thermal Energies= -1816.362799
Sum of electronic and thermal Enthalpies= -1816.361854
Sum of electronic and thermal Free Energies= -1816.467935

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.890267	1.473299	-0.001001
2	6	0	-5.204514	1.792245	-0.328920
3	6	0	-5.467257	2.874200	-1.165995
4	6	0	-4.398328	3.615841	-1.664435
5	6	0	-3.080593	3.282353	-1.338277
6	6	0	-2.816231	2.201139	-0.501432
7	6	0	-3.830835	0.268304	0.910906
8	6	0	-5.303157	-0.286785	0.925050
9	6	0	-6.175588	0.843265	0.326810
10	1	0	-6.488129	3.131325	-1.432423
11	1	0	-4.590405	4.458828	-2.320511
12	1	0	-2.260290	3.866714	-1.741601
13	1	0	-1.794103	1.923604	-0.253606
14	1	0	-5.600423	-0.525863	1.946273
15	1	0	-6.905500	0.421855	-0.371280
16	1	0	-3.504645	0.535027	1.919806
17	1	0	-6.739456	1.346143	1.119019
18	6	0	-3.269322	-1.580249	-0.610242
19	6	0	-1.582556	-0.879436	0.657806
20	7	0	-2.255951	-2.286854	-1.008979
21	7	0	-2.904360	-0.731323	0.400987
22	7	0	-1.227977	-1.827716	-0.213838
23	6	0	-4.714950	-1.605847	-0.985375
24	1	0	-4.956606	-0.779560	-1.668650
25	1	0	-4.974781	-2.549852	-1.464122
26	8	0	-5.447354	-1.514499	0.225249
27	6	0	0.093435	-2.363214	-0.371168
28	6	0	0.384240	-3.593394	0.225731
29	6	0	1.023947	-1.635159	-1.111057
30	6	0	1.675740	-4.088266	0.073727
31	6	0	2.308652	-2.170536	-1.231534
32	6	0	2.649453	-3.387043	-0.643527
33	1	0	1.930730	-5.042476	0.529442
34	1	0	3.057514	-1.621266	-1.796893

35	6	0	-0.663613	-4.324831	1.017549
36	1	0	-0.969165	-3.701301	1.863181
37	1	0	-1.546298	-4.535949	0.406517
38	1	0	-0.269424	-5.269731	1.396366
39	6	0	4.046710	-3.938682	-0.764884
40	1	0	4.610332	-3.416905	-1.541518
41	1	0	4.591443	-3.818415	0.177833
42	1	0	4.030066	-5.006518	-0.999786
43	6	0	0.666006	-0.316665	-1.744134
44	1	0	-0.340759	-0.337961	-2.171711
45	1	0	0.697603	0.487319	-0.998434
46	1	0	1.378106	-0.069545	-2.534146
47	6	0	2.759532	1.230436	1.201198
48	6	0	1.733907	0.232141	1.665763
49	1	0	3.353834	1.551580	2.064993
50	6	0	0.429221	0.464776	1.764543
51	1	0	2.114209	-0.743562	1.963573
52	1	0	-0.001911	1.422686	1.480329
53	6	0	-0.509525	-0.576721	2.312957
54	8	0	-0.091421	-1.684335	2.705393
55	1	0	-1.381217	-0.104827	2.818954
56	6	0	3.714056	0.662836	0.161397
57	6	0	4.618734	-0.327186	0.551542
58	6	0	3.726978	1.115891	-1.156896
59	6	0	5.526544	-0.853172	-0.361595
60	1	0	4.620445	-0.681627	1.579569
61	6	0	4.637793	0.588921	-2.072870
62	1	0	3.024159	1.878909	-1.478144
63	6	0	5.539811	-0.395217	-1.678878
64	1	0	6.227909	-1.618217	-0.043461
65	1	0	4.640365	0.952528	-3.095626
66	1	0	6.251112	-0.801586	-2.390759
67	8	0	2.052324	2.368651	0.687085
68	6	0	2.674823	3.543785	0.545778
69	8	0	2.134054	4.486257	0.025282
70	8	0	3.914828	3.538049	1.032643
71	6	0	4.627676	4.770624	0.870765
72	1	0	4.104628	5.577599	1.385027
73	1	0	5.606732	4.602392	1.312997
74	1	0	4.719342	5.010997	-0.189437

Si-TS1

Total energy= -1817.00830144

Sum of electronic and zero-point Energies= -1816.399548
Sum of electronic and thermal Energies= -1816.363055
Sum of electronic and thermal Enthalpies= -1816.362111
Sum of electronic and thermal Free Energies= -1816.472246

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.150529	-2.172008	-0.184100
2	6	0	-4.124597	-2.624748	0.705788
3	6	0	-3.829881	-3.655808	1.593353
4	6	0	-2.550858	-4.209977	1.581001
5	6	0	-1.579645	-3.746168	0.689966
6	6	0	-1.873733	-2.721828	-0.207820
7	6	0	-3.674526	-1.041086	-1.037158
8	6	0	-5.209515	-1.087227	-0.775895
9	6	0	-5.406920	-1.847739	0.556903
10	1	0	-4.581811	-4.021843	2.286261
11	1	0	-2.308459	-5.013649	2.269505
12	1	0	-0.590345	-4.193845	0.692053
13	1	0	-1.149827	-2.353577	-0.929432
14	1	0	-5.654273	-1.669544	-1.585346
15	1	0	-5.536431	-1.160388	1.400005
16	1	0	-3.406009	-1.143131	-2.090126
17	1	0	-6.296150	-2.481638	0.524473
18	6	0	-3.892478	1.248530	-0.010943
19	6	0	-1.843825	0.640699	-0.608867
20	7	0	-3.142433	2.243199	0.361515
21	7	0	-3.142781	0.256977	-0.588770
22	7	0	-1.883667	1.837999	-0.014207
23	6	0	-5.380353	1.123029	0.090355
24	1	0	-5.672663	0.858389	1.113787
25	1	0	-5.845858	2.078277	-0.157152
26	8	0	-5.839603	0.178107	-0.853717
27	6	0	-0.737248	2.651204	0.269380
28	6	0	0.148977	2.220079	1.264889
29	6	0	-0.527346	3.806532	-0.484535
30	6	0	1.298525	2.977584	1.474199
31	6	0	0.628548	4.544224	-0.222862
32	6	0	1.550566	4.141785	0.742638
33	1	0	2.021132	2.630496	2.208123
34	1	0	0.818002	5.445586	-0.800622
35	6	0	-0.111253	0.969636	2.063235
36	1	0	0.661452	0.847853	2.824174

37	1	0	-1.091386	1.013830	2.549078
38	1	0	-0.098652	0.082183	1.421744
39	6	0	2.797223	4.945771	1.007398
40	1	0	2.960003	5.694885	0.229773
41	1	0	2.725023	5.466412	1.967454
42	1	0	3.676192	4.297471	1.054025
43	6	0	-1.510611	4.229547	-1.543793
44	1	0	-1.729595	3.406117	-2.231221
45	1	0	-2.460650	4.535029	-1.096069
46	1	0	-1.114914	5.065720	-2.122316
47	6	0	2.588575	-1.410001	-0.208936
48	6	0	1.375233	-1.238545	-1.078950
49	1	0	2.496941	-2.333673	0.371236
50	6	0	0.664091	-0.117329	-1.157382
51	1	0	1.091113	-2.102207	-1.677028
52	1	0	0.959014	0.764608	-0.595866
53	6	0	-0.559044	0.004124	-2.018130
54	8	0	-1.031309	-0.976189	-2.634013
55	1	0	-0.639461	1.020082	-2.466608
56	6	0	3.875530	-1.449386	-1.011296
57	6	0	4.733981	-2.543896	-0.935307
58	6	0	4.204783	-0.369310	-1.832889
59	6	0	5.910585	-2.565527	-1.682253
60	1	0	4.483112	-3.377130	-0.284342
61	6	0	5.384865	-0.383315	-2.567703
62	1	0	3.527631	0.478645	-1.892281
63	6	0	6.237706	-1.485015	-2.496967
64	1	0	6.572961	-3.423164	-1.622975
65	1	0	5.638057	0.460618	-3.201261
66	1	0	7.154979	-1.499338	-3.076795
67	8	0	2.607121	-0.289830	0.707215
68	6	0	3.327476	-0.344303	1.825854
69	8	0	3.368806	0.576209	2.605985
70	8	0	3.966490	-1.504613	1.979391
71	6	0	4.758590	-1.604428	3.168929
72	1	0	4.123051	-1.521824	4.051669
73	1	0	5.229735	-2.583752	3.123957
74	1	0	5.510850	-0.814797	3.184855

Re-M1

Total energy= -1817.01516503

Sum of electronic and zero-point Energies= -1816.404403

Sum of electronic and thermal Energies= -1816.368721

Sum of electronic and thermal Enthalpies= -1816.367777
Sum of electronic and thermal Free Energies= -1816.472322

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.009077	1.411796	0.047935
2	6	0	-5.344790	1.664741	-0.251818
3	6	0	-5.681579	2.755734	-1.048882
4	6	0	-4.663911	3.571916	-1.538876
5	6	0	-3.324682	3.303163	-1.244089
6	6	0	-2.986487	2.213720	-0.444949
7	6	0	-3.875573	0.187596	0.925991
8	6	0	-5.301966	-0.475222	0.890906
9	6	0	-6.247737	0.637520	0.383350
10	1	0	-6.719299	2.962365	-1.292583
11	1	0	-4.913619	4.423019	-2.164078
12	1	0	-2.545178	3.944125	-1.641742
13	1	0	-1.945733	1.988770	-0.225699
14	1	0	-5.579426	-0.821042	1.886734
15	1	0	-6.980651	0.216175	-0.311010
16	1	0	-3.594914	0.442883	1.950256
17	1	0	-6.804136	1.071408	1.220520
18	6	0	-3.157848	-1.540671	-0.665391
19	6	0	-1.564179	-0.888420	0.701574
20	7	0	-2.109152	-2.205386	-1.043442
21	7	0	-2.869212	-0.732192	0.402434
22	7	0	-1.125838	-1.779941	-0.189379
23	6	0	-4.584929	-1.601831	-1.101530
24	1	0	-4.842920	-0.738546	-1.729375
25	1	0	-4.774178	-2.518856	-1.658790
26	8	0	-5.358098	-1.644220	0.085347
27	6	0	0.199058	-2.329313	-0.300306
28	6	0	0.483873	-3.501542	0.406298
29	6	0	1.109215	-1.698098	-1.145225
30	6	0	1.767893	-4.021093	0.275968
31	6	0	2.386151	-2.255298	-1.236036
32	6	0	2.731162	-3.405913	-0.529382
33	1	0	2.023908	-4.929220	0.816912
34	1	0	3.126037	-1.773571	-1.870128
35	6	0	-0.561847	-4.144527	1.271861
36	1	0	-0.847618	-3.421029	2.044024
37	1	0	-1.448154	-4.408075	0.684982
38	1	0	-0.173151	-5.053427	1.734974

39	6	0	4.117838	-3.987465	-0.627301
40	1	0	4.699808	-3.490653	-1.406546
41	1	0	4.654206	-3.866702	0.319769
42	1	0	4.079546	-5.058290	-0.846919
43	6	0	0.736141	-0.462641	-1.919769
44	1	0	-0.250548	-0.565310	-2.381119
45	1	0	0.711344	0.410627	-1.258082
46	1	0	1.470179	-0.270453	-2.704541
47	6	0	2.680302	1.287886	1.124804
48	6	0	1.560863	0.359379	1.504141
49	1	0	3.226269	1.568519	2.033004
50	6	0	0.265180	0.634129	1.417788
51	1	0	1.842953	-0.607653	1.918908
52	1	0	-0.083116	1.587697	1.022669
53	6	0	-0.767709	-0.372348	1.941696
54	8	0	-0.302037	-1.403287	2.616157
55	1	0	-1.535056	0.264971	2.464448
56	6	0	3.671901	0.666803	0.152473
57	6	0	4.561000	-0.304363	0.617852
58	6	0	3.728685	1.057755	-1.184798
59	6	0	5.500718	-0.868442	-0.238786
60	1	0	4.525302	-0.611551	1.660437
61	6	0	4.671273	0.493518	-2.043469
62	1	0	3.038823	1.807778	-1.559739
63	6	0	5.561188	-0.468772	-1.573541
64	1	0	6.192607	-1.615412	0.137634
65	1	0	4.710238	0.811665	-3.080695
66	1	0	6.299341	-0.902550	-2.240674
67	8	0	2.091807	2.472115	0.562316
68	6	0	2.805505	3.597665	0.464896
69	8	0	2.371199	4.576322	-0.088148
70	8	0	4.005831	3.505197	1.036611
71	6	0	4.810045	4.686842	0.938261
72	1	0	4.304838	5.525998	1.417813
73	1	0	5.738743	4.451445	1.452849
74	1	0	4.999290	4.923314	-0.109683

Si-M1

Total energy= -1817.02100788

Sum of electronic and zero-point Energies= -1816.411552

Sum of electronic and thermal Energies= -1816.375984

Sum of electronic and thermal Enthalpies= -1816.375040

Sum of electronic and thermal Free Energies= -1816.481899

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.902261	2.466378	-0.128793
2	6	0	-1.461838	3.705485	-0.437239
3	6	0	-2.443689	4.253498	0.383618
4	6	0	-2.840420	3.553024	1.522045
5	6	0	-2.255661	2.326202	1.842966
6	6	0	-1.278083	1.772047	1.017082
7	6	0	0.120867	2.074437	-1.174584
8	6	0	0.403928	3.407582	-1.945625
9	6	0	-0.847654	4.274122	-1.693161
10	1	0	-2.882621	5.218940	0.150065
11	1	0	-3.597792	3.973607	2.176301
12	1	0	-2.551363	1.800060	2.746327
13	1	0	-0.818838	0.821893	1.271072
14	1	0	0.553740	3.203781	-3.006509
15	1	0	-0.565179	5.326483	-1.602602
16	1	0	-0.222696	1.293031	-1.859841
17	1	0	-1.539481	4.189686	-2.538300
18	6	0	2.300457	2.396089	-0.070122
19	6	0	1.814155	0.303661	-0.506598
20	7	0	3.341353	1.731056	0.338402
21	7	0	1.353711	1.562985	-0.590765
22	7	0	3.010902	0.424185	0.065630
23	6	0	2.031738	3.859273	-0.204278
24	1	0	1.279605	4.183756	0.526689
25	1	0	2.946855	4.432346	-0.057744
26	8	0	1.602602	4.065776	-1.539992
27	6	0	3.939519	-0.638431	0.332522
28	6	0	4.111533	-1.052407	1.654033
29	6	0	4.621161	-1.202087	-0.750007
30	6	0	5.019868	-2.083842	1.885064
31	6	0	5.511583	-2.236200	-0.465056
32	6	0	5.721297	-2.687765	0.839705
33	1	0	5.177909	-2.427159	2.904284
34	1	0	6.058059	-2.697559	-1.283724
35	6	0	3.341920	-0.403298	2.773046
36	1	0	3.636278	0.643145	2.895072
37	1	0	2.266189	-0.416237	2.568718
38	1	0	3.519110	-0.925069	3.714413
39	6	0	6.668625	-3.827457	1.111560
40	1	0	7.104018	-3.749454	2.110147

41	1	0	6.142466	-4.785739	1.052719
42	1	0	7.479045	-3.850628	0.379600
43	6	0	4.406957	-0.697613	-2.153711
44	1	0	3.360067	-0.786206	-2.473084
45	1	0	4.676420	0.362121	-2.221133
46	1	0	5.034822	-1.252793	-2.852461
47	6	0	-2.682730	-1.106596	-0.338312
48	6	0	-1.335064	-1.047425	-0.989515
49	1	0	-3.207966	-0.169651	-0.550593
50	6	0	-0.158778	-1.140681	-0.379595
51	1	0	-1.327631	-0.867052	-2.063600
52	1	0	-0.083517	-1.337723	0.689813
53	6	0	1.129832	-0.911559	-1.173884
54	8	0	0.990514	-0.612276	-2.462538
55	1	0	1.807192	-1.767239	-0.927921
56	6	0	-3.530709	-2.272326	-0.804238
57	6	0	-4.838165	-2.070524	-1.242158
58	6	0	-3.004145	-3.565519	-0.777457
59	6	0	-5.614102	-3.151107	-1.658113
60	1	0	-5.248654	-1.064478	-1.251713
61	6	0	-3.780740	-4.645867	-1.181832
62	1	0	-1.980796	-3.715350	-0.443448
63	6	0	-5.086728	-4.439120	-1.626047
64	1	0	-6.629742	-2.986604	-2.003595
65	1	0	-3.367121	-5.648967	-1.157544
66	1	0	-5.690461	-5.282034	-1.946960
67	8	0	-2.473914	-1.196639	1.092103
68	6	0	-3.368716	-0.688317	1.937265
69	8	0	-3.188740	-0.689698	3.130839
70	8	0	-4.445184	-0.189592	1.326888
71	6	0	-5.412199	0.404978	2.198755
72	1	0	-4.979036	1.271256	2.702760
73	1	0	-6.235690	0.710529	1.557199
74	1	0	-5.747762	-0.320688	2.940313

Re-TS2^{D}

Total energy= -1816.94391617

Sum of electronic and zero-point Energies= -1816.338308

Sum of electronic and thermal Energies= -1816.302216

Sum of electronic and thermal Enthalpies= -1816.301271

Sum of electronic and thermal Free Energies= -1816.408208

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.510271	3.018536	0.380598
2	6	0	-0.746546	4.382926	0.536988
3	6	0	-1.628010	4.831801	1.515622
4	6	0	-2.260316	3.897605	2.333788
5	6	0	-2.007292	2.532840	2.184647
6	6	0	-1.122843	2.081380	1.207419
7	6	0	0.474271	2.775170	-0.746777
8	6	0	1.076293	4.198113	-1.047406
9	6	0	0.057857	5.192244	-0.448088
10	1	0	-1.813366	5.893790	1.645749
11	1	0	-2.948990	4.234867	3.101689
12	1	0	-2.499194	1.817535	2.835282
13	1	0	-0.915146	1.019947	1.102833
14	1	0	1.190853	4.334854	-2.123351
15	1	0	0.583216	6.035089	0.010167
16	1	0	-0.010035	2.389618	-1.648592
17	1	0	-0.584816	5.596287	-1.237427
18	6	0	2.597061	2.245918	0.363837
19	6	0	1.705866	0.518137	-0.686380
20	7	0	3.445968	1.289994	0.552289
21	7	0	1.523725	1.836996	-0.380803
22	7	0	2.881186	0.205996	-0.092883
23	6	0	2.669622	3.701285	0.683951
24	1	0	1.961053	3.965934	1.479884
25	1	0	3.678336	3.973323	0.992912
26	8	0	2.385167	4.385415	-0.525796
27	6	0	3.507689	-1.074259	0.062347
28	6	0	4.807422	-1.228699	-0.422320
29	6	0	2.824806	-2.094294	0.733714
30	6	0	5.436788	-2.455648	-0.207134
31	6	0	3.496410	-3.299308	0.922665
32	6	0	4.801243	-3.497687	0.465077
33	1	0	6.446422	-2.598526	-0.584216
34	1	0	2.984037	-4.107855	1.439128
35	6	0	5.502227	-0.123550	-1.173821
36	1	0	4.838427	0.311730	-1.926694
37	1	0	5.802641	0.684797	-0.501783
38	1	0	6.392067	-0.507864	-1.675611
39	6	0	5.498251	-4.812878	0.701686
40	1	0	4.878508	-5.650944	0.363556
41	1	0	6.454261	-4.855048	0.171260
42	1	0	5.695377	-4.962450	1.770281

43	6	0	1.404670	-1.917112	1.196747
44	1	0	1.252195	-0.946168	1.680346
45	1	0	0.738014	-1.982411	0.329361
46	1	0	1.130673	-2.701501	1.905751
47	6	0	-2.773263	-1.443420	-1.275308
48	6	0	-1.302216	-1.357415	-1.557778
49	1	0	-3.336695	-1.663065	-2.188667
50	6	0	-0.550825	-0.268426	-1.364189
51	1	0	-0.822966	-2.275243	-1.886177
52	1	0	-1.026609	0.647508	-1.028716
53	6	0	0.909789	-0.310818	-1.551883
54	8	0	1.470624	-1.579357	-1.899761
55	1	0	1.397326	-0.445690	-2.612807
56	6	0	-3.063026	-2.515210	-0.239829
57	6	0	-3.908668	-3.583779	-0.526649
58	6	0	-2.459044	-2.432752	1.016920
59	6	0	-4.142658	-4.570447	0.430140
60	1	0	-4.389019	-3.639870	-1.499942
61	6	0	-2.701063	-3.408607	1.977164
62	1	0	-1.793836	-1.599482	1.230769
63	6	0	-3.540773	-4.483196	1.682373
64	1	0	-4.798254	-5.403608	0.197809
65	1	0	-2.230446	-3.336833	2.952725
66	1	0	-3.723402	-5.249959	2.428461
67	8	0	-3.187822	-0.150838	-0.775996
68	6	0	-4.483029	0.147360	-0.669776
69	8	0	-4.861893	1.171920	-0.160408
70	8	0	-5.277339	-0.790210	-1.191124
71	6	0	-6.678817	-0.516186	-1.086568
72	1	0	-6.926846	0.393119	-1.635881
73	1	0	-7.178198	-1.377508	-1.524781
74	1	0	-6.961267	-0.398435	-0.039545

Si-TS2^{D}

Total energy= -1816.95282175

Sum of electronic and zero-point Energies= -1816.347357

Sum of electronic and thermal Energies= -1816.310725

Sum of electronic and thermal Enthalpies= -1816.309781

Sum of electronic and thermal Free Energies= -1816.420147

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

1	6	0	-3.718818	-1.790914	0.115149
2	6	0	-4.962907	-1.996194	0.706587
3	6	0	-5.065810	-2.778509	1.854697
4	6	0	-3.909921	-3.339752	2.392931
5	6	0	-2.667067	-3.137724	1.785326
6	6	0	-2.558962	-2.362363	0.633274
7	6	0	-3.819174	-0.888659	-1.091451
8	6	0	-5.358114	-0.619907	-1.254553
9	6	0	-6.064762	-1.309236	-0.058127
10	1	0	-6.031133	-2.948685	2.322525
11	1	0	-3.975077	-3.947806	3.289898
12	1	0	-1.780617	-3.596506	2.211785
13	1	0	-1.611602	-2.228730	0.113109
14	1	0	-5.679387	-1.072692	-2.192894
15	1	0	-6.606233	-0.579529	0.553234
16	1	0	-3.366190	-1.338353	-1.973070
17	1	0	-6.810471	-2.023920	-0.417362
18	6	0	-3.710437	1.508150	-0.380821
19	6	0	-1.752771	0.572790	-0.757014
20	7	0	-2.857219	2.404847	-0.003761
21	7	0	-3.098867	0.376257	-0.857734
22	7	0	-1.635465	1.818214	-0.234326
23	6	0	-5.202238	1.568159	-0.360740
24	1	0	-5.576432	1.250358	0.621701
25	1	0	-5.540323	2.588455	-0.544665
26	8	0	-5.692846	0.750947	-1.400697
27	6	0	-0.420747	2.495167	0.100489
28	6	0	0.026282	2.425616	1.425366
29	6	0	0.313615	3.098814	-0.918747
30	6	0	1.272717	2.970888	1.712101
31	6	0	1.558697	3.634196	-0.582916
32	6	0	2.056952	3.565907	0.717669
33	1	0	1.662434	2.900606	2.724445
34	1	0	2.157881	4.099453	-1.361653
35	6	0	-0.791698	1.708157	2.464887
36	1	0	-1.790237	2.145084	2.554806
37	1	0	-0.921382	0.654204	2.190508
38	1	0	-0.301374	1.750463	3.438465
39	6	0	3.425811	4.089520	1.062003
40	1	0	3.917193	4.525217	0.189833
41	1	0	3.366700	4.854886	1.841561
42	1	0	4.044930	3.272582	1.445050
43	6	0	-0.208212	3.119793	-2.330061
44	1	0	-0.237745	2.103297	-2.738452

45	1	0	-1.226166	3.518393	-2.367294
46	1	0	0.429825	3.730910	-2.970086
47	6	0	2.698101	-1.536764	0.067063
48	6	0	1.353065	-1.446592	-0.597372
49	1	0	2.726734	-2.380154	0.765406
50	6	0	0.564789	-0.368459	-0.536785
51	1	0	1.051299	-2.307300	-1.187015
52	1	0	0.888521	0.485801	0.046006
53	6	0	-0.720240	-0.300314	-1.246379
54	8	0	-1.159606	-1.496526	-1.915791
55	1	0	-0.731487	-0.345253	-2.428641
56	6	0	3.818188	-1.693798	-0.944857
57	6	0	4.664577	-2.799239	-0.910970
58	6	0	4.001248	-0.714210	-1.923736
59	6	0	5.682955	-2.933883	-1.853318
60	1	0	4.529693	-3.552063	-0.138898
61	6	0	5.025015	-0.840057	-2.856221
62	1	0	3.333507	0.143466	-1.944926
63	6	0	5.865183	-1.953677	-2.825014
64	1	0	6.335980	-3.800246	-1.824229
65	1	0	5.165894	-0.074465	-3.612517
66	1	0	6.659307	-2.055638	-3.557730
67	8	0	2.884525	-0.312196	0.814475
68	6	0	3.850516	-0.210906	1.723840
69	8	0	4.089092	0.827311	2.291349
70	8	0	4.491261	-1.362378	1.936071
71	6	0	5.545082	-1.294816	2.902947
72	1	0	5.148049	-0.989438	3.871987
73	1	0	5.958608	-2.299454	2.956029
74	1	0	6.305238	-0.582541	2.579085

Re-M01^{B}

Total energy= -2081.46820798

Sum of electronic and zero-point Energies= -2080.828404

Sum of electronic and thermal Energies= -2080.787716

Sum of electronic and thermal Enthalpies= -2080.786771

Sum of electronic and thermal Free Energies= -2080.904989

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.950940	2.164320	0.193525
2	6	0	-2.958167	2.967689	-0.952324

3	6	0	-2.364454	4.223936	-0.925254
4	6	0	-1.789745	4.667450	0.266837
5	6	0	-1.841657	3.886068	1.422909
6	6	0	-2.435467	2.624618	1.399568
7	6	0	-3.667071	0.865720	-0.083829
8	6	0	-4.588670	1.292972	-1.248186
9	6	0	-3.733802	2.295746	-2.060204
10	1	0	-2.362606	4.856409	-1.807769
11	1	0	-1.322148	5.646546	0.303617
12	1	0	-1.426026	4.268501	2.349417
13	1	0	-2.519754	2.006460	2.289223
14	1	0	-5.429544	1.829280	-0.802125
15	1	0	-3.058145	1.776920	-2.752202
16	1	0	-4.156141	0.433720	0.792578
17	1	0	-4.344684	2.984474	-2.647420
18	6	0	-3.052034	-0.901541	-1.765430
19	6	0	-1.610118	-0.686505	-0.131603
20	7	0	-2.147901	-1.805853	-1.998808
21	7	0	-2.761167	-0.185614	-0.631778
22	7	0	-1.258579	-1.655251	-0.974553
23	6	0	-4.236840	-0.598031	-2.630603
24	1	0	-3.888701	-0.126004	-3.558997
25	1	0	-4.745237	-1.527719	-2.891568
26	8	0	-5.164619	0.216090	-1.953447
27	6	0	-0.093576	-2.499529	-0.945080
28	6	0	-0.174026	-3.712011	-0.256145
29	6	0	1.014293	-2.115614	-1.699780
30	6	0	0.944733	-4.540326	-0.298328
31	6	0	2.102553	-2.991024	-1.723108
32	6	0	2.092761	-4.191560	-1.014438
33	1	0	0.916570	-5.485263	0.238687
34	1	0	2.978108	-2.721859	-2.310868
35	6	0	-1.423768	-4.090778	0.484788
36	1	0	-1.613226	-3.358466	1.275632
37	1	0	-2.286802	-4.099489	-0.189514
38	1	0	-1.322444	-5.084209	0.925443
39	6	0	3.305464	-5.085992	-1.005436
40	1	0	3.905910	-4.948362	-1.908114
41	1	0	3.941365	-4.855846	-0.144073
42	1	0	3.022385	-6.138816	-0.933623
43	6	0	1.048727	-0.807209	-2.445098
44	1	0	0.113458	-0.630452	-2.984037
45	1	0	1.199748	0.028636	-1.750996
46	1	0	1.868782	-0.801256	-3.165994

47	6	0	2.716778	1.265019	0.924427
48	6	0	1.526253	0.385793	1.193606
49	1	0	2.835948	1.996532	1.730282
50	6	0	0.297958	0.599787	0.734056
51	1	0	1.682630	-0.475562	1.839227
52	1	0	0.074050	1.453290	0.092420
53	6	0	-0.852646	-0.307600	1.153986
54	8	0	-0.504635	-1.407090	1.845905
55	1	0	-1.708461	-1.759887	2.734912
56	6	0	4.003004	0.479552	0.775981
57	6	0	5.165630	0.867597	1.439674
58	6	0	4.023249	-0.656508	-0.034885
59	6	0	6.337043	0.126538	1.295693
60	1	0	5.151431	1.753847	2.067762
61	6	0	5.191260	-1.395533	-0.184381
62	1	0	3.108044	-0.969874	-0.528943
63	6	0	6.352272	-1.003990	0.482257
64	1	0	7.236930	0.430796	1.820743
65	1	0	5.192809	-2.282849	-0.811367
66	1	0	7.264561	-1.582100	0.373530
67	8	0	2.430628	1.989581	-0.301579
68	6	0	3.099006	3.098942	-0.611685
69	8	0	2.929564	3.674987	-1.657527
70	8	0	3.945206	3.487576	0.345914
71	6	0	4.680895	4.679310	0.049364
72	1	0	3.998374	5.521191	-0.075543
73	1	0	5.335664	4.839481	0.903277
74	1	0	5.263189	4.543662	-0.863042
75	6	0	-3.586948	-1.347425	3.228887
76	8	0	-2.481003	-2.146944	3.288074
77	8	0	-4.605641	-1.773338	3.806900
78	8	0	-3.474135	-0.250103	2.596539
79	1	0	-1.587137	0.319914	1.680609

Si-M01^{B}

Total energy= -2081.47086945

Sum of electronic and zero-point Energies= -2080.831046

Sum of electronic and thermal Energies= -2080.790409

Sum of electronic and thermal Enthalpies= -2080.789465

Sum of electronic and thermal Free Energies= -2080.907764

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

1	6	0	-3.892148	-1.367780	-0.013684
2	6	0	-4.839148	-2.216607	-0.578456
3	6	0	-6.187326	-2.049490	-0.271013
4	6	0	-6.554805	-1.025757	0.601645
5	6	0	-5.592218	-0.178998	1.159683
6	6	0	-4.242078	-0.341048	0.855823
7	6	0	-2.498060	-1.726249	-0.465058
8	6	0	-2.707773	-2.797569	-1.594561
9	6	0	-4.186080	-3.243752	-1.469569
10	1	0	-6.939670	-2.702294	-0.704387
11	1	0	-7.602621	-0.883496	0.848403
12	1	0	-5.890834	0.610879	1.842344
13	1	0	-3.487654	0.317289	1.284334
14	1	0	-2.021852	-3.631721	-1.444473
15	1	0	-4.639307	-3.309131	-2.464193
16	1	0	-1.882713	-2.077477	0.362383
17	1	0	-4.243280	-4.242357	-1.024461
18	6	0	-2.027375	-0.116247	-2.279996
19	6	0	-1.011061	0.364240	-0.401826
20	7	0	-1.392987	0.988966	-2.533113
21	7	0	-1.808706	-0.539224	-0.996938
22	7	0	-0.772650	1.279154	-1.347565
23	6	0	-2.831734	-1.007854	-3.166368
24	1	0	-3.905905	-0.882752	-2.971743
25	1	0	-2.629638	-0.784635	-4.213807
26	8	0	-2.397590	-2.328336	-2.902551
27	6	0	0.064751	2.441545	-1.232651
28	6	0	1.389803	2.344258	-1.676770
29	6	0	-0.482281	3.602609	-0.686433
30	6	0	2.200207	3.462145	-1.508052
31	6	0	0.372290	4.700153	-0.552399
32	6	0	1.708831	4.643438	-0.942340
33	1	0	3.240721	3.407472	-1.818739
34	1	0	-0.022766	5.620070	-0.129225
35	6	0	1.914570	1.080078	-2.304271
36	1	0	1.633463	0.201930	-1.714731
37	1	0	1.508094	0.952097	-3.312562
38	1	0	3.004330	1.107381	-2.355720
39	6	0	2.622188	5.827221	-0.756327
40	1	0	2.063542	6.716287	-0.457616
41	1	0	3.367658	5.619657	0.017536
42	1	0	3.164266	6.052731	-1.678738
43	6	0	-1.926760	3.667602	-0.270022

44	1	0	-2.570911	3.240260	-1.045063
45	1	0	-2.114960	3.116279	0.660586
46	1	0	-2.223266	4.707068	-0.115651
47	6	0	3.194875	-0.972948	1.265425
48	6	0	1.702581	-0.826884	1.387318
49	1	0	3.684361	-0.759893	2.221745
50	6	0	1.021784	0.217844	0.932028
51	1	0	1.164011	-1.630571	1.882772
52	1	0	1.545782	1.045640	0.462617
53	6	0	-0.496770	0.308157	1.054682
54	8	0	-1.086165	-0.693568	1.726738
55	1	0	-0.745125	1.318992	1.445189
56	6	0	3.599532	-2.356257	0.798435
57	6	0	4.464994	-3.140580	1.557753
58	6	0	3.102148	-2.851614	-0.409237
59	6	0	4.827336	-4.413157	1.120637
60	1	0	4.860435	-2.748689	2.490935
61	6	0	3.471880	-4.116670	-0.853335
62	1	0	2.422903	-2.237733	-0.995568
63	6	0	4.333661	-4.900927	-0.086463
64	1	0	5.498337	-5.020155	1.719983
65	1	0	3.085017	-4.495005	-1.794192
66	1	0	4.618883	-5.890137	-0.430144
67	8	0	3.623939	0.016998	0.297921
68	6	0	4.908727	0.336343	0.169826
69	8	0	5.297234	1.078636	-0.699330
70	8	0	5.685877	-0.234510	1.092656
71	6	0	7.078096	0.080912	0.982344
72	1	0	7.228236	1.157284	1.074766
73	1	0	7.563828	-0.446556	1.800234
74	1	0	7.464911	-0.260611	0.021202
75	6	0	-3.037711	1.445440	3.442989
76	8	0	-2.670569	2.018291	2.372676
77	8	0	-3.819962	1.893190	4.305572
78	8	0	-2.533689	0.195935	3.673212
79	1	0	-1.960010	-0.093059	2.885611

Re-TS2^{B}

Total energy= -2081.45201034

Sum of electronic and zero-point Energies=	-2080.816778
Sum of electronic and thermal Energies=	-2080.777159
Sum of electronic and thermal Enthalpies=	-2080.776215
Sum of electronic and thermal Free Energies=	-2080.891639

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.025906	1.297773	-0.214639
2	6	0	-3.197419	1.892638	-1.469843
3	6	0	-2.894227	3.236638	-1.650296
4	6	0	-2.447953	3.975691	-0.553314
5	6	0	-2.337845	3.387979	0.708660
6	6	0	-2.632318	2.037989	0.893206
7	6	0	-3.419527	-0.156864	-0.280630
8	6	0	-4.400231	-0.133249	-1.474571
9	6	0	-3.783067	0.900685	-2.446311
10	1	0	-3.017609	3.709422	-2.619889
11	1	0	-2.200851	5.024417	-0.686659
12	1	0	-2.027189	3.984303	1.560786
13	1	0	-2.559149	1.562572	1.866052
14	1	0	-5.345834	0.262886	-1.097196
15	1	0	-2.995846	0.449605	-3.063432
16	1	0	-3.823163	-0.543444	0.656884
17	1	0	-4.525899	1.333898	-3.119282
18	6	0	-2.416620	-2.011418	-1.651610
19	6	0	-1.084519	-1.230149	-0.088092
20	7	0	-1.364408	-2.770608	-1.706674
21	7	0	-2.295877	-1.051233	-0.678290
22	7	0	-0.543974	-2.269686	-0.733952
23	6	0	-3.610926	-2.088513	-2.552517
24	1	0	-3.344698	-1.683272	-3.537980
25	1	0	-3.902221	-3.132053	-2.681029
26	8	0	-4.710033	-1.405748	-1.995616
27	6	0	0.786276	-2.796388	-0.600740
28	6	0	0.975358	-3.924339	0.199874
29	6	0	1.811296	-2.182953	-1.319169
30	6	0	2.266807	-4.438016	0.280947
31	6	0	3.087019	-2.741747	-1.211637
32	6	0	3.333103	-3.856209	-0.410685
33	1	0	2.447208	-5.312565	0.901448
34	1	0	3.902626	-2.290935	-1.772438
35	6	0	-0.180644	-4.528460	0.946056
36	1	0	-0.614260	-3.797351	1.639272
37	1	0	-0.970260	-4.838651	0.253684
38	1	0	0.142459	-5.404162	1.511855
39	6	0	4.729891	-4.405245	-0.271840
40	1	0	5.254235	-3.912445	0.553992

41	1	0	4.716664	-5.476601	-0.059190
42	1	0	5.312783	-4.237785	-1.180917
43	6	0	1.567972	-0.954051	-2.154553
44	1	0	0.622501	-1.018386	-2.700982
45	1	0	1.529034	-0.061776	-1.518194
46	1	0	2.375693	-0.816537	-2.876226
47	6	0	2.214661	2.206369	0.798844
48	6	0	1.338155	1.075753	1.237917
49	1	0	2.382538	2.906812	1.622670
50	6	0	0.186014	0.709618	0.671764
51	1	0	1.731582	0.462662	2.043451
52	1	0	-0.229767	1.297005	-0.146483
53	6	0	-0.539567	-0.520168	1.093904
54	8	0	0.269017	-1.378029	1.849384
55	1	0	-0.420548	-1.799689	2.514911
56	6	0	3.577414	1.748014	0.292745
57	6	0	4.527163	2.717895	-0.041863
58	6	0	3.907919	0.400286	0.159322
59	6	0	5.784628	2.349235	-0.505069
60	1	0	4.273494	3.770536	0.059480
61	6	0	5.174003	0.028776	-0.294209
62	1	0	3.176724	-0.363141	0.410756
63	6	0	6.112679	0.998809	-0.629237
64	1	0	6.512315	3.112619	-0.762227
65	1	0	5.422899	-1.025195	-0.378815
66	1	0	7.097443	0.707445	-0.980701
67	8	0	1.618046	2.947125	-0.298057
68	6	0	0.965929	4.090098	-0.091311
69	8	0	0.603429	4.789845	-1.005203
70	8	0	0.783430	4.372513	1.201907
71	6	0	0.236801	5.668650	1.460386
72	1	0	-0.732559	5.779232	0.972540
73	1	0	0.131861	5.733024	2.541343
74	1	0	0.914564	6.441245	1.092577
75	6	0	-2.628653	-1.655230	3.286871
76	8	0	-1.534164	-2.354266	3.241136
77	8	0	-3.643429	-2.027022	3.910409
78	8	0	-2.648280	-0.496251	2.627157
79	1	0	-1.613080	-0.367748	1.853234

Si-TS2^{B}

Total energy= -2081.45644970

Sum of electronic and zero-point Energies= -2080.824304

Sum of electronic and thermal Energies= -2080.784050
Sum of electronic and thermal Enthalpies= -2080.783105
Sum of electronic and thermal Free Energies= -2080.900939

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.391906	-0.994496	0.121570
2	6	0	-5.664984	-1.344976	-0.317819
3	6	0	-6.752601	-1.227560	0.543768
4	6	0	-6.536388	-0.754300	1.837584
5	6	0	-5.253853	-0.400458	2.265632
6	6	0	-4.162370	-0.519024	1.407631
7	6	0	-3.360937	-1.215654	-0.958907
8	6	0	-4.203330	-1.500645	-2.253249
9	6	0	-5.628343	-1.832582	-1.745035
10	1	0	-7.752636	-1.494546	0.214238
11	1	0	-7.375260	-0.655618	2.519736
12	1	0	-5.101578	-0.033218	3.275683
13	1	0	-3.162778	-0.236679	1.728223
14	1	0	-3.768894	-2.334824	-2.805287
15	1	0	-6.373403	-1.353822	-2.388561
16	1	0	-2.688606	-2.033704	-0.704542
17	1	0	-5.804952	-2.912186	-1.793837
18	6	0	-2.964036	1.035236	-1.865552
19	6	0	-1.309441	0.306342	-0.598117
20	7	0	-2.117669	2.014431	-1.865789
21	7	0	-2.514111	-0.031822	-1.134149
22	7	0	-1.090319	1.556566	-1.072318
23	6	0	-4.247856	0.860409	-2.605550
24	1	0	-5.105972	0.971262	-1.927948
25	1	0	-4.328469	1.595083	-3.406628
26	8	0	-4.205764	-0.428493	-3.190082
27	6	0	0.019617	2.414993	-0.785094
28	6	0	1.163041	2.317231	-1.585579
29	6	0	-0.070331	3.269031	0.314737
30	6	0	2.265563	3.086654	-1.230565
31	6	0	1.058745	4.031689	0.623769
32	6	0	2.232529	3.939681	-0.122685
33	1	0	3.186981	2.987841	-1.797788
34	1	0	1.022467	4.695716	1.483964
35	6	0	1.220326	1.334527	-2.722612
36	1	0	1.287908	0.313401	-2.327323
37	1	0	0.325217	1.390599	-3.348205

38	1	0	2.098390	1.516842	-3.344423
39	6	0	3.458278	4.734462	0.244499
40	1	0	4.334764	4.080961	0.261867
41	1	0	3.646484	5.522262	-0.491885
42	1	0	3.348558	5.205357	1.223720
43	6	0	-1.321797	3.331050	1.149555
44	1	0	-2.212103	3.386624	0.516384
45	1	0	-1.413991	2.441707	1.784898
46	1	0	-1.301751	4.210580	1.796255
47	6	0	3.230351	-1.228092	0.619848
48	6	0	1.733129	-1.363241	0.566878
49	1	0	3.579796	-1.210421	1.657563
50	6	0	0.909978	-0.336394	0.347336
51	1	0	1.326653	-2.354638	0.744451
52	1	0	1.341902	0.648275	0.207480
53	6	0	-0.573990	-0.465713	0.403649
54	8	0	-1.064583	-1.735731	0.589168
55	1	0	-0.880539	0.145175	1.498036
56	6	0	3.950170	-2.337636	-0.120330
57	6	0	4.935888	-3.091717	0.512771
58	6	0	3.633421	-2.603033	-1.454623
59	6	0	5.597858	-4.106810	-0.175846
60	1	0	5.188364	-2.874861	1.547253
61	6	0	4.300235	-3.608158	-2.147780
62	1	0	2.857143	-2.017320	-1.940232
63	6	0	5.282492	-4.363656	-1.507391
64	1	0	6.362258	-4.691684	0.325891
65	1	0	4.051089	-3.808418	-3.185166
66	1	0	5.798903	-5.152000	-2.045997
67	8	0	3.561189	0.050672	0.012041
68	6	0	4.742184	0.620016	0.227570
69	8	0	5.069687	1.648977	-0.314374
70	8	0	5.503665	-0.056823	1.092173
71	6	0	6.784658	0.525528	1.350430
72	1	0	6.666763	1.517269	1.789377
73	1	0	7.275745	-0.147440	2.050096
74	1	0	7.356518	0.602225	0.424478
75	6	0	-1.461828	-0.579475	3.551695
76	8	0	-1.262112	0.450011	2.767412
77	8	0	-1.667624	-0.460571	4.767108
78	8	0	-1.450386	-1.782933	2.991498
79	1	0	-1.289696	-1.774258	1.891337

Re-M01^{W}

Total energy= -1893.42721973

Sum of electronic and zero-point Energies= -1892.792124

Sum of electronic and thermal Energies= -1892.753500

Sum of electronic and thermal Enthalpies= -1892.752556

Sum of electronic and thermal Free Energies= -1892.865955

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.961430	-1.680495	-0.142261
2	6	0	-4.102822	-2.407996	-0.478413
3	6	0	-5.167212	-1.782160	-1.119682
4	6	0	-5.070941	-0.423781	-1.416506
5	6	0	-3.921528	0.297362	-1.088409
6	6	0	-2.849653	-0.328272	-0.454417
7	6	0	-1.965127	-2.577394	0.572380
8	6	0	-2.479188	-4.029212	0.270072
9	6	0	-3.974658	-3.849576	-0.055239
10	1	0	-6.056119	-2.344543	-1.388637
11	1	0	-5.895131	0.077805	-1.913235
12	1	0	-3.862974	1.356587	-1.315633
13	1	0	-1.957475	0.242129	-0.213651
14	1	0	-2.317261	-4.678362	1.131143
15	1	0	-4.279385	-4.560884	-0.827685
16	1	0	-1.946507	-2.394211	1.650630
17	1	0	-4.580201	-4.049758	0.835272
18	6	0	-0.270647	-2.917945	-1.164713
19	6	0	0.467808	-1.776546	0.557929
20	7	0	0.952249	-2.609486	-1.473047
21	7	0	-0.606626	-2.419839	0.064819
22	7	0	1.395499	-1.889666	-0.392060
23	6	0	-1.275629	-3.812070	-1.815615
24	1	0	-2.073790	-3.228293	-2.290787
25	1	0	-0.795604	-4.441806	-2.564008
26	8	0	-1.769417	-4.659340	-0.790433
27	6	0	2.692414	-1.263016	-0.464900
28	6	0	3.794724	-1.921423	0.073465
29	6	0	2.769552	-0.040652	-1.133467
30	6	0	5.029803	-1.284700	-0.046820
31	6	0	4.023836	0.560180	-1.216101
32	6	0	5.161022	-0.047127	-0.678499
33	1	0	5.910612	-1.769994	0.366372
34	1	0	4.114475	1.521182	-1.718684

35	6	0	3.638694	-3.238760	0.776867
36	1	0	3.085368	-3.098084	1.712304
37	1	0	3.082734	-3.951966	0.160230
38	1	0	4.615186	-3.671222	1.004283
39	6	0	6.503434	0.631665	-0.786847
40	1	0	6.728432	0.885550	-1.829750
41	1	0	6.511903	1.566362	-0.212334
42	1	0	7.303737	-0.012028	-0.409036
43	6	0	1.551940	0.577965	-1.765263
44	1	0	1.231364	-0.005591	-2.634609
45	1	0	0.714316	0.613039	-1.061446
46	1	0	1.759754	1.600685	-2.086440
47	6	0	-0.211980	2.703787	1.279599
48	6	0	0.444959	1.379151	1.548161
49	1	0	-0.019551	3.395102	2.107841
50	6	0	-0.185245	0.228699	1.755522
51	1	0	1.533959	1.367916	1.547414
52	1	0	-1.271537	0.174383	1.786340
53	6	0	0.624689	-1.061298	1.920246
54	8	0	1.909474	-0.898258	2.234279
55	1	0	0.049975	-1.721599	2.616026
56	6	0	0.328861	3.309513	-0.008021
57	6	0	1.642562	3.781028	-0.032205
58	6	0	-0.436748	3.359273	-1.172650
59	6	0	2.183060	4.301228	-1.204747
60	1	0	2.246031	3.743762	0.871396
61	6	0	0.101932	3.887247	-2.344711
62	1	0	-1.453956	2.978365	-1.173465
63	6	0	1.411687	4.358849	-2.365356
64	1	0	3.205149	4.666531	-1.210346
65	1	0	-0.504320	3.924497	-3.244109
66	1	0	1.830349	4.768076	-3.278961
67	8	0	-1.624894	2.470620	1.185612
68	6	0	-2.478777	3.501006	1.189335
69	8	0	-3.650416	3.351825	0.951170
70	8	0	-1.889508	4.658926	1.480152
71	6	0	-2.763313	5.795292	1.474402
72	1	0	-3.551429	5.665675	2.216895
73	1	0	-2.135643	6.647452	1.723575
74	1	0	-3.207226	5.918713	0.485708
75	8	0	2.158092	-2.831825	3.879179
76	1	0	3.067265	-2.847682	4.194837
77	1	0	2.126531	-2.019372	3.266083

Si-M01^{W}

Total energy= -1893.43439267

Sum of electronic and zero-point Energies= -1892.799757

Sum of electronic and thermal Energies= -1892.760683

Sum of electronic and thermal Enthalpies= -1892.759739

Sum of electronic and thermal Free Energies= -1892.874331

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.000606	2.551376	-0.204570
2	6	0	-1.579361	3.774542	-0.541087
3	6	0	-2.579286	4.317963	0.260256
4	6	0	-2.972162	3.631159	1.408581
5	6	0	-2.365878	2.423132	1.758917
6	6	0	-1.370935	1.871948	0.951666
7	6	0	0.047199	2.168543	-1.231262
8	6	0	0.333815	3.506987	-1.986148
9	6	0	-0.953876	4.333789	-1.796113
10	1	0	-3.033387	5.270986	0.005882
11	1	0	-3.742249	4.049930	2.048915
12	1	0	-2.654517	1.912853	2.673565
13	1	0	-0.892754	0.938023	1.230579
14	1	0	0.547988	3.313383	-3.037920
15	1	0	-0.715090	5.398362	-1.729645
16	1	0	-0.277212	1.385009	-1.922486
17	1	0	-1.616809	4.195251	-2.657413
18	6	0	2.152240	2.527028	-0.010514
19	6	0	1.751565	0.429191	-0.491978
20	7	0	3.164355	1.879430	0.489562
21	7	0	1.271838	1.676584	-0.613115
22	7	0	2.887560	0.568664	0.187032
23	6	0	1.859433	3.985639	-0.154376
24	1	0	1.069812	4.291675	0.543929
25	1	0	2.755690	4.575105	0.037230
26	8	0	1.489355	4.193772	-1.507493
27	6	0	3.780861	-0.479635	0.596373
28	6	0	3.763148	-0.865461	1.939009
29	6	0	4.624776	-1.047157	-0.360594
30	6	0	4.638411	-1.879120	2.320823
31	6	0	5.480283	-2.059254	0.074533
32	6	0	5.496882	-2.488384	1.402409
33	1	0	4.648698	-2.201415	3.358922

34	1	0	6.152997	-2.520002	-0.644327
35	6	0	2.842047	-0.197840	2.925074
36	1	0	3.137902	0.842106	3.092750
37	1	0	1.809259	-0.185901	2.561016
38	1	0	2.861001	-0.720955	3.881944
39	6	0	6.408797	-3.607194	1.833704
40	1	0	6.681801	-3.511006	2.886815
41	1	0	5.913573	-4.575108	1.706107
42	1	0	7.323073	-3.623257	1.236498
43	6	0	4.597099	-0.598464	-1.797054
44	1	0	3.756642	-1.056154	-2.334428
45	1	0	4.502763	0.488636	-1.872568
46	1	0	5.518086	-0.898965	-2.300264
47	6	0	-2.682551	-1.103202	-0.265562
48	6	0	-1.347824	-1.010288	-0.939667
49	1	0	-3.246814	-0.194619	-0.499219
50	6	0	-0.161804	-1.069420	-0.344104
51	1	0	-1.365953	-0.840959	-2.014944
52	1	0	-0.068984	-1.255073	0.725721
53	6	0	1.110012	-0.801966	-1.145847
54	8	0	0.925198	-0.515088	-2.448989
55	1	0	1.819480	-1.635532	-0.944785
56	6	0	-3.491711	-2.314036	-0.683178
57	6	0	-4.816586	-2.173784	-1.092754
58	6	0	-2.914369	-3.584516	-0.636789
59	6	0	-5.560457	-3.294150	-1.457949
60	1	0	-5.265603	-1.184651	-1.119215
61	6	0	-3.658715	-4.704489	-0.991387
62	1	0	-1.877740	-3.686413	-0.326655
63	6	0	-4.982937	-4.559713	-1.405138
64	1	0	-6.590054	-3.178084	-1.780922
65	1	0	-3.205698	-5.689868	-0.951678
66	1	0	-5.561809	-5.433212	-1.687658
67	8	0	-2.447061	-1.138317	1.162940
68	6	0	-3.349714	-0.640146	2.006715
69	8	0	-3.147220	-0.586753	3.195265
70	8	0	-4.459523	-0.217855	1.399094
71	6	0	-5.441830	0.359443	2.265979
72	1	0	-5.058180	1.284301	2.701418
73	1	0	-6.303376	0.565925	1.634961
74	1	0	-5.700905	-0.340722	3.060536
75	8	0	2.271141	-2.409823	-3.525737
76	1	0	1.696288	-1.651992	-3.173962
77	1	0	2.724924	-2.022993	-4.281496

Re-TS2^{W}

Total energy= -1893.39069142

Sum of electronic and zero-point Energies= -1892.759421

Sum of electronic and thermal Energies= -1892.721047

Sum of electronic and thermal Enthalpies= -1892.720103

Sum of electronic and thermal Free Energies= -1892.834696

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.695487	3.045093	-0.393446
2	6	0	0.976131	4.392967	-0.610228
3	6	0	1.965356	4.761776	-1.516078
4	6	0	2.658215	3.764706	-2.201081
5	6	0	2.360095	2.416844	-1.993175
6	6	0	1.367771	2.044965	-1.088964
7	6	0	-0.409604	2.895322	0.634556
8	6	0	-1.022034	4.336798	0.751249
9	6	0	0.086746	5.274715	0.229593
10	1	0	2.187400	5.809555	-1.694149
11	1	0	3.432019	4.039229	-2.910698
12	1	0	2.903003	1.651528	-2.537645
13	1	0	1.129504	0.995772	-0.935116
14	1	0	-1.285401	4.552014	1.787205
15	1	0	-0.356571	6.104450	-0.327794
16	1	0	-0.038281	2.569023	1.609844
17	1	0	0.643350	5.702663	1.070098
18	6	0	-2.351357	2.297306	-0.741973
19	6	0	-1.655507	0.656455	0.544970
20	7	0	-3.147552	1.311265	-1.013991
21	7	0	-1.427467	1.944563	0.204257
22	7	0	-2.694336	0.287993	-0.213623
23	6	0	-2.366549	3.732267	-1.156478
24	1	0	-1.557904	3.945197	-1.867545
25	1	0	-3.323108	3.984506	-1.613277
26	8	0	-2.241677	4.489202	0.036142
27	6	0	-3.303741	-1.008038	-0.359201
28	6	0	-4.498561	-1.251713	0.313985
29	6	0	-2.676945	-1.942598	-1.179515
30	6	0	-5.112175	-2.483087	0.097148
31	6	0	-3.327146	-3.161708	-1.365655
32	6	0	-4.548615	-3.440848	-0.749688

33	1	0	-6.043671	-2.705383	0.611798
34	1	0	-2.863285	-3.913695	-1.999255
35	6	0	-5.029362	-0.242795	1.294521
36	1	0	-4.291810	-0.098482	2.093672
37	1	0	-5.203535	0.727757	0.820670
38	1	0	-5.963736	-0.586575	1.740444
39	6	0	-5.251852	-4.749807	-1.000191
40	1	0	-5.835131	-5.057346	-0.129307
41	1	0	-5.942154	-4.661129	-1.845544
42	1	0	-4.538692	-5.542413	-1.237310
43	6	0	-1.321658	-1.657901	-1.768137
44	1	0	-1.302428	-0.697517	-2.294030
45	1	0	-0.570830	-1.616324	-0.968191
46	1	0	-1.027512	-2.442288	-2.467626
47	6	0	2.608606	-1.542058	1.255563
48	6	0	1.133787	-1.373036	1.487393
49	1	0	3.111456	-1.855032	2.177140
50	6	0	0.479452	-0.214560	1.421508
51	1	0	0.582055	-2.286385	1.691744
52	1	0	1.038195	0.696677	1.225418
53	6	0	-0.997535	-0.111406	1.621360
54	8	0	-1.632154	-1.344214	1.813429
55	1	0	-1.372970	0.391019	2.699311
56	6	0	2.863652	-2.573566	0.172469
57	6	0	3.458102	-3.794917	0.477705
58	6	0	2.468726	-2.307351	-1.140051
59	6	0	3.651228	-4.749713	-0.519467
60	1	0	3.776166	-3.996259	1.497279
61	6	0	2.670635	-3.254330	-2.138707
62	1	0	2.005327	-1.351448	-1.372596
63	6	0	3.259414	-4.479996	-1.827877
64	1	0	4.114207	-5.700357	-0.274881
65	1	0	2.365815	-3.039785	-3.158225
66	1	0	3.412908	-5.221784	-2.604940
67	8	0	3.126794	-0.256486	0.856181
68	6	0	4.445905	-0.057992	0.787699
69	8	0	4.914211	0.963585	0.353315
70	8	0	5.149403	-1.090439	1.254566
71	6	0	6.570561	-0.924029	1.192105
72	1	0	6.874492	-0.065058	1.791643
73	1	0	6.990003	-1.843252	1.594462
74	1	0	6.885293	-0.777067	0.157990
75	8	0	-2.200747	0.017384	3.835163
76	1	0	-2.974088	0.588010	3.753970

77	1	0	-2.084608	-1.125439	2.697093

Si-TS2^{W}

Total energy= -1893.39838080

Sum of electronic and zero-point Energies= -1892.766145

Sum of electronic and thermal Energies= -1892.728039

Sum of electronic and thermal Enthalpies= -1892.727094

Sum of electronic and thermal Free Energies= -1892.839645

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.481405	-1.917605	0.077204
2	6	0	4.694879	-2.430427	-0.371919
3	6	0	4.708324	-3.512406	-1.249777
4	6	0	3.496084	-4.059423	-1.663436
5	6	0	2.282101	-3.540287	-1.203434
6	6	0	2.264284	-2.462286	-0.322556
7	6	0	3.687401	-0.735103	0.992886
8	6	0	5.243976	-0.497254	1.001931
9	6	0	5.862706	-1.682136	0.217220
10	1	0	5.648206	-3.919745	-1.610297
11	1	0	3.492644	-4.899746	-2.350353
12	1	0	1.347964	-3.982720	-1.534185
13	1	0	1.325736	-2.055804	0.048304
14	1	0	5.592586	-0.482666	2.034079
15	1	0	6.559605	-1.310185	-0.541274
16	1	0	3.294972	-0.912760	1.991221
17	1	0	6.441572	-2.321607	0.890115
18	6	0	3.563192	1.275238	-0.457336
19	6	0	1.679224	0.800186	0.558264
20	7	0	2.721468	2.142547	-0.924433
21	7	0	2.980284	0.445294	0.466502
22	7	0	1.550085	1.837320	-0.282485
23	6	0	5.017606	1.094330	-0.738848
24	1	0	5.165158	0.309479	-1.494312
25	1	0	5.451944	2.024270	-1.105923
26	8	0	5.636204	0.765575	0.487071
27	6	0	0.362071	2.606648	-0.525770
28	6	0	-0.410637	2.276350	-1.643888
29	6	0	0.016896	3.610641	0.381381
30	6	0	-1.594437	2.983166	-1.835031
31	6	0	-1.172790	4.297728	0.136772

32	6	0	-1.987945	3.995509	-0.955630
33	1	0	-2.233274	2.718620	-2.672668
34	1	0	-1.472430	5.085474	0.823356
35	6	0	-0.001507	1.157763	-2.563891
36	1	0	0.958074	1.371682	-3.043942
37	1	0	0.110596	0.218545	-2.008956
38	1	0	-0.758513	1.004379	-3.334393
39	6	0	-3.260207	4.765637	-1.195909
40	1	0	-3.733627	5.050182	-0.249874
41	1	0	-3.050979	5.687761	-1.754364
42	1	0	-3.972622	4.174352	-1.780766
43	6	0	0.884383	3.927295	1.572134
44	1	0	0.795689	3.165172	2.358956
45	1	0	1.938056	3.983471	1.281826
46	1	0	0.596950	4.890694	1.997476
47	6	0	-2.525746	-1.611318	0.120787
48	6	0	-1.261475	-1.278147	0.865982
49	1	0	-2.415564	-2.576618	-0.384013
50	6	0	-0.606437	-0.128945	0.704667
51	1	0	-0.906956	-2.026887	1.569382
52	1	0	-1.013651	0.602772	0.017266
53	6	0	0.629348	0.250252	1.441998
54	8	0	1.129706	-0.747015	2.294023
55	1	0	0.438972	1.087902	2.334269
56	6	0	-3.740152	-1.663852	1.028424
57	6	0	-4.531449	-2.808814	1.089774
58	6	0	-4.069477	-0.554932	1.810634
59	6	0	-5.639988	-2.852954	1.933231
60	1	0	-4.281092	-3.664659	0.469159
61	6	0	-5.183276	-0.592389	2.642665
62	1	0	-3.443784	0.332752	1.765773
63	6	0	-5.967871	-1.743983	2.708635
64	1	0	-6.249523	-3.749761	1.979038
65	1	0	-5.437288	0.273568	3.246197
66	1	0	-6.833194	-1.774160	3.362974
67	8	0	-2.695669	-0.583549	-0.883820
68	6	0	-3.511980	-0.764917	-1.920129
69	8	0	-3.682555	0.089942	-2.754236
70	8	0	-4.085420	-1.969722	-1.927723
71	6	0	-4.985425	-2.199853	-3.017802
72	1	0	-4.453749	-2.126660	-3.967216
73	1	0	-5.373510	-3.205279	-2.869457
74	1	0	-5.794783	-1.468809	-2.995741
75	8	0	0.705940	1.255813	3.745210

76	1	0	1.067703	-0.211417	3.160759
77	1	0	-0.168867	1.221659	4.150897

Re-M2

Total energy= -1893.39838080
Sum of electronic and zero-point Energies= -1816.414583
Sum of electronic and thermal Energies= -1816.378043
Sum of electronic and thermal Enthalpies= -1816.377099
Sum of electronic and thermal Free Energies= -1816.484881

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.435725	-2.538374	0.997768
2	6	0	-1.330056	-3.238646	0.178223
3	6	0	-2.692362	-3.203846	0.447945
4	6	0	-3.139372	-2.475484	1.552926
5	6	0	-2.241679	-1.798152	2.378961
6	6	0	-0.873866	-1.827174	2.105437
7	6	0	0.965263	-2.716386	0.480495
8	6	0	0.822722	-4.079526	-0.239717
9	6	0	-0.574816	-3.990922	-0.892438
10	1	0	-3.400330	-3.730427	-0.184244
11	1	0	-4.201427	-2.445000	1.780399
12	1	0	-2.609617	-1.248182	3.239572
13	1	0	-0.167256	-1.289560	2.731789
14	1	0	0.782758	-4.844319	0.541950
15	1	0	-0.533558	-3.410300	-1.822017
16	1	0	1.733384	-2.725584	1.263924
17	1	0	-0.995055	-4.973110	-1.118606
18	6	0	2.446341	-2.153729	-1.303947
19	6	0	1.745171	-0.398481	-0.141508
20	7	0	3.480969	-1.399968	-1.243298
21	7	0	1.340206	-1.695231	-0.559013
22	7	0	3.116926	-0.335650	-0.434433
23	6	0	2.320109	-3.468451	-1.991442
24	1	0	1.599786	-3.381856	-2.816384
25	1	0	3.284806	-3.783036	-2.390007
26	8	0	1.903472	-4.456279	-1.061080
27	6	0	4.058902	0.650694	-0.063165
28	6	0	4.726214	1.387568	-1.060253
29	6	0	4.299880	0.878629	1.302371
30	6	0	5.642318	2.353608	-0.657583

31	6	0	5.207297	1.880718	1.652853
32	6	0	5.891687	2.622005	0.692697
33	1	0	6.163413	2.930915	-1.418077
34	1	0	5.393945	2.069879	2.707308
35	6	0	4.435557	1.151073	-2.517899
36	1	0	4.870855	0.208599	-2.860388
37	1	0	3.357249	1.084223	-2.690713
38	1	0	4.840066	1.963696	-3.124211
39	6	0	6.871316	3.697438	1.082757
40	1	0	7.868165	3.487117	0.678130
41	1	0	6.559236	4.671106	0.684243
42	1	0	6.950903	3.787107	2.170092
43	6	0	3.603568	0.058157	2.354977
44	1	0	2.543402	0.324488	2.430371
45	1	0	3.655806	-1.006807	2.108003
46	1	0	4.067341	0.214145	3.330358
47	6	0	-2.887969	1.246619	0.454083
48	6	0	-1.399025	1.377608	0.599341
49	1	0	-3.337195	1.011906	1.425964
50	6	0	-0.525497	0.474898	0.140241
51	1	0	-1.060226	2.262798	1.130189
52	1	0	-0.887475	-0.410415	-0.371592
53	6	0	0.913810	0.609534	0.226406
54	8	0	1.358231	1.831645	0.677210
55	1	0	2.289759	1.957961	0.452783
56	6	0	-3.529068	2.502543	-0.104502
57	6	0	-4.613561	3.103677	0.531067
58	6	0	-3.030319	3.055038	-1.286666
59	6	0	-5.191323	4.254200	-0.004312
60	1	0	-5.007892	2.665537	1.444045
61	6	0	-3.610929	4.196666	-1.827069
62	1	0	-2.181607	2.582320	-1.773865
63	6	0	-4.691696	4.800140	-1.183528
64	1	0	-6.032501	4.721194	0.497948
65	1	0	-3.219672	4.620060	-2.746602
66	1	0	-5.141820	5.694946	-1.601487
67	8	0	-3.135760	0.141821	-0.445645
68	6	0	-4.325118	-0.454366	-0.473400
69	8	0	-4.603743	-1.291392	-1.295214
70	8	0	-5.146417	-0.034338	0.494792
71	6	0	-6.438932	-0.648630	0.487618
72	1	0	-6.345701	-1.725478	0.641985
73	1	0	-6.986907	-0.189147	1.307327
74	1	0	-6.938653	-0.462354	-0.463890

Si-M2

Total energy= -1817.03606407

Sum of electronic and zero-point Energies= -1816.426589

Sum of electronic and thermal Energies= -1816.389653

Sum of electronic and thermal Enthalpies= -1816.388709

Sum of electronic and thermal Free Energies= -1816.498476

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.268678	-1.375328	0.510277
2	6	0	-5.653481	-1.471801	0.622336
3	6	0	-6.237436	-1.744560	1.856935
4	6	0	-5.416231	-1.912214	2.970027
5	6	0	-4.027761	-1.809724	2.853595
6	6	0	-3.441659	-1.542045	1.618422
7	6	0	-3.851669	-1.065060	-0.910829
8	6	0	-5.201979	-0.781184	-1.666355
9	6	0	-6.325753	-1.250591	-0.709292
10	1	0	-7.316801	-1.818291	1.953328
11	1	0	-5.859559	-2.118928	3.938992
12	1	0	-3.402820	-1.937975	3.731544
13	1	0	-2.362919	-1.445662	1.525168
14	1	0	-5.221990	-1.337576	-2.603696
15	1	0	-7.121859	-0.499913	-0.668528
16	1	0	-3.332728	-1.906403	-1.366882
17	1	0	-6.777253	-2.176834	-1.078701
18	6	0	-3.489120	1.361907	-0.888415
19	6	0	-1.606351	0.183822	-0.703212
20	7	0	-2.597928	2.263046	-0.670995
21	7	0	-2.966725	0.092849	-0.988260
22	7	0	-1.407342	1.550499	-0.591976
23	6	0	-4.963385	1.506797	-1.077854
24	1	0	-5.491871	1.334758	-0.128281
25	1	0	-5.206648	2.506620	-1.438113
26	8	0	-5.356641	0.572999	-2.064593
27	6	0	-0.190689	2.230730	-0.313416
28	6	0	0.021629	2.723935	0.979866
29	6	0	0.774340	2.341402	-1.320199
30	6	0	1.244270	3.331357	1.256036
31	6	0	1.988696	2.946046	-0.995051
32	6	0	2.243945	3.438565	0.285446

33	1	0	1.431798	3.709327	2.258428
34	1	0	2.754596	3.034026	-1.762469
35	6	0	-1.036875	2.554080	2.036651
36	1	0	-1.930530	3.136249	1.794533
37	1	0	-1.349665	1.505917	2.103170
38	1	0	-0.664533	2.870078	3.012532
39	6	0	3.584904	4.027693	0.634649
40	1	0	3.480707	4.861004	1.334100
41	1	0	4.204462	3.263264	1.114869
42	1	0	4.106981	4.384504	-0.256124
43	6	0	0.519962	1.774299	-2.689718
44	1	0	0.572530	0.679333	-2.664848
45	1	0	-0.478360	2.042879	-3.046176
46	1	0	1.260968	2.138764	-3.403663
47	6	0	2.931198	-1.636358	0.440891
48	6	0	1.534860	-1.737831	-0.101820
49	1	0	3.098562	-2.394434	1.214357
50	6	0	0.645688	-0.728019	-0.102669
51	1	0	1.295982	-2.697290	-0.553220
52	1	0	0.947051	0.216255	0.335576
53	6	0	-0.703616	-0.843986	-0.587712
54	8	0	-1.149792	-2.114543	-0.958453
55	1	0	-1.019463	-2.702150	-0.198885
56	6	0	3.972172	-1.814543	-0.649653
57	6	0	4.842808	-2.900760	-0.628221
58	6	0	4.047677	-0.888503	-1.692658
59	6	0	5.780632	-3.070613	-1.645428
60	1	0	4.790893	-3.611203	0.192783
61	6	0	4.993992	-1.047475	-2.699396
62	1	0	3.360061	-0.045223	-1.702659
63	6	0	5.859220	-2.142511	-2.679684
64	1	0	6.453404	-3.922008	-1.624639
65	1	0	5.055329	-0.322105	-3.504585
66	1	0	6.593108	-2.269203	-3.469142
67	8	0	3.068571	-0.329538	1.043634
68	6	0	4.109751	-0.060027	1.829833
69	8	0	4.309690	1.043972	2.273924
70	8	0	4.871273	-1.128529	2.073274
71	6	0	6.007226	-0.878733	2.908056
72	1	0	5.684112	-0.508605	3.881945
73	1	0	6.512363	-1.836845	3.008224
74	1	0	6.663526	-0.144550	2.438770

Re-TS3

Total energy= -1817.01695763

Sum of electronic and zero-point Energies= -1816.408862

Sum of electronic and thermal Energies= -1816.372719

Sum of electronic and thermal Enthalpies= -1816.371775

Sum of electronic and thermal Free Energies= -1816.479502

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.944166	-2.952231	0.447766
2	6	0	-2.719329	-4.109779	0.431407
3	6	0	-2.818866	-4.897096	1.574252
4	6	0	-2.143879	-4.500580	2.727814
5	6	0	-1.389392	-3.325777	2.745660
6	6	0	-1.286670	-2.536606	1.601757
7	6	0	-1.990091	-2.261188	-0.900305
8	6	0	-3.175260	-2.965369	-1.655530
9	6	0	-3.372387	-4.306262	-0.913579
10	1	0	-3.423386	-5.798971	1.571763
11	1	0	-2.216480	-5.103426	3.627219
12	1	0	-0.884812	-3.021187	3.656308
13	1	0	-0.718908	-1.609502	1.624197
14	1	0	-2.912979	-3.117754	-2.703025
15	1	0	-4.437766	-4.544466	-0.847479
16	1	0	-1.064775	-2.393152	-1.468499
17	1	0	-2.888869	-5.117470	-1.467927
18	6	0	-3.492677	-0.357663	-0.540571
19	6	0	-1.381361	0.239767	-0.804192
20	7	0	-3.516637	0.931531	-0.446791
21	7	0	-2.227888	-0.833664	-0.771690
22	7	0	-2.198880	1.306497	-0.607033
23	6	0	-4.597274	-1.361204	-0.569751
24	1	0	-4.622788	-1.941312	0.362256
25	1	0	-5.557207	-0.865680	-0.710614
26	8	0	-4.362666	-2.186055	-1.698672
27	6	0	-1.819473	2.648144	-0.273264
28	6	0	-1.346985	2.899152	1.014980
29	6	0	-1.979205	3.648295	-1.234238
30	6	0	-1.032348	4.221049	1.336865
31	6	0	-1.652740	4.950823	-0.867563
32	6	0	-1.177449	5.254433	0.411266
33	1	0	-0.672509	4.446292	2.338451
34	1	0	-1.769114	5.748161	-1.597592

35	6	0	-1.170793	1.782520	2.011093
36	1	0	-0.272072	1.193612	1.785868
37	1	0	-1.059736	2.182530	3.020827
38	1	0	-2.027407	1.100925	2.002081
39	6	0	-0.807709	6.670230	0.771067
40	1	0	-0.784048	6.810505	1.853751
41	1	0	0.183843	6.919747	0.379931
42	1	0	-1.517333	7.383352	0.344649
43	6	0	-2.457573	3.300044	-2.616392
44	1	0	-1.751552	2.611822	-3.092401
45	1	0	-3.430995	2.802156	-2.584115
46	1	0	-2.542273	4.194956	-3.234819
47	6	0	3.156284	-1.351446	-0.218883
48	6	0	2.232206	-0.719578	-1.070127
49	1	0	2.800704	-2.233557	0.313073
50	6	0	0.874455	-0.785099	-0.778348
51	1	0	2.589482	0.072693	-1.717466
52	1	0	0.514684	-1.634452	-0.198994
53	6	0	0.007274	0.268784	-1.039958
54	8	0	0.507645	1.481614	-1.462051
55	1	0	1.285165	1.676346	-0.898921
56	6	0	4.595867	-1.390451	-0.576631
57	6	0	5.299180	-2.593262	-0.493767
58	6	0	5.255877	-0.237221	-1.017381
59	6	0	6.639093	-2.654829	-0.870992
60	1	0	4.792289	-3.486826	-0.139291
61	6	0	6.594634	-0.298399	-1.385640
62	1	0	4.712323	0.703669	-1.030203
63	6	0	7.287981	-1.508001	-1.319261
64	1	0	7.175203	-3.596553	-0.809560
65	1	0	7.104111	0.600125	-1.719677
66	1	0	8.333250	-1.551833	-1.608456
67	8	0	3.223319	-0.403153	1.365318
68	6	0	2.822837	0.811442	1.312099
69	8	0	2.831489	1.589571	0.353747
70	8	0	2.333715	1.222558	2.519861
71	6	0	2.061305	2.616674	2.616359
72	1	0	1.385024	2.944364	1.823714
73	1	0	1.599904	2.766603	3.593073
74	1	0	2.986640	3.195561	2.548778

Si-TS3

Total energy= -1817.02037264

Sum of electronic and zero-point Energies= -1816.412461
Sum of electronic and thermal Energies= -1816.376319
Sum of electronic and thermal Enthalpies= -1816.375375
Sum of electronic and thermal Free Energies= -1816.482816

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.640932	-1.605191	-0.805486
2	6	0	4.974403	-1.975079	-0.655651
3	6	0	5.742159	-2.281968	-1.776725
4	6	0	5.153042	-2.209319	-3.036738
5	6	0	3.812638	-1.839589	-3.179277
6	6	0	3.041855	-1.535511	-2.060077
7	6	0	3.003386	-1.298985	0.530762
8	6	0	4.191798	-1.361410	1.564552
9	6	0	5.380576	-1.989079	0.795787
10	1	0	6.784197	-2.568833	-1.671025
11	1	0	5.741017	-2.442727	-3.918628
12	1	0	3.370154	-1.790571	-4.168807
13	1	0	1.995824	-1.257617	-2.157521
14	1	0	3.898257	-1.974728	2.416369
15	1	0	6.294519	-1.419622	0.993514
16	1	0	2.232812	-2.023110	0.786221
17	1	0	5.559393	-3.011587	1.142576
18	6	0	3.136977	1.152382	0.750631
19	6	0	1.123223	0.447905	0.168748
20	7	0	2.459713	2.241369	0.597598
21	7	0	2.380738	0.029519	0.528991
22	7	0	1.206507	1.805625	0.224256
23	6	0	4.544104	0.956328	1.205079
24	1	0	5.201479	0.734893	0.352227
25	1	0	4.906111	1.851039	1.711120
26	8	0	4.521859	-0.106331	2.138109
27	6	0	0.205262	2.768835	-0.111902
28	6	0	0.070452	3.140564	-1.452671
29	6	0	-0.596696	3.285520	0.907097
30	6	0	-0.915250	4.073126	-1.764105
31	6	0	-1.567899	4.220060	0.547598
32	6	0	-1.737608	4.624655	-0.777547
33	1	0	-1.045735	4.377601	-2.799795
34	1	0	-2.211172	4.634790	1.319527
35	6	0	0.945528	2.515554	-2.504922
36	1	0	2.004074	2.618211	-2.247879

37	1	0	0.731193	1.444125	-2.592438
38	1	0	0.775666	2.979501	-3.477374
39	6	0	-2.779504	5.648710	-1.146415
40	1	0	-3.342150	5.333625	-2.032471
41	1	0	-3.484937	5.810201	-0.325791
42	1	0	-2.306662	6.610235	-1.382233
43	6	0	-0.451103	2.787506	2.320301
44	1	0	-0.805174	1.751001	2.399160
45	1	0	0.593649	2.806830	2.642461
46	1	0	-1.041316	3.396780	3.006496
47	6	0	-3.606432	-0.580687	-0.034132
48	6	0	-2.332186	-0.788653	-0.620965
49	1	0	-3.880492	0.455964	0.159389
50	6	0	-1.293850	0.068084	-0.290057
51	1	0	-2.106651	-1.776123	-1.008848
52	1	0	-1.545357	1.071676	0.043899
53	6	0	0.030681	-0.359437	-0.197698
54	8	0	0.303730	-1.711088	-0.333986
55	1	0	-0.335123	-2.171405	0.250392
56	6	0	-4.736851	-1.453909	-0.444247
57	6	0	-5.917550	-0.893941	-0.932395
58	6	0	-4.610265	-2.845462	-0.374147
59	6	0	-6.954917	-1.714635	-1.371726
60	1	0	-6.022057	0.186807	-0.975983
61	6	0	-5.647950	-3.662470	-0.805911
62	1	0	-3.701589	-3.263990	0.051188
63	6	0	-6.820969	-3.098699	-1.310886
64	1	0	-7.868464	-1.272274	-1.756074
65	1	0	-5.548028	-4.741603	-0.743513
66	1	0	-7.630762	-3.738571	-1.646794
67	8	0	-3.478390	-0.957782	1.720536
68	6	0	-2.329728	-1.443921	2.041491
69	8	0	-1.778389	-2.440809	1.575256
70	8	0	-1.702700	-0.682972	2.978279
71	6	0	-0.405620	-1.128925	3.353732
72	1	0	0.277003	-1.077047	2.497343
73	1	0	-0.068502	-0.453997	4.139900
74	1	0	-0.434582	-2.157368	3.719353

M3$_{endo}$

Total energy= -1512.84369393

Sum of electronic and zero-point Energies= -1512.305670

Sum of electronic and thermal Energies= -1512.274736

Sum of electronic and thermal Enthalpies= -1512.273792

Sum of electronic and thermal Free Energies= -1512.371350

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.046539	-1.964248	0.231811
2	6	0	-4.356669	-2.418755	0.349684
3	6	0	-4.726195	-3.192362	1.447992
4	6	0	-3.768642	-3.490376	2.414575
5	6	0	-2.456131	-3.026046	2.290390
6	6	0	-2.081811	-2.256944	1.191586
7	6	0	-2.862990	-1.141324	-1.021956
8	6	0	-4.313664	-0.976857	-1.608390
9	6	0	-5.200314	-1.967921	-0.815459
10	1	0	-5.745224	-3.552439	1.552534
11	1	0	-4.045097	-4.088293	3.277029
12	1	0	-1.724500	-3.267341	3.054348
13	1	0	-1.062770	-1.888875	1.088581
14	1	0	-4.305927	-1.208418	-2.673012
15	1	0	-6.129560	-1.476398	-0.509644
16	1	0	-2.169199	-1.592236	-1.734178
17	1	0	-5.480161	-2.815637	-1.448241
18	6	0	-3.070453	1.204223	-0.242836
19	6	0	-1.012343	0.538833	-0.567304
20	7	0	-2.339773	2.215767	0.123322
21	7	0	-2.299250	0.170783	-0.690274
22	7	0	-1.056235	1.782338	-0.080531
23	6	0	-4.551106	1.028000	-0.329690
24	1	0	-4.922634	0.461224	0.535667
25	1	0	-5.051368	1.995541	-0.363437
26	8	0	-4.801252	0.357654	-1.549826
27	6	0	0.048258	2.671114	0.154365
28	6	0	0.372800	2.977025	1.475696
29	6	0	0.733492	3.187293	-0.949608
30	6	0	1.444164	3.846289	1.683060
31	6	0	1.796598	4.046430	-0.687004
32	6	0	2.164797	4.385779	0.618308
33	1	0	1.723012	4.100281	2.702329
34	1	0	2.350960	4.465364	-1.523258
35	6	0	-0.396885	2.378534	2.623055
36	1	0	-1.416209	2.773540	2.660387
37	1	0	-0.474310	1.290384	2.520936
38	1	0	0.095613	2.600241	3.570737
39	6	0	3.322670	5.319295	0.857853

40	1	0	3.482006	5.488412	1.924383
41	1	0	4.244527	4.910190	0.434738
42	1	0	3.146392	6.287426	0.380266
43	6	0	0.337810	2.825258	-2.356701
44	1	0	0.551387	1.773102	-2.573070
45	1	0	-0.733145	2.984156	-2.517596
46	1	0	0.886937	3.437253	-3.073514
47	6	0	3.522618	-1.149812	0.338891
48	6	0	2.407709	-1.086909	-0.423923
49	1	0	3.551949	-0.569793	1.261419
50	6	0	1.246049	-0.296299	-0.142013
51	1	0	2.344606	-1.673932	-1.339410
52	1	0	1.231380	0.341560	0.737086
53	6	0	0.154672	-0.318018	-0.990890
54	8	0	-0.045298	-0.964663	-2.058733
55	6	0	4.720459	-1.941235	0.053903
56	6	0	5.737805	-2.023109	1.019332
57	6	0	4.917328	-2.630018	-1.156944
58	6	0	6.893621	-2.763605	0.794589
59	1	0	5.610400	-1.496379	1.961837
60	6	0	6.070253	-3.370774	-1.380828
61	1	0	4.164152	-2.574817	-1.936736
62	6	0	7.067656	-3.445045	-0.407627
63	1	0	7.660748	-2.809374	1.561949
64	1	0	6.196182	-3.889632	-2.326478
65	1	0	7.968947	-4.021755	-0.588303

M3$_{exo}$

Total energy= -1512.84218718

Sum of electronic and zero-point Energies= -1512.304110

Sum of electronic and thermal Energies= -1512.273254

Sum of electronic and thermal Enthalpies= -1512.272310

Sum of electronic and thermal Free Energies= -1512.368542

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.943434	-2.650346	0.578185
2	6	0	-2.833036	-3.702244	0.383003
3	6	0	-3.439499	-4.307059	1.481737
4	6	0	-3.140076	-3.836705	2.758180
5	6	0	-2.248431	-2.775688	2.941936
6	6	0	-1.636984	-2.168051	1.848138

7	6	0	-1.411761	-2.137102	-0.740248
8	6	0	-2.241670	-2.901468	-1.836260
9	6	0	-2.989735	-4.026949	-1.080790
10	1	0	-4.139375	-5.125970	1.345909
11	1	0	-3.608841	-4.296970	3.622086
12	1	0	-2.031964	-2.422684	3.944771
13	1	0	-0.947400	-1.334700	1.981102
14	1	0	-1.568082	-3.304203	-2.592076
15	1	0	-4.034647	-4.063889	-1.405081
16	1	0	-0.337761	-2.299330	-0.852969
17	1	0	-2.546581	-4.999344	-1.316399
18	6	0	-2.851933	-0.176401	-1.214726
19	6	0	-0.889044	0.323275	-0.391272
20	7	0	-2.889139	1.110845	-1.031113
21	7	0	-1.639649	-0.693047	-0.847705
22	7	0	-1.658962	1.401235	-0.506333
23	6	0	-3.848470	-1.132988	-1.785293
24	1	0	-4.406408	-1.628876	-0.978768
25	1	0	-4.551084	-0.614273	-2.436925
26	8	0	-3.117071	-2.056033	-2.569210
27	6	0	-1.306376	2.750780	-0.157320
28	6	0	-1.675580	3.215580	1.103351
29	6	0	-0.622721	3.521008	-1.099750
30	6	0	-1.348652	4.536178	1.411031
31	6	0	-0.316657	4.831660	-0.743127
32	6	0	-0.675646	5.353722	0.502733
33	1	0	-1.621567	4.930529	2.386340
34	1	0	0.215752	5.459993	-1.453008
35	6	0	-2.358521	2.303316	2.083760
36	1	0	-3.296973	1.913715	1.677399
37	1	0	-1.698957	1.454786	2.295979
38	1	0	-2.575653	2.829332	3.014522
39	6	0	-0.327872	6.777689	0.851767
40	1	0	-0.683942	7.039762	1.849640
41	1	0	0.754973	6.929603	0.823992
42	1	0	-0.772939	7.473692	0.134920
43	6	0	-0.224195	2.936242	-2.428269
44	1	0	0.511962	2.136897	-2.287662
45	1	0	-1.086971	2.505630	-2.945769
46	1	0	0.217799	3.700620	-3.068549
47	6	0	3.870878	-0.830448	-0.788847
48	6	0	2.822325	-0.380269	-0.064245
49	1	0	3.697495	-1.099336	-1.831125
50	6	0	1.479234	-0.228111	-0.547690

51	1	0	2.961872	-0.098002	0.978891
52	1	0	1.246758	-0.473905	-1.581471
53	6	0	0.471671	0.247932	0.269354
54	8	0	0.476823	0.603465	1.480167
55	6	0	5.247153	-1.001666	-0.320881
56	6	0	6.221176	-1.467389	-1.219637
57	6	0	5.658477	-0.725547	0.996002
58	6	0	7.543412	-1.649307	-0.828500
59	1	0	5.927788	-1.688216	-2.242943
60	6	0	6.978708	-0.907106	1.386935
61	1	0	4.937201	-0.364658	1.722641
62	6	0	7.932594	-1.370097	0.479316
63	1	0	8.271604	-2.011377	-1.548102
64	1	0	7.267218	-0.685502	2.410228
65	1	0	8.962934	-1.510675	0.789367

TS4$_{endo}$

Total energy= -1512.82518661

Sum of electronic and zero-point Energies= -1512.287771

Sum of electronic and thermal Energies= -1512.257351

Sum of electronic and thermal Enthalpies= -1512.256406

Sum of electronic and thermal Free Energies= -1512.353633

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.261628	-2.463338	0.171724
2	6	0	-3.390486	-3.277177	0.192755
3	6	0	-3.571956	-4.188322	1.230164
4	6	0	-2.612377	-4.262396	2.236830
5	6	0	-1.483013	-3.438679	2.210968
6	6	0	-1.296270	-2.529193	1.172804
7	6	0	-2.266276	-1.556893	-1.037782
8	6	0	-3.679941	-1.775392	-1.695763
9	6	0	-4.277835	-3.020136	-0.997379
10	1	0	-4.449976	-4.826633	1.256493
11	1	0	-2.742924	-4.966762	3.052094
12	1	0	-0.746314	-3.511468	3.004253
13	1	0	-0.421146	-1.882383	1.141971
14	1	0	-3.564123	-1.931483	-2.767938
15	1	0	-5.320343	-2.829085	-0.723120
16	1	0	-1.443308	-1.757150	-1.728656
17	1	0	-4.277878	-3.875784	-1.679477

18	6	0	-3.157314	0.601398	-0.199060
19	6	0	-0.988231	0.565723	-0.493183
20	7	0	-2.758688	1.778312	0.184320
21	7	0	-2.110686	-0.157703	-0.637255
22	7	0	-1.399930	1.736468	-0.000202
23	6	0	-4.520161	0.007602	-0.343384
24	1	0	-4.729947	-0.689342	0.479959
25	1	0	-5.280907	0.787747	-0.354530
26	8	0	-4.531557	-0.640400	-1.601841
27	6	0	-0.603843	2.909366	0.230947
28	6	0	-0.365035	3.298657	1.550807
29	6	0	-0.121121	3.604769	-0.878108
30	6	0	0.401967	4.443939	1.746409
31	6	0	0.645058	4.743027	-0.627267
32	6	0	0.916888	5.173563	0.671381
33	1	0	0.606651	4.772576	2.762516
34	1	0	1.034057	5.308278	-1.470113
35	6	0	-0.913926	2.500859	2.703632
36	1	0	-2.003751	2.581956	2.753011
37	1	0	-0.673090	1.437582	2.597425
38	1	0	-0.497350	2.855507	3.647323
39	6	0	1.764756	6.393274	0.922335
40	1	0	1.272584	7.076514	1.619478
41	1	0	2.723762	6.109319	1.366955
42	1	0	1.969055	6.931913	-0.004760
43	6	0	-0.424085	3.146181	-2.280588
44	1	0	0.037481	2.176834	-2.497962
45	1	0	-1.503258	3.034917	-2.429030
46	1	0	-0.052114	3.871734	-3.005318
47	6	0	3.271456	-1.265791	0.157047
48	6	0	2.771378	-0.096690	-0.259563
49	1	0	2.615422	-1.929767	0.720560
50	6	0	1.376662	0.333938	-0.017085
51	1	0	3.423034	0.591809	-0.804228
52	1	0	1.152489	0.916835	0.873010
53	6	0	0.380829	0.087618	-0.921306
54	8	0	0.377303	-0.503748	-2.046701
55	6	0	4.645349	-1.762892	-0.042400
56	6	0	5.065069	-2.890895	0.674381
57	6	0	5.558135	-1.161341	-0.921364
58	6	0	6.355114	-3.394779	0.535511
59	1	0	4.366600	-3.373836	1.352919
60	6	0	6.846827	-1.662481	-1.061250
61	1	0	5.254350	-0.303307	-1.512781

62	6	0	7.253541	-2.780151	-0.332028
63	1	0	6.657029	-4.268020	1.105304
64	1	0	7.536579	-1.183799	-1.749570
65	1	0	8.259315	-3.171272	-0.446610

TS4$_{endo}$

Total energy= -1512.82518661

Sum of electronic and zero-point Energies= -1512.287771

Sum of electronic and thermal Energies= -1512.257351

Sum of electronic and thermal Enthalpies= -1512.256406

Sum of electronic and thermal Free Energies= -1512.353633

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.261628	-2.463338	0.171724
2	6	0	-3.390486	-3.277177	0.192755
3	6	0	-3.571956	-4.188322	1.230164
4	6	0	-2.612377	-4.262396	2.236830
5	6	0	-1.483013	-3.438679	2.210968
6	6	0	-1.296270	-2.529193	1.172804
7	6	0	-2.266276	-1.556893	-1.037782
8	6	0	-3.679941	-1.775392	-1.695763
9	6	0	-4.277835	-3.020136	-0.997379
10	1	0	-4.449976	-4.826633	1.256493
11	1	0	-2.742924	-4.966762	3.052094
12	1	0	-0.746314	-3.511468	3.004253
13	1	0	-0.421146	-1.882383	1.141971
14	1	0	-3.564123	-1.931483	-2.767938
15	1	0	-5.320343	-2.829085	-0.723120
16	1	0	-1.443308	-1.757150	-1.728656
17	1	0	-4.277878	-3.875784	-1.679477
18	6	0	-3.157314	0.601398	-0.199060
19	6	0	-0.988231	0.565723	-0.493183
20	7	0	-2.758688	1.778312	0.184320
21	7	0	-2.110686	-0.157703	-0.637255
22	7	0	-1.399930	1.736468	-0.000202
23	6	0	-4.520161	0.007602	-0.343384
24	1	0	-4.729947	-0.689342	0.479959
25	1	0	-5.280907	0.787747	-0.354530
26	8	0	-4.531557	-0.640400	-1.601841
27	6	0	-0.603843	2.909366	0.230947
28	6	0	-0.365035	3.298657	1.550807

29	6	0	-0.121121	3.604769	-0.878108
30	6	0	0.401967	4.443939	1.746409
31	6	0	0.645058	4.743027	-0.627267
32	6	0	0.916888	5.173563	0.671381
33	1	0	0.606651	4.772576	2.762516
34	1	0	1.034057	5.308278	-1.470113
35	6	0	-0.913926	2.500859	2.703632
36	1	0	-2.003751	2.581956	2.753011
37	1	0	-0.673090	1.437582	2.597425
38	1	0	-0.497350	2.855507	3.647323
39	6	0	1.764756	6.393274	0.922335
40	1	0	1.272584	7.076514	1.619478
41	1	0	2.723762	6.109319	1.366955
42	1	0	1.969055	6.931913	-0.004760
43	6	0	-0.424085	3.146181	-2.280588
44	1	0	0.037481	2.176834	-2.497962
45	1	0	-1.503258	3.034917	-2.429030
46	1	0	-0.052114	3.871734	-3.005318
47	6	0	3.271456	-1.265791	0.157047
48	6	0	2.771378	-0.096690	-0.259563
49	1	0	2.615422	-1.929767	0.720560
50	6	0	1.376662	0.333938	-0.017085
51	1	0	3.423034	0.591809	-0.804228
52	1	0	1.152489	0.916835	0.873010
53	6	0	0.380829	0.087618	-0.921306
54	8	0	0.377303	-0.503748	-2.046701
55	6	0	4.645349	-1.762892	-0.042400
56	6	0	5.065069	-2.890895	0.674381
57	6	0	5.558135	-1.161341	-0.921364
58	6	0	6.355114	-3.394779	0.535511
59	1	0	4.366600	-3.373836	1.352919
60	6	0	6.846827	-1.662481	-1.061250
61	1	0	5.254350	-0.303307	-1.512781
62	6	0	7.253541	-2.780151	-0.332028
63	1	0	6.657029	-4.268020	1.105304
64	1	0	7.536579	-1.183799	-1.749570
65	1	0	8.259315	-3.171272	-0.446610

TS4$_{exo}$

Total energy= -1512.82407795

Sum of electronic and zero-point Energies= -1512.286615

Sum of electronic and thermal Energies= -1512.256209

Sum of electronic and thermal Enthalpies= -1512.255265

Sum of electronic and thermal Free Energies= -1512.351697

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.492493	-3.027481	0.446465
2	6	0	-0.856085	-4.364419	0.319867
3	6	0	-0.905422	-5.176780	1.450592
4	6	0	-0.591723	-4.622728	2.689580
5	6	0	-0.234673	-3.275969	2.805134
6	6	0	-0.179926	-2.458476	1.678499
7	6	0	-0.509672	-2.330962	-0.894236
8	6	0	-1.129778	-3.380811	-1.888074
9	6	0	-1.150724	-4.721966	-1.114848
10	1	0	-1.190268	-6.221459	1.369661
11	1	0	-0.629277	-5.243597	3.579031
12	1	0	0.000567	-2.864192	3.781091
13	1	0	0.084535	-1.403453	1.757381
14	1	0	-0.516066	-3.443986	-2.786278
15	1	0	-2.121178	-5.211498	-1.245195
16	1	0	0.483378	-2.002455	-1.209143
17	1	0	-0.393258	-5.402523	-1.515357
18	6	0	-2.712341	-1.195148	-0.937168
19	6	0	-1.027239	0.114076	-0.450784
20	7	0	-3.256992	-0.046293	-0.663470
21	7	0	-1.349698	-1.133202	-0.832289
22	7	0	-2.189726	0.752437	-0.351098
23	6	0	-3.293095	-2.495046	-1.390218
24	1	0	-3.403034	-3.182247	-0.539603
25	1	0	-4.267910	-2.342569	-1.852495
26	8	0	-2.412872	-3.007200	-2.372604
27	6	0	-2.379694	2.129891	0.011656
28	6	0	-2.666739	2.422121	1.345944
29	6	0	-2.274387	3.096549	-0.987643
30	6	0	-2.873909	3.760804	1.668984
31	6	0	-2.487884	4.422403	-0.612714
32	6	0	-2.788570	4.769382	0.705385
33	1	0	-3.100809	4.023447	2.699278
34	1	0	-2.414490	5.200713	-1.367930
35	6	0	-2.708451	1.324890	2.372596
36	1	0	-3.471556	0.579954	2.126154
37	1	0	-1.733222	0.825693	2.392080
38	1	0	-2.925618	1.729779	3.362205
39	6	0	-2.984592	6.211973	1.093484

40	1	0	-3.277370	6.817008	0.232840
41	1	0	-3.750467	6.312290	1.866058
42	1	0	-2.055590	6.629774	1.494526
43	6	0	-1.926695	2.710324	-2.400292
44	1	0	-0.922188	2.274316	-2.438148
45	1	0	-2.627260	1.966012	-2.791043
46	1	0	-1.947737	3.582753	-3.054710
47	6	0	3.653680	0.227036	-0.477201
48	6	0	2.665199	1.066758	-0.807589
49	1	0	3.404320	-0.822659	-0.319504
50	6	0	1.264480	0.637954	-1.022644
51	1	0	2.898296	2.127983	-0.926326
52	1	0	0.951046	0.347448	-2.023893
53	6	0	0.333305	0.631067	-0.021478
54	8	0	0.388339	0.928570	1.210749
55	6	0	5.071074	0.579663	-0.271873
56	6	0	5.905948	-0.318667	0.405037
57	6	0	5.629330	1.778366	-0.739569
58	6	0	7.247851	-0.024609	0.628379
59	1	0	5.490720	-1.256179	0.765727
60	6	0	6.969050	2.074405	-0.516582
61	1	0	5.013364	2.476739	-1.297831
62	6	0	7.784954	1.175702	0.170280
63	1	0	7.874387	-0.734167	1.159906
64	1	0	7.381552	3.006884	-0.889326
65	1	0	8.831647	1.406816	0.339886

M4$_{endo}$

Total energy= -1512.84233870
Sum of electronic and zero-point Energies= -1512.304646
Sum of electronic and thermal Energies= -1512.273544
Sum of electronic and thermal Enthalpies= -1512.272600
Sum of electronic and thermal Free Energies= -1512.371219

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.628777	-2.175815	0.365919
2	6	0	-3.861531	-2.820566	0.396983
3	6	0	-4.256669	-3.507307	1.542846
4	6	0	-3.403133	-3.528521	2.643605
5	6	0	-2.168839	-2.873916	2.605600
6	6	0	-1.768461	-2.190525	1.460467

7	6	0	-2.400562	-1.493961	-0.963125
8	6	0	-3.767314	-1.642706	-1.729150
9	6	0	-4.599901	-2.656881	-0.906905
10	1	0	-5.216571	-4.013625	1.580297
11	1	0	-3.700770	-4.058006	3.543009
12	1	0	-1.518455	-2.900125	3.473485
13	1	0	-0.810720	-1.674769	1.424208
14	1	0	-3.581766	-2.002643	-2.740769
15	1	0	-5.621265	-2.284046	-0.778656
16	1	0	-1.559090	-1.913232	-1.517595
17	1	0	-4.671809	-3.609630	-1.440240
18	6	0	-3.053901	0.862485	-0.557028
19	6	0	-0.893734	0.509626	-0.534463
20	7	0	-2.539467	2.015668	-0.248286
21	7	0	-2.083586	-0.076059	-0.761364
22	7	0	-1.189835	1.778863	-0.234813
23	6	0	-4.466489	0.436665	-0.788253
24	1	0	-4.862979	-0.074576	0.100461
25	1	0	-5.094742	1.297609	-1.014843
26	8	0	-4.448026	-0.409346	-1.921058
27	6	0	-0.280895	2.859279	0.031404
28	6	0	-0.215139	3.347088	1.336312
29	6	0	0.480484	3.370469	-1.023877
30	6	0	0.664683	4.402213	1.578483
31	6	0	1.344976	4.420297	-0.727769
32	6	0	1.449698	4.947157	0.563149
33	1	0	0.741014	4.800846	2.586652
34	1	0	1.952222	4.840670	-1.525681
35	6	0	-1.049941	2.742003	2.433551
36	1	0	-2.109683	2.973508	2.293008
37	1	0	-0.955411	1.650414	2.443535
38	1	0	-0.736923	3.123390	3.406360
39	6	0	2.400518	6.082299	0.840086
40	1	0	2.369256	6.378916	1.890493
41	1	0	3.428069	5.795607	0.596014
42	1	0	2.151634	6.955351	0.229323
43	6	0	0.373245	2.800950	-2.413336
44	1	0	0.801901	1.794129	-2.462962
45	1	0	-0.671472	2.731632	-2.731725
46	1	0	0.908203	3.431970	-3.124404
47	6	0	3.204194	-1.421393	-0.397604
48	6	0	2.660557	-0.484707	0.417728
49	1	0	2.625737	-1.755830	-1.253271
50	6	0	1.361689	0.122649	0.305787

51	1	0	3.253956	-0.129897	1.260328
52	1	0	1.099887	0.884720	1.031601
53	6	0	0.430195	-0.202255	-0.663120
54	8	0	0.477491	-1.035714	-1.613076
55	6	0	4.534264	-2.014205	-0.233786
56	6	0	5.036671	-2.848449	-1.246688
57	6	0	5.350641	-1.800272	0.891635
58	6	0	6.296708	-3.430364	-1.151718
59	1	0	4.421326	-3.035312	-2.123194
60	6	0	6.609875	-2.378520	0.986320
61	1	0	4.994082	-1.181445	1.709233
62	6	0	7.094847	-3.196734	-0.034556
63	1	0	6.655572	-4.068560	-1.953744
64	1	0	7.217264	-2.193697	1.867567
65	1	0	8.078258	-3.648685	0.044840

M4$_{exo}$

Total energy= -1512.84091106

Sum of electronic and zero-point Energies= -1512.301800

Sum of electronic and thermal Energies= -1512.271158

Sum of electronic and thermal Enthalpies= -1512.270214

Sum of electronic and thermal Free Energies= -1512.365528

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.296840	-2.382151	0.431401
2	6	0	-3.416229	-3.206940	0.379433
3	6	0	-3.847294	-3.861520	1.530970
4	6	0	-3.143418	-3.668187	2.717152
5	6	0	-2.023654	-2.831987	2.759477
6	6	0	-1.585702	-2.177207	1.611155
7	6	0	-2.009775	-1.771075	-0.920837
8	6	0	-3.233330	-2.184454	-1.819944
9	6	0	-4.004474	-3.253305	-1.007665
10	1	0	-4.720949	-4.505700	1.506727
11	1	0	-3.470792	-4.169412	3.622489
12	1	0	-1.492614	-2.692142	3.695137
13	1	0	-0.719546	-1.516877	1.637254
14	1	0	-2.873210	-2.582797	-2.767984
15	1	0	-5.076944	-3.034073	-1.026705
16	1	0	-1.060891	-2.110741	-1.340939
17	1	0	-3.872177	-4.241000	-1.459417

18	6	0	-3.050267	0.474672	-0.782523
19	6	0	-0.884199	0.464073	-0.480875
20	7	0	-2.753977	1.703423	-0.476737
21	7	0	-1.930618	-0.311453	-0.811825
22	7	0	-1.400303	1.673668	-0.280901
23	6	0	-4.342930	-0.177838	-1.149858
24	1	0	-4.777876	-0.682749	-0.275941
25	1	0	-5.053153	0.558107	-1.525391
26	8	0	-4.051673	-1.085044	-2.195441
27	6	0	-0.679136	2.873169	0.047904
28	6	0	-0.600365	3.246756	1.388074
29	6	0	-0.106794	3.602019	-0.996169
30	6	0	0.076276	4.432337	1.675265
31	6	0	0.559769	4.776090	-0.657237
32	6	0	0.655638	5.206294	0.669397
33	1	0	0.156013	4.753252	2.710530
34	1	0	1.017546	5.368068	-1.446020
35	6	0	-1.195149	2.375411	2.459426
36	1	0	-2.269903	2.236978	2.305904
37	1	0	-0.715050	1.391201	2.422847
38	1	0	-1.040332	2.815240	3.445634
39	6	0	1.382646	6.485269	0.995202
40	1	0	1.374002	6.684854	2.068201
41	1	0	2.423999	6.433710	0.664980
42	1	0	0.920416	7.335137	0.484765
43	6	0	-0.198728	3.113859	-2.417281
44	1	0	0.352070	2.173566	-2.533614
45	1	0	-1.238136	2.928262	-2.705482
46	1	0	0.225241	3.846856	-3.104707
47	6	0	3.367419	-1.063363	-0.164306
48	6	0	2.546702	-1.022406	-1.240804
49	1	0	2.985927	-0.697058	0.783744
50	6	0	1.196344	-0.521451	-1.280005
51	1	0	2.916891	-1.414512	-2.188198
52	1	0	0.656908	-0.573912	-2.221717
53	6	0	0.541926	0.039603	-0.201291
54	8	0	0.903906	0.240784	0.992210
55	6	0	4.735995	-1.587740	-0.157277
56	6	0	5.388484	-1.761240	1.075103
57	6	0	5.449863	-1.927279	-1.320792
58	6	0	6.683233	-2.263930	1.148760
59	1	0	4.858939	-1.498391	1.987283
60	6	0	6.742495	-2.431258	-1.248399
61	1	0	4.994130	-1.784176	-2.295933

62	6	0	7.369575	-2.605780	-0.014114
63	1	0	7.157041	-2.388887	2.117928
64	1	0	7.269945	-2.683877	-2.163549
65	1	0	8.380447	-2.996952	0.038221

$TS5R_{endo}$

Total energy= -2314.81187008

Sum of electronic and zero-point Energies= -2313.985841

Sum of electronic and thermal Energies= -2313.937281

Sum of electronic and thermal Enthalpies= -2313.936337

Sum of electronic and thermal Free Energies= -2314.067819

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.237803	-2.138913	-0.544440
2	6	0	5.545599	-2.599161	-0.419533
3	6	0	6.070479	-3.468825	-1.372399
4	6	0	5.268421	-3.860260	-2.441761
5	6	0	3.955848	-3.395401	-2.559573
6	6	0	3.426932	-2.530031	-1.605675
7	6	0	3.875180	-1.217329	0.598440
8	6	0	5.232912	-0.978992	1.362871
9	6	0	6.204173	-2.053284	0.820304
10	1	0	7.089395	-3.833407	-1.284938
11	1	0	5.666812	-4.535077	-3.192477
12	1	0	3.344448	-3.712940	-3.397524
13	1	0	2.402383	-2.174504	-1.685210
14	1	0	5.072727	-1.081479	2.435755
15	1	0	7.184759	-1.606191	0.629798
16	1	0	3.112074	-1.634031	1.258217
17	1	0	6.349173	-2.842468	1.564449
18	6	0	4.172780	1.053209	-0.334520
19	6	0	2.081619	0.454252	-0.120020
20	7	0	3.489258	2.054459	-0.802602
21	7	0	3.347382	0.060059	0.105110
22	7	0	2.183477	1.665103	-0.673740
23	6	0	5.635524	0.873916	-0.093665
24	1	0	6.080293	0.214684	-0.851635
25	1	0	6.145393	1.836653	-0.110909
26	8	0	5.746314	0.337046	1.211406
27	6	0	1.161305	2.661846	-0.904032
28	6	0	0.412767	2.651862	-2.074931

29	6	0	1.047065	3.660982	0.075034
30	6	0	-0.536791	3.666940	-2.230438
31	6	0	0.089676	4.644635	-0.131443
32	6	0	-0.720767	4.656041	-1.272867
33	1	0	-1.146760	3.668909	-3.130216
34	1	0	-0.027912	5.426160	0.615469
35	6	0	0.587751	1.640417	-3.173658
36	1	0	1.485177	1.030753	-3.044698
37	1	0	-0.290715	0.989723	-3.200588
38	1	0	0.664495	2.148677	-4.138393
39	6	0	-1.764266	5.728405	-1.448729
40	1	0	-1.331349	6.723427	-1.311597
41	1	0	-2.216417	5.683024	-2.441471
42	1	0	-2.561261	5.614324	-0.707819
43	6	0	1.960723	3.703739	1.270068
44	1	0	2.093377	2.710787	1.702977
45	1	0	2.941346	4.102020	0.990286
46	1	0	1.534069	4.345652	2.042463
47	6	0	-1.861242	-1.607572	0.381016
48	6	0	-1.071538	-1.561500	-0.787265
49	1	0	-1.361685	-1.445363	1.330592
50	6	0	0.110318	-0.850595	-0.872932
51	1	0	-1.533975	-1.873202	-1.723082
52	1	0	0.465203	-0.551857	-1.852170
53	6	0	0.900812	-0.446398	0.238337
54	8	0	0.925406	-0.863977	1.404714
55	6	0	-3.087259	-2.432558	0.464446
56	6	0	-4.041058	-2.129360	1.444654
57	6	0	-3.314456	-3.518810	-0.385549
58	6	0	-5.198360	-2.888274	1.562992
59	1	0	-3.860773	-1.268093	2.082441
60	6	0	-4.473693	-4.283939	-0.263844
61	1	0	-2.568563	-3.785599	-1.129230
62	6	0	-5.419942	-3.969576	0.707696
63	1	0	-5.933738	-2.638309	2.321918
64	1	0	-4.632922	-5.129435	-0.926234
65	1	0	-6.323185	-4.564302	0.802033
66	7	0	-2.398170	0.276159	0.339161
67	7	0	-1.373971	1.065413	0.547928
68	6	0	-2.882899	0.431245	-1.008118
69	8	0	-2.355540	1.058067	-1.896665
70	8	0	-4.056167	-0.199632	-1.081079
71	6	0	-1.001273	1.111985	1.891571
72	8	0	-0.039008	1.766217	2.253071

73	8	0	-1.769187	0.386408	2.729572
74	6	0	-1.471185	0.331048	4.151223
75	6	0	-0.098108	-0.290629	4.386464
76	6	0	-1.593184	1.719573	4.773916
77	6	0	-2.563327	-0.586602	4.691215
78	1	0	-0.038491	-1.258970	3.883077
79	1	0	0.692447	0.349099	3.997127
80	1	0	0.047257	-0.439901	5.460894
81	1	0	-2.568401	2.152683	4.532681
82	1	0	-1.514595	1.634631	5.861794
83	1	0	-0.807739	2.381151	4.410403
84	1	0	-2.447006	-0.711721	5.771128
85	1	0	-3.551787	-0.162074	4.492353
86	1	0	-2.502191	-1.569747	4.215219
87	6	0	-4.761662	-0.330268	-2.346344
88	6	0	-5.159507	1.044079	-2.876913
89	6	0	-3.907967	-1.111198	-3.341083
90	6	0	-5.994909	-1.137065	-1.957322
91	1	0	-5.696583	1.599028	-2.102343
92	1	0	-4.285456	1.617562	-3.184750
93	1	0	-5.826918	0.917917	-3.734268
94	1	0	-3.669028	-2.097202	-2.929691
95	1	0	-4.471424	-1.253992	-4.267645
96	1	0	-2.984083	-0.578162	-3.572870
97	1	0	-6.608301	-1.332427	-2.841014
98	1	0	-5.691905	-2.088793	-1.510752
99	1	0	-6.593794	-0.584783	-1.227850

TS5S$_{endo}$

Total energy= -2314.83255218

Sum of electronic and zero-point Energies= -2314.006490

Sum of electronic and thermal Energies= -2313.958058

Sum of electronic and thermal Enthalpies= -2313.957114

Sum of electronic and thermal Free Energies= -2314.087822

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.237088	3.862617	-0.410030
2	6	0	0.272880	4.922343	0.340425
3	6	0	0.425295	6.175034	-0.243221
4	6	0	0.050423	6.348889	-1.576270
5	6	0	-0.472857	5.287964	-2.316188

6	6	0	-0.621839	4.028611	-1.734058
7	6	0	-0.279319	2.611825	0.437810
8	6	0	-0.181098	3.138907	1.897254
9	6	0	0.582185	4.469766	1.748673
10	1	0	0.816572	7.009270	0.331461
11	1	0	0.156837	7.324249	-2.040094
12	1	0	-0.771365	5.444700	-3.347420
13	1	0	-1.048314	3.204400	-2.301457
14	1	0	0.349590	2.408483	2.509972
15	1	0	0.272324	5.180005	2.519331
16	1	0	0.563452	1.939945	0.263369
17	1	0	1.656967	4.290168	1.865496
18	6	0	-2.669528	2.306718	0.816408
19	6	0	-1.790623	0.692182	-0.355738
20	7	0	-3.660025	1.497140	0.573057
21	7	0	-1.514295	1.858815	0.248216
22	7	0	-3.097960	0.499578	-0.164804
23	6	0	-2.569713	3.512633	1.692854
24	1	0	-2.485304	4.424461	1.087965
25	1	0	-3.451401	3.583977	2.329375
26	8	0	-1.446487	3.320044	2.534001
27	6	0	-3.928592	-0.567742	-0.655883
28	6	0	-4.056304	-0.734699	-2.038732
29	6	0	-4.604986	-1.358431	0.277009
30	6	0	-4.880202	-1.765963	-2.482899
31	6	0	-5.413132	-2.378476	-0.225561
32	6	0	-5.556815	-2.602623	-1.594137
33	1	0	-5.000051	-1.914676	-3.553207
34	1	0	-5.945561	-3.013713	0.477963
35	6	0	-3.345780	0.153814	-3.026272
36	1	0	-3.372257	1.204301	-2.720500
37	1	0	-2.296257	-0.138605	-3.138109
38	1	0	-3.816795	0.074125	-4.007286
39	6	0	-6.408249	-3.734094	-2.107633
40	1	0	-5.779580	-4.574931	-2.418696
41	1	0	-7.092960	-4.096234	-1.338313
42	1	0	-6.992930	-3.424797	-2.977399
43	6	0	-4.489979	-1.130207	1.761995
44	1	0	-3.465303	-0.879872	2.049310
45	1	0	-5.137710	-0.306426	2.075958
46	1	0	-4.795357	-2.030662	2.299458
47	6	0	1.824325	-1.611168	-0.996459
48	6	0	1.527537	-0.445720	-1.725523
49	1	0	0.995476	-2.170662	-0.578328

50	6	0	0.342722	0.252007	-1.587228
51	1	0	2.347493	0.059704	-2.234839
52	1	0	0.308616	1.294497	-1.892251
53	6	0	-0.829985	-0.303603	-0.980485
54	8	0	-1.178283	-1.485432	-0.919902
55	6	0	3.062069	-2.387784	-1.181071
56	6	0	3.444497	-3.282666	-0.171585
57	6	0	3.851779	-2.295087	-2.333135
58	6	0	4.591320	-4.053425	-0.304956
59	1	0	2.834162	-3.331760	0.726554
60	6	0	4.998560	-3.075768	-2.470644
61	1	0	3.548760	-1.637454	-3.143281
62	6	0	5.374185	-3.953765	-1.456971
63	1	0	4.879320	-4.735802	0.488913
64	1	0	5.592083	-3.005079	-3.377055
65	1	0	6.266777	-4.562048	-1.564526
66	7	0	1.955876	-0.687418	0.871149
67	7	0	0.810068	-0.144059	1.180272
68	6	0	2.907753	0.345346	0.574598
69	8	0	2.669068	1.532087	0.481656
70	8	0	4.107229	-0.217224	0.479190
71	6	0	-0.122939	-1.054092	1.689714
72	8	0	-1.218248	-0.657320	2.057832
73	8	0	0.276098	-2.329089	1.712959
74	6	0	-0.598763	-3.388169	2.203896
75	6	0	-1.024694	-3.110808	3.643452
76	6	0	-1.790311	-3.551697	1.267939
77	6	0	0.300904	-4.617645	2.146753
78	1	0	-0.148930	-2.865123	4.251450
79	1	0	-1.738326	-2.289284	3.696366
80	1	0	-1.485911	-4.012605	4.056225
81	1	0	-1.450852	-3.817403	0.263970
82	1	0	-2.438948	-4.347632	1.647724
83	1	0	-2.357902	-2.624840	1.195179
84	1	0	-0.259032	-5.504103	2.456161
85	1	0	0.664874	-4.771279	1.126857
86	1	0	1.160317	-4.494615	2.812094
87	6	0	5.275175	0.560881	0.087215
88	6	0	6.373071	-0.494313	0.045796
89	6	0	5.058615	1.162854	-1.297561
90	6	0	5.578591	1.622358	1.139991
91	1	0	6.517501	-0.931640	1.037397
92	1	0	6.091928	-1.290471	-0.649386
93	1	0	7.313465	-0.042774	-0.280955

94	1	0	4.245129	1.889944	-1.289599
95	1	0	5.975945	1.663642	-1.619836
96	1	0	4.830922	0.366824	-2.013204
97	1	0	6.543772	2.084688	0.914414
98	1	0	4.809936	2.395112	1.156143
99	1	0	5.643617	1.158272	2.128273

$TS5R_{exo}$

Total energy= -2314.83479111

Sum of electronic and zero-point Energies= -2314.007829

Sum of electronic and thermal Energies= -2313.959556

Sum of electronic and thermal Enthalpies= -2313.958612

Sum of electronic and thermal Free Energies= -2314.089461

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.988603	3.752386	-0.080883
2	6	0	-0.973070	4.908799	0.695983
3	6	0	-1.067185	6.156622	0.086349
4	6	0	-1.180868	6.220744	-1.301511
5	6	0	-1.192110	5.055859	-2.073284
6	6	0	-1.091930	3.805173	-1.466766
7	6	0	-0.852229	2.528217	0.792774
8	6	0	-1.069235	3.051561	2.250566
9	6	0	-0.823288	4.574203	2.159961
10	1	0	-1.058809	7.064834	0.681555
11	1	0	-1.263056	7.187118	-1.788874
12	1	0	-1.277788	5.127112	-3.152752
13	1	0	-1.080580	2.888363	-2.049463
14	1	0	-0.364755	2.555851	2.919528
15	1	0	-1.523664	5.109794	2.807406
16	1	0	0.127076	2.060123	0.710560
17	1	0	0.189383	4.808901	2.504904
18	6	0	-3.135003	1.615854	0.914508
19	6	0	-1.757027	0.379827	-0.234512
20	7	0	-3.859748	0.616369	0.501308
21	7	0	-1.850198	1.513578	0.470630
22	7	0	-2.986119	-0.141526	-0.227170
23	6	0	-3.423114	2.733519	1.863253
24	1	0	-3.515960	3.685960	1.324319
25	1	0	-4.343872	2.538314	2.412222
26	8	0	-2.353482	2.747159	2.790362

27	6	0	-3.451153	-1.306876	-0.926853
28	6	0	-3.912265	-2.389013	-0.169096
29	6	0	-3.415342	-1.304244	-2.324436
30	6	0	-4.319058	-3.523077	-0.868872
31	6	0	-3.836305	-2.465706	-2.971363
32	6	0	-4.284522	-3.581245	-2.263769
33	1	0	-4.669162	-4.385277	-0.306748
34	1	0	-3.815415	-2.494780	-4.057664
35	6	0	-3.972806	-2.330942	1.333699
36	1	0	-3.064074	-1.888493	1.752726
37	1	0	-4.819070	-1.718397	1.658715
38	1	0	-4.099702	-3.334891	1.743406
39	6	0	-4.755235	-4.814726	-2.988672
40	1	0	-4.526440	-5.717493	-2.417748
41	1	0	-5.839632	-4.782643	-3.135256
42	1	0	-4.289001	-4.897902	-3.972520
43	6	0	-2.945419	-0.109399	-3.114317
44	1	0	-3.302954	0.827399	-2.676321
45	1	0	-1.852336	-0.059184	-3.160293
46	1	0	-3.317534	-0.170437	-4.138154
47	6	0	2.171271	-1.271398	-1.161726
48	6	0	1.011689	-2.044403	-1.058287
49	1	0	2.106800	-0.320319	-1.671200
50	6	0	-0.247374	-1.497888	-0.886265
51	1	0	1.123891	-3.110656	-0.866391
52	1	0	-1.066012	-2.144199	-0.584263
53	6	0	-0.485827	-0.085875	-0.903732
54	8	0	0.207361	0.808531	-1.415904
55	6	0	3.502367	-1.898799	-1.079901
56	6	0	4.483501	-1.640268	-2.043240
57	6	0	3.803817	-2.767030	-0.024972
58	6	0	5.725696	-2.264709	-1.972790
59	1	0	4.263095	-0.955642	-2.857761
60	6	0	5.044842	-3.391501	0.047030
61	1	0	3.059599	-2.899965	0.753132
62	6	0	6.008711	-3.146221	-0.929810
63	1	0	6.475118	-2.064080	-2.732527
64	1	0	5.265948	-4.059375	0.874749
65	1	0	6.979071	-3.629517	-0.873067
66	7	0	1.959237	-0.279059	0.771672
67	7	0	0.734062	-0.204366	1.193564
68	6	0	2.473591	1.033495	0.563959
69	8	0	2.159581	1.989814	1.247970
70	8	0	3.434667	1.044125	-0.356634

71	6	0	0.205116	-1.340210	1.819030
72	8	0	-0.940124	-1.311505	2.244192
73	8	0	1.036536	-2.383680	1.931658
74	6	0	0.573486	-3.625567	2.546129
75	6	0	1.788061	-4.542760	2.451542
76	6	0	0.209846	-3.385614	4.008796
77	6	0	-0.587622	-4.210087	1.746343
78	1	0	2.038605	-4.747552	1.406834
79	1	0	2.652773	-4.082486	2.938424
80	1	0	1.571514	-5.492397	2.947283
81	1	0	-0.674170	-2.755735	4.097720
82	1	0	0.012497	-4.347317	4.490676
83	1	0	1.046643	-2.907512	4.525880
84	1	0	-0.834229	-5.198638	2.144631
85	1	0	-1.470979	-3.574471	1.806756
86	1	0	-0.299411	-4.329300	0.697136
87	6	0	4.040410	2.310939	-0.755643
88	6	0	2.961878	3.294376	-1.208636
89	6	0	4.897119	2.859452	0.379936
90	6	0	4.913089	1.906596	-1.937980
91	1	0	2.259560	2.788681	-1.878921
92	1	0	2.406150	3.703161	-0.364699
93	1	0	3.436012	4.115572	-1.753829
94	1	0	5.640087	2.115836	0.681799
95	1	0	5.424603	3.752926	0.033607
96	1	0	4.282339	3.123781	1.239923
97	1	0	5.483063	2.770141	-2.290150
98	1	0	5.608363	1.115739	-1.643924
99	1	0	4.292067	1.538152	-2.759790

TS5S$_{exo}$

Total energy= -2314.81490589
Sum of electronic and zero-point Energies= -2313.988234
Sum of electronic and thermal Energies= -2313.940040
Sum of electronic and thermal Enthalpies= -2313.939096
Sum of electronic and thermal Free Energies= -2314.070011

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.371582	-1.106007	-1.258340
2	6	0	5.694491	-1.528376	-1.171426
3	6	0	6.569514	-1.278360	-2.226007

4	6	0	6.095393	-0.603110	-3.348340
5	6	0	4.764626	-0.182176	-3.425572
6	6	0	3.885661	-0.433285	-2.375304
7	6	0	3.605484	-1.472596	-0.008496
8	6	0	4.695685	-1.998835	0.994434
9	6	0	5.959063	-2.237652	0.132614
10	1	0	7.605519	-1.598507	-2.172232
11	1	0	6.768936	-0.397555	-4.174017
12	1	0	4.415123	0.342525	-4.308353
13	1	0	2.848278	-0.107668	-2.429927
14	1	0	4.348846	-2.916120	1.469464
15	1	0	6.845112	-1.865722	0.656398
16	1	0	2.853427	-2.235168	-0.199779
17	1	0	6.107200	-3.309642	-0.029774
18	6	0	3.677062	0.654777	1.209390
19	6	0	1.766257	0.308570	0.203182
20	7	0	3.034508	1.777416	1.316586
21	7	0	2.936369	-0.278044	0.536617
22	7	0	1.852515	1.554494	0.668268
23	6	0	5.025719	0.247659	1.708327
24	1	0	5.787262	0.415173	0.933986
25	1	0	5.289631	0.824081	2.594695
26	8	0	4.930860	-1.112501	2.076777
27	6	0	0.959834	2.680669	0.531273
28	6	0	1.016557	3.420841	-0.653346
29	6	0	0.247189	3.085185	1.660959
30	6	0	0.255399	4.587597	-0.705720
31	6	0	-0.487661	4.264413	1.556232
32	6	0	-0.506137	5.019140	0.382287
33	1	0	0.271863	5.183096	-1.615179
34	1	0	-1.049356	4.606168	2.422332
35	6	0	1.886407	3.004285	-1.807858
36	1	0	2.892601	2.734548	-1.468764
37	1	0	1.451402	2.133291	-2.304548
38	1	0	1.977533	3.818213	-2.528559
39	6	0	-1.349710	6.262153	0.281783
40	1	0	-1.499160	6.720653	1.261850
41	1	0	-0.895097	6.998343	-0.385206
42	1	0	-2.338424	6.015695	-0.123502
43	6	0	0.310300	2.306685	2.943666
44	1	0	0.111334	1.246078	2.766609
45	1	0	1.304199	2.395263	3.395350
46	1	0	-0.422609	2.691212	3.655109
47	6	0	-1.747838	-1.715341	-1.557772

48	6	0	-0.716218	-2.355080	-0.865081
49	1	0	-1.498521	-0.863214	-2.173193
50	6	0	0.368920	-1.670301	-0.347264
51	1	0	-0.887260	-3.368291	-0.504186
52	1	0	0.968034	-2.157280	0.415022
53	6	0	0.645300	-0.293801	-0.627690
54	8	0	0.167705	0.429305	-1.508994
55	6	0	-2.984883	-2.439256	-1.904309
56	6	0	-3.523845	-2.364403	-3.193500
57	6	0	-3.643165	-3.211114	-0.941661
58	6	0	-4.669487	-3.081967	-3.522837
59	1	0	-3.036080	-1.740526	-3.937215
60	6	0	-4.790535	-3.927605	-1.268493
61	1	0	-3.258863	-3.196017	0.072539
62	6	0	-5.303183	-3.871715	-2.563464
63	1	0	-5.073282	-3.021831	-4.528946
64	1	0	-5.292951	-4.518583	-0.507847
65	1	0	-6.198953	-4.428040	-2.821173
66	7	0	-2.320441	-0.433708	0.026795
67	7	0	-1.380310	-0.127318	0.868557
68	6	0	-2.881059	0.658881	-0.680758
69	8	0	-3.239774	0.607748	-1.838521
70	8	0	-3.140684	1.674415	0.153071
71	6	0	-1.140444	-1.092058	1.860491
72	8	0	-0.251994	-0.923590	2.682838
73	8	0	-1.958157	-2.156249	1.848992
74	6	0	-1.814178	-3.194251	2.865297
75	6	0	-0.432148	-3.837594	2.783786
76	6	0	-2.107163	-2.616447	4.247152
77	6	0	-2.883996	-4.213772	2.488188
78	1	0	-0.231051	-4.155422	1.755417
79	1	0	0.347304	-3.148837	3.106662
80	1	0	-0.412671	-4.725521	3.422400
81	1	0	-3.091571	-2.139636	4.249271
82	1	0	-2.116493	-3.427467	4.980953
83	1	0	-1.353158	-1.885523	4.536310
84	1	0	-2.930815	-4.997321	3.248820
85	1	0	-3.863520	-3.731601	2.421148
86	1	0	-2.654137	-4.681255	1.526349
87	6	0	-3.999024	2.768171	-0.291121
88	6	0	-3.354524	3.515067	-1.455177
89	6	0	-5.388051	2.240377	-0.639892
90	6	0	-4.069884	3.660887	0.942289
91	1	0	-2.313895	3.748427	-1.210827

92	1	0	-3.378647	2.921234	-2.368018
93	1	0	-3.893897	4.452421	-1.624656
94	1	0	-5.790356	1.663352	0.197893
95	1	0	-6.054950	3.087486	-0.824804
96	1	0	-5.361204	1.611429	-1.529298
97	1	0	-4.696161	4.532963	0.735004
98	1	0	-4.498337	3.111948	1.785080
99	1	0	-3.068155	3.998703	1.218730

M5R$_{endo}$

Total energy= -2314.86850676

Sum of electronic and zero-point Energies= -2314.038542

Sum of electronic and thermal Energies= -2313.990593

Sum of electronic and thermal Enthalpies= -2313.989648

Sum of electronic and thermal Free Energies= -2314.118996

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.616100	-0.800329	1.214732
2	6	0	-5.941231	-1.122677	0.934286
3	6	0	-6.898347	-1.077187	1.945205
4	6	0	-6.504088	-0.704094	3.228335
5	6	0	-5.168888	-0.394593	3.504099
6	6	0	-4.208005	-0.445360	2.497240
7	6	0	-3.757439	-0.901582	-0.024652
8	6	0	-4.777935	-1.135689	-1.198545
9	6	0	-6.112663	-1.512764	-0.511752
10	1	0	-7.935339	-1.323279	1.736198
11	1	0	-7.240903	-0.656532	4.024171
12	1	0	-4.879594	-0.118510	4.513084
13	1	0	-3.156536	-0.247938	2.686272
14	1	0	-4.408832	-1.932684	-1.844177
15	1	0	-6.943802	-1.000205	-1.006188
16	1	0	-3.014167	-1.692985	0.043214
17	1	0	-6.296350	-2.588087	-0.604179
18	6	0	-3.577063	1.411785	-0.862138
19	6	0	-1.734395	0.673127	0.048105
20	7	0	-2.741223	2.401726	-0.976959
21	7	0	-3.002878	0.340964	-0.242371
22	7	0	-1.600204	1.926749	-0.391324
23	6	0	-4.948165	1.230954	-1.421504
24	1	0	-5.708771	1.275812	-0.629867

25	1	0	-5.156394	2.000095	-2.164804
26	8	0	-4.932628	-0.024325	-2.073059
27	6	0	-0.419447	2.747623	-0.412824
28	6	0	-0.203971	3.664297	0.619365
29	6	0	0.407984	2.646997	-1.535215
30	6	0	0.944615	4.450291	0.542312
31	6	0	1.539018	3.459856	-1.564407
32	6	0	1.826719	4.357489	-0.535315
33	1	0	1.143537	5.165255	1.337559
34	1	0	2.204707	3.394819	-2.421015
35	6	0	-1.177700	3.862080	1.753343
36	1	0	-1.977513	3.118723	1.758544
37	1	0	-0.661900	3.823026	2.716828
38	1	0	-1.645272	4.847548	1.671750
39	6	0	3.036960	5.252596	-0.608534
40	1	0	3.524855	5.336490	0.366229
41	1	0	3.765465	4.874057	-1.329110
42	1	0	2.749284	6.262050	-0.919529
43	6	0	0.040088	1.766870	-2.698283
44	1	0	-0.263803	0.769397	-2.374396
45	1	0	-0.796056	2.212246	-3.248903
46	1	0	0.890081	1.658965	-3.371870
47	6	0	1.702300	-1.088119	1.675295
48	6	0	1.162233	0.140432	2.376918
49	1	0	0.944829	-1.872868	1.807681
50	6	0	0.014842	0.606813	1.888486
51	1	0	1.682875	0.619709	3.199101
52	1	0	-0.482648	1.472941	2.312121
53	6	0	-0.750788	-0.233370	0.849874
54	8	0	-1.388505	-1.232812	1.383292
55	6	0	3.025002	-1.686021	2.103956
56	6	0	3.649923	-2.610524	1.259953
57	6	0	3.594578	-1.412605	3.344573
58	6	0	4.835477	-3.227274	1.639752
59	1	0	3.197637	-2.828903	0.294995
60	6	0	4.782306	-2.037000	3.729972
61	1	0	3.119188	-0.715800	4.026897
62	6	0	5.410272	-2.939883	2.879241
63	1	0	5.311656	-3.936569	0.969442
64	1	0	5.215191	-1.812000	4.699793
65	1	0	6.335582	-3.421737	3.178325
66	7	0	1.624904	-0.797167	0.232392
67	7	0	0.311263	-0.674730	-0.212242
68	6	0	2.538999	0.006453	-0.435207

69	8	0	2.413042	0.331580	-1.598101
70	8	0	3.567066	0.299688	0.362532
71	6	0	-0.112907	-1.525895	-1.203676
72	8	0	-1.247804	-1.469686	-1.655956
73	8	0	0.852371	-2.342815	-1.628531
74	6	0	0.759135	-2.967997	-2.941689
75	6	0	-0.333751	-4.030759	-2.946357
76	6	0	0.539734	-1.894058	-4.003286
77	6	0	2.135336	-3.603550	-3.101374
78	1	0	-0.163782	-4.746021	-2.136654
79	1	0	-1.316409	-3.576492	-2.821055
80	1	0	-0.307227	-4.572973	-3.896126
81	1	0	1.274736	-1.095053	-3.865809
82	1	0	0.671435	-2.332719	-4.996177
83	1	0	-0.463268	-1.470716	-3.933288
84	1	0	2.208078	-4.103152	-4.070743
85	1	0	2.911583	-2.835555	-3.038101
86	1	0	2.306795	-4.341547	-2.312846
87	6	0	4.862396	0.684461	-0.183775
88	6	0	5.318771	-0.327898	-1.229224
89	6	0	4.773940	2.098534	-0.743316
90	6	0	5.767270	0.628390	1.041041
91	1	0	5.303358	-1.334541	-0.799950
92	1	0	4.680833	-0.301620	-2.113183
93	1	0	6.344922	-0.094634	-1.526656
94	1	0	4.371966	2.773404	0.018223
95	1	0	5.771720	2.445732	-1.027558
96	1	0	4.120473	2.123994	-1.616520
97	1	0	6.784718	0.918795	0.766222
98	1	0	5.401797	1.311608	1.812751
99	1	0	5.779795	-0.386280	1.451394

M5S$_{endo}$

Total energy= -2314.86054869

Sum of electronic and zero-point Energies= -2314.030578

Sum of electronic and thermal Energies= -2313.982722

Sum of electronic and thermal Enthalpies= -2313.981778

Sum of electronic and thermal Free Energies= -2314.110666

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.315657	3.478426	-0.875311

2	6	0	0.216143	4.605099	-0.248571
3	6	0	0.332679	5.799898	-0.949934
4	6	0	-0.101546	5.849207	-2.274919
5	6	0	-0.648495	4.721992	-2.890034
6	6	0	-0.760281	3.520753	-2.190469
7	6	0	-0.311760	2.309369	0.086591
8	6	0	-0.158009	2.977559	1.485559
9	6	0	0.582534	4.294614	1.183654
10	1	0	0.740474	6.684931	-0.470913
11	1	0	-0.025516	6.778291	-2.830609
12	1	0	-0.994975	4.782265	-3.916343
13	1	0	-1.205406	2.647510	-2.660260
14	1	0	0.402004	2.319875	2.152219
15	1	0	0.288324	5.072903	1.892340
16	1	0	0.527535	1.636805	-0.085481
17	1	0	1.663205	4.140125	1.282791
18	6	0	-2.692820	2.075133	0.549050
19	6	0	-1.817293	0.287916	-0.355804
20	7	0	-3.686468	1.248447	0.420781
21	7	0	-1.544053	1.538967	0.042973
22	7	0	-3.129501	0.143029	-0.166163
23	6	0	-2.549394	3.360943	1.298349
24	1	0	-2.451306	4.213117	0.615265
25	1	0	-3.411551	3.515199	1.946796
26	8	0	-1.409670	3.205001	2.132260
27	6	0	-4.009040	-0.952069	-0.493443
28	6	0	-4.677343	-1.592228	0.550915
29	6	0	-4.232039	-1.256759	-1.840062
30	6	0	-5.586625	-2.594808	0.207389
31	6	0	-5.152250	-2.260495	-2.126190
32	6	0	-5.838669	-2.940969	-1.117710
33	1	0	-6.108887	-3.117337	1.005052
34	1	0	-5.337109	-2.519288	-3.166203
35	6	0	-4.440012	-1.231849	1.993503
36	1	0	-3.379463	-1.054185	2.184794
37	1	0	-4.985292	-0.321155	2.259489
38	1	0	-4.789527	-2.038708	2.640897
39	6	0	-6.839331	-4.012201	-1.466215
40	1	0	-7.742624	-3.573470	-1.901893
41	1	0	-6.427883	-4.708830	-2.201485
42	1	0	-7.134337	-4.580602	-0.581866
43	6	0	-3.480025	-0.571121	-2.946700
44	1	0	-3.379887	0.505329	-2.770571
45	1	0	-2.476839	-1.003490	-3.013529

46	1	0	-3.987625	-0.714496	-3.902144
47	6	0	1.665996	-1.821998	-1.251311
48	6	0	1.130730	-0.903589	-2.333510
49	1	0	0.906858	-2.598284	-1.095119
50	6	0	-0.042316	-0.331825	-2.061067
51	1	0	1.702452	-0.672257	-3.226655
52	1	0	-0.505347	0.386096	-2.733237
53	6	0	-0.826047	-0.813731	-0.821543
54	8	0	-1.390620	-1.960161	-0.930117
55	6	0	2.992976	-2.519246	-1.456392
56	6	0	3.670825	-3.042242	-0.350152
57	6	0	3.521353	-2.719218	-2.729005
58	6	0	4.867594	-3.728678	-0.514673
59	1	0	3.254796	-2.890670	0.642763
60	6	0	4.722077	-3.411090	-2.895476
61	1	0	3.000955	-2.344470	-3.604574
62	6	0	5.402208	-3.912447	-1.791375
63	1	0	5.385857	-4.122457	0.354394
64	1	0	5.123508	-3.554874	-3.893729
65	1	0	6.338472	-4.445707	-1.920903
66	7	0	1.596835	-1.029662	-0.003669
67	7	0	0.275337	-0.756363	0.352936
68	6	0	2.470418	0.027236	0.231341
69	8	0	2.281832	0.869553	1.091883
70	8	0	3.522070	-0.042245	-0.577498
71	6	0	-0.101046	-0.957004	1.652181
72	8	0	-1.214722	-0.649300	2.055331
73	8	0	0.878909	-1.460133	2.408772
74	6	0	0.812133	-1.341438	3.859579
75	6	0	0.667156	0.127320	4.247611
76	6	0	-0.310259	-2.210598	4.417497
77	6	0	2.172087	-1.873462	4.296428
78	1	0	1.466678	0.706685	3.775876
79	1	0	-0.299496	0.525410	3.933555
80	1	0	0.753501	0.226576	5.333266
81	1	0	-0.213912	-3.231082	4.036089
82	1	0	-0.233785	-2.241754	5.508420
83	1	0	-1.286878	-1.816790	4.137328
84	1	0	2.264839	-1.816711	5.383962
85	1	0	2.290230	-2.915754	3.987691
86	1	0	2.970226	-1.280231	3.841073
87	6	0	4.769418	0.653281	-0.274482
88	6	0	5.710560	0.108333	-1.341872
89	6	0	4.571255	2.156877	-0.425654

90	6	0	5.249196	0.263345	1.118991
91	1	0	5.785817	-0.980137	-1.254375
92	1	0	5.332824	0.350926	-2.339045
93	1	0	6.703449	0.549812	-1.223783
94	1	0	3.899820	2.539806	0.343376
95	1	0	5.538548	2.659699	-0.338419
96	1	0	4.153333	2.381076	-1.411309
97	1	0	6.242356	0.688149	1.288282
98	1	0	4.571725	0.636383	1.888597
99	1	0	5.319943	-0.826298	1.194511

$M5R_{exo}$

Total energy= -2314.87829507

Sum of electronic and zero-point Energies= -2314.048284

Sum of electronic and thermal Energies= -2314.000148

Sum of electronic and thermal Enthalpies= -2313.999204

Sum of electronic and thermal Free Energies= -2314.131349

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.758110	3.291071	-0.106467
2	6	0	-2.037415	4.492705	0.540587
3	6	0	-2.388502	5.617456	-0.200968
4	6	0	-2.455860	5.512058	-1.589357
5	6	0	-2.166839	4.304012	-2.229031
6	6	0	-1.807946	3.176089	-1.492358
7	6	0	-1.395431	2.215561	0.896009
8	6	0	-1.802020	2.830137	2.282612
9	6	0	-1.879278	4.351839	2.034096
10	1	0	-2.611707	6.558365	0.293429
11	1	0	-2.735293	6.379019	-2.179920
12	1	0	-2.219389	4.245265	-3.311646
13	1	0	-1.552471	2.226825	-1.957696
14	1	0	-1.062878	2.574172	3.042897
15	1	0	-2.703551	4.785374	2.608052
16	1	0	-0.330045	1.979420	0.856100
17	1	0	-0.955478	4.834309	2.371030
18	6	0	-3.475319	0.914758	0.995193
19	6	0	-1.832625	-0.171324	0.047718
20	7	0	-4.010047	-0.201631	0.604505
21	7	0	-2.151498	0.981249	0.662250
22	7	0	-2.971212	-0.862121	-0.003574

23	6	0	-4.018231	2.030168	1.826201
24	1	0	-4.251091	2.904772	1.204888
25	1	0	-4.919306	1.709586	2.348512
26	8	0	-3.026858	2.314421	2.796223
27	6	0	-3.236499	-2.110747	-0.664413
28	6	0	-3.338596	-3.266537	0.112593
29	6	0	-3.383399	-2.096057	-2.053281
30	6	0	-3.577420	-4.462951	-0.560543
31	6	0	-3.619375	-3.320489	-2.677723
32	6	0	-3.717801	-4.507797	-1.950164
33	1	0	-3.649792	-5.383115	0.013995
34	1	0	-3.727554	-3.345223	-3.759037
35	6	0	-3.173935	-3.208187	1.606631
36	1	0	-2.230633	-2.721962	1.874303
37	1	0	-3.981004	-2.624754	2.060618
38	1	0	-3.192407	-4.212676	2.032432
39	6	0	-3.999053	-5.813890	-2.646469
40	1	0	-3.495451	-6.643788	-2.145494
41	1	0	-5.072653	-6.028027	-2.640861
42	1	0	-3.671309	-5.785446	-3.687711
43	6	0	-3.261196	-0.813503	-2.832103
44	1	0	-3.948344	-0.056048	-2.439546
45	1	0	-2.246006	-0.404262	-2.755612
46	1	0	-3.499510	-0.982845	-3.883214
47	6	0	2.204770	-1.015963	-1.134349
48	6	0	1.163002	-2.115791	-1.175716
49	1	0	2.200689	-0.558777	-2.131329
50	6	0	-0.129816	-1.876304	-0.961603
51	1	0	1.521014	-3.104599	-1.446499
52	1	0	-0.869989	-2.663750	-1.046701
53	6	0	-0.485818	-0.417951	-0.642565
54	8	0	-0.382158	0.408421	-1.645833
55	6	0	3.606104	-1.544822	-0.874779
56	6	0	4.183717	-2.390193	-1.825949
57	6	0	4.339524	-1.202625	0.259894
58	6	0	5.465034	-2.899901	-1.639796
59	1	0	3.627001	-2.646745	-2.724651
60	6	0	5.624558	-1.711206	0.446688
61	1	0	3.894124	-0.544696	0.998877
62	6	0	6.190664	-2.562434	-0.498495
63	1	0	5.898515	-3.556398	-2.387738
64	1	0	6.183616	-1.438632	1.337197
65	1	0	7.190817	-2.957221	-0.351247
66	7	0	1.812946	0.050472	-0.180372

67	7	0	0.596985	-0.087607	0.455359
68	6	0	2.177123	1.364427	-0.416545
69	8	0	1.717450	2.317784	0.180980
70	8	0	3.151287	1.403495	-1.328089
71	6	0	0.559803	-0.818673	1.625840
72	8	0	-0.502040	-1.214591	2.082667
73	8	0	1.756568	-0.992091	2.179387
74	6	0	1.889022	-1.752161	3.423553
75	6	0	3.392149	-1.732219	3.674363
76	6	0	1.148381	-1.042782	4.552340
77	6	0	1.406171	-3.182797	3.207553
78	1	0	3.922086	-2.238641	2.863415
79	1	0	3.753593	-0.702019	3.741465
80	1	0	3.614352	-2.242879	4.614677
81	1	0	0.071713	-1.051973	4.385431
82	1	0	1.365991	-1.550550	5.496147
83	1	0	1.493085	-0.007756	4.632504
84	1	0	1.687666	-3.790387	4.072046
85	1	0	0.324209	-3.223712	3.082326
86	1	0	1.886956	-3.602308	2.318534
87	6	0	3.820987	2.657565	-1.652340
88	6	0	2.825034	3.641732	-2.256469
89	6	0	4.510043	3.210430	-0.409116
90	6	0	4.850167	2.222165	-2.688511
91	1	0	2.291232	3.167919	-3.085114
92	1	0	2.101254	3.976153	-1.513461
93	1	0	3.368021	4.508290	-2.644505
94	1	0	5.167811	2.449157	0.021116
95	1	0	5.119189	4.074204	-0.689171
96	1	0	3.778975	3.519400	0.338314
97	1	0	5.448781	3.081194	-3.001646
98	1	0	5.513981	1.462965	-2.265689
99	1	0	4.352383	1.801541	-3.566224

M5S$_{exo}$

Total energy= -2314.86906292
Sum of electronic and zero-point Energies= -2314.038564
Sum of electronic and thermal Energies= -2313.991043
Sum of electronic and thermal Enthalpies= -2313.990099
Sum of electronic and thermal Free Energies= -2314.118374

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

1	6	0	-4.422972	-1.371855	0.473118
2	6	0	-5.728913	-1.784525	0.217723
3	6	0	-6.628420	-1.935232	1.269230
4	6	0	-6.197125	-1.660487	2.565863
5	6	0	-4.884395	-1.249521	2.811179
6	6	0	-3.976615	-1.104637	1.763425
7	6	0	-3.637894	-1.265273	-0.819034
8	6	0	-4.734394	-1.344642	-1.938156
9	6	0	-5.945121	-2.015679	-1.256992
10	1	0	-7.650072	-2.252250	1.082062
11	1	0	-6.890394	-1.765984	3.394464
12	1	0	-4.568110	-1.044902	3.829008
13	1	0	-2.939935	-0.816613	1.919950
14	1	0	-4.371690	-1.915076	-2.794133
15	1	0	-6.876187	-1.587911	-1.639375
16	1	0	-2.900427	-2.063213	-0.907374
17	1	0	-5.958300	-3.087201	-1.483486
18	6	0	-3.668391	1.164872	-1.085215
19	6	0	-1.672067	0.381023	-0.620198
20	7	0	-2.937266	2.219610	-0.900775
21	7	0	-2.940882	0.022688	-0.908490
22	7	0	-1.695515	1.714978	-0.599927
23	6	0	-5.079386	1.002209	-1.552078
24	1	0	-5.755487	0.813576	-0.708508
25	1	0	-5.406518	1.897491	-2.080525
26	8	0	-5.066582	-0.069679	-2.478540
27	6	0	-0.681386	2.652138	-0.197885
28	6	0	-0.334807	2.688230	1.154313
29	6	0	-0.189064	3.553628	-1.146472
30	6	0	0.600617	3.648254	1.540663
31	6	0	0.751434	4.482074	-0.707270
32	6	0	1.167926	4.533688	0.624729
33	1	0	0.879911	3.717140	2.587564
34	1	0	1.166414	5.185534	-1.425482
35	6	0	-0.979025	1.759084	2.147574
36	1	0	-2.069722	1.773886	2.039023
37	1	0	-0.644871	0.724974	2.001808
38	1	0	-0.740961	2.068774	3.166789
39	6	0	2.220486	5.519487	1.059581
40	1	0	2.135361	6.459983	0.509973
41	1	0	2.146136	5.732715	2.128246
42	1	0	3.221257	5.116354	0.870365
43	6	0	-0.676204	3.548996	-2.569565

44	1	0	-0.695223	2.532278	-2.967180
45	1	0	-1.688486	3.959634	-2.630695
46	1	0	-0.020756	4.159421	-3.194259
47	6	0	1.465640	-2.541844	-0.201182
48	6	0	0.530432	-2.534757	-1.390356
49	1	0	1.035953	-3.217291	0.548879
50	6	0	-0.492612	-1.689636	-1.465616
51	1	0	0.730707	-3.265537	-2.168088
52	1	0	-1.161251	-1.671229	-2.322478
53	6	0	-0.662830	-0.737396	-0.266969
54	8	0	-1.075677	-1.315533	0.829497
55	6	0	2.842800	-3.075050	-0.573486
56	6	0	2.949309	-4.388287	-1.039465
57	6	0	3.998887	-2.305161	-0.458237
58	6	0	4.183898	-4.917045	-1.402836
59	1	0	2.056982	-5.006262	-1.111694
60	6	0	5.237127	-2.834036	-0.821060
61	1	0	3.920075	-1.285772	-0.094472
62	6	0	5.334821	-4.138078	-1.297905
63	1	0	4.248001	-5.938895	-1.763392
64	1	0	6.130583	-2.223210	-0.725965
65	1	0	6.299639	-4.547548	-1.579568
66	7	0	1.540167	-1.209460	0.440877
67	7	0	0.775117	-0.178788	-0.089998
68	6	0	1.876038	-1.212478	1.776294
69	8	0	2.230191	-2.236770	2.331947
70	8	0	1.862818	0.007228	2.321278
71	6	0	1.340453	0.447389	-1.199769
72	8	0	0.658123	0.841899	-2.126918
73	8	0	2.659599	0.582984	-1.089131
74	6	0	3.443130	1.079971	-2.221698
75	6	0	3.280204	0.125718	-3.400120
76	6	0	3.048199	2.514136	-2.558242
77	6	0	4.872559	1.040725	-1.694374
78	1	0	3.502557	-0.896131	-3.075177
79	1	0	2.267122	0.163242	-3.801784
80	1	0	3.984859	0.401590	-4.189634
81	1	0	3.111478	3.138012	-1.661758
82	1	0	3.745182	2.907108	-3.304107
83	1	0	2.033792	2.565661	-2.953900
84	1	0	5.551214	1.458942	-2.441872
85	1	0	4.953843	1.629886	-0.776885
86	1	0	5.177841	0.012599	-1.485768
87	6	0	2.478083	0.186830	3.635527

88	6	0	1.689919	-0.569544	4.700434
89	6	0	3.948295	-0.224451	3.587262
90	6	0	2.371580	1.687249	3.869357
91	1	0	0.630542	-0.304034	4.633288
92	1	0	1.796504	-1.646720	4.579775
93	1	0	2.055007	-0.280255	5.690267
94	1	0	4.452143	0.299471	2.768958
95	1	0	4.430245	0.062942	4.525922
96	1	0	4.059410	-1.298968	3.447843
97	1	0	2.868228	1.949117	4.807088
98	1	0	2.843616	2.237729	3.050750
99	1	0	1.323378	1.986226	3.936097

$TS6R_{endo}$

Total energy= -2314.85030339

Sum of electronic and zero-point Energies= -2314.022100

Sum of electronic and thermal Energies= -2313.974136

Sum of electronic and thermal Enthalpies= -2313.973192

Sum of electronic and thermal Free Energies= -2314.105151

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.678292	-0.518530	1.208796
2	6	0	-5.969949	-0.977744	0.962739
3	6	0	-6.981551	-0.746319	1.891253
4	6	0	-6.676758	-0.048159	3.058779
5	6	0	-5.377682	0.405981	3.300650
6	6	0	-4.363221	0.169817	2.374986
7	6	0	-3.749629	-0.874931	0.069786
8	6	0	-4.707588	-1.367147	-1.070315
9	6	0	-6.037705	-1.705513	-0.357698
10	1	0	-7.992846	-1.097268	1.707120
11	1	0	-7.456902	0.144243	3.788652
12	1	0	-5.158232	0.943427	4.217641
13	1	0	-3.341351	0.492424	2.554290
14	1	0	-4.273897	-2.235695	-1.567777
15	1	0	-6.885004	-1.404043	-0.980881
16	1	0	-3.041481	-1.652800	0.347100
17	1	0	-6.118261	-2.786378	-0.199174
18	6	0	-3.568548	1.233139	-1.153162
19	6	0	-1.705983	0.672818	-0.069473
20	7	0	-2.761081	2.220657	-1.390505

21	7	0	-2.973407	0.283845	-0.367787
22	7	0	-1.626091	1.854024	-0.701390
23	6	0	-4.926276	0.932568	-1.694960
24	1	0	-5.703027	1.106582	-0.937973
25	1	0	-5.134896	1.551790	-2.567421
26	8	0	-4.896575	-0.419764	-2.116257
27	6	0	-0.499458	2.737656	-0.745860
28	6	0	-0.307248	3.660685	0.284647
29	6	0	0.311160	2.692640	-1.885498
30	6	0	0.786016	4.522143	0.179318
31	6	0	1.373395	3.590075	-1.953788
32	6	0	1.636912	4.496605	-0.924135
33	1	0	0.963776	5.243067	0.974868
34	1	0	2.012027	3.581521	-2.833556
35	6	0	-1.262748	3.795550	1.442504
36	1	0	-1.950298	2.950590	1.516028
37	1	0	-0.717295	3.887486	2.385293
38	1	0	-1.867157	4.700371	1.323661
39	6	0	2.825695	5.422069	-0.994610
40	1	0	3.650306	5.033127	-0.380577
41	1	0	3.185173	5.519773	-2.025181
42	1	0	2.571140	6.417697	-0.612380
43	6	0	-0.001675	1.738809	-3.007593
44	1	0	-0.131476	0.722869	-2.625740
45	1	0	-0.924909	2.035489	-3.513918
46	1	0	0.812027	1.727280	-3.735401
47	6	0	2.014035	-0.866970	2.003884
48	6	0	1.318178	0.377120	2.520288
49	1	0	1.489625	-1.731262	2.435123
50	6	0	0.074165	0.572816	2.083401
51	1	0	1.793105	1.060965	3.215736
52	1	0	-0.543252	1.399077	2.414890
53	6	0	-0.623400	-0.503149	1.282756
54	8	0	-1.518557	-1.165541	1.819614
55	6	0	3.481429	-1.099264	2.303422
56	6	0	4.123149	-2.164454	1.662011
57	6	0	4.181488	-0.359034	3.250721
58	6	0	5.446789	-2.470651	1.951723
59	1	0	3.571976	-2.743821	0.923847
60	6	0	5.509851	-0.670586	3.547844
61	1	0	3.706809	0.465520	3.771024
62	6	0	6.147428	-1.722193	2.899717
63	1	0	5.932704	-3.297868	1.442617
64	1	0	6.043444	-0.084271	4.289143

65	1	0	7.180493	-1.961335	3.130411
66	7	0	1.672707	-0.959646	0.572647
67	7	0	0.315149	-1.193249	0.392366
68	6	0	2.286125	-0.201721	-0.422206
69	8	0	1.852456	-0.126881	-1.552484
70	8	0	3.413971	0.340227	0.032165
71	6	0	-0.094441	-2.124644	-0.541293
72	8	0	-1.244805	-2.206535	-0.924953
73	8	0	0.927293	-2.876489	-0.952346
74	6	0	0.812539	-3.657159	-2.180262
75	6	0	-0.171540	-4.804831	-1.982417
76	6	0	0.424531	-2.742785	-3.338141
77	6	0	2.229748	-4.185370	-2.366222
78	1	0	0.115031	-5.399737	-1.110530
79	1	0	-1.184198	-4.427768	-1.841744
80	1	0	-0.150526	-5.452659	-2.863569
81	1	0	1.084061	-1.870351	-3.349822
82	1	0	0.534958	-3.288634	-4.279571
83	1	0	-0.608628	-2.405452	-3.245751
84	1	0	2.283446	-4.801767	-3.266993
85	1	0	2.931677	-3.352591	-2.464188
86	1	0	2.524286	-4.793285	-1.506450
87	6	0	4.530332	0.610839	-0.874550
88	6	0	4.857886	-0.647942	-1.670940
89	6	0	4.192727	1.787675	-1.778899
90	6	0	5.661120	0.956352	0.085227
91	1	0	5.051628	-1.482295	-0.989809
92	1	0	4.039201	-0.908755	-2.343800
93	1	0	5.757864	-0.470995	-2.266103
94	1	0	3.900438	2.650994	-1.174670
95	1	0	5.073516	2.056342	-2.369524
96	1	0	3.368652	1.534163	-2.447439
97	1	0	6.567728	1.188596	-0.479460
98	1	0	5.390579	1.825462	0.690572
99	1	0	5.860716	0.113059	0.753573

TS6S$_{endo}$

Total energy= -2314.84693059
Sum of electronic and zero-point Energies= -2314.019784
Sum of electronic and thermal Energies= -2313.971597
Sum of electronic and thermal Enthalpies= -2313.970652
Sum of electronic and thermal Free Energies= -2314.101855

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.062425	3.706322	0.168739
2	6	0	-0.534508	4.725602	-0.570588
3	6	0	-0.609382	6.012428	-0.045647
4	6	0	-0.068094	6.259301	1.215420
5	6	0	0.548758	5.237813	1.941015
6	6	0	0.619561	3.947686	1.418558
7	6	0	0.014170	2.398524	-0.592273
8	6	0	-0.335008	2.829001	-2.057457
9	6	0	-1.002364	4.213796	-1.912143
10	1	0	-1.068498	6.815667	-0.614241
11	1	0	-0.114088	7.260195	1.632499
12	1	0	0.980835	5.450937	2.913160
13	1	0	1.120278	3.153044	1.965685
14	1	0	-0.987874	2.084490	-2.512817
15	1	0	-0.710788	4.858209	-2.746240
16	1	0	-0.756431	1.734106	-0.195499
17	1	0	-2.093301	4.117857	-1.939497
18	6	0	2.328844	2.163847	-1.303789
19	6	0	1.700133	0.649585	0.204746
20	7	0	3.406418	1.484688	-1.067540
21	7	0	1.282813	1.691936	-0.556679
22	7	0	2.997014	0.561837	-0.128763
23	6	0	2.029197	3.236130	-2.298535
24	1	0	1.975244	4.221047	-1.815850
25	1	0	2.793832	3.261366	-3.074979
26	8	0	0.801834	2.879607	-2.913693
27	6	0	3.993111	-0.336907	0.383037
28	6	0	4.568950	-1.258565	-0.494226
29	6	0	4.408915	-0.195169	1.710170
30	6	0	5.566005	-2.092620	0.013459
31	6	0	5.411901	-1.047808	2.166431
32	6	0	5.993741	-2.008089	1.337279
33	1	0	6.021946	-2.823873	-0.650090
34	1	0	5.751148	-0.955322	3.195601
35	6	0	4.177496	-1.332991	-1.945930
36	1	0	3.115532	-1.124506	-2.077689
37	1	0	4.748371	-0.607662	-2.534018
38	1	0	4.384261	-2.330991	-2.339542
39	6	0	7.050700	-2.941380	1.869648
40	1	0	7.673444	-2.446224	2.618814
41	1	0	6.591199	-3.812569	2.347831

42	1	0	7.697205	-3.306389	1.068349
43	6	0	3.796338	0.832957	2.622122
44	1	0	3.670927	1.795345	2.116030
45	1	0	2.812619	0.482858	2.948216
46	1	0	4.423988	0.985072	3.502456
47	6	0	-1.957924	-1.228579	1.879111
48	6	0	-1.367994	-0.008390	2.560084
49	1	0	-1.430773	-2.105871	2.279241
50	6	0	-0.104402	0.282605	2.247742
51	1	0	-1.930837	0.584099	3.273302
52	1	0	0.432336	1.106070	2.706384
53	6	0	0.728871	-0.673354	1.413269
54	8	0	1.600733	-1.342922	1.973542
55	6	0	-3.433454	-1.543403	2.021550
56	6	0	-3.973931	-2.542386	1.204327
57	6	0	-4.240420	-0.944212	2.983493
58	6	0	-5.304220	-2.919929	1.335759
59	1	0	-3.338087	-3.009952	0.455364
60	6	0	-5.575731	-1.328703	3.121152
61	1	0	-3.844769	-0.176574	3.639475
62	6	0	-6.112971	-2.311803	2.298034
63	1	0	-5.711691	-3.690970	0.689203
64	1	0	-6.193907	-0.852028	3.875298
65	1	0	-7.151848	-2.606714	2.404271
66	7	0	-1.489363	-1.174699	0.482020
67	7	0	-0.115763	-1.343357	0.397850
68	6	0	-2.055794	-0.367678	-0.492720
69	8	0	-1.543910	-0.179755	-1.580550
70	8	0	-3.215028	0.127561	-0.065476
71	6	0	0.400994	-2.252749	-0.502988
72	8	0	1.582920	-2.312104	-0.765382
73	8	0	-0.569616	-3.004672	-1.032276
74	6	0	-0.316100	-3.778694	-2.240414
75	6	0	0.206500	-2.863752	-3.343990
76	6	0	0.634928	-4.930955	-1.936047
77	6	0	-1.704845	-4.299143	-2.591986
78	1	0	-0.428596	-1.975558	-3.411237
79	1	0	1.233208	-2.553658	-3.146471
80	1	0	0.174989	-3.396103	-4.298633
81	1	0	0.245405	-5.530263	-1.108181
82	1	0	0.717466	-5.573544	-2.817481
83	1	0	1.624692	-4.557583	-1.672649
84	1	0	-1.657839	-4.914969	-3.493540
85	1	0	-2.101051	-4.905671	-1.772826

86	1	0	-2.385862	-3.461708	-2.769949
87	6	0	-4.269417	0.529292	-0.995148
88	6	0	-5.464896	0.727037	-0.072446
89	6	0	-3.878615	1.833811	-1.675416
90	6	0	-4.534580	-0.592301	-1.992265
91	1	0	-5.694733	-0.205905	0.450382
92	1	0	-5.247550	1.499263	0.670781
93	1	0	-6.335664	1.036154	-0.656317
94	1	0	-3.057892	1.673657	-2.375379
95	1	0	-4.736043	2.233271	-2.224344
96	1	0	-3.580079	2.568231	-0.920203
97	1	0	-5.396959	-0.325671	-2.609008
98	1	0	-3.674558	-0.754060	-2.644242
99	1	0	-4.763847	-1.518225	-1.455768

$TS6R_{exo}$

Total energy= -2314.84138949

Sum of electronic and zero-point Energies= -2314.013669

Sum of electronic and thermal Energies= -2313.965217

Sum of electronic and thermal Enthalpies= -2313.964273

Sum of electronic and thermal Free Energies= -2314.099406

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.108566	3.292633	-0.557661
2	6	0	-2.240385	4.542553	0.039267
3	6	0	-2.917535	5.562480	-0.625770
4	6	0	-3.454365	5.304019	-1.885310
5	6	0	-3.314472	4.045863	-2.479148
6	6	0	-2.635562	3.025662	-1.816801
7	6	0	-1.353706	2.332128	0.331177
8	6	0	-1.187022	3.102673	1.690222
9	6	0	-1.568579	4.573574	1.389211
10	1	0	-3.031177	6.541459	-0.169303
11	1	0	-3.988203	6.088680	-2.412197
12	1	0	-3.737371	3.866425	-3.462430
13	1	0	-2.506497	2.042457	-2.263332
14	1	0	-0.154981	3.015653	2.034895
15	1	0	-2.213267	4.962536	2.184094
16	1	0	-0.377829	2.073116	-0.088139
17	1	0	-0.672217	5.201389	1.365232
18	6	0	-3.120141	1.017224	1.434273

19	6	0	-2.084991	-0.031323	-0.254238
20	7	0	-3.765767	-0.101352	1.322747
21	7	0	-2.103924	1.093269	0.517238
22	7	0	-3.110126	-0.720348	0.273080
23	6	0	-3.264726	2.148331	2.398060
24	1	0	-3.832083	2.974708	1.945790
25	1	0	-3.775109	1.824673	3.305376
26	8	0	-1.956037	2.558856	2.757515
27	6	0	-3.553047	-1.995975	-0.196365
28	6	0	-3.548982	-3.087734	0.679785
29	6	0	-3.963751	-2.110470	-1.530431
30	6	0	-3.981677	-4.317784	0.186146
31	6	0	-4.377068	-3.366331	-1.977639
32	6	0	-4.399849	-4.477297	-1.135284
33	1	0	-3.978956	-5.178161	0.851381
34	1	0	-4.698197	-3.474010	-3.011035
35	6	0	-3.057864	-2.954114	2.096950
36	1	0	-2.069447	-2.484660	2.106476
37	1	0	-3.726363	-2.328344	2.693172
38	1	0	-2.986207	-3.937090	2.566659
39	6	0	-4.886667	-5.814483	-1.632024
40	1	0	-4.367403	-6.634471	-1.130231
41	1	0	-5.957337	-5.934610	-1.436460
42	1	0	-4.734140	-5.916210	-2.708951
43	6	0	-3.962876	-0.929411	-2.468103
44	1	0	-4.423603	-0.053556	-2.000915
45	1	0	-2.943578	-0.640508	-2.743945
46	1	0	-4.516500	-1.169811	-3.377730
47	6	0	2.535598	-1.239908	-1.529702
48	6	0	1.342037	-2.090920	-1.937174
49	1	0	3.019132	-0.923921	-2.462981
50	6	0	0.092401	-1.624634	-2.000221
51	1	0	1.576850	-3.105299	-2.244985
52	1	0	-0.751603	-2.198266	-2.365168
53	6	0	-0.042086	-0.194308	-1.612263
54	8	0	-0.269396	0.723927	-2.363067
55	6	0	3.580309	-2.021121	-0.736555
56	6	0	4.183167	-3.134532	-1.327876
57	6	0	3.996195	-1.621500	0.532238
58	6	0	5.171379	-3.846505	-0.655146
59	1	0	3.891190	-3.441966	-2.329203
60	6	0	4.988358	-2.333270	1.206091
61	1	0	3.541003	-0.753024	0.998169
62	6	0	5.577225	-3.448102	0.617338

63	1	0	5.630421	-4.708208	-1.128905
64	1	0	5.300907	-2.008986	2.194550
65	1	0	6.351702	-3.998759	1.141053
66	7	0	2.095996	-0.004972	-0.846431
67	7	0	0.777715	0.059034	-0.404772
68	6	0	2.831918	1.163880	-0.818847
69	8	0	2.442871	2.201756	-0.330519
70	8	0	4.023638	0.932429	-1.378690
71	6	0	0.566276	-0.654863	0.806705
72	8	0	-0.234741	-1.544355	0.960932
73	8	0	1.357776	-0.139558	1.743633
74	6	0	1.244074	-0.591469	3.134277
75	6	0	2.305982	0.245844	3.835891
76	6	0	-0.147925	-0.252523	3.658307
77	6	0	1.562948	-2.077954	3.254049
78	1	0	3.296348	0.032665	3.421827
79	1	0	2.095790	1.310990	3.708928
80	1	0	2.316479	0.012920	4.903304
81	1	0	-0.912357	-0.869590	3.182219
82	1	0	-0.176408	-0.433520	4.736570
83	1	0	-0.385195	0.799613	3.475590
84	1	0	1.606652	-2.341686	4.314549
85	1	0	0.800051	-2.688800	2.771807
86	1	0	2.535213	-2.297013	2.803984
87	6	0	5.121325	1.882871	-1.215224
88	6	0	4.795489	3.187515	-1.932582
89	6	0	5.402204	2.085220	0.269947
90	6	0	6.282820	1.162507	-1.888302
91	1	0	4.531556	2.985218	-2.974326
92	1	0	3.967386	3.703848	-1.447310
93	1	0	5.677776	3.833644	-1.920251
94	1	0	5.580259	1.117610	0.749429
95	1	0	6.300246	2.698223	0.385267
96	1	0	4.568748	2.584992	0.764888
97	1	0	7.187213	1.772308	-1.822866
98	1	0	6.465710	0.202460	-1.397106
99	1	0	6.058068	0.980325	-2.942490

TS6S$_{exo}$

Total energy= -2314.83835992

Sum of electronic and zero-point Energies= -2314.010501

Sum of electronic and thermal Energies= -2313.962525

Sum of electronic and thermal Enthalpies= -2313.961581

Sum of electronic and thermal Free Energies= -2314.093798

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.552845	-1.633543	0.275065
2	6	0	-5.870040	-2.045567	0.095779
3	6	0	-6.640831	-2.410611	1.197208
4	6	0	-6.069722	-2.351892	2.466767
5	6	0	-4.745908	-1.937089	2.637175
6	6	0	-3.971620	-1.572773	1.537673
7	6	0	-3.908125	-1.261296	-1.043214
8	6	0	-5.097308	-1.277484	-2.073746
9	6	0	-6.251906	-2.023209	-1.362836
10	1	0	-7.671365	-2.728948	1.070133
11	1	0	-6.660489	-2.628369	3.334366
12	1	0	-4.319108	-1.897785	3.634179
13	1	0	-2.937220	-1.256605	1.652304
14	1	0	-4.795049	-1.785331	-2.990253
15	1	0	-7.200729	-1.512965	-1.555739
16	1	0	-3.135377	-1.978747	-1.328236
17	1	0	-6.346196	-3.040332	-1.757219
18	6	0	-4.077601	1.176964	-1.037210
19	6	0	-2.014494	0.384892	-0.621697
20	7	0	-3.389916	2.236897	-0.756224
21	7	0	-3.292573	0.055326	-0.974916
22	7	0	-2.130569	1.720976	-0.500635
23	6	0	-5.492660	1.004063	-1.481844
24	1	0	-6.135090	0.704173	-0.641814
25	1	0	-5.880347	1.928129	-1.910602
26	8	0	-5.480644	0.021292	-2.504462
27	6	0	-1.131282	2.625101	-0.019978
28	6	0	-0.696470	2.512382	1.301965
29	6	0	-0.673452	3.631618	-0.879253
30	6	0	0.237937	3.449216	1.755564
31	6	0	0.238927	4.551630	-0.374040
32	6	0	0.712663	4.471325	0.938829
33	1	0	0.582408	3.386077	2.784927
34	1	0	0.609040	5.338460	-1.028418
35	6	0	-1.209302	1.440077	2.227171
36	1	0	-2.257522	1.203179	2.024087
37	1	0	-0.632630	0.515023	2.110125
38	1	0	-1.128391	1.772891	3.264945
39	6	0	1.729985	5.463266	1.441744

40	1	0	1.413764	6.490309	1.238796
41	1	0	1.887839	5.358126	2.517281
42	1	0	2.694544	5.315902	0.944395
43	6	0	-1.135689	3.686324	-2.309665
44	1	0	-0.990623	2.708730	-2.780766
45	1	0	-2.199185	3.930767	-2.375525
46	1	0	-0.568368	4.434700	-2.867218
47	6	0	2.124912	-2.539682	-0.451526
48	6	0	1.003111	-2.629336	-1.470511
49	1	0	2.014899	-3.404103	0.218055
50	6	0	-0.176106	-2.033133	-1.287191
51	1	0	1.185794	-3.252927	-2.339335
52	1	0	-1.011563	-2.126334	-1.968062
53	6	0	-0.244072	-1.256904	-0.013148
54	8	0	-0.751088	-1.641850	1.013170
55	6	0	3.510645	-2.650336	-1.079169
56	6	0	3.785803	-3.721037	-1.935223
57	6	0	4.533406	-1.756653	-0.769394
58	6	0	5.049201	-3.875761	-2.497088
59	1	0	3.013900	-4.453059	-2.157908
60	6	0	5.801253	-1.913761	-1.328503
61	1	0	4.331223	-0.925579	-0.102683
62	6	0	6.062616	-2.967796	-2.198589
63	1	0	5.242736	-4.710104	-3.163626
64	1	0	6.588633	-1.208708	-1.078056
65	1	0	7.049427	-3.087308	-2.633765
66	7	0	1.974922	-1.340295	0.408909
67	7	0	0.980768	-0.415869	0.076093
68	6	0	2.425059	-1.425933	1.713082
69	8	0	3.068139	-2.387816	2.089570
70	8	0	2.119214	-0.342250	2.418236
71	6	0	1.331370	0.444238	-0.990273
72	8	0	0.550972	0.808537	-1.837532
73	8	0	2.610921	0.800403	-0.889864
74	6	0	3.250463	1.553394	-1.974225
75	6	0	3.235767	0.710418	-3.244939
76	6	0	2.579743	2.909003	-2.160632
77	6	0	4.674114	1.750111	-1.467320
78	1	0	3.690023	-0.266217	-3.050529
79	1	0	2.217334	0.569832	-3.610061
80	1	0	3.818223	1.217508	-4.019233
81	1	0	2.523379	3.430381	-1.201316
82	1	0	3.184192	3.508536	-2.847676
83	1	0	1.572608	2.808455	-2.564401

84	1	0	5.234295	2.357644	-2.182512
85	1	0	4.664127	2.264870	-0.502594
86	1	0	5.183238	0.791280	-1.355153
87	6	0	2.593013	-0.216327	3.795909
88	6	0	1.963977	-1.303387	4.659934
89	6	0	4.117894	-0.241784	3.833817
90	6	0	2.077574	1.158574	4.200174
91	1	0	0.876102	-1.282561	4.546674
92	1	0	2.335049	-2.290057	4.382897
93	1	0	2.206293	-1.114127	5.709369
94	1	0	4.519547	0.492930	3.129518
95	1	0	4.453376	0.027676	4.839137
96	1	0	4.506607	-1.228234	3.584249
97	1	0	2.375174	1.379322	5.228263
98	1	0	2.489965	1.925564	3.539124
99	1	0	0.986964	1.188358	4.134489

M6R$_{endo}$

Total energy= -2314.86751560

Sum of electronic and zero-point Energies= -2314.039385

Sum of electronic and thermal Energies= -2313.989985

Sum of electronic and thermal Enthalpies= -2313.989040

Sum of electronic and thermal Free Energies= -2314.126132

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.374969	-0.748122	1.120528
2	6	0	-5.606184	-1.349945	0.878185
3	6	0	-6.603758	-1.310536	1.849812
4	6	0	-6.345373	-0.657805	3.053851
5	6	0	-5.106701	-0.053376	3.288814
6	6	0	-4.108415	-0.094966	2.318735
7	6	0	-3.443714	-0.896373	-0.060991
8	6	0	-4.354933	-1.475501	-1.200344
9	6	0	-5.634227	-1.984148	-0.490514
10	1	0	-7.570461	-1.772677	1.671182
11	1	0	-7.116162	-0.613297	3.817127
12	1	0	-4.925679	0.450416	4.232990
13	1	0	-3.135223	0.362305	2.477639
14	1	0	-3.834126	-2.283431	-1.716355
15	1	0	-6.519012	-1.713987	-1.075725
16	1	0	-2.624281	-1.581363	0.161820

17	1	0	-5.618035	-3.076448	-0.414053
18	6	0	-3.600911	1.268132	-1.182623
19	6	0	-1.688236	0.948402	-0.022255
20	7	0	-2.977038	2.395299	-1.311957
21	7	0	-2.866138	0.383939	-0.440036
22	7	0	-1.815336	2.172344	-0.590401
23	6	0	-4.885376	0.783308	-1.769674
24	1	0	-5.693917	0.813444	-1.024902
25	1	0	-5.173476	1.390449	-2.628081
26	8	0	-4.653426	-0.537797	-2.228801
27	6	0	-0.873317	3.244154	-0.512675
28	6	0	-0.590998	3.818145	0.730824
29	6	0	-0.294281	3.714112	-1.696956
30	6	0	0.307156	4.886041	0.766794
31	6	0	0.575638	4.799797	-1.614098
32	6	0	0.894680	5.393040	-0.392418
33	1	0	0.539311	5.342816	1.726239
34	1	0	1.036380	5.174080	-2.525963
35	6	0	-1.242408	3.310378	1.989707
36	1	0	-0.925039	2.286017	2.200392
37	1	0	-0.987451	3.947489	2.838524
38	1	0	-2.331841	3.287256	1.883159
39	6	0	1.888738	6.523735	-0.323471
40	1	0	2.908643	6.133197	-0.238804
41	1	0	1.847154	7.143611	-1.222036
42	1	0	1.705131	7.160151	0.545288
43	6	0	-0.567573	3.034935	-3.012998
44	1	0	-0.483860	1.948337	-2.902823
45	1	0	-1.579211	3.245688	-3.368698
46	1	0	0.148301	3.366347	-3.768141
47	6	0	2.582353	-1.419295	1.948230
48	6	0	1.814316	-0.456831	2.828658
49	1	0	2.405879	-2.430399	2.343213
50	6	0	0.489898	-0.410592	2.662787
51	1	0	2.303252	0.139761	3.591145
52	1	0	-0.164384	0.205835	3.267774
53	6	0	-0.216249	-1.367938	1.765291
54	8	0	-1.351819	-1.727823	1.977931
55	6	0	4.089717	-1.282880	1.829812
56	6	0	4.743378	-2.025731	0.841363
57	6	0	4.842946	-0.505918	2.704534
58	6	0	6.126630	-1.977057	0.721063
59	1	0	4.151482	-2.629627	0.157736
60	6	0	6.233416	-0.463496	2.589063

61	1	0	4.365525	0.077485	3.483786
62	6	0	6.879126	-1.193164	1.597667
63	1	0	6.620113	-2.552147	-0.056158
64	1	0	6.808311	0.148685	3.276532
65	1	0	7.959696	-1.154929	1.506374
66	7	0	1.895316	-1.430415	0.648999
67	7	0	0.598722	-1.928096	0.759825
68	6	0	2.016577	-0.396115	-0.293286
69	8	0	1.283029	-0.308287	-1.252321
70	8	0	3.050335	0.372542	0.012125
71	6	0	0.140112	-2.807372	-0.244038
72	8	0	-1.025923	-3.070496	-0.411392
73	8	0	1.172445	-3.281882	-0.925061
74	6	0	0.960145	-3.968350	-2.201155
75	6	0	0.293394	-5.316555	-1.956885
76	6	0	0.159917	-3.073209	-3.141093
77	6	0	2.383260	-4.145155	-2.714869
78	1	0	0.882441	-5.904686	-1.247489
79	1	0	-0.715949	-5.187716	-1.565551
80	1	0	0.240371	-5.867393	-2.900087
81	1	0	0.596769	-2.070847	-3.151784
82	1	0	0.201669	-3.490974	-4.150588
83	1	0	-0.883625	-3.001399	-2.833885
84	1	0	2.368177	-4.665096	-3.675826
85	1	0	2.857760	-3.168802	-2.848512
86	1	0	2.975127	-4.732233	-2.007524
87	6	0	3.687272	1.231095	-0.987696
88	6	0	4.080967	0.396483	-2.200827
89	6	0	2.745053	2.371658	-1.337757
90	6	0	4.923470	1.727783	-0.250544
91	1	0	4.696283	-0.452126	-1.885926
92	1	0	3.200645	0.029674	-2.730808
93	1	0	4.668199	1.015818	-2.884203
94	1	0	2.408038	2.878532	-0.428115
95	1	0	3.264958	3.101446	-1.966367
96	1	0	1.869232	2.002657	-1.873117
97	1	0	5.501861	2.388180	-0.901895
98	1	0	4.633735	2.282698	0.645967
99	1	0	5.548284	0.881044	0.050356

M6S$_{endo}$

Total energy= -2314.87643456

Sum of electronic and zero-point Energies= -2314.047244

Sum of electronic and thermal Energies= -2313.998661
Sum of electronic and thermal Enthalpies= -2313.997717
Sum of electronic and thermal Free Energies= -2314.129554

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.346194	-1.198526	1.264191
2	6	0	4.702707	-1.373351	0.998195
3	6	0	5.619639	-1.378637	2.044623
4	6	0	5.153832	-1.215651	3.350124
5	6	0	3.790613	-1.054835	3.608632
6	6	0	2.871508	-1.047829	2.559920
7	6	0	2.545730	-1.221138	-0.017357
8	6	0	3.526970	-1.839975	-1.059312
9	6	0	4.929108	-1.537954	-0.486860
10	1	0	6.679352	-1.519919	1.852608
11	1	0	5.857962	-1.225244	4.176227
12	1	0	3.445570	-0.942175	4.631556
13	1	0	1.805325	-0.941115	2.741342
14	1	0	3.360492	-1.384543	-2.036333
15	1	0	5.628182	-2.339567	-0.739969
16	1	0	2.259720	-0.210777	-0.318519
17	1	0	5.316358	-0.609002	-0.922094
18	6	0	1.401348	-3.370498	0.052122
19	6	0	0.042720	-1.576123	0.172511
20	7	0	0.214767	-3.891738	0.103894
21	7	0	1.333547	-2.005014	0.093158
22	7	0	-0.596832	-2.771576	0.177461
23	6	0	2.745777	-3.972215	-0.194003
24	1	0	3.364807	-3.939454	0.712338
25	1	0	2.650610	-5.007471	-0.522583
26	8	0	3.334860	-3.241917	-1.260684
27	6	0	-2.014829	-2.923415	0.083931
28	6	0	-2.545472	-3.650484	-0.993244
29	6	0	-2.838632	-2.282424	1.016667
30	6	0	-3.932506	-3.731457	-1.108165
31	6	0	-4.221782	-2.391778	0.852321
32	6	0	-4.788571	-3.112277	-0.197077
33	1	0	-4.355202	-4.282535	-1.945447
34	1	0	-4.871375	-1.897578	1.572202
35	6	0	-1.669056	-4.298645	-2.035845
36	1	0	-0.815686	-3.664689	-2.295709
37	1	0	-1.255318	-5.242645	-1.673091

38	1	0	-2.249071	-4.497640	-2.939706
39	6	0	-6.283641	-3.237090	-0.336946
40	1	0	-6.637399	-4.179642	0.093491
41	1	0	-6.798482	-2.423348	0.178305
42	1	0	-6.583567	-3.224869	-1.387769
43	6	0	-2.283524	-1.461558	2.150027
44	1	0	-1.417109	-1.946692	2.608969
45	1	0	-1.947565	-0.485218	1.785365
46	1	0	-3.049202	-1.308403	2.914831
47	6	0	-1.964719	1.597034	-1.450193
48	6	0	-2.348185	0.237946	-1.987796
49	1	0	-1.883602	2.280288	-2.309422
50	6	0	-1.412961	-0.642306	-2.337133
51	1	0	-3.403028	0.012063	-2.116039
52	1	0	-1.653232	-1.620515	-2.737060
53	6	0	0.032542	-0.306891	-2.338358
54	8	0	0.864940	-1.017135	-2.856641
55	6	0	-3.007286	2.193992	-0.522963
56	6	0	-3.119079	3.581315	-0.433650
57	6	0	-3.892407	1.387847	0.193564
58	6	0	-4.111884	4.159421	0.353301
59	1	0	-2.427284	4.209413	-0.990006
60	6	0	-4.889641	1.963854	0.975204
61	1	0	-3.800695	0.304773	0.148306
62	6	0	-5.006352	3.350278	1.052083
63	1	0	-4.195617	5.240021	0.409969
64	1	0	-5.575507	1.327153	1.525755
65	1	0	-5.788846	3.799114	1.655562
66	7	0	-0.595223	1.506951	-0.914440
67	7	0	0.311538	0.981590	-1.829211
68	6	0	-0.110336	1.545323	0.383881
69	8	0	1.079397	1.466287	0.624271
70	8	0	-1.072783	1.754435	1.272081
71	6	0	1.505681	1.686827	-2.079996
72	8	0	2.500906	1.165183	-2.522360
73	8	0	1.336051	2.969966	-1.788861
74	6	0	2.495865	3.859714	-1.696375
75	6	0	3.505154	3.300735	-0.698894
76	6	0	3.096161	4.071574	-3.081269
77	6	0	1.875945	5.147531	-1.169007
78	1	0	3.003369	3.059675	0.241781
79	1	0	3.986218	2.400278	-1.083021
80	1	0	4.272801	4.056926	-0.513106
81	1	0	2.326361	4.418583	-3.776216

82	1	0	3.875170	4.836800	-3.020149
83	1	0	3.534733	3.149399	-3.462302
84	1	0	2.648037	5.912125	-1.054690
85	1	0	1.116045	5.516970	-1.862805
86	1	0	1.408043	4.970434	-0.196588
87	6	0	-0.751950	2.280284	2.599533
88	6	0	-2.127046	2.421187	3.237152
89	6	0	0.111465	1.299609	3.385015
90	6	0	-0.083586	3.641648	2.443097
91	1	0	-2.761099	3.068238	2.625544
92	1	0	-2.608674	1.442346	3.321151
93	1	0	-2.027660	2.852438	4.236623
94	1	0	1.127893	1.264096	2.994612
95	1	0	0.138249	1.613805	4.432605
96	1	0	-0.325681	0.297104	3.339065
97	1	0	0.052691	4.095530	3.428335
98	1	0	0.894501	3.542892	1.967796
99	1	0	-0.716207	4.300178	1.839894

M6R$_{exo}$

Total energy= -2314.88456174

Sum of electronic and zero-point Energies= -2314.055569

Sum of electronic and thermal Energies= -2314.006531

Sum of electronic and thermal Enthalpies= -2314.005587

Sum of electronic and thermal Free Energies= -2314.138145

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.954442	-2.019073	-0.658871
2	6	0	5.043928	-2.824432	-0.341504
3	6	0	5.891973	-3.277036	-1.349912
4	6	0	5.630667	-2.904420	-2.667359
5	6	0	4.537514	-2.089542	-2.977249
6	6	0	3.688522	-1.639283	-1.969430
7	6	0	3.177486	-1.628278	0.577963
8	6	0	4.097384	-2.078192	1.765685
9	6	0	5.108364	-3.073865	1.145634
10	1	0	6.748873	-3.901385	-1.113909
11	1	0	6.287101	-3.245175	-3.461966
12	1	0	4.353366	-1.806508	-4.008830
13	1	0	2.835284	-1.000162	-2.185522
14	1	0	3.499460	-2.547055	2.548442

15	1	0	6.103348	-2.913006	1.572045
16	1	0	2.209297	-2.127648	0.623291
17	1	0	4.817186	-4.103413	1.379633
18	6	0	3.950895	0.650874	0.968044
19	6	0	1.864377	0.505799	0.115641
20	7	0	3.616552	1.886713	0.776201
21	7	0	2.936057	-0.193776	0.604643
22	7	0	2.340577	1.768585	0.253065
23	6	0	5.177888	0.047866	1.568953
24	1	0	5.855321	-0.324536	0.787072
25	1	0	5.710258	0.780129	2.176638
26	8	0	4.747680	-0.996411	2.424963
27	6	0	1.662363	2.974195	-0.103594
28	6	0	1.436180	3.937075	0.888018
29	6	0	1.289197	3.180762	-1.439053
30	6	0	0.807409	5.126786	0.513386
31	6	0	0.655728	4.380390	-1.758907
32	6	0	0.404121	5.362921	-0.799735
33	1	0	0.621506	5.881571	1.274045
34	1	0	0.353400	4.553634	-2.789339
35	6	0	1.850218	3.714221	2.319592
36	1	0	1.718140	2.669694	2.613351
37	1	0	2.907256	3.954995	2.462495
38	1	0	1.258591	4.345450	2.986029
39	6	0	-0.320900	6.628976	-1.175986
40	1	0	0.045405	7.026089	-2.126226
41	1	0	-1.392599	6.436169	-1.293628
42	1	0	-0.200310	7.398263	-0.410406
43	6	0	1.557538	2.151327	-2.505312
44	1	0	2.573297	1.753438	-2.423080
45	1	0	0.873250	1.301417	-2.412001
46	1	0	1.432107	2.593047	-3.495849
47	6	0	-2.521312	-0.581982	-1.881963
48	6	0	-1.379499	-0.734628	-2.845411
49	1	0	-3.430274	-0.847808	-2.427888
50	6	0	-0.349068	-1.551537	-2.614222
51	1	0	-1.450322	-0.172033	-3.772139
52	1	0	0.442312	-1.712982	-3.337583
53	6	0	-0.118974	-2.174859	-1.289117
54	8	0	0.883414	-2.792254	-1.017601
55	6	0	-2.697076	0.819345	-1.328498
56	6	0	-3.955284	1.418774	-1.394151
57	6	0	-1.637236	1.492133	-0.716059
58	6	0	-4.162211	2.687243	-0.857367

59	1	0	-4.774593	0.885044	-1.868734
60	6	0	-1.848572	2.758703	-0.175961
61	1	0	-0.653765	1.025313	-0.631218
62	6	0	-3.105348	3.358848	-0.247767
63	1	0	-5.143476	3.147315	-0.917252
64	1	0	-1.026472	3.280212	0.302937
65	1	0	-3.257281	4.347836	0.174155
66	7	0	-2.379126	-1.607282	-0.848170
67	7	0	-1.118760	-1.871922	-0.338285
68	6	0	-3.429678	-2.229462	-0.208185
69	8	0	-3.284393	-3.015972	0.703112
70	8	0	-4.586217	-1.819386	-0.739733
71	6	0	-0.802067	-1.498272	0.987764
72	8	0	0.186391	-1.887707	1.558588
73	8	0	-1.742752	-0.693612	1.453991
74	6	0	-1.624235	-0.098628	2.784167
75	6	0	-2.893363	0.738675	2.878496
76	6	0	-1.616944	-1.195905	3.841876
77	6	0	-0.383949	0.787547	2.833035
78	1	0	-2.912724	1.274337	3.831005
79	1	0	-2.928356	1.463097	2.059354
80	1	0	-3.775144	0.094635	2.819514
81	1	0	-0.692252	-1.771731	3.812081
82	1	0	-1.720729	-0.740776	4.830722
83	1	0	-2.463338	-1.869466	3.678356
84	1	0	-0.374416	1.338091	3.778545
85	1	0	0.530575	0.196985	2.753024
86	1	0	-0.410466	1.507474	2.007501
87	6	0	-5.855789	-2.200165	-0.120441
88	6	0	-6.040124	-3.712703	-0.170412
89	6	0	-5.907076	-1.644751	1.298419
90	6	0	-6.882318	-1.505641	-1.006060
91	1	0	-5.904799	-4.071266	-1.194758
92	1	0	-5.332260	-4.219940	0.483974
93	1	0	-7.057792	-3.956926	0.146446
94	1	0	-5.719269	-0.566797	1.277967
95	1	0	-6.901473	-1.815276	1.719730
96	1	0	-5.165295	-2.127728	1.936146
97	1	0	-6.800647	-1.861591	-2.036528
98	1	0	-7.889413	-1.720057	-0.640263
99	1	0	-6.728989	-0.423290	-0.990993

M6S$_{exo}$

Total energy= -2314.87931914
Sum of electronic and zero-point Energies= -2314.051035
Sum of electronic and thermal Energies= -2314.002001
Sum of electronic and thermal Enthalpies= -2314.001057
Sum of electronic and thermal Free Energies= -2314.134966

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.931724	-1.500951	-0.040697
2	6	0	5.039211	-2.246848	-0.436443
3	6	0	4.877069	-3.349354	-1.268654
4	6	0	3.596811	-3.674127	-1.712253
5	6	0	2.493759	-2.901478	-1.337033
6	6	0	2.649395	-1.802756	-0.491948
7	6	0	4.345242	-0.347923	0.852103
8	6	0	5.900270	-0.272041	0.669463
9	6	0	6.307953	-1.664291	0.138517
10	1	0	5.735376	-3.935554	-1.586965
11	1	0	3.453832	-4.521771	-2.376112
12	1	0	1.510657	-3.140048	-1.729135
13	1	0	1.799916	-1.176558	-0.223482
14	1	0	6.386498	-0.045704	1.618039
15	1	0	7.113281	-1.566372	-0.597385
16	1	0	4.083787	-0.535074	1.896131
17	1	0	6.688119	-2.285367	0.959349
18	6	0	4.139977	1.552347	-0.662078
19	6	0	2.558500	1.444456	0.948412
20	7	0	3.351219	2.539046	-0.941761
21	7	0	3.710368	0.889581	0.457731
22	7	0	2.387565	2.439748	0.049449
23	6	0	5.427581	1.090904	-1.266975
24	1	0	5.259454	0.221558	-1.917751
25	1	0	5.890848	1.885997	-1.852848
26	8	0	6.308218	0.778544	-0.198387
27	6	0	1.263908	3.320191	0.017724
28	6	0	0.417307	3.296193	-1.101769
29	6	0	1.022285	4.159379	1.110519
30	6	0	-0.702272	4.126657	-1.086404
31	6	0	-0.110972	4.976571	1.075567
32	6	0	-0.986408	4.969128	-0.007460
33	1	0	-1.375139	4.112088	-1.939500
34	1	0	-0.311290	5.624961	1.921787
35	6	0	0.679957	2.392706	-2.275859

36	1	0	1.552143	2.726803	-2.844996
37	1	0	0.859098	1.365900	-1.948686
38	1	0	-0.188412	2.384408	-2.942602
39	6	0	-2.211475	5.844850	-0.029815
40	1	0	-2.127133	6.619739	-0.800323
41	1	0	-3.107323	5.259734	-0.256971
42	1	0	-2.360740	6.341567	0.932085
43	6	0	1.928975	4.167880	2.313757
44	1	0	1.786911	3.259565	2.907908
45	1	0	2.980777	4.187724	2.018076
46	1	0	1.720955	5.035896	2.939257
47	6	0	-2.700627	-3.295551	-0.547939
48	6	0	-1.962366	-3.830867	-1.748377
49	1	0	-3.723413	-3.677965	-0.542784
50	6	0	-1.190576	-3.021217	-2.481983
51	1	0	-2.066200	-4.885281	-1.994440
52	1	0	-0.656165	-3.355067	-3.365687
53	6	0	-0.851013	-1.645340	-2.033163
54	8	0	0.089317	-1.029095	-2.478921
55	6	0	-2.031402	-3.594377	0.784565
56	6	0	-0.652976	-3.760744	0.899102
57	6	0	-2.822727	-3.593072	1.939708
58	6	0	-0.067748	-3.933400	2.153639
59	1	0	-0.027048	-3.763018	0.011893
60	6	0	-2.238751	-3.768608	3.189919
61	1	0	-3.894208	-3.436026	1.847784
62	6	0	-0.859091	-3.939920	3.297618
63	1	0	1.009509	-4.056815	2.228944
64	1	0	-2.860637	-3.772265	4.078769
65	1	0	-0.402669	-4.077936	4.274050
66	7	0	-2.821110	-1.855655	-0.733344
67	7	0	-1.633086	-1.185964	-0.952063
68	6	0	-4.026601	-1.211202	-0.913227
69	8	0	-5.090794	-1.764506	-0.720524
70	8	0	-3.822173	0.047803	-1.285874
71	6	0	-1.169161	-0.276872	0.023054
72	8	0	-0.132261	0.325596	-0.094281
73	8	0	-2.027498	-0.221254	1.030867
74	6	0	-1.682966	0.540986	2.240544
75	6	0	-0.337809	0.073635	2.789701
76	6	0	-1.703148	2.029530	1.915924
77	6	0	-2.804726	0.162435	3.197661
78	1	0	-0.320406	-1.023399	2.828819
79	1	0	0.503407	0.434755	2.194309

80	1	0	-0.234611	0.451643	3.812448
81	1	0	-2.719695	2.354899	1.655201
82	1	0	-1.380795	2.594064	2.800346
83	1	0	-1.025484	2.267776	1.088283
84	1	0	-2.689275	0.716321	4.132850
85	1	0	-3.782819	0.401376	2.766786
86	1	0	-2.770975	-0.910060	3.415715
87	6	0	-4.905421	1.030062	-1.252458
88	6	0	-5.952358	0.683330	-2.306688
89	6	0	-5.490957	1.097924	0.151874
90	6	0	-4.178790	2.322663	-1.597419
91	1	0	-5.477690	0.583042	-3.286780
92	1	0	-6.461483	-0.247917	-2.057234
93	1	0	-6.688924	1.489216	-2.359776
94	1	0	-4.683739	1.259245	0.873097
95	1	0	-6.185345	1.937733	0.215065
96	1	0	-6.019149	0.177323	0.408728
97	1	0	-4.884322	3.158994	-1.594504
98	1	0	-3.388527	2.519108	-0.865571
99	1	0	-3.721625	2.251414	-2.589692

PR

Total energy= -1262.94724656
Sum of electronic and zero-point Energies= -1262.503887
Sum of electronic and thermal Energies= -1262.477123
Sum of electronic and thermal Enthalpies= -1262.476179
Sum of electronic and thermal Free Energies= -1262.561287

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.207023	1.695260	0.932232
2	6	0	0.119829	3.117126	0.553055
3	1	0	-1.121590	1.694769	1.527541
4	6	0	0.462152	3.430958	-0.698814
5	1	0	0.060164	3.875958	1.328152
6	1	0	0.674449	4.445701	-1.014595
7	6	0	0.762272	2.384867	-1.711893
8	8	0	1.340861	2.618329	-2.745339
9	6	0	0.887874	0.978380	1.710647
10	6	0	2.217448	1.393546	1.680755
11	6	0	0.540302	-0.167568	2.433048
12	6	0	3.189277	0.683558	2.387964

13	1	0	2.498416	2.276005	1.113264
14	6	0	1.507374	-0.875137	3.136901
15	1	0	-0.495754	-0.499631	2.433162
16	6	0	2.835877	-0.444742	3.120734
17	1	0	4.221838	1.016313	2.364096
18	1	0	1.228127	-1.759221	3.701399
19	1	0	3.591887	-0.992956	3.673574
20	7	0	-0.527884	0.982768	-0.300417
21	7	0	0.418215	1.074012	-1.301537
22	6	0	-1.700311	0.321089	-0.600672
23	8	0	-1.934441	-0.154706	-1.689122
24	8	0	-2.481518	0.272332	0.484486
25	6	0	1.222858	-0.051360	-1.595850
26	8	0	2.164449	-0.003843	-2.346934
27	8	0	0.772393	-1.100404	-0.924803
28	6	0	1.506077	-2.366944	-0.946931
29	6	0	0.659042	-3.247394	-0.037129
30	6	0	1.544526	-2.926562	-2.363833
31	6	0	2.892990	-2.151629	-0.353527
32	1	0	0.585347	-2.795392	0.956138
33	1	0	-0.347063	-3.362373	-0.449573
34	1	0	1.117742	-4.234864	0.055269
35	1	0	2.169705	-2.316012	-3.014826
36	1	0	1.949711	-3.941689	-2.332078
37	1	0	0.532078	-2.971113	-2.774761
38	1	0	3.387182	-3.119964	-0.235179
39	1	0	3.505027	-1.520900	-0.999334
40	1	0	2.802832	-1.682424	0.631405
41	6	0	-3.739802	-0.475230	0.453464
42	6	0	-4.689489	0.136838	-0.570235
43	6	0	-3.451714	-1.946974	0.178807
44	6	0	-4.275009	-0.283773	1.866822
45	1	0	-4.806578	1.207197	-0.378564
46	1	0	-4.322257	-0.008771	-1.585722
47	1	0	-5.669852	-0.337882	-0.474342
48	1	0	-2.728715	-2.328239	0.906296
49	1	0	-4.378043	-2.518807	0.280973
50	1	0	-3.056498	-2.088617	-0.827428
51	1	0	-5.227143	-0.808525	1.975603
52	1	0	-3.569225	-0.683168	2.600140
53	1	0	-4.435357	0.777610	2.073479

PS

Total energy= -1262.93737628
Sum of electronic and zero-point Energies= -1262.495212
Sum of electronic and thermal Energies= -1262.468456
Sum of electronic and thermal Enthalpies= -1262.467512
Sum of electronic and thermal Free Energies= -1262.551387

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.684336	-1.361299	-0.816443
2	6	0	-0.633569	-2.866962	-0.687234
3	1	0	-0.280331	-1.040277	-1.788104
4	6	0	0.130124	-3.501342	0.203927
5	1	0	-1.329178	-3.414997	-1.316148
6	1	0	0.086967	-4.573681	0.353416
7	6	0	1.253037	-2.809488	0.874534
8	8	0	2.126236	-3.384306	1.476887
9	6	0	-2.163068	-1.003213	-0.737674
10	6	0	-2.839051	-0.591350	-1.881988
11	6	0	-2.865349	-1.179520	0.456002
12	6	0	-4.211084	-0.345451	-1.834197
13	1	0	-2.293534	-0.453917	-2.811461
14	6	0	-4.230457	-0.919174	0.507321
15	1	0	-2.334460	-1.511567	1.344968
16	6	0	-4.908198	-0.504493	-0.640285
17	1	0	-4.731345	-0.022728	-2.730303
18	1	0	-4.768077	-1.048022	1.441377
19	1	0	-5.974631	-0.308067	-0.601567
20	7	0	0.096005	-0.800699	0.291314
21	7	0	1.306861	-1.425001	0.579181
22	6	0	-0.004061	0.485583	0.815375
23	8	0	0.682585	0.871774	1.736626
24	8	0	-0.917066	1.186309	0.153948
25	6	0	2.517483	-0.814733	0.185045
26	8	0	3.597861	-1.217731	0.533592
27	8	0	2.258747	0.217267	-0.611891
28	6	0	3.309528	1.193088	-0.919158
29	6	0	2.550059	2.247762	-1.711737
30	6	0	3.850491	1.776844	0.380612
31	6	0	4.390258	0.541436	-1.772690
32	1	0	2.115599	1.808901	-2.613838
33	1	0	1.745758	2.666511	-1.101250
34	1	0	3.228552	3.052692	-2.004065
35	1	0	4.426696	1.037183	0.937476

36	1	0	4.497779	2.626888	0.149179
37	1	0	3.018241	2.122737	1.000459
38	1	0	5.090438	1.310921	-2.109457
39	1	0	4.937823	-0.212311	-1.207684
40	1	0	3.941913	0.075317	-2.654623
41	6	0	-1.502368	2.394227	0.741262
42	6	0	-2.000752	2.106662	2.153418
43	6	0	-0.480544	3.523227	0.704514
44	6	0	-2.674123	2.675655	-0.189258
45	1	0	-2.663713	1.236083	2.142157
46	1	0	-1.174857	1.925368	2.841399
47	1	0	-2.571894	2.969139	2.507388
48	1	0	-0.176591	3.722988	-0.326927
49	1	0	-0.932827	4.433627	1.107946
50	1	0	0.397755	3.270509	1.300573
51	1	0	-3.184953	3.589488	0.125010
52	1	0	-2.321065	2.804845	-1.216027
53	1	0	-3.381146	1.841033	-0.164744

Re-M01^{2W}

Total energy= -1969.84394663

Sum of electronic and zero-point Energies= -1969.183390

Sum of electronic and thermal Energies= -1969.142224

Sum of electronic and thermal Enthalpies= -1969.141280

Sum of electronic and thermal Free Energies= -1969.259413

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.678312	-0.283105	0.681680
2	6	0	-6.021294	-0.384240	0.326689
3	6	0	-7.010722	0.001526	1.226899
4	6	0	-6.630627	0.492527	2.474339
5	6	0	-5.281287	0.597208	2.822014
6	6	0	-4.289614	0.208338	1.924354
7	6	0	-3.787903	-0.753341	-0.448606
8	6	0	-4.755967	-0.837489	-1.683150
9	6	0	-6.169298	-0.932621	-1.070402
10	1	0	-8.060320	-0.069132	0.958185
11	1	0	-7.391149	0.803406	3.183419
12	1	0	-5.003857	0.984031	3.796814
13	1	0	-3.238410	0.275397	2.191116
14	1	0	-4.512377	-1.705539	-2.296329

15	1	0	-6.882647	-0.376715	-1.685156
16	1	0	-3.314328	-1.719340	-0.244556
17	1	0	-6.500941	-1.976141	-1.045412
18	6	0	-2.968639	1.371188	-1.384747
19	6	0	-1.421044	0.177800	-0.394013
20	7	0	-1.886996	2.084612	-1.492413
21	7	0	-2.723679	0.205259	-0.719954
22	7	0	-0.933362	1.328504	-0.857543
23	6	0	-4.330865	1.520128	-1.979829
24	1	0	-5.066854	1.806260	-1.217366
25	1	0	-4.321576	2.269141	-2.771056
26	8	0	-4.632460	0.267357	-2.572201
27	6	0	0.419853	1.810746	-0.778928
28	6	0	1.348772	1.323541	-1.696134
29	6	0	0.729902	2.726049	0.229559
30	6	0	2.654839	1.798444	-1.581244
31	6	0	2.049627	3.158587	0.309944
32	6	0	3.021945	2.701979	-0.583971
33	1	0	3.406816	1.432086	-2.275302
34	1	0	2.330752	3.856183	1.094898
35	6	0	0.954387	0.303577	-2.729235
36	1	0	0.515852	-0.584240	-2.255575
37	1	0	0.208577	0.714198	-3.418465
38	1	0	1.826046	-0.004749	-3.309474
39	6	0	4.447822	3.165183	-0.439192
40	1	0	4.507242	4.257163	-0.422125
41	1	0	4.862540	2.799431	0.506702
42	1	0	5.071204	2.801300	-1.259774
43	6	0	-0.324946	3.193819	1.196426
44	1	0	-1.141234	3.701765	0.674376
45	1	0	-0.762766	2.349087	1.740383
46	1	0	0.101658	3.882705	1.926501
47	6	0	3.087599	-1.337729	0.798048
48	6	0	1.674121	-1.505016	0.309435
49	1	0	3.299248	-2.093227	1.564173
50	6	0	0.636371	-0.779177	0.704956
51	1	0	1.498099	-2.291097	-0.420976
52	1	0	0.749197	0.017478	1.438245
53	6	0	-0.751225	-1.076343	0.171553
54	8	0	-0.818836	-2.000369	-0.825160
55	1	0	-1.380400	-1.336079	1.053794
56	6	0	4.101601	-1.499999	-0.323757
57	6	0	4.219835	-2.742181	-0.951588
58	6	0	4.918022	-0.450155	-0.737739

59	6	0	5.133460	-2.926729	-1.984543
60	1	0	3.596632	-3.572187	-0.627617
61	6	0	5.834560	-0.634031	-1.771705
62	1	0	4.830023	0.522151	-0.263534
63	6	0	5.943786	-1.871052	-2.399774
64	1	0	5.216345	-3.897583	-2.462529
65	1	0	6.463401	0.194492	-2.083541
66	1	0	6.658776	-2.015010	-3.203137
67	8	0	3.182510	-0.037670	1.401227
68	6	0	4.207617	0.263950	2.199338
69	8	0	4.387588	1.385594	2.607078
70	8	0	4.977925	-0.786610	2.480624
71	6	0	6.102709	-0.500375	3.320455
72	1	0	5.765230	-0.093562	4.274424
73	1	0	6.609008	-1.451924	3.464429
74	1	0	6.762208	0.216969	2.829562
75	8	0	-3.020598	-2.557089	2.363040
76	1	0	-2.786701	-3.098277	1.572735
77	1	0	-3.947386	-2.325362	2.241838
78	8	0	-2.216330	-3.802684	0.118992
79	1	0	-2.840628	-4.075663	-0.560873
80	1	0	-1.587907	-3.080328	-0.331022

Si-M01^{2W}

Total energy= -1969.84597035

Sum of electronic and zero-point Energies= -1969.184645

Sum of electronic and thermal Energies= -1969.143402

Sum of electronic and thermal Enthalpies= -1969.142458

Sum of electronic and thermal Free Energies= -1969.260419

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.385381	2.546314	-0.211695
2	6	0	-2.025594	3.682587	-0.705763
3	6	0	-3.125273	4.213469	-0.039233
4	6	0	-3.563310	3.600145	1.133198
5	6	0	-2.906335	2.475250	1.636872
6	6	0	-1.807793	1.936911	0.965908
7	6	0	-0.246955	2.153271	-1.131518
8	6	0	-0.016669	3.425192	-2.017066
9	6	0	-1.365562	4.169038	-1.971383
10	1	0	-3.625391	5.099078	-0.419670

11	1	0	-4.414402	4.009208	1.668820
12	1	0	-3.240844	2.018150	2.563664
13	1	0	-1.295900	1.065429	1.362123
14	1	0	0.259061	3.132830	-3.031015
15	1	0	-1.202540	5.249604	-1.993141
16	1	0	-0.480853	1.289995	-1.759620
17	1	0	-1.967547	3.907019	-2.848345
18	6	0	1.809876	2.785006	0.069407
19	6	0	1.578116	0.629369	-0.226507
20	7	0	2.898777	2.270317	0.561619
21	7	0	0.981868	1.815656	-0.421840
22	7	0	2.728089	0.920439	0.376506
23	6	0	1.400373	4.195212	-0.200207
24	1	0	0.562545	4.488467	0.444831
25	1	0	2.236009	4.875228	-0.038634
26	8	0	1.061836	4.248407	-1.576496
27	6	0	3.807555	0.007080	0.636850
28	6	0	3.972266	-0.502611	1.923521
29	6	0	4.644681	-0.312065	-0.437284
30	6	0	5.041647	-1.375294	2.128298
31	6	0	5.699582	-1.185852	-0.181002
32	6	0	5.911235	-1.725160	1.092693
33	1	0	5.196030	-1.793248	3.119411
34	1	0	6.369135	-1.455750	-0.993525
35	6	0	3.021389	-0.130696	3.028391
36	1	0	2.939710	0.955357	3.128098
37	1	0	2.018463	-0.519478	2.823692
38	1	0	3.357451	-0.543462	3.980247
39	6	0	7.032048	-2.703504	1.326530
40	1	0	7.308464	-2.743836	2.381832
41	1	0	6.725148	-3.708932	1.021004
42	1	0	7.915940	-2.436033	0.743256
43	6	0	4.398412	0.274155	-1.801831
44	1	0	3.392504	0.024903	-2.160054
45	1	0	4.478242	1.365855	-1.771788
46	1	0	5.132515	-0.102020	-2.516505
47	6	0	-2.760968	-1.223591	-0.244156
48	6	0	-1.373435	-1.088185	-0.795114
49	1	0	-3.357691	-0.379744	-0.605902
50	6	0	-0.259669	-0.972397	-0.080814
51	1	0	-1.291088	-1.046368	-1.879611
52	1	0	-0.276454	-1.030628	1.006513
53	6	0	1.077452	-0.708230	-0.760136
54	8	0	1.036703	-0.598432	-2.114157

55	1	0	1.797621	-1.463115	-0.382862
56	6	0	-3.437858	-2.521819	-0.631861
57	6	0	-4.696866	-2.517959	-1.228424
58	6	0	-2.798319	-3.736598	-0.374509
59	6	0	-5.313221	-3.719717	-1.572460
60	1	0	-5.195844	-1.571452	-1.418044
61	6	0	-3.417094	-4.936422	-0.707225
62	1	0	-1.811854	-3.732423	0.081821
63	6	0	-4.674989	-4.928877	-1.309972
64	1	0	-6.291945	-3.710613	-2.041490
65	1	0	-2.916571	-5.877777	-0.504734
66	1	0	-5.155071	-5.865252	-1.575925
67	8	0	-2.666451	-1.131074	1.196593
68	6	0	-3.683685	-0.648977	1.909658
69	8	0	-3.608863	-0.503813	3.105340
70	8	0	-4.749862	-0.348677	1.166899
71	6	0	-5.852719	0.206853	1.891495
72	1	0	-5.573668	1.175881	2.310670
73	1	0	-6.651346	0.323643	1.162484
74	1	0	-6.154486	-0.467088	2.693759
75	8	0	3.158317	-3.436234	-0.157788
76	1	0	3.009180	-3.130613	-1.081510
77	1	0	3.839917	-2.841931	0.175559
78	8	0	2.607400	-2.477617	-2.657904
79	1	0	3.362256	-2.095827	-3.116751
80	1	0	1.931924	-1.701823	-2.530528

Re-TS2^{2W}

Total energy= -1969.82575807
Sum of electronic and zero-point Energies= -1969.169141
Sum of electronic and thermal Energies= -1969.128827
Sum of electronic and thermal Enthalpies= -1969.127883
Sum of electronic and thermal Free Energies= -1969.244426

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.648101	-0.504298	0.565602
2	6	0	-5.923177	-0.926482	0.193540
3	6	0	-7.044232	-0.391149	0.820063
4	6	0	-6.864489	0.570760	1.813393
5	6	0	-5.583318	0.993935	2.173218
6	6	0	-4.454305	0.461106	1.550043

7	6	0	-3.593804	-1.235422	-0.239909
8	6	0	-4.397356	-1.897064	-1.413465
9	6	0	-5.852093	-1.962635	-0.900263
10	1	0	-8.042120	-0.709420	0.533591
11	1	0	-7.730176	1.001394	2.306530
12	1	0	-5.461550	1.748608	2.943329
13	1	0	-3.458728	0.799664	1.836357
14	1	0	-3.996765	-2.886086	-1.638210
15	1	0	-6.549727	-1.780025	-1.722525
16	1	0	-3.072921	-1.990923	0.344536
17	1	0	-6.065508	-2.961254	-0.503923
18	6	0	-2.906939	0.498459	-1.819726
19	6	0	-1.335469	0.024853	-0.352567
20	7	0	-1.952514	1.328703	-2.095889
21	7	0	-2.579916	-0.318943	-0.768994
22	7	0	-0.981124	1.029354	-1.172074
23	6	0	-4.197094	0.223077	-2.520010
24	1	0	-5.044380	0.647955	-1.966165
25	1	0	-4.176914	0.645937	-3.524176
26	8	0	-4.291940	-1.184844	-2.640611
27	6	0	0.235588	1.790670	-1.167179
28	6	0	1.294359	1.354391	-1.965737
29	6	0	0.301264	2.917365	-0.345709
30	6	0	2.474886	2.093311	-1.915528
31	6	0	1.507889	3.616230	-0.324048
32	6	0	2.602974	3.215381	-1.092390
33	1	0	3.318161	1.783053	-2.528839
34	1	0	1.593844	4.494415	0.310910
35	6	0	1.167052	0.105782	-2.795402
36	1	0	1.127590	-0.776622	-2.144777
37	1	0	0.255156	0.118720	-3.398783
38	1	0	2.025186	-0.004548	-3.461529
39	6	0	3.910475	3.956616	-1.010190
40	1	0	3.754992	5.004315	-0.743304
41	1	0	4.539831	3.496122	-0.242196
42	1	0	4.448415	3.914740	-1.960201
43	6	0	-0.874771	3.324971	0.501199
44	1	0	-1.783225	3.401542	-0.104827
45	1	0	-1.071552	2.593085	1.296750
46	1	0	-0.689654	4.295117	0.965736
47	6	0	3.169030	-1.214791	1.233334
48	6	0	1.677610	-1.348090	1.095963
49	1	0	3.498613	-1.624624	2.194363
50	6	0	0.842459	-0.335401	0.871900

51	1	0	1.294844	-2.361624	1.177095
52	1	0	1.235183	0.674542	0.813971
53	6	0	-0.644780	-0.505219	0.835816
54	8	0	-1.048122	-1.837350	1.065533
55	1	0	-1.072624	0.241751	1.769125
56	6	0	3.873794	-1.949916	0.108347
57	6	0	4.403663	-3.221233	0.312764
58	6	0	3.943999	-1.365530	-1.156964
59	6	0	4.998374	-3.909026	-0.743730
60	1	0	4.355102	-3.672391	1.300594
61	6	0	4.547257	-2.046880	-2.209056
62	1	0	3.527881	-0.371172	-1.300768
63	6	0	5.072617	-3.322692	-2.004612
64	1	0	5.411440	-4.899161	-0.579418
65	1	0	4.606369	-1.584888	-3.189980
66	1	0	5.542039	-3.855435	-2.825316
67	8	0	3.483586	0.189332	1.193130
68	6	0	4.714993	0.607000	1.489382
69	8	0	5.046471	1.759355	1.359782
70	8	0	5.500607	-0.369305	1.943969
71	6	0	6.835983	0.035808	2.267931
72	1	0	6.818867	0.785187	3.060458
73	1	0	7.341973	-0.866975	2.602359
74	1	0	7.326028	0.448322	1.385010
75	8	0	-1.611866	0.922714	2.853265
76	1	0	-2.127153	-0.424517	3.249960
77	1	0	-0.863539	1.175047	3.408130
78	8	0	-2.432501	-1.414257	3.278253
79	1	0	-3.379875	-1.389312	3.099757
80	1	0	-1.536129	-1.832820	1.932442

Si-TS2^{2W}

Total energy= -1969.81507520
Sum of electronic and zero-point Energies= -1969.159457
Sum of electronic and thermal Energies= -1969.118729
Sum of electronic and thermal Enthalpies= -1969.117785
Sum of electronic and thermal Free Energies= -1969.235832

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.074465	2.809957	-0.237676
2	6	0	-1.581862	4.076555	-0.524031

3	6	0	-2.614554	4.606072	0.244430
4	6	0	-3.114795	3.858644	1.309342
5	6	0	-2.585460	2.601445	1.608586
6	6	0	-1.558425	2.064449	0.832688
7	6	0	0.028609	2.453318	-1.216923
8	6	0	0.402886	3.825301	-1.873057
9	6	0	-0.857139	4.695423	-1.693969
10	1	0	-3.012454	5.593141	0.028611
11	1	0	-3.911492	4.265257	1.924414
12	1	0	-2.959738	2.039665	2.459484
13	1	0	-1.143684	1.089923	1.070930
14	1	0	0.664999	3.688971	-2.922856
15	1	0	-0.575898	5.739312	-1.531042
16	1	0	-0.287115	1.725116	-1.968180
17	1	0	-1.472259	4.656091	-2.599554
18	6	0	2.028021	2.687676	0.188930
19	6	0	1.618109	0.619439	-0.424435
20	7	0	2.947612	1.982874	0.781978
21	7	0	1.198755	1.894921	-0.547751
22	7	0	2.670955	0.698126	0.391930
23	6	0	1.802211	4.161276	0.078543
24	1	0	0.965368	4.474667	0.715609
25	1	0	2.698484	4.709158	0.367611
26	8	0	1.559251	4.425857	-1.293297
27	6	0	3.519276	-0.382051	0.814000
28	6	0	3.311945	-0.931747	2.080850
29	6	0	4.521006	-0.809561	-0.058168
30	6	0	4.150045	-1.975017	2.466628
31	6	0	5.338018	-1.853829	0.377546
32	6	0	5.161200	-2.450533	1.627710
33	1	0	4.011910	-2.425674	3.446114
34	1	0	6.128769	-2.209101	-0.278150
35	6	0	2.233356	-0.400655	2.986538
36	1	0	2.406200	0.653946	3.220781
37	1	0	1.247687	-0.471862	2.515602
38	1	0	2.203987	-0.963347	3.920204
39	6	0	6.032840	-3.599622	2.062377
40	1	0	6.255540	-3.542199	3.130386
41	1	0	5.526413	-4.553161	1.882320
42	1	0	6.974639	-3.612784	1.510257
43	6	0	4.680815	-0.193974	-1.421261
44	1	0	3.882244	-0.533723	-2.091463
45	1	0	4.644961	0.898148	-1.372008
46	1	0	5.634313	-0.488907	-1.862322

47	6	0	-2.769446	-1.183301	-0.427622
48	6	0	-1.440836	-0.957991	-1.087211
49	1	0	-3.458508	-0.396100	-0.746276
50	6	0	-0.275307	-0.862581	-0.444132
51	1	0	-1.466038	-0.840167	-2.167101
52	1	0	-0.247919	-0.995662	0.637203
53	6	0	1.025490	-0.570719	-1.105695
54	8	0	0.843729	-0.200407	-2.464372
55	1	0	1.788299	-1.683555	-1.052969
56	6	0	-3.390202	-2.535264	-0.721018
57	6	0	-4.750539	-2.641179	-1.009309
58	6	0	-2.606128	-3.689625	-0.663634
59	6	0	-5.324500	-3.889766	-1.241066
60	1	0	-5.359422	-1.742034	-1.045366
61	6	0	-3.179668	-4.936948	-0.886345
62	1	0	-1.543728	-3.598925	-0.453842
63	6	0	-4.540076	-5.038551	-1.176537
64	1	0	-6.382819	-3.964785	-1.469891
65	1	0	-2.565461	-5.830580	-0.841199
66	1	0	-4.986233	-6.011823	-1.355078
67	8	0	-2.569399	-1.060399	1.004936
68	6	0	-3.516261	-0.556772	1.791492
69	8	0	-3.342840	-0.403400	2.976753
70	8	0	-4.635523	-0.239578	1.137702
71	6	0	-5.664404	0.338866	1.948181
72	1	0	-5.333647	1.302626	2.340225
73	1	0	-6.517692	0.470222	1.286511
74	1	0	-5.912984	-0.327643	2.774427
75	8	0	2.376617	-2.790035	-1.309449
76	1	0	2.607241	-2.348570	-2.686891
77	1	0	3.198774	-2.810242	-0.804668
78	8	0	2.625635	-1.840819	-3.599316
79	1	0	2.171265	-2.410511	-4.229517
80	1	0	1.486450	-0.738488	-2.993576