SUPPORTING INFORMATION FOR

Insights to the isothiourea-catalyzed asymmetric [4 + 2] annulation of phenylacetic acid with alkylidene pyrazolone

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CONTENT

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Part 1: Different conformers of *Si*-TS3 and *Si*-M3

We have additionally optimized and calculated the energies of different conformers of **M3** (*i.e.* ***Si*-M3** (E) and ***Si*-M3'** (Z)) and the corresponding transition states (*i.e.* ***Si*-TS3** (E), ***Si*-TS3a** (E), ***Si*-TS3b** (Z), and ***Si*-TS3c** (Z)). The optimized structures were provided in Fig. S1, and the relative energies were summarized in Table S1. As shown in Table S1, the conformers ***Si*-M3** (6.9 kcal/mol) and ***Si*-TS3** (14.3 kcal/mol) have the lowest energies compared to their conformers respectively, so they are the most energy favorable conformers, and we only discussed them in the main text of the manuscript.

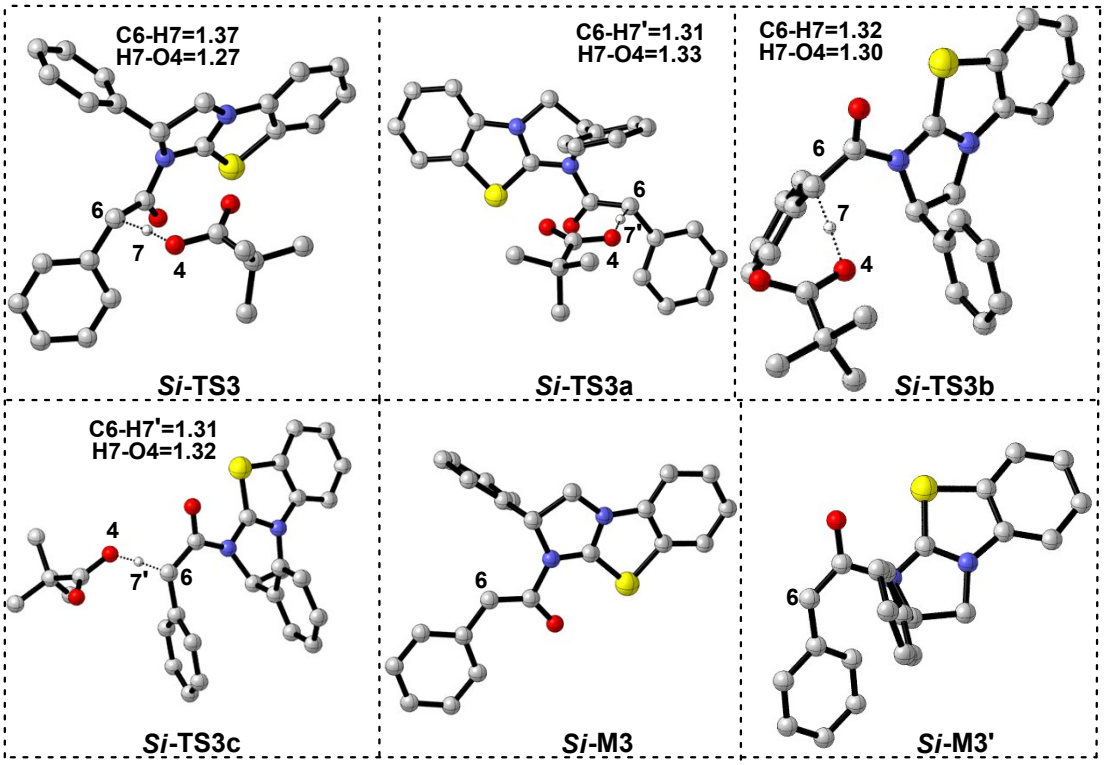


Fig. S1 Different conformers of the ***Si*-M3** and ***Si*-TS3** (the hydrogen atoms which are not involved in the reaction are omitted and distance is shown in Å)

Table S1 The relatively energies (**ΔG**) of the different conformers of ***Si*-M3** and ***Si*-TS3** with the energy of **R1'+R2+Cat** as 0.0 kcal/mol (unit: kcal/mol)

	***Si*-TS3** (E)	***Si*-TS3a** (E)	***Si*-TS3b** (Z)	***Si*-TS3c** (Z)	***Si*-M3** (E)	**Si-M3'** (Z)
ΔG (kcal/mol)	14.3	19.1	24.0	26.2	6.9	14.7

Part 2: Different configurations of TS4s

In Pathway A, the enolate intermediate ***Si*-M3** reacts with the reactant **R2** for the formation of intermediate **M4** *via* transition state **TS4.** Different conformational possibilities of the transition states for the nucleophilic addition of reactant **R2** to the enolate intermediate ***Si*-M3**. we have considered and investigated the different conformations of **TS4**s in the C–C bond formation step in the revised manuscript. By rotating dihedral angle Φ_1(C2-C6-C8-C10) from 0-360° at intervals of 90° in the four transition states **TS4*RR&SR&RS&SS***, so there should be sixteen (4 × 4) possible conformations obtained in theory. Actually, we have only obtained twelve conformations (*i.e.* **TS4*RR&SR&RS&SS***, **TS4*′RR&SR&RS&SS***, and **TS4*′′RR&SR&RS&SS***), because the original conformations by rotating the dihedral Φ_1 at 90° would lead to the same conformations of those at 0/360° after the structural optimizations. The optimized structures of the twelve conformations have been depicted in Fig. S2, and the corresponding energy barriers have been summarized in Table S2. As shown in Table S2, the conformers **TS4*RR*** (8.1 kcal/mol), **TS4*RS*** (10.7 kcal/mol), **TS4*SR*** (17.4 kcal/mol) and **TS4*SS*** (19.1 kcal/mol) have the lowest energies compared to their conformers respectively, so they should be the most energy favorable conformers, and we only discussed them in the main text of the manuscript.

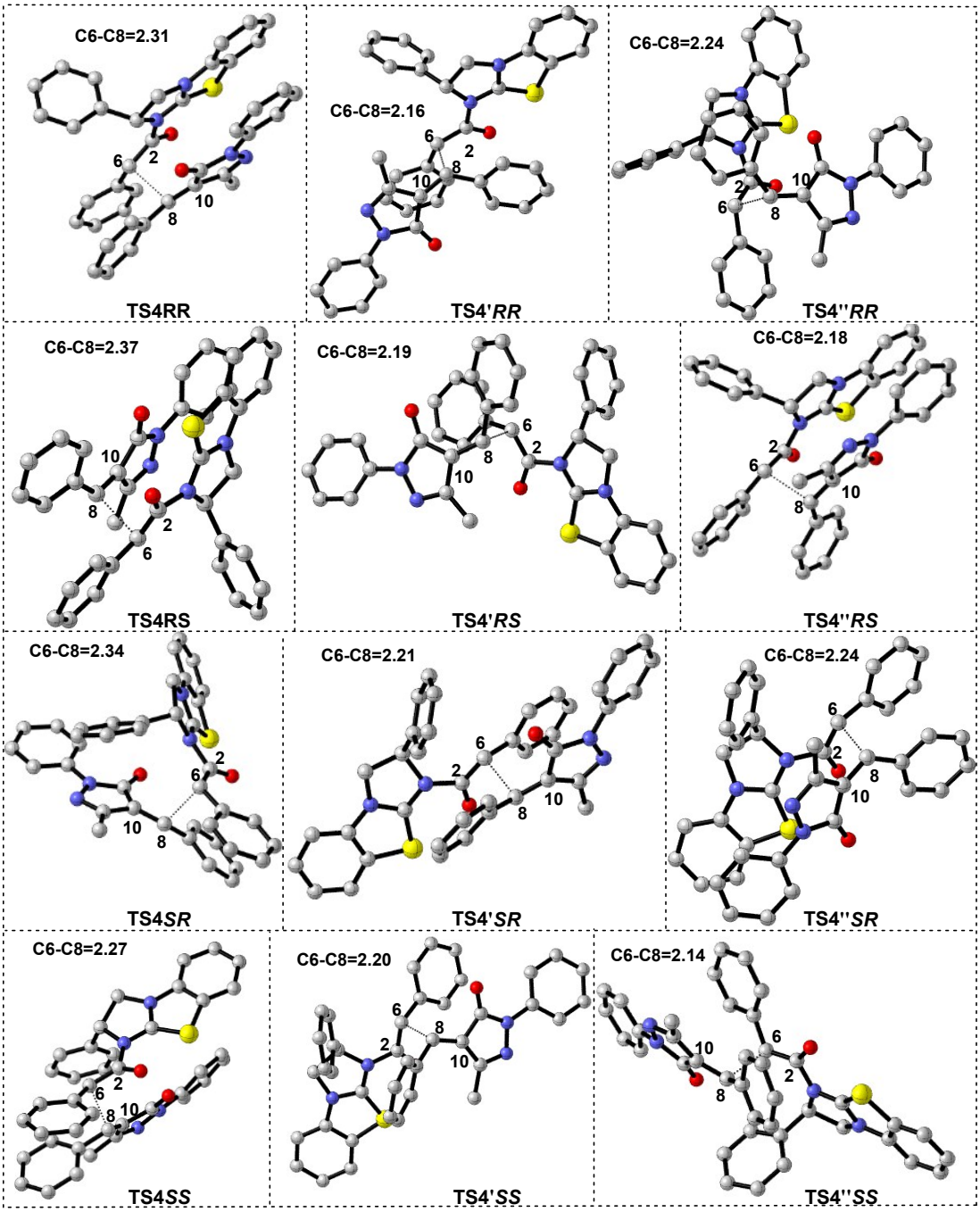


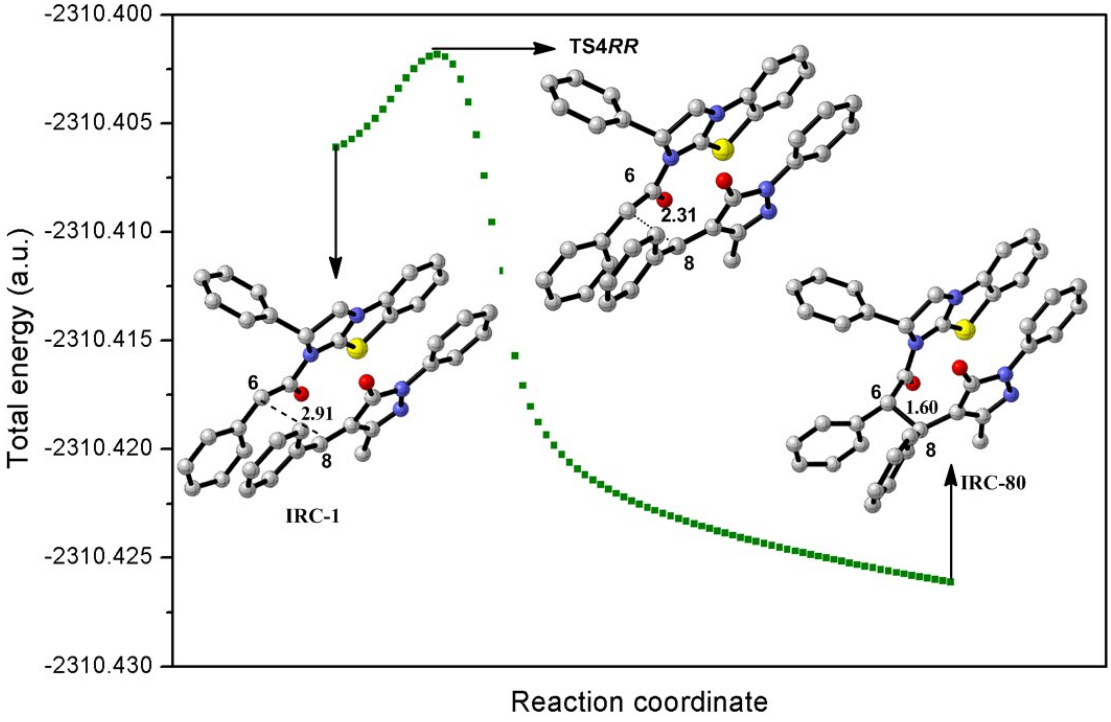
Fig. S2 The optimized structures of transition states **TS4*RR&SR&RS&SS***, **TS4′*RR&SR&RS&SS***, and **TS4′′*RR&SR&RS&SS*** (the hydrogen atoms which are not involved in the reaction are omitted)

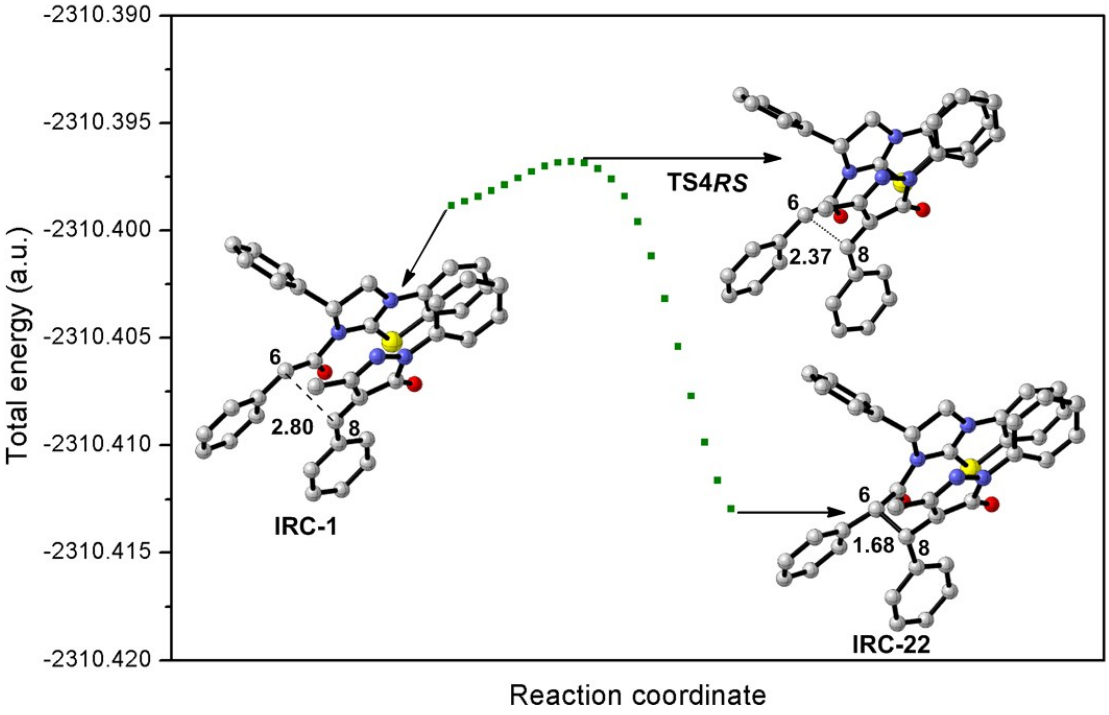
Table S2 The relative Gibbs free energies (**ΔG**) for different conformations of **TS4*RR&SR&RS&SS***, **TS4′*RR&SR&RS&SS***, and **TS4′′*RR&SR&RS&SS*** with the energy of **R1'+R2+Cat** as 0.0 kcal/mol (unit: kcal/mol)

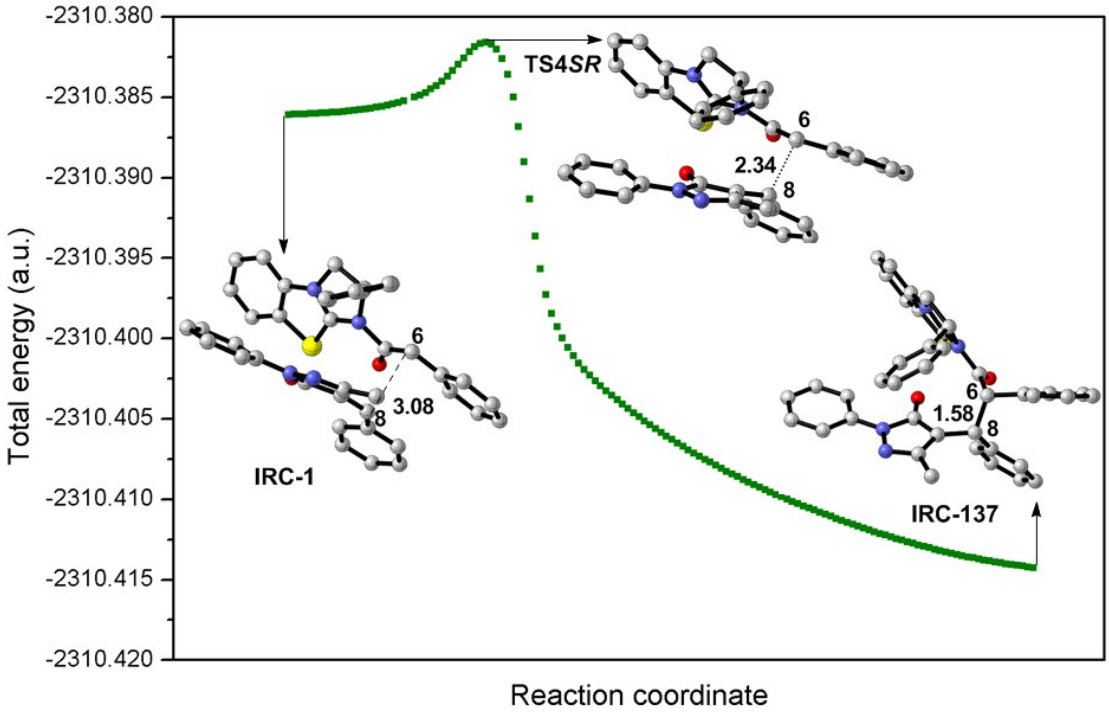
SP	Energy
TS4(*RR*)	8.1
TS4′(*RR*)	17.8

TS4″(*RR*)	12.5
TS4(*RS*)	10.7
TS4′(*RS*)	18.3
TS4″(*RS*)	14.2
TS4(*SR*)	19.1
TS4′(*SR*)	21.2
TS4″(*SR*)	23.4
TS4(*SS*)	17.4
TS4′(*SS*)	22.6
TS4″(*SS*)	18.8

Part 3: IRC results of TS4*RR*, TS4*RS*, TS4*SR*, and TS4*SS*




-2310.390
-2310.395
-2310.400
-2310.405
-2310.410
-2310.415
-2310.420
Total energy (a.u.)
TS4RS
6
2.37
8
6
2.80
8
IRC-1
6
1.68
8
IRC-22
Reaction coordinate


-2310.380
-2310.385
-2310.390
-2310.395
-2310.400
-2310.405
-2310.410
-2310.415
-2310.420
Total energy (a.u.)
TS4SR
6
2.34
8
6
3.08
8
IRC-1
6
1.58
8
IRC-137
Reaction coordinate

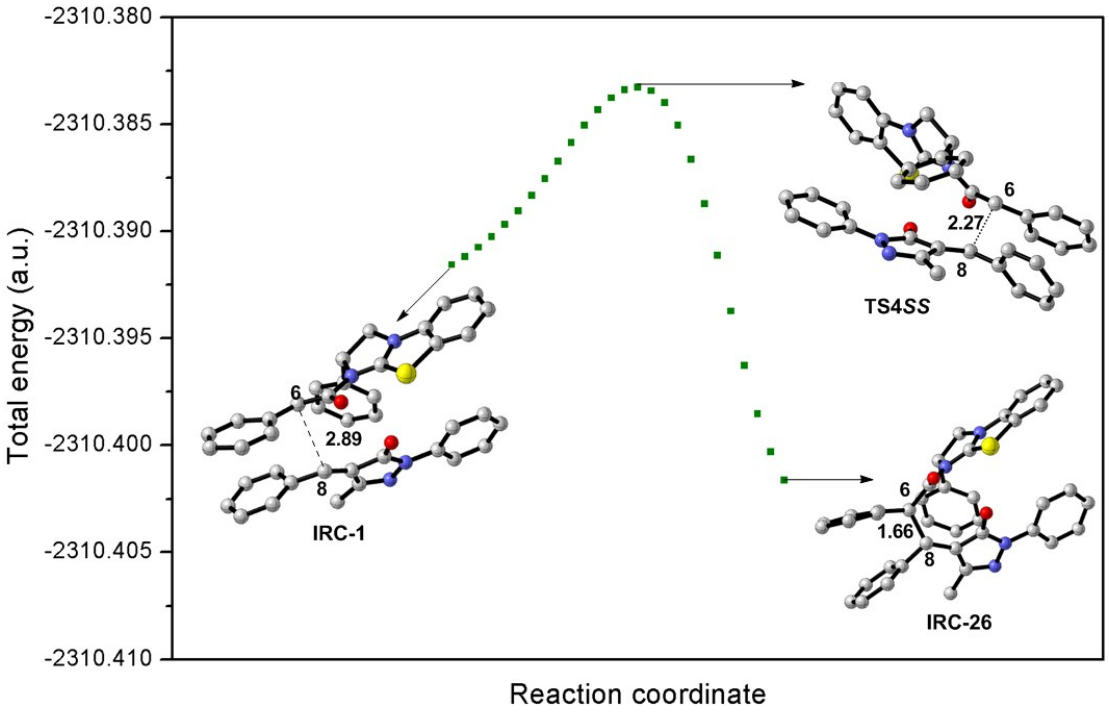
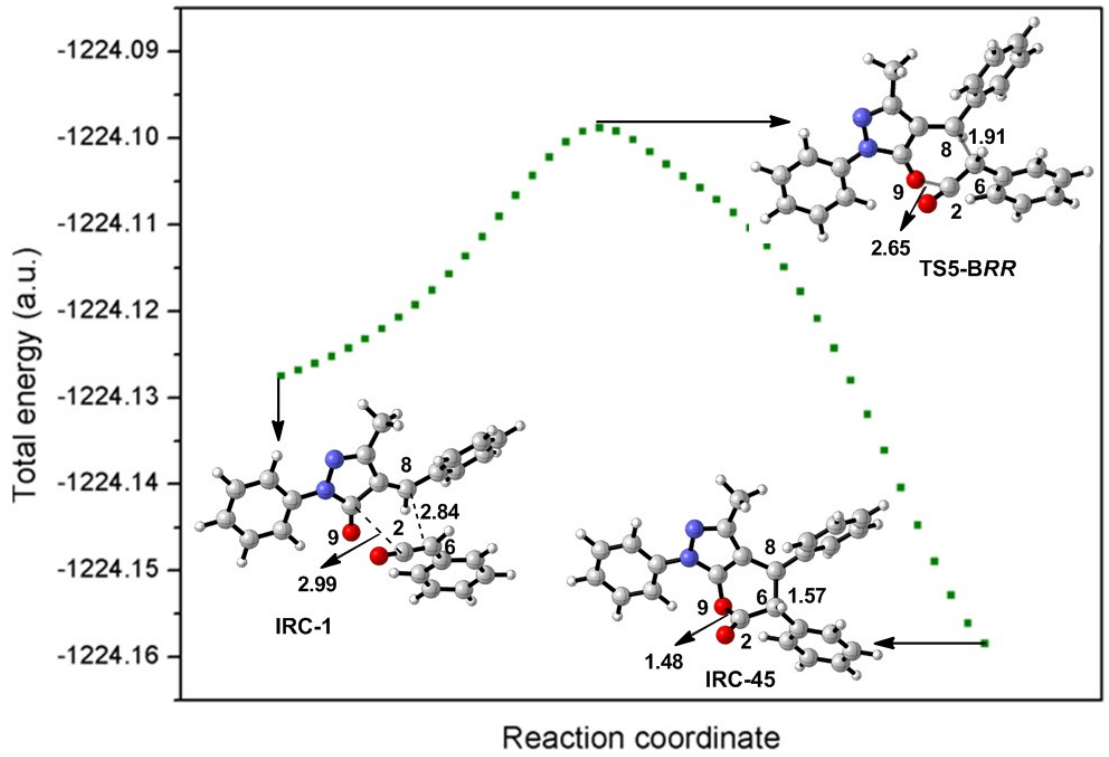
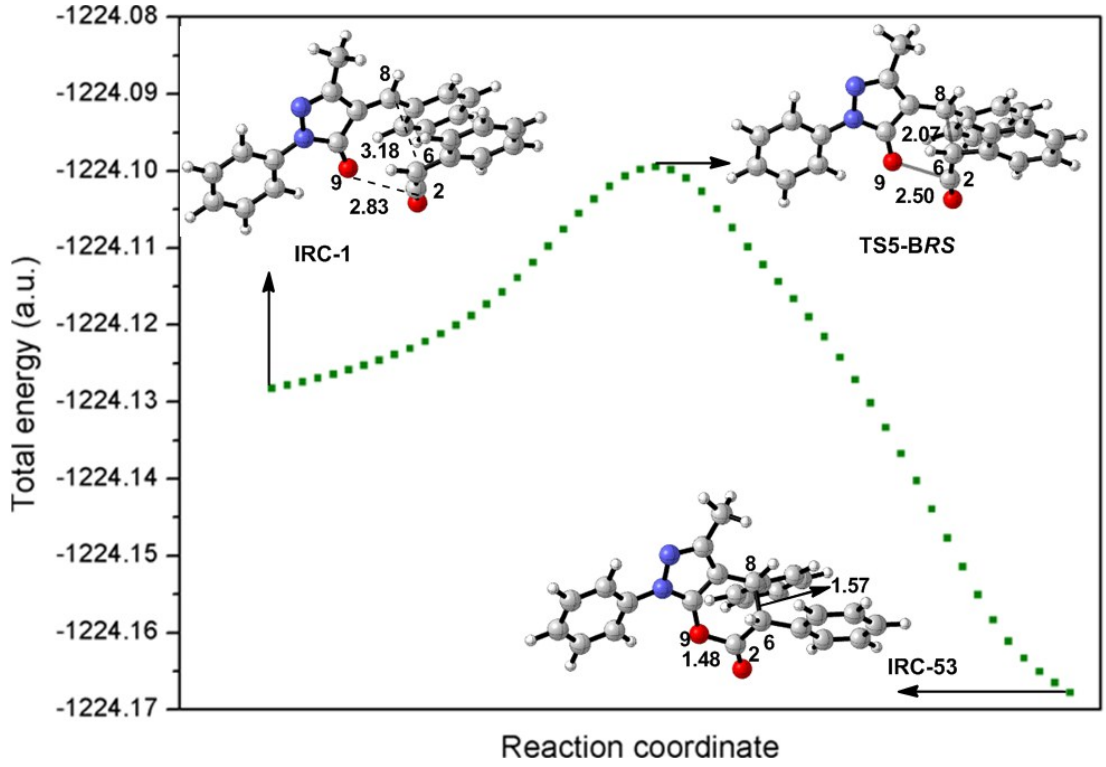
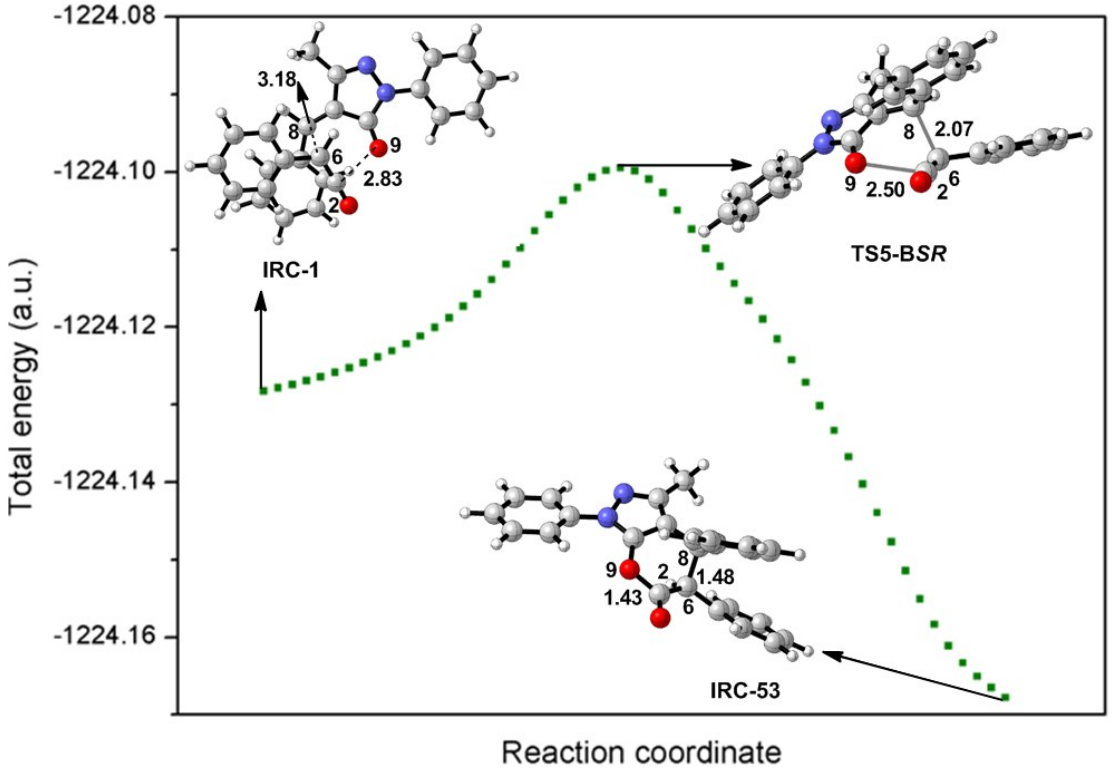


Fig. S3 IRC results of **TS4*RR***, **TS4*RS***, **TS4*SR***, and **TS4*SS***

Part 4: IRC results of TS5B-*RR*, TS5B-*RS*, TS5B-*SR*, and TS5B-*SS*




-1224.08
-1224.09
-1224.10
-1224.11
-1224.12
-1224.13
-1224.14
-1224.15
-1224.16
-1224.17
Total energy (a.u.)
Reaction coordinate
IRC-1
TS5-B*RS*
IRC-53
3.18
2.83
2.07
2.50
1.57
1.48


-1224.08
-1224.10
-1224.12
-1224.14
-1224.16
Total energy (a.u.)
Reaction coordinate
IRC-1
TS5-B*SR*
IRC-53
3.18
2.83
2.07
2.50
1.43
1.48

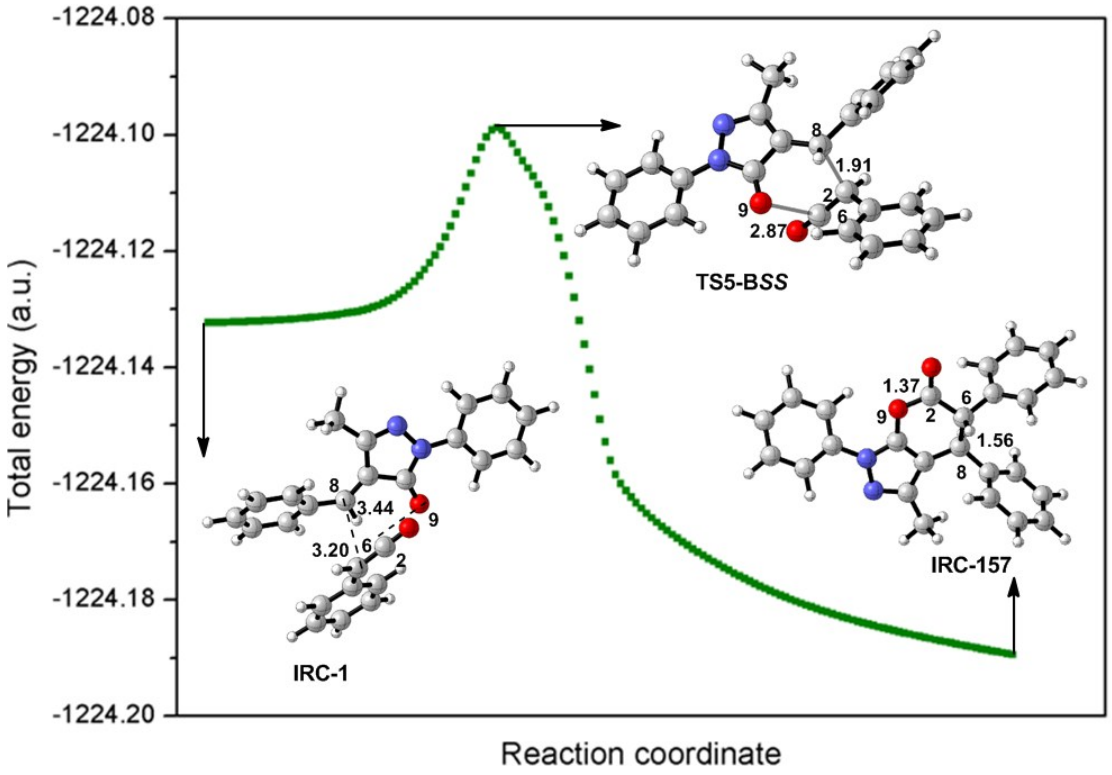


Fig. S4 IRC results of **TS5B-*RR***, **TS5B-*RS***, **TS5B-*SR***, and **TS5B-*SS***

Part 5: The $\Delta\Delta G^{\neq}$ of the TS4s calculated at the M06-2X/6-31++G(2df, 2pd) and M06-2X-D3/6-311++G(2df, 2pd) levels

We have compared the $\Delta\Delta G^{\neq}$ of the **TS4**s calculated at the M06-2X/6-311++G(2df, 2pd) and M06-2X-D3/6-311++G(2df, 2pd) levels. As shown in Table S3, there are tiny differences for the $\Delta\Delta G^{\neq}$ of the key transition states **TS4**s, indicating the selected method is proper and reliable in this kind of reaction system.

Table S3 The $\Delta\Delta G^{\neq}$ calculated at the M06-2X/6-31++G(2df, 2pd) level and M06-2X-D3/6-311++G(2df, 2pd) level of the **TS4**s (unit in kcal/mol)

	$\Delta\Delta G^{\neq}_{TS4RR}$	$\Delta\Delta G^{\neq}_{TS4RS}$	$\Delta\Delta G^{\neq}_{TS4SR}$	$\Delta\Delta G^{\neq}_{TS4SS}$
M06-2X/6-311++G(2df, 2pd)	0.0	1.1	1.0	3.1
M06-2X-D3/6-311++G(2df, 2pd)	0.0	1.0	0.9	3.0

Part 6: List of the energies and Cartesian coordinates of all the structures involved in the reaction

R1

Total Energy= -730.43156416
Sum of electronic and zero-point Energies= -730.163895
Sum of electronic and thermal Energies= -730.147865
Sum of electronic and thermal Enthalpies= -730.146921
Sum of electronic and thermal Free Energies= -730.210377

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.013198	-1.892202	0.322770
2	8	0	-0.421014	-2.885730	-0.203418
3	6	0	1.323469	-1.727032	1.011340
4	1	0	1.127489	-1.607264	2.082136
5	1	0	1.875561	-2.656439	0.862877
6	6	0	2.077602	-0.528420	0.479713
7	6	0	2.014075	0.700877	1.137786
8	6	0	2.809347	-0.629532	-0.704917
9	6	0	2.669766	1.814398	0.619760
10	1	0	1.446646	0.783152	2.061348
11	6	0	3.467687	0.482511	-1.223906
12	1	0	2.863261	-1.584080	-1.222158
13	6	0	3.397467	1.707158	-0.563521
14	1	0	2.613550	2.764701	1.141151
15	1	0	4.034684	0.392323	-2.144921
16	1	0	3.909775	2.573964	-0.968297
17	8	0	-0.742393	-0.727341	0.430931
18	6	0	-1.722209	-0.386082	-0.483700
19	8	0	-1.862921	-0.950537	-1.530181
20	6	0	-2.503623	0.819347	0.011023
21	6	0	-3.596260	1.139161	-1.007751
22	1	0	-4.157993	2.016200	-0.675011
23	1	0	-3.166044	1.352071	-1.989301
24	1	0	-4.290138	0.301382	-1.114879
25	6	0	-1.526903	2.000922	0.139384
26	1	0	-2.078542	2.884768	0.472721
27	1	0	-0.737853	1.785866	0.863844
28	1	0	-1.059534	2.231067	-0.822905
29	6	0	-3.119315	0.497173	1.380575
30	1	0	-3.796326	-0.360005	1.318121
31	1	0	-2.346370	0.280006	2.121123
32	1	0	-3.694992	1.361472	1.724166

R2

Total Energy= -840.62228852
Sum of electronic and zero-point Energies= -840.348965
Sum of electronic and thermal Energies= -840.332824
Sum of electronic and thermal Enthalpies= -840.331879
Sum of electronic and thermal Free Energies= -840.394320

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.297799	-0.166451	0.004929
2	6	0	-0.649735	0.983244	-0.006614
3	6	0	0.223941	2.156710	-0.049582
4	7	0	1.470465	1.827624	-0.070488
5	7	0	1.542769	0.437896	-0.053207
6	6	0	2.815807	-0.176272	-0.027817
7	6	0	3.936488	0.602004	0.282190
8	6	0	2.966965	-1.536193	-0.320430
9	6	0	5.197566	0.018064	0.301206
10	1	0	3.807243	1.654484	0.499450
11	6	0	4.237881	-2.102910	-0.289213
12	1	0	2.102474	-2.135516	-0.566727
13	6	0	5.358154	-1.336703	0.019446
14	1	0	6.060118	0.630607	0.543615
15	1	0	4.347385	-3.158541	-0.516704
16	1	0	6.344309	-1.788219	0.039199
17	6	0	-0.206880	3.584321	-0.073031
18	1	0	-0.798829	3.826714	0.814190
19	1	0	0.672425	4.228183	-0.098417
20	1	0	-0.822495	3.790862	-0.953369
21	6	0	-2.001624	1.071112	-0.010714
22	1	0	-2.368232	2.097875	-0.052773
23	6	0	-3.083127	0.094975	0.019869
24	6	0	-4.387549	0.609887	-0.099773
25	6	0	-2.913904	-1.293187	0.166796
26	6	0	-5.491621	-0.230374	-0.084800
27	1	0	-4.527333	1.681892	-0.207973
28	6	0	-4.024080	-2.128526	0.186812
29	1	0	-1.916033	-1.701177	0.263661
30	6	0	-5.310475	-1.604811	0.059476
31	1	0	-6.489344	0.183760	-0.182504
32	1	0	-3.884815	-3.198364	0.302796
33	1	0	-6.170519	-2.266509	0.074331

34	8	0	0.094672	-1.371753	0.054323

Cat

Total Energy= -1086.21727870

Sum of electronic and zero-point Energies= -1085.978961

Sum of electronic and thermal Energies= -1085.965362

Sum of electronic and thermal Enthalpies= -1085.964418

Sum of electronic and thermal Free Energies= -1086.021707

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.535755	-1.070978	0.522392
2	6	0	-0.393088	1.012277	0.634557
3	6	0	-1.379985	-0.139747	1.023736
4	6	0	2.125506	0.599261	0.148117
5	6	0	2.893826	-0.545091	-0.130548
6	6	0	4.207562	-0.434824	-0.554499
7	1	0	4.796579	-1.320371	-0.767941
8	6	0	4.751411	0.842214	-0.714981
9	6	0	3.985217	1.976546	-0.452919
10	6	0	2.664816	1.870336	-0.015702
11	1	0	-0.375877	1.817020	1.371346
12	1	0	5.776778	0.945904	-1.051643
13	1	0	4.419550	2.961408	-0.587691
14	1	0	2.067904	2.750623	0.197836
15	16	0	1.959359	-2.037456	0.131685
16	7	0	0.860828	0.271255	0.601032
17	7	0	-0.680164	-1.406285	0.706796
18	6	0	-2.713770	-0.006043	0.327491
19	6	0	-2.921175	-0.570554	-0.932601
20	6	0	-3.736457	0.737169	0.918196
21	6	0	-4.135045	-0.393494	-1.590771
22	1	0	-2.127811	-1.158597	-1.384242
23	6	0	-4.949455	0.920268	0.258341
24	1	0	-3.583733	1.172277	1.902934
25	6	0	-5.151246	0.354460	-0.998357
26	1	0	-4.289210	-0.841886	-2.567306
27	1	0	-5.738411	1.498318	0.729015
28	1	0	-6.097869	0.491286	-1.511153
29	1	0	-0.619926	1.426126	-0.356286
30	1	0	-1.545597	-0.108400	2.108650

PivOH

Total Energy= -346.88654388
Sum of electronic and zero-point Energies= -346.738244
Sum of electronic and thermal Energies= -346.730114
Sum of electronic and thermal Enthalpies= -346.729170
Sum of electronic and thermal Free Energies= -346.770350

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.602109	0.986575	0.000050
2	6	0	-0.938088	-0.183223	0.000032
3	8	0	-1.514636	-1.246378	-0.000005
4	6	0	0.570470	0.009823	0.000000
5	6	0	1.244130	-1.360626	0.000300
6	1	0	2.330448	-1.234289	0.000382
7	1	0	0.959401	-1.936277	0.884594
8	1	0	0.959554	-1.936605	-0.883821
9	6	0	0.962987	0.802407	1.256637
10	1	0	2.048289	0.938850	1.272481
11	1	0	0.488468	1.786297	1.264672
12	1	0	0.673413	0.267351	2.166103
13	6	0	0.962955	0.801878	-1.256998
14	1	0	0.673522	0.266370	-2.166241
15	1	0	0.488292	1.785698	-1.265519
16	1	0	2.048234	0.938472	-1.272830
17	1	0	-2.550385	0.781001	-0.000016

***Re*-TS1**

Total Energy= -1816.64891938
Sum of electronic and zero-point Energies= -1816.140843
Sum of electronic and thermal Energies= -1816.111022
Sum of electronic and thermal Enthalpies= -1816.110078
Sum of electronic and thermal Free Energies= -1816.204139

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.331644	0.016395	-0.377988
2	6	0	2.468253	1.107983	1.295480
3	6	0	1.026994	1.672102	1.122454
4	6	0	3.522352	-0.716812	-0.261009

5	6	0	3.009421	-1.591645	-1.230242
6	6	0	3.810890	-2.566898	-1.804695
7	1	0	3.414208	-3.244339	-2.552565
8	6	0	5.138864	-2.654715	-1.388785
9	6	0	5.645180	-1.785261	-0.420133
10	6	0	4.845544	-0.802145	0.156142
11	1	0	2.588576	0.556630	2.231217
12	1	0	5.783107	-3.410011	-1.824334
13	1	0	6.680343	-1.873356	-0.109308
14	1	0	5.232974	-0.121949	0.906710
15	16	0	1.289163	-1.276459	-1.542595
16	7	0	2.556139	0.179494	0.167541
17	7	0	0.415640	0.813330	0.080845
18	6	0	0.954205	3.120940	0.689369
19	6	0	-0.072151	3.930910	1.176303
20	6	0	1.857374	3.644636	-0.239386
21	6	0	-0.181113	5.255275	0.757465
22	1	0	-0.793414	3.504326	1.866975
23	6	0	1.748593	4.966798	-0.659323
24	1	0	2.648465	3.017114	-0.644845
25	6	0	0.731095	5.776389	-0.157294
26	1	0	-0.979377	5.880281	1.144996
27	1	0	2.456927	5.365218	-1.378576
28	1	0	0.648047	6.808574	-0.482165
29	1	0	3.230469	1.886001	1.223246
30	1	0	0.433754	1.520748	2.025846
31	6	0	-1.249701	0.503312	0.263697
32	8	0	-1.663915	1.065680	1.285445
33	6	0	-1.827467	0.847290	-1.114337
34	1	0	-1.730013	1.932603	-1.214324
35	1	0	-1.233359	0.375099	-1.903706
36	6	0	-3.266829	0.410114	-1.203841
37	6	0	-4.263330	1.118900	-0.527404
38	6	0	-3.619868	-0.742282	-1.909189
39	6	0	-5.586364	0.687125	-0.561718
40	1	0	-3.986750	2.003104	0.038869
41	6	0	-4.942912	-1.176989	-1.946784
42	1	0	-2.846870	-1.302460	-2.429878
43	6	0	-5.930168	-0.462182	-1.271916
44	1	0	-6.351395	1.246805	-0.032327
45	1	0	-5.202594	-2.072634	-2.502667
46	1	0	-6.962085	-0.797750	-1.299718
47	8	0	-1.246064	-0.985533	0.284017
48	6	0	-0.706706	-1.626962	1.329166

49	8	0	0.145380	-1.156061	2.053982
50	6	0	-1.300254	-3.023826	1.489273
51	6	0	-2.788164	-2.848082	1.835830
52	1	0	-3.249919	-3.831092	1.970602
53	1	0	-2.909611	-2.282367	2.764864
54	1	0	-3.311834	-2.317774	1.035868
55	6	0	-0.570466	-3.758963	2.611135
56	1	0	-0.999499	-4.757415	2.737040
57	1	0	0.493777	-3.864042	2.382721
58	1	0	-0.660543	-3.218896	3.556824
59	6	0	-1.167356	-3.792687	0.167315
60	1	0	-1.683264	-3.268754	-0.640908
61	1	0	-0.116317	-3.918282	-0.112269
62	1	0	-1.611446	-4.786810	0.279566

_Si_-TS1

Total Energy= -1816.65220125
Sum of electronic and zero-point Energies= -1816.144950
Sum of electronic and thermal Energies= -1816.114876
Sum of electronic and thermal Enthalpies= -1816.113932
Sum of electronic and thermal Free Energies= -1816.208984

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.784862	-0.085917	-0.513759
2	6	0	2.269492	1.527477	1.047896
3	6	0	0.731707	1.348433	0.843766
4	6	0	4.057170	-0.029011	-0.060786
5	6	0	4.011058	-1.000596	-1.071899
6	6	0	5.176383	-1.599572	-1.527304
7	1	0	5.143310	-2.353720	-2.306513
8	6	0	6.389993	-1.201208	-0.966726
9	6	0	6.429684	-0.227856	0.032949
10	6	0	5.262832	0.371141	0.502823
11	1	0	2.567341	1.444172	2.093958
12	1	0	7.311539	-1.652663	-1.316846
13	1	0	7.383511	0.070554	0.454356
14	1	0	5.286837	1.124978	1.282394
15	16	0	2.346185	-1.318482	-1.609379
16	7	0	2.782382	0.414185	0.255688
17	7	0	0.619467	0.445849	-0.324692
18	6	0	-0.006630	2.647601	0.628136

19	6	0	-0.987950	3.069453	1.522807
20	6	0	0.274210	3.423448	-0.499986
21	6	0	-1.679825	4.259801	1.297492
22	1	0	-1.216436	2.461944	2.394988
23	6	0	-0.414573	4.609000	-0.726405
24	1	0	1.021896	3.081449	-1.211656
25	6	0	-1.393979	5.029662	0.173895
26	1	0	-2.443678	4.581391	1.998060
27	1	0	-0.192958	5.203157	-1.606997
28	1	0	-1.934089	5.953816	-0.004277
29	1	0	2.628043	2.478804	0.639773
30	1	0	0.305073	0.829032	1.711940
31	6	0	-0.850726	-0.582339	-0.792779
32	8	0	-0.441202	-1.536127	-1.448325
33	6	0	-1.768530	0.480418	-1.390284
34	1	0	-1.821114	1.345319	-0.726171
35	1	0	-1.310635	0.790576	-2.333595
36	6	0	-3.143492	-0.103754	-1.608635
37	6	0	-4.197462	0.223421	-0.753077
38	6	0	-3.368996	-1.021610	-2.637946
39	6	0	-5.456876	-0.347439	-0.925929
40	1	0	-4.025123	0.931945	0.053811
41	6	0	-4.626151	-1.592787	-2.814417
42	1	0	-2.544120	-1.293786	-3.290027
43	6	0	-5.674075	-1.256528	-1.958919
44	1	0	-6.268118	-0.081649	-0.255183
45	1	0	-4.788216	-2.303978	-3.618435
46	1	0	-6.654588	-1.701353	-2.096395
47	8	0	-1.351083	-0.807621	0.550051
48	6	0	-0.704327	-1.622011	1.405543
49	8	0	0.447081	-1.967712	1.279570
50	6	0	-1.606495	-1.998316	2.577407
51	6	0	-2.004143	-0.708910	3.313905
52	1	0	-2.652362	-0.956683	4.160050
53	1	0	-1.121218	-0.192083	3.706702
54	1	0	-2.543695	-0.029250	2.649105
55	6	0	-0.843953	-2.931668	3.514798
56	1	0	-1.478474	-3.198729	4.364814
57	1	0	-0.550343	-3.848839	2.997817
58	1	0	0.062939	-2.452805	3.892715
59	6	0	-2.863155	-2.690927	2.029017
60	1	0	-3.417482	-2.027302	1.360317
61	1	0	-2.600800	-3.598386	1.476535
62	1	0	-3.513628	-2.975190	2.861965

***Re*-M1**

Total Energy= -1816.64949412

Sum of electronic and zero-point Energies= -1816.141750

Sum of electronic and thermal Energies= -1816.111204

Sum of electronic and thermal Enthalpies= -1816.110259

Sum of electronic and thermal Free Energies= -1816.205823

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.490387	-0.047136	-0.273098
2	6	0	2.566877	1.663261	0.819420
3	6	0	1.019055	1.800412	0.937803
4	6	0	3.769228	-0.420118	-0.231241
5	6	0	3.336447	-1.521540	-0.983823
6	6	0	4.245496	-2.443894	-1.481621
7	1	0	3.912891	-3.297852	-2.061332
8	6	0	5.599495	-2.236572	-1.222826
9	6	0	6.026802	-1.134843	-0.478205
10	6	0	5.118039	-0.210662	0.030708
11	1	0	3.065487	1.676739	1.789160
12	1	0	6.327233	-2.941421	-1.608503
13	1	0	7.085285	-0.992792	-0.290372
14	1	0	5.442376	0.645081	0.612451
15	16	0	1.567723	-1.543919	-1.150272
16	7	0	2.692671	0.353520	0.179427
17	7	0	0.510981	0.766625	0.008929
18	6	0	0.516653	3.180227	0.590237
19	6	0	0.021828	4.018366	1.587243
20	6	0	0.575645	3.639675	-0.727483
21	6	0	-0.403385	5.307204	1.273971
22	1	0	-0.039804	3.654478	2.608895
23	6	0	0.142547	4.923824	-1.043569
24	1	0	0.949549	2.980805	-1.507977
25	6	0	-0.344604	5.761428	-0.041269
26	1	0	-0.788545	5.953524	2.056019
27	1	0	0.184413	5.271119	-2.070922
28	1	0	-0.681489	6.763418	-0.286658
29	1	0	2.995464	2.434146	0.171063
30	1	0	0.673391	1.512973	1.935108
31	6	0	-1.077185	0.409259	0.123769
32	8	0	-1.577167	0.973897	1.111329

33	6	0	-1.654254	0.653835	-1.281222
34	1	0	-1.625468	1.738036	-1.431025
35	1	0	-1.019929	0.182580	-2.039629
36	6	0	-3.060697	0.120627	-1.356360
37	6	0	-4.094797	0.766985	-0.673227
38	6	0	-3.342445	-1.065290	-2.037969
39	6	0	-5.382808	0.238676	-0.674476
40	1	0	-3.869859	1.674648	-0.122339
41	6	0	-4.630244	-1.596721	-2.042106
42	1	0	-2.539832	-1.579359	-2.561409
43	6	0	-5.654811	-0.945401	-1.358321
44	1	0	-6.176712	0.750313	-0.138828
45	1	0	-4.833266	-2.519560	-2.576985
46	1	0	-6.659377	-1.356770	-1.359308
47	8	0	-1.028724	-1.104955	0.181091
48	6	0	-0.676428	-1.672497	1.341119
49	8	0	0.133105	-1.194317	2.108635
50	6	0	-1.428242	-2.978162	1.575467
51	6	0	-0.899320	-3.653571	2.837590
52	1	0	-1.447739	-4.582727	3.019458
53	1	0	0.163239	-3.892154	2.736786
54	1	0	-1.016838	-3.002514	3.707308
55	6	0	-1.255495	-3.894724	0.356940
56	1	0	-1.802645	-4.828310	0.522060
57	1	0	-1.645856	-3.415800	-0.544525
58	1	0	-0.201197	-4.141930	0.194250
59	6	0	-2.912985	-2.606954	1.733035
60	1	0	-3.057307	-1.923108	2.575679
61	1	0	-3.285382	-2.121083	0.825822
62	1	0	-3.499747	-3.511943	1.920256

***Si*-M1**

Total Energy= -1816.65582558
Sum of electronic and zero-point Energies= -1816.146433
Sum of electronic and thermal Energies= -1816.116482
Sum of electronic and thermal Enthalpies= -1816.115538
Sum of electronic and thermal Free Energies= -1816.209554

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.864433	-0.070199	-0.519250
2	6	0	2.246441	1.860381	0.663822

3	6	0	0.741893	1.495816	0.656430
4	6	0	4.111828	0.156925	-0.063762
5	6	0	4.101670	-1.022760	-0.819840
6	6	0	5.289450	-1.690339	-1.090436
7	1	0	5.290884	-2.607222	-1.669846
8	6	0	6.477576	-1.149982	-0.602814
9	6	0	6.477076	0.032154	0.143081
10	6	0	5.291655	0.704019	0.426449
11	1	0	2.619361	2.053561	1.669645
12	1	0	7.414821	-1.655422	-0.807076
13	1	0	7.414458	0.433934	0.511676
14	1	0	5.281554	1.618334	1.009476
15	16	0	2.452776	-1.491461	-1.296797
16	7	0	2.817029	0.634282	0.107355
17	7	0	0.666767	0.468783	-0.421573
18	6	0	-0.205947	2.650380	0.473252
19	6	0	-1.274311	2.789946	1.358021
20	6	0	-0.076328	3.540610	-0.595601
21	6	0	-2.206519	3.810117	1.182624
22	1	0	-1.384641	2.083675	2.176316
23	6	0	-1.007268	4.559336	-0.772519
24	1	0	0.735059	3.420878	-1.308883
25	6	0	-2.074174	4.694682	0.115631
26	1	0	-3.035989	3.909292	1.875057
27	1	0	-0.905784	5.244116	-1.608038
28	1	0	-2.801957	5.486628	-0.027515
29	1	0	2.479944	2.708761	0.012117
30	1	0	0.507713	0.978599	1.594664
31	6	0	-0.563490	-0.411256	-0.784522
32	8	0	-0.194090	-1.492482	-1.321326
33	6	0	-1.582626	0.455235	-1.551732
34	1	0	-1.738565	1.414394	-1.054929
35	1	0	-1.131703	0.642774	-2.531760
36	6	0	-2.897766	-0.268273	-1.684736
37	6	0	-4.009185	0.147665	-0.947663
38	6	0	-3.017724	-1.392249	-2.506171
39	6	0	-5.217715	-0.540981	-1.028517
40	1	0	-3.917549	1.016868	-0.299399
41	6	0	-4.223215	-2.084194	-2.588398
42	1	0	-2.147049	-1.728597	-3.059488
43	6	0	-5.327493	-1.660632	-1.850534
44	1	0	-6.072691	-0.204964	-0.449488
45	1	0	-4.300911	-2.957379	-3.229277
46	1	0	-6.267772	-2.199207	-1.916425

47	8	0	-1.255591	-0.558388	0.568546
48	6	0	-0.695798	-1.328850	1.496480
49	8	0	0.495914	-1.563725	1.566611
50	6	0	-1.735215	-1.860755	2.481800
51	6	0	-2.456792	-0.667494	3.125808
52	1	0	-3.206870	-1.029956	3.835915
53	1	0	-1.752725	-0.031999	3.675077
54	1	0	-2.958303	-0.061733	2.366635
55	6	0	-1.041960	-2.703539	3.549252
56	1	0	-1.782365	-3.089499	4.256356
57	1	0	-0.516868	-3.549026	3.097702
58	1	0	-0.309259	-2.109816	4.102537
59	6	0	-2.743614	-2.707049	1.688651
60	1	0	-3.230190	-2.105566	0.915145
61	1	0	-2.246736	-3.553748	1.204380
62	1	0	-3.506003	-3.101294	2.368211

***Re*-TS2**

Total Energy= -1816.64580370
Sum of electronic and zero-point Energies= -1816.138323
Sum of electronic and thermal Energies= -1816.109116
Sum of electronic and thermal Enthalpies= -1816.108172
Sum of electronic and thermal Free Energies= -1816.200427

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.436569	-0.038739	-0.394511
2	6	0	2.490400	1.642749	0.775063
3	6	0	0.947658	1.766399	0.909356
4	6	0	3.710483	-0.392165	-0.334900
5	6	0	3.292968	-1.476835	-1.116533
6	6	0	4.216023	-2.385766	-1.617963
7	1	0	3.898225	-3.230623	-2.218530
8	6	0	5.562472	-2.174809	-1.332311
9	6	0	5.973119	-1.086681	-0.555876
10	6	0	5.052705	-0.178671	-0.042642
11	1	0	2.989368	1.599687	1.743535
12	1	0	6.300969	-2.867168	-1.720191
13	1	0	7.027753	-0.944943	-0.347927
14	1	0	5.362030	0.666448	0.562150
15	16	0	1.528580	-1.517104	-1.280690
16	7	0	2.621262	0.371129	0.064767

17	7	0	0.452718	0.794339	-0.099801
18	6	0	0.440249	3.165063	0.663253
19	6	0	-0.062732	3.918848	1.721274
20	6	0	0.500797	3.725855	-0.614524
21	6	0	-0.494858	5.225702	1.509026
22	1	0	-0.125857	3.476084	2.711207
23	6	0	0.060636	5.028132	-0.829326
24	1	0	0.882073	3.134973	-1.444393
25	6	0	-0.435079	5.781680	0.233698
26	1	0	-0.886397	5.805426	2.338627
27	1	0	0.104593	5.455368	-1.825964
28	1	0	-0.778085	6.797551	0.066395
29	1	0	2.917816	2.448098	0.170021
30	1	0	0.615930	1.394134	1.882057
31	6	0	-1.014752	0.515178	-0.125510
32	8	0	-1.646133	1.040089	0.773006
33	6	0	-1.543820	0.374215	-1.547166
34	1	0	-1.472623	1.381853	-1.977360
35	1	0	-0.894474	-0.283870	-2.129727
36	6	0	-2.968788	-0.110780	-1.569195
37	6	0	-4.014872	0.771525	-1.292791
38	6	0	-3.265574	-1.450350	-1.828705
39	6	0	-5.334273	0.325623	-1.278880
40	1	0	-3.788170	1.812469	-1.080243
41	6	0	-4.583644	-1.899198	-1.820023
42	1	0	-2.451533	-2.142541	-2.023279
43	6	0	-5.622193	-1.011531	-1.543366
44	1	0	-6.137685	1.022939	-1.062285
45	1	0	-4.800172	-2.942972	-2.026356
46	1	0	-6.650145	-1.360163	-1.535239
47	8	0	-0.934065	-1.367622	0.161449
48	6	0	-0.550902	-1.683259	1.355164
49	8	0	0.359283	-1.118538	1.973302
50	6	0	-1.358365	-2.825916	1.994345
51	6	0	-0.743298	-3.234171	3.329826
52	1	0	-1.338346	-4.028277	3.793443
53	1	0	0.278103	-3.601979	3.194456
54	1	0	-0.702288	-2.382215	4.012860
55	6	0	-1.394972	-4.017176	1.030596
56	1	0	-1.988236	-4.832176	1.459549
57	1	0	-1.841300	-3.719915	0.078479
58	1	0	-0.386038	-4.398179	0.836750
59	6	0	-2.784027	-2.291814	2.199561
60	1	0	-2.782305	-1.424211	2.868016

61	1	0	-3.214294	-1.984197	1.241868
62	1	0	-3.418316	-3.066299	2.644658

_Si_-TS2

Total Energy= -1816.65336459
Sum of electronic and zero-point Energies= -1816.144417
Sum of electronic and thermal Energies= -1816.114824
Sum of electronic and thermal Enthalpies= -1816.113880
Sum of electronic and thermal Free Energies= -1816.206581

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.510401	0.071552	-0.580707
2	6	0	2.101287	1.366847	1.229550
3	6	0	0.570463	1.500511	0.939813
4	6	0	3.756787	-0.115253	-0.153255
5	6	0	3.602072	-1.039011	-1.194683
6	6	0	4.692427	-1.762671	-1.660812
7	1	0	4.579832	-2.482948	-2.463638
8	6	0	5.931467	-1.541693	-1.064380
9	6	0	6.075792	-0.618938	-0.023765
10	6	0	4.989744	0.111164	0.447532
11	1	0	2.296102	0.882595	2.188074
12	1	0	6.795435	-2.096572	-1.412583
13	1	0	7.050824	-0.467205	0.425809
14	1	0	5.093732	0.830751	1.251910
15	16	0	1.913178	-1.141076	-1.735407
16	7	0	2.543185	0.493529	0.143942
17	7	0	0.368695	0.661700	-0.264830
18	6	0	0.135456	2.933292	0.733180
19	6	0	-0.518283	3.609410	1.762721
20	6	0	0.410810	3.600192	-0.462664
21	6	0	-0.892565	4.941788	1.602124
22	1	0	-0.740898	3.088419	2.690213
23	6	0	0.032263	4.928994	-0.625244
24	1	0	0.908334	3.071093	-1.271548
25	6	0	-0.619095	5.602633	0.407690
26	1	0	-1.404531	5.458954	2.407000
27	1	0	0.241911	5.439190	-1.559753
28	1	0	-0.916639	6.638062	0.278175
29	1	0	2.612534	2.330407	1.178546
30	1	0	-0.001905	1.036698	1.747114

31	6	0	-0.909488	-0.007261	-0.638915
32	8	0	-0.774744	-0.851853	-1.537912
33	6	0	-2.074242	0.984333	-0.652884
34	1	0	-2.109810	1.539716	0.287217
35	1	0	-1.851774	1.697755	-1.455389
36	6	0	-3.380597	0.283246	-0.911821
37	6	0	-4.235598	-0.045467	0.142230
38	6	0	-3.744021	-0.079085	-2.210511
39	6	0	-5.431497	-0.718528	-0.095226
40	1	0	-3.947645	0.217627	1.156409
41	6	0	-4.938911	-0.751918	-2.452933
42	1	0	-3.077657	0.163483	-3.033101
43	6	0	-5.787168	-1.073172	-1.395277
44	1	0	-6.085192	-0.966768	0.735460
45	1	0	-5.207907	-1.025656	-3.468562
46	1	0	-6.719953	-1.595647	-1.582795
47	8	0	-1.312040	-0.773683	0.869957
48	6	0	-0.473695	-1.646570	1.362771
49	8	0	0.728274	-1.438525	1.532434
50	6	0	-1.102772	-3.011414	1.663036
51	6	0	-2.469538	-2.835248	2.332456
52	1	0	-2.921749	-3.816240	2.513042
53	1	0	-2.374574	-2.323728	3.296295
54	1	0	-3.136798	-2.251300	1.694048
55	6	0	-0.174298	-3.846979	2.540263
56	1	0	-0.601905	-4.842620	2.696736
57	1	0	0.807337	-3.954664	2.073692
58	1	0	-0.031801	-3.377586	3.518653
59	6	0	-1.288341	-3.674019	0.287320
60	1	0	-1.886471	-3.030725	-0.364542
61	1	0	-0.320058	-3.838679	-0.197190
62	1	0	-1.787869	-4.641742	0.401964

***Re*-M2**

Total Energy= -1816.65679597

Sum of electronic and zero-point Energies= -1816.147745

Sum of electronic and thermal Energies= -1816.117129

Sum of electronic and thermal Enthalpies= -1816.116185

Sum of electronic and thermal Free Energies= -1816.211300

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

1	6	0	1.244815	0.003562	-0.694059
2	6	0	2.157488	1.030120	1.162821
3	6	0	0.659923	1.419333	1.042769
4	6	0	3.485926	-0.432308	-0.523718
5	6	0	3.149409	-1.223209	-1.627381
6	6	0	4.105738	-2.002873	-2.266960
7	1	0	3.846199	-2.616853	-3.121619
8	6	0	5.403219	-1.973625	-1.766983
9	6	0	5.734562	-1.185220	-0.658479
10	6	0	4.782693	-0.399165	-0.021161
11	1	0	2.326831	0.361061	2.006751
12	1	0	6.168459	-2.574976	-2.244406
13	1	0	6.753456	-1.186251	-0.288133
14	1	0	5.032456	0.214426	0.837076
15	16	0	1.432416	-1.083934	-2.013040
16	7	0	2.382360	0.274583	-0.069028
17	7	0	0.206580	0.662628	-0.162878
18	6	0	0.417316	2.900102	0.863602
19	6	0	-0.492752	3.569189	1.678139
20	6	0	1.103681	3.605277	-0.128516
21	6	0	-0.707857	4.935805	1.512406
22	1	0	-1.039774	3.014595	2.435054
23	6	0	0.885858	4.968066	-0.298823
24	1	0	1.809941	3.086522	-0.774696
25	6	0	-0.019387	5.635813	0.525072
26	1	0	-1.417334	5.451391	2.151243
27	1	0	1.420804	5.508639	-1.072671
28	1	0	-0.189252	6.699559	0.394132
29	1	0	2.810235	1.903557	1.198128
30	1	0	0.098393	1.029413	1.893566
31	6	0	-1.182401	0.517615	-0.400201
32	8	0	-1.937694	1.017871	0.396492
33	6	0	-1.589886	-0.164733	-1.686349
34	1	0	-1.242400	0.453369	-2.523692
35	1	0	-1.081403	-1.131376	-1.713547
36	6	0	-3.079517	-0.386861	-1.742039
37	6	0	-3.907580	0.426061	-2.513100
38	6	0	-3.636355	-1.427386	-0.992484
39	6	0	-5.283632	0.202821	-2.541373
40	1	0	-3.475666	1.235517	-3.095961
41	6	0	-5.009756	-1.647931	-1.019725
42	1	0	-2.968216	-2.041636	-0.391296
43	6	0	-5.836433	-0.833990	-1.794831
44	1	0	-5.921258	0.838239	-3.147943

45	1	0	-5.438547	-2.457403	-0.436706
46	1	0	-6.907404	-1.009316	-1.817066
47	8	0	-0.752847	-2.090428	0.309968
48	6	0	-0.165001	-1.952258	1.416922
49	8	0	1.012183	-1.537762	1.571061
50	6	0	-0.998861	-2.290452	2.682795
51	6	0	-0.141988	-2.222282	3.944305
52	1	0	-0.745877	-2.450366	4.830365
53	1	0	0.683552	-2.937996	3.894687
54	1	0	0.292480	-1.226253	4.063822
55	6	0	-1.594059	-3.693316	2.525184
56	1	0	-2.230492	-3.941209	3.382587
57	1	0	-2.193164	-3.746869	1.613120
58	1	0	-0.804606	-4.450513	2.460466
59	6	0	-2.139364	-1.268027	2.771603
60	1	0	-1.749211	-0.250992	2.895040
61	1	0	-2.740723	-1.280665	1.858303
62	1	0	-2.786647	-1.489364	3.628605

_Si_-M2

Total Energy= -1816.66673579
Sum of electronic and zero-point Energies= -1816.157134
Sum of electronic and thermal Energies= -1816.126785
Sum of electronic and thermal Enthalpies= -1816.125841
Sum of electronic and thermal Free Energies= -1816.219284

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.268379	0.372527	-0.642356
2	6	0	1.700447	1.705992	1.186218
3	6	0	0.157301	1.588294	0.984367
4	6	0	3.512965	0.543423	-0.290234
5	6	0	3.473814	-0.380075	-1.342340
6	6	0	4.647052	-0.922735	-1.854164
7	1	0	4.621833	-1.637451	-2.669014
8	6	0	5.851079	-0.523406	-1.283859
9	6	0	5.882383	0.396505	-0.229079
10	6	0	4.714163	0.947399	0.282867
11	1	0	2.012981	1.193922	2.095906
12	1	0	6.779631	-0.934156	-1.663783
13	1	0	6.835608	0.687732	0.197748
14	1	0	4.729799	1.661512	1.098608

15	16	0	1.810263	-0.717398	-1.848286
16	7	0	2.231912	0.966707	0.039300
17	7	0	0.045558	0.737593	-0.235481
18	6	0	-0.524999	2.922812	0.800367
19	6	0	-1.387225	3.409465	1.781000
20	6	0	-0.282406	3.684216	-0.345869
21	6	0	-2.001774	4.650514	1.619463
22	1	0	-1.584001	2.813519	2.668183
23	6	0	-0.900120	4.919029	-0.510145
24	1	0	0.384562	3.304143	-1.116597
25	6	0	-1.760726	5.404221	0.474511
26	1	0	-2.674537	5.022618	2.385030
27	1	0	-0.711146	5.502501	-1.405218
28	1	0	-2.243504	6.367415	0.345951
29	1	0	2.044277	2.741469	1.160939
30	1	0	-0.274274	0.999952	1.798742
31	6	0	-1.109583	0.110076	-0.739446
32	8	0	-0.981869	-0.677986	-1.651365
33	6	0	-2.418270	0.561401	-0.138449
34	1	0	-2.295289	0.567230	0.947505
35	1	0	-2.588445	1.594259	-0.466790
36	6	0	-3.557862	-0.336168	-0.544709
37	6	0	-3.738898	-1.560538	0.105092
38	6	0	-4.429790	0.035433	-1.566310
39	6	0	-4.784605	-2.399763	-0.269606
40	1	0	-3.036610	-1.834268	0.890505
41	6	0	-5.477460	-0.804332	-1.939786
42	1	0	-4.291002	0.988515	-2.070146
43	6	0	-5.656323	-2.023476	-1.291422
44	1	0	-4.921750	-3.350396	0.236872
45	1	0	-6.153243	-0.504717	-2.734673
46	1	0	-6.472945	-2.677894	-1.579705
47	8	0	-0.939216	-1.233021	1.677515
48	6	0	0.216332	-1.733463	1.585448
49	8	0	1.296047	-1.091936	1.643927
50	6	0	0.288457	-3.266961	1.357763
51	6	0	-0.473198	-3.963811	2.490583
52	1	0	-0.486633	-5.048970	2.336067
53	1	0	-0.003289	-3.766717	3.460733
54	1	0	-1.503031	-3.600163	2.529721
55	6	0	1.737469	-3.746849	1.322718
56	1	0	1.778572	-4.829587	1.155288
57	1	0	2.289850	-3.246832	0.521492
58	1	0	2.246591	-3.520092	2.263656

59	6	0	-0.395331	-3.580971	0.021837
60	1	0	-1.425336	-3.214710	0.020635
61	1	0	0.130125	-3.097370	-0.808528
62	1	0	-0.402606	-4.662191	-0.160665

_Si_-TS3

Total Energy= -1816.64439969
Sum of electronic and zero-point Energies= -1816.141188
Sum of electronic and thermal Energies= -1816.110615
Sum of electronic and thermal Enthalpies= -1816.109671
Sum of electronic and thermal Free Energies= -1816.206965

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.389689	-0.496510	-0.901603
2	6	0	-1.749421	-1.197479	1.264306
3	6	0	-0.238951	-1.348270	0.900164
4	6	0	-3.602174	-0.303991	-0.348828
5	6	0	-3.591970	0.267657	-1.626689
6	6	0	-4.763544	0.762762	-2.187531
7	1	0	-4.763379	1.208240	-3.176057
8	6	0	-5.934080	0.672308	-1.440298
9	6	0	-5.934231	0.102745	-0.162245
10	6	0	-4.767574	-0.396832	0.404269
11	1	0	-1.905921	-0.433572	2.027621
12	1	0	-6.859896	1.052343	-1.857137
13	1	0	-6.860369	0.048774	0.398882
14	1	0	-4.758683	-0.840877	1.393610
15	16	0	-1.961970	0.272651	-2.325813
16	7	0	-2.328614	-0.735354	0.003633
17	7	0	-0.174103	-0.878950	-0.509601
18	6	0	0.277126	-2.759628	1.055451
19	6	0	1.103695	-3.072795	2.133896
20	6	0	-0.098873	-3.762340	0.159220
21	6	0	1.547580	-4.380085	2.321253
22	1	0	1.403429	-2.289802	2.825776
23	6	0	0.347693	-5.066569	0.344122
24	1	0	-0.732969	-3.518394	-0.689738
25	6	0	1.170153	-5.377495	1.426951
26	1	0	2.191729	-4.616069	3.161834
27	1	0	0.056372	-5.841224	-0.357646
28	1	0	1.519340	-6.395016	1.568624

29	1	0	-2.196320	-2.145951	1.567237
30	1	0	0.348897	-0.655537	1.505923
31	6	0	0.983900	-0.301170	-1.145582
32	8	0	0.792836	0.191091	-2.249740
33	6	0	2.163104	-0.274409	-0.318854
34	1	0	1.793554	0.702368	0.568814
35	1	0	2.265920	-1.161769	0.307407
36	6	0	3.436198	0.172016	-0.939921
37	6	0	3.506226	1.361385	-1.680896
38	6	0	4.620057	-0.547882	-0.737468
39	6	0	4.713601	1.799350	-2.214752
40	1	0	2.600894	1.939923	-1.834636
41	6	0	5.830982	-0.105573	-1.264243
42	1	0	4.587563	-1.467609	-0.158610
43	6	0	5.883725	1.069563	-2.010020
44	1	0	4.742727	2.721151	-2.788221
45	1	0	6.734804	-0.682619	-1.092163
46	1	0	6.825795	1.415843	-2.423106
47	8	0	1.563059	1.646086	1.385039
48	6	0	0.362136	2.119598	1.323378
49	8	0	-0.587547	1.568762	0.751429
50	6	0	0.175071	3.464365	2.046640
51	6	0	-1.258447	3.962482	1.879451
52	1	0	-1.387693	4.915499	2.402972
53	1	0	-1.499430	4.110875	0.823435
54	1	0	-1.972281	3.241223	2.285594
55	6	0	1.163022	4.475464	1.449505
56	1	0	1.064514	5.441046	1.956721
57	1	0	2.189218	4.119422	1.562911
58	1	0	0.967893	4.630886	0.383205
59	6	0	0.493858	3.256056	3.533569
60	1	0	-0.195266	2.534036	3.984748
61	1	0	1.513832	2.885578	3.659117
62	1	0	0.394443	4.203105	4.074370

***Si*-TS3a**

Total Energy= -1816.6392292

Sum of electronic and zero-point Energies= -1816.135935

Sum of electronic and thermal Energies= -1816.105700

Sum of electronic and thermal Enthalpies= -1816.104755

Sum of electronic and thermal Free Energies= -1816.198564

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	1.675626	-1.137168	0.231935
2	6	0	2.248722	-0.358443	2.323743
3	6	0	0.697370	-0.333555	2.159036
4	6	0	3.935964	-0.764527	0.350263
5	6	0	3.809169	-1.291171	-0.941690
6	6	0	4.929078	-1.447866	-1.750037
7	1	0	4.839703	-1.853117	-2.751732
8	6	0	6.165497	-1.069515	-1.235727
9	6	0	6.282039	-0.548152	0.057646
10	6	0	5.167715	-0.386336	0.872354
11	1	0	2.587962	-1.134714	3.013668
12	1	0	7.052119	-1.181555	-1.849536
13	1	0	7.258030	-0.262333	0.433464
14	1	0	5.248771	0.018243	1.875106
15	16	0	2.126454	-1.703590	-1.323839
16	7	0	2.690981	-0.688612	0.966884
17	7	0	0.511132	-1.062156	0.868795
18	6	0	0.143919	1.075446	2.142889
19	6	0	-0.834480	1.448272	3.062009
20	6	0	0.660764	2.027385	1.260300
21	6	0	-1.304850	2.759481	3.098063
22	1	0	-1.230827	0.711331	3.756285
23	6	0	0.193426	3.335645	1.297732
24	1	0	1.405017	1.741790	0.521727
25	6	0	-0.789563	3.704495	2.216433
26	1	0	-2.069790	3.039408	3.814759
27	1	0	0.597714	4.072057	0.610032
28	1	0	-1.152516	4.727056	2.241229
29	1	0	2.636105	0.612984	2.632284
30	1	0	0.223253	-0.914122	2.952827
31	6	0	-0.693173	-1.536253	0.237386
32	8	0	-0.528437	-2.197990	-0.774822
33	6	0	-1.926273	-1.076027	0.831454
34	1	0	-1.998871	0.098850	0.245931
35	6	0	-3.175647	-1.784840	0.440725
36	6	0	-3.510219	-1.970373	-0.908443
37	6	0	-4.083318	-2.220006	1.413082
38	6	0	-4.701786	-2.593201	-1.266140
39	1	0	-2.823347	-1.620778	-1.672276
40	6	0	-5.280842	-2.834500	1.055634
41	1	0	-3.844410	-2.074188	2.463669
42	6	0	-5.593912	-3.029169	-0.287259

43	1	0	-4.939887	-2.731612	-2.316708
44	1	0	-5.968072	-3.165200	1.828780
45	1	0	-6.524557	-3.511437	-0.569185
46	8	0	-0.183456	0.763530	-1.314780
47	6	0	-1.219190	1.442136	-1.243062
48	8	0	-2.202402	1.213323	-0.448640
49	6	0	-1.424823	2.622578	-2.216520
50	6	0	-2.237586	3.741116	-1.561967
51	1	0	-2.409403	4.550515	-2.280364
52	1	0	-3.201584	3.363424	-1.216097
53	1	0	-1.710172	4.156578	-0.697066
54	6	0	-2.205587	2.056572	-3.413669
55	1	0	-2.380453	2.839159	-4.160232
56	1	0	-1.647144	1.244553	-3.890393
57	1	0	-3.174153	1.664692	-3.088472
58	6	0	-0.071105	3.152959	-2.685930
59	1	0	0.509311	3.537647	-1.840267
60	1	0	0.511188	2.358636	-3.156934
61	1	0	-0.209053	3.967355	-3.405522
62	1	0	-1.850240	-0.883212	1.901199

_Si_-TS3b

Total Energy= -1816.629969
Sum of electronic and zero-point Energies= -1816.126785
Sum of electronic and thermal Energies= -1816.096423
Sum of electronic and thermal Enthalpies= -1816.095478
Sum of electronic and thermal Free Energies= -1816.190392

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.248100	0.185426	-0.617008
2	6	0	-1.923671	0.241196	1.656347
3	6	0	-0.558870	0.209850	0.916397
4	6	0	-4.196457	-0.358548	0.458771
5	6	0	-4.612343	-0.349412	-0.879099
6	6	0	-5.934843	-0.618659	-1.211480
7	1	0	-6.262279	-0.613816	-2.244968
8	6	0	-6.823854	-0.889430	-0.176272
9	6	0	-6.401477	-0.892768	1.158117
10	6	0	-5.079915	-0.629467	1.497944
11	1	0	-2.166366	1.231440	2.052179
12	1	0	-7.861206	-1.100433	-0.409813

13	1	0	-7.117220	-1.104354	1.944440
14	1	0	-4.744006	-0.631806	2.528786
15	16	0	-3.273340	0.023685	-1.982413
16	7	0	-2.837535	-0.069778	0.548230
17	7	0	-0.971081	0.543545	-0.471110
18	6	0	0.086819	-1.162542	0.994295
19	6	0	0.705555	-1.520840	2.193984
20	6	0	0.040336	-2.076240	-0.055694
21	6	0	1.265817	-2.784148	2.345120
22	1	0	0.754554	-0.804782	3.011103
23	6	0	0.601562	-3.342976	0.097458
24	1	0	-0.411486	-1.806324	-1.006161
25	6	0	1.214421	-3.699662	1.294416
26	1	0	1.750475	-3.051435	3.278656
27	1	0	0.564571	-4.047560	-0.727077
28	1	0	1.655673	-4.684468	1.408686
29	1	0	-1.983500	-0.512629	2.440878
30	1	0	0.113027	0.979814	1.298305
31	6	0	-0.160503	0.925948	-1.609121
32	8	0	-0.640055	0.645514	-2.698740
33	6	0	1.116219	1.524210	-1.305850
34	1	0	1.600621	1.811055	-2.241401
35	6	0	1.184329	2.602521	-0.260742
36	6	0	0.077576	3.375754	0.118907
37	6	0	2.414969	2.861862	0.359368
38	6	0	0.188520	4.354105	1.105059
39	1	0	-0.883737	3.218089	-0.364901
40	6	0	2.529047	3.851944	1.331108
41	1	0	3.282945	2.285942	0.048419
42	6	0	1.415415	4.596036	1.717694
43	1	0	-0.684367	4.937122	1.383310
44	1	0	3.493075	4.038378	1.795202
45	1	0	1.505411	5.361450	2.481917
46	1	0	1.910664	0.555267	-0.877108
47	8	0	2.727486	-0.351203	-0.412415
48	6	0	3.949475	-0.177327	-0.784512
49	8	0	4.380452	0.822878	-1.369780
50	6	0	4.887300	-1.352658	-0.434819
51	6	0	4.836145	-1.577006	1.081737
52	1	0	5.471181	-2.425402	1.360767
53	1	0	5.195441	-0.693407	1.620831
54	1	0	3.810775	-1.783216	1.399468
55	6	0	6.314834	-1.043936	-0.877813
56	1	0	6.974939	-1.884427	-0.636945

57	1	0	6.357125	-0.863519	-1.955058
58	1	0	6.693941	-0.149017	-0.376968
59	6	0	4.369041	-2.607799	-1.148712
60	1	0	3.341015	-2.819369	-0.843609
61	1	0	4.388765	-2.476962	-2.236142
62	1	0	4.996581	-3.471100	-0.900144

_Si_-TS3c

Total Energy= -1816.6261477
Sum of electronic and zero-point Energies= -1816.123153
Sum of electronic and thermal Energies= -1816.093585
Sum of electronic and thermal Enthalpies= -1816.092641
Sum of electronic and thermal Free Energies= -1816.186064

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.827396	-0.879714	-0.231459
2	6	0	2.198089	0.479518	1.586820
3	6	0	1.050319	1.055319	0.709623
4	6	0	3.795763	-1.454292	0.796333
5	6	0	3.728078	-2.408847	-0.225821
6	6	0	4.723739	-3.369081	-0.365133
7	1	0	4.677292	-4.108908	-1.156538
8	6	0	5.775049	-3.353542	0.544924
9	6	0	5.833079	-2.398864	1.567149
10	6	0	4.845121	-1.431643	1.709346
11	1	0	1.834870	0.055752	2.526072
12	1	0	6.561100	-4.095122	0.459300
13	1	0	6.664214	-2.411398	2.263163
14	1	0	4.884345	-0.688781	2.498150
15	16	0	2.294069	-2.184005	-1.243527
16	7	0	2.699411	-0.598171	0.731221
17	7	0	0.748695	-0.084133	-0.206752
18	6	0	1.463072	2.293324	-0.062918
19	6	0	1.424509	3.522771	0.600524
20	6	0	1.891973	2.240721	-1.388616
21	6	0	1.812350	4.686073	-0.052865
22	1	0	1.065011	3.569191	1.625754
23	6	0	2.276595	3.410301	-2.044088
24	1	0	1.912480	1.299093	-1.930369
25	6	0	2.239086	4.631465	-1.380029
26	1	0	1.769756	5.637045	0.467914

27	1	0	2.601237	3.361587	-3.078165
28	1	0	2.533605	5.539992	-1.894877
29	1	0	2.975077	1.219769	1.779785
30	1	0	0.185009	1.275542	1.331884
31	6	0	-0.205185	-0.154052	-1.303891
32	8	0	0.142212	-0.876951	-2.231354
33	6	0	-1.498165	0.469711	-1.180155
34	1	0	-2.229576	-0.594230	-0.951409
35	6	0	-1.840790	1.437976	-0.092795
36	6	0	-2.265348	0.961150	1.155725
37	6	0	-1.778401	2.821032	-0.290245
38	6	0	-2.575120	1.841827	2.188383
39	1	0	-2.350530	-0.112970	1.300569
40	6	0	-2.100770	3.705447	0.736778
41	1	0	-1.447438	3.203374	-1.252838
42	6	0	-2.489863	3.218886	1.982828
43	1	0	-2.896147	1.454753	3.150929
44	1	0	-2.033846	4.775794	0.566409
45	1	0	-2.735984	3.907251	2.785244
46	1	0	-1.836237	0.771594	-2.172084
47	8	0	-2.971695	-1.621060	-0.573594
48	6	0	-4.214711	-1.262615	-0.581126
49	8	0	-4.648987	-0.232869	-1.100650
50	6	0	-5.157070	-2.230580	0.164789
51	6	0	-4.995519	-3.639197	-0.417813
52	1	0	-5.623739	-4.350995	0.129203
53	1	0	-5.294302	-3.663951	-1.471191
54	1	0	-3.954782	-3.963346	-0.349554
55	6	0	-6.605062	-1.766016	0.034307
56	1	0	-7.271364	-2.447864	0.574154
57	1	0	-6.727731	-0.759570	0.442125
58	1	0	-6.912415	-1.738137	-1.014859
59	6	0	-4.736121	-2.236426	1.640969
60	1	0	-3.699920	-2.570538	1.739075
61	1	0	-4.817473	-1.232527	2.073423
62	1	0	-5.379165	-2.909052	2.219391

***Si*-M3**

Total Energy= -1469.74898850
Sum of electronic and zero-point Energies= -1469.390447
Sum of electronic and thermal Energies= -1469.369085
Sum of electronic and thermal Enthalpies= -1469.368141
Sum of electronic and thermal Free Energies= -1469.443655

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.324963	-0.611057	-0.205392
2	6	0	-1.734555	1.332092	-1.380503
3	6	0	-0.202214	1.165544	-1.113654
4	6	0	-3.587681	-0.220625	-0.358659
5	6	0	-3.566285	-1.449042	0.315021
6	6	0	-4.752935	-2.070487	0.681068
7	1	0	-4.744316	-3.020627	1.204055
8	6	0	-5.953154	-1.441345	0.357579
9	6	0	-5.964443	-0.217711	-0.317654
10	6	0	-4.780318	0.413367	-0.686399
11	1	0	-1.989954	1.220392	-2.437105
12	1	0	-6.890259	-1.910901	0.634649
13	1	0	-6.911294	0.252083	-0.559683
14	1	0	-4.781549	1.362807	-1.210282
15	16	0	-1.905508	-2.030182	0.584476
16	7	0	-2.293391	0.217214	-0.616285
17	7	0	-0.114917	-0.176227	-0.491115
18	6	0	0.349446	2.251059	-0.213545
19	6	0	1.003905	3.342383	-0.783311
20	6	0	0.155947	2.204898	1.167838
21	6	0	1.460454	4.384267	0.020719
22	1	0	1.162369	3.374403	-1.858291
23	6	0	0.614187	3.244928	1.970168
24	1	0	-0.335899	1.347929	1.621067
25	6	0	1.264992	4.337198	1.398295
26	1	0	1.973200	5.227616	-0.430005
27	1	0	0.467609	3.200436	3.044314
28	1	0	1.623760	5.145481	2.026932
29	1	0	-2.107855	2.286307	-1.006250
30	1	0	0.347202	1.147896	-2.057772
31	6	0	1.084420	-0.966735	-0.148638
32	8	0	0.795401	-2.049522	0.415396
33	6	0	2.278205	-0.390121	-0.510803
34	1	0	2.267136	0.591341	-0.969054
35	6	0	3.580696	-0.989273	-0.293045
36	6	0	4.734899	-0.281124	-0.690075
37	6	0	3.777727	-2.256321	0.298204
38	6	0	6.009728	-0.801219	-0.510325
39	1	0	4.614696	0.698687	-1.146924
40	6	0	5.057840	-2.770881	0.475264

41	1	0	2.908866	-2.821580	0.612378
42	6	0	6.185719	-2.055160	0.075623
43	1	0	6.873315	-0.223439	-0.828383
44	1	0	5.175790	-3.749470	0.933445
45	1	0	7.180577	-2.465016	0.217259

***Si*-M3'**

Total Energy= -1469.7394009

Sum of electronic and zero-point Energies= -1469.380468

Sum of electronic and thermal Energies= -1469.359499

Sum of electronic and thermal Enthalpies= -1469.358555

Sum of electronic and thermal Free Energies= -1469.431870

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.093937	0.540431	-0.477460
2	6	0	-0.570977	-0.136685	1.650655
3	6	0	0.633912	-0.342597	0.690329
4	6	0	-3.007820	0.358025	0.782689
5	6	0	-3.520602	0.848016	-0.426498
6	6	0	-4.880250	1.094659	-0.567015
7	1	0	-5.283656	1.469396	-1.501348
8	6	0	-5.707876	0.854664	0.527204
9	6	0	-5.187080	0.372457	1.731820
10	6	0	-3.827912	0.114369	1.878249
11	1	0	-0.427317	0.716962	2.319737
12	1	0	-6.771368	1.046431	0.440657
13	1	0	-5.852299	0.194388	2.569418
14	1	0	-3.417477	-0.261987	2.808807
15	16	0	-2.248568	1.039996	-1.653244
16	7	0	-1.632857	0.170673	0.689602
17	7	0	0.226800	0.465738	-0.487805
18	6	0	0.839877	-1.802129	0.326508
19	6	0	1.469868	-2.626208	1.262622
20	6	0	0.385828	-2.348082	-0.875069
21	6	0	1.635144	-3.983504	1.008284
22	1	0	1.835493	-2.201136	2.194470
23	6	0	0.555568	-3.708566	-1.127672
24	1	0	-0.069444	-1.713036	-1.630948
25	6	0	1.174846	-4.528669	-0.189240
26	1	0	2.128419	-4.613864	1.741046
27	1	0	0.204498	-4.124397	-2.066578

28	1	0	1.306196	-5.586632	-0.391615
29	1	0	-0.803091	-1.034383	2.224224
30	1	0	1.542132	0.068760	1.130876
31	6	0	0.973430	0.622595	-1.765442
32	8	0	0.238597	0.478008	-2.771746
33	6	0	2.325600	0.848584	-1.673308
34	1	0	2.849078	0.736920	-2.617704
35	6	0	3.117862	1.301913	-0.537865
36	6	0	2.610119	2.114489	0.497757
37	6	0	4.492368	0.992706	-0.483781
38	6	0	3.416910	2.543831	1.546835
39	1	0	1.569694	2.427455	0.461900
40	6	0	5.301617	1.438511	0.553674
41	1	0	4.919723	0.384513	-1.276893
42	6	0	4.769582	2.210396	1.586648
43	1	0	2.988214	3.165857	2.327722
44	1	0	6.355744	1.175952	0.559954
45	1	0	5.399721	2.554694	2.400028

M04*RR*

Total Energy= -2310.40690773
Sum of electronic and zero-point Energies= -2309.773498
Sum of electronic and thermal Energies= -2309.734928
Sum of electronic and thermal Enthalpies= -2309.733984
Sum of electronic and thermal Free Energies= -2309.845708

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.038819	0.466841	-1.417778
2	6	0	1.248583	1.950191	0.341575
3	6	0	-0.255212	1.588825	0.114777
4	6	0	3.251677	0.949840	-1.019117
5	6	0	3.354287	0.083333	-2.114207
6	6	0	4.600097	-0.235660	-2.641197
7	1	0	4.689953	-0.911447	-3.484772
8	6	0	5.726001	0.344484	-2.063049
9	6	0	5.609841	1.216830	-0.975841
10	6	0	4.369934	1.530364	-0.432485
11	1	0	1.578426	1.693583	1.350662
12	1	0	6.707082	0.113381	-2.463109
13	1	0	6.503222	1.646956	-0.536450
14	1	0	4.272314	2.185340	0.426434

15	16	0	1.762238	-0.485030	-2.659763
16	7	0	1.921248	1.110225	-0.648252
17	7	0	-0.219611	0.718011	-1.091061
18	6	0	-1.124405	2.814138	-0.042635
19	6	0	-1.978130	3.178014	0.997480
20	6	0	-1.058839	3.600968	-1.193906
21	6	0	-2.761562	4.324938	0.891596
22	1	0	-2.040418	2.550539	1.883925
23	6	0	-1.846021	4.742731	-1.301393
24	1	0	-0.404159	3.309830	-2.011841
25	6	0	-2.696558	5.107587	-0.257986
26	1	0	-3.426359	4.601052	1.703408
27	1	0	-1.800849	5.346495	-2.201843
28	1	0	-3.311198	5.997657	-0.344637
29	1	0	1.447434	3.003989	0.129963
30	1	0	-0.623896	0.985462	0.951629
31	6	0	-1.309588	-0.081206	-1.665532
32	8	0	-0.908677	-0.897525	-2.530830
33	6	0	-2.562003	0.169102	-1.151515
34	1	0	-2.685554	0.978508	-0.444763
35	6	0	-3.750555	-0.595624	-1.466579
36	6	0	-4.991222	-0.156613	-0.957185
37	6	0	-3.744615	-1.805293	-2.194380
38	6	0	-6.156625	-0.887403	-1.143750
39	1	0	-5.020309	0.767536	-0.384381
40	6	0	-4.915537	-2.535932	-2.372675
41	1	0	-2.808305	-2.156148	-2.612583
42	6	0	-6.129435	-2.091004	-1.849439
43	1	0	-7.091921	-0.519128	-0.731041
44	1	0	-4.878738	-3.468026	-2.930184
45	1	0	-7.037707	-2.667263	-1.993395
46	6	0	0.879380	-1.049607	1.745336
47	6	0	-0.153964	-1.775786	0.972076
48	6	0	0.615374	-2.584575	0.029584
49	7	0	1.888462	-2.421299	0.182429
50	7	0	2.072431	-1.489970	1.203195
51	6	0	3.392338	-1.112214	1.541902
52	6	0	4.456262	-1.680697	0.829572
53	6	0	3.651429	-0.182817	2.557693
54	6	0	5.761599	-1.320379	1.135117
55	1	0	4.248235	-2.391412	0.040924
56	6	0	4.969938	0.166229	2.843604
57	1	0	2.836283	0.248074	3.120280
58	6	0	6.030977	-0.394453	2.141372

59	1	0	6.575654	-1.764890	0.570893
60	1	0	5.159335	0.886383	3.633590
61	1	0	7.053580	-0.115999	2.373435
62	6	0	0.067990	-3.533940	-0.980881
63	1	0	-0.558214	-2.987847	-1.692374
64	1	0	0.893211	-4.008241	-1.513704
65	1	0	-0.534161	-4.308087	-0.495740
66	6	0	-1.515945	-1.772784	1.007479
67	1	0	-1.973350	-2.388516	0.230042
68	6	0	-2.503518	-1.173847	1.897398
69	6	0	-3.845190	-1.523992	1.658383
70	6	0	-2.212315	-0.303699	2.965688
71	6	0	-4.867280	-1.015534	2.449314
72	1	0	-4.083329	-2.189080	0.832782
73	6	0	-3.240387	0.204023	3.749637
74	1	0	-1.182780	-0.037983	3.171533
75	6	0	-4.567499	-0.146860	3.495629
76	1	0	-5.895898	-1.289416	2.238696
77	1	0	-3.005266	0.875361	4.569405
78	1	0	-5.363512	0.255764	4.113989
79	8	0	0.771046	-0.198954	2.629476

M04*RS*

Total Energy= -2310.4003468
Sum of electronic and zero-point Energies= -2309.767890
Sum of electronic and thermal Energies= -2309.729094
Sum of electronic and thermal Enthalpies= -2309.728150
Sum of electronic and thermal Free Energies= -2309.840619

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.805755	0.341108	-1.276804
2	6	0	1.736456	1.898740	0.156605
3	6	0	0.175570	1.943637	0.243723
4	6	0	3.100433	0.308778	-1.417971
5	6	0	2.751445	-0.654197	-2.373952
6	6	0	3.738804	-1.327144	-3.082186
7	1	0	3.480285	-2.079560	-3.819296
8	6	0	5.069460	-1.005469	-2.822637
9	6	0	5.404487	-0.033636	-1.875381
10	6	0	4.423445	0.640457	-1.156459
11	1	0	2.197695	1.646705	1.114518

12	1	0	5.855083	-1.520421	-3.364194
13	1	0	6.447918	0.190825	-1.682275
14	1	0	4.674948	1.370798	-0.394469
15	16	0	0.989811	-0.837515	-2.518170
16	7	0	1.961134	0.833347	-0.818716
17	7	0	-0.251528	0.880166	-0.695301
18	6	0	-0.395134	3.295604	-0.120823
19	6	0	-0.794842	4.167187	0.890531
20	6	0	-0.474451	3.699487	-1.454657
21	6	0	-1.268059	5.438527	0.572972
22	1	0	-0.740994	3.848092	1.928787
23	6	0	-0.951901	4.966680	-1.771244
24	1	0	-0.177801	3.015965	-2.246513
25	6	0	-1.347243	5.839150	-0.757826
26	1	0	-1.580896	6.111040	1.364907
27	1	0	-1.019494	5.272826	-2.810003
28	1	0	-1.721356	6.826715	-1.007062
29	1	0	2.146080	2.840157	-0.217106
30	1	0	-0.144087	1.670500	1.252376
31	6	0	-1.611226	0.401442	-0.988368
32	8	0	-1.651013	-0.384904	-1.958508
33	6	0	-2.581243	0.857396	-0.116362
34	1	0	-2.291595	1.554903	0.661498
35	6	0	-3.975389	0.470802	-0.152949
36	6	0	-4.820769	0.872433	0.903455
37	6	0	-4.546458	-0.321326	-1.170218
38	6	0	-6.158200	0.501557	0.948265
39	1	0	-4.404332	1.482954	1.702547
40	6	0	-5.887991	-0.684482	-1.121648
41	1	0	-3.913898	-0.659801	-1.982018
42	6	0	-6.706844	-0.282829	-0.067440
43	1	0	-6.777259	0.826400	1.779993
44	1	0	-6.297475	-1.301521	-1.917310
45	1	0	-7.751781	-0.574628	-0.036012
46	6	0	0.920711	-1.527564	1.270433
47	6	0	-0.365371	-1.102695	1.855998
48	6	0	0.012087	-0.145774	2.885911
49	7	0	1.295640	0.018559	2.957041
50	7	0	1.866477	-0.814669	2.000602
51	6	0	3.271240	-0.828226	1.852935
52	6	0	4.026107	0.186477	2.454637
53	6	0	3.915655	-1.841038	1.129914
54	6	0	5.411530	0.189475	2.323892
55	1	0	3.523347	0.949648	3.036185

56	6	0	5.301256	-1.819471	1.013597
57	1	0	3.335456	-2.622887	0.662208
58	6	0	6.058609	-0.809580	1.601612
59	1	0	5.984266	0.980251	2.798183
60	1	0	5.791256	-2.605742	0.447751
61	1	0	7.138867	-0.803545	1.501768
62	6	0	-0.918796	0.610122	3.774812
63	1	0	-1.493817	-0.071578	4.408005
64	1	0	-0.349566	1.289335	4.410267
65	1	0	-1.636209	1.190271	3.182749
66	6	0	-1.666173	-1.412236	1.574107
67	1	0	-2.388157	-0.899562	2.211651
68	6	0	-2.296340	-2.364652	0.677676
69	6	0	-3.661453	-2.623916	0.901448
70	6	0	-1.643027	-3.028723	-0.376625
71	6	0	-4.345269	-3.555442	0.133720
72	1	0	-4.185832	-2.075934	1.680111
73	6	0	-2.336872	-3.950888	-1.149115
74	1	0	-0.601194	-2.814161	-0.574475
75	6	0	-3.680280	-4.225794	-0.891066
76	1	0	-5.397246	-3.742660	0.321352
77	1	0	-1.827127	-4.459514	-1.960960
78	1	0	-4.211541	-4.952794	-1.497656
79	8	0	1.183402	-2.291159	0.345353

M04*SR*

Total Energy= -2310.38608062
Sum of electronic and zero-point Energies= -2309.753124
Sum of electronic and thermal Energies= -2309.714181
Sum of electronic and thermal Enthalpies= -2309.713236
Sum of electronic and thermal Free Energies= -2309.826913

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.757298	1.143010	-0.979696
2	8	0	-2.036764	2.167012	-0.326976
3	6	0	-2.510532	0.056940	-1.375363
4	1	0	-2.003367	-0.792327	-1.815316
5	6	0	-3.932154	-0.070548	-1.130658
6	6	0	-4.546130	-1.335565	-1.252978
7	6	0	-4.755801	1.008858	-0.747332
8	6	0	-5.895539	-1.520474	-0.978129
9	1	0	-3.937588	-2.185031	-1.557841

10	6	0	-6.107705	0.819598	-0.482934
11	1	0	-4.306001	1.987745	-0.633858
12	6	0	-6.691239	-0.443036	-0.584769
13	1	0	-6.330424	-2.511792	-1.072164
14	1	0	-6.713117	1.671330	-0.183750
15	1	0	-7.744999	-0.585945	-0.368205
16	6	0	0.760597	-1.115540	1.499349
17	6	0	-0.597278	-1.654420	1.277098
18	6	0	-0.373743	-3.064807	0.988066
19	7	0	0.867459	-3.397836	1.125667
20	7	0	1.574597	-2.237097	1.424988
21	6	0	2.980007	-2.309313	1.519070
22	6	0	3.582623	-3.570363	1.623983
23	6	0	3.778157	-1.157708	1.489287
24	6	0	4.966125	-3.672983	1.699208
25	1	0	2.957650	-4.453934	1.639108
26	6	0	5.162793	-1.284078	1.571346
27	1	0	3.316922	-0.183895	1.409664
28	6	0	5.767270	-2.532829	1.675784
29	1	0	5.419040	-4.655983	1.781434
30	1	0	5.771898	-0.385833	1.549546
31	1	0	6.846867	-2.618266	1.737921
32	6	0	-1.406627	-4.067779	0.600334
33	1	0	-2.174621	-4.170558	1.372185
34	1	0	-1.900386	-3.757683	-0.326440
35	1	0	-0.931620	-5.036200	0.439881
36	6	0	-1.842284	-1.111819	1.391422
37	1	0	-2.645283	-1.779659	1.072680
38	6	0	-2.342261	0.115739	1.983838
39	6	0	-3.739210	0.244758	2.077996
40	6	0	-1.530387	1.131839	2.519024
41	6	0	-4.311249	1.347594	2.698885
42	1	0	-4.377273	-0.527111	1.653862
43	6	0	-2.107720	2.228220	3.143031
44	1	0	-0.453575	1.048633	2.439037
45	6	0	-3.495784	2.340047	3.236377
46	1	0	-5.391637	1.432971	2.755493
47	1	0	-1.471828	3.005209	3.555969
48	1	0	-3.940277	3.202152	3.724194
49	8	0	1.156897	0.036485	1.661941
50	6	0	0.535144	1.971928	-0.934557
51	6	0	1.543440	1.243377	-2.876743
52	6	0	0.223386	0.446030	-2.621642
53	6	0	2.601126	2.953231	-1.198228

54	6	0	2.125876	3.615542	-0.058613
55	6	0	2.903638	4.578839	0.571009
56	1	0	2.541931	5.095390	1.453342
57	6	0	4.158672	4.862485	0.038034
58	6	0	4.621936	4.201888	-1.103534
59	6	0	3.849879	3.235185	-1.740184
60	1	0	1.471065	1.915990	-3.734924
61	1	0	4.782759	5.608517	0.517019
62	1	0	5.601255	4.442985	-1.501910
63	1	0	4.203886	2.716775	-2.624553
64	16	0	0.482921	3.098482	0.368574
65	7	0	1.666814	2.028017	-1.649152
66	7	0	-0.327938	1.083019	-1.388975
67	6	0	0.482839	-1.039920	-2.501533
68	6	0	1.497596	-1.517973	-1.668035
69	6	0	-0.230247	-1.934905	-3.298328
70	6	0	1.803518	-2.874311	-1.650415
71	1	0	2.058552	-0.829534	-1.034721
72	6	0	0.061117	-3.297214	-3.263163
73	1	0	-1.014189	-1.561889	-3.952576
74	6	0	1.083260	-3.766325	-2.443612
75	1	0	2.597851	-3.238750	-1.006537
76	1	0	-0.502403	-3.985273	-3.884876
77	1	0	1.321928	-4.824722	-2.421207
78	1	0	2.398077	0.577699	-3.002485
79	1	0	-0.500281	0.623397	-3.420760

M04*SS*

Total Energy= -2310.39595510
Sum of electronic and zero-point Energies= -2309.762247
Sum of electronic and thermal Energies= -2309.723897
Sum of electronic and thermal Enthalpies= -2309.722953
Sum of electronic and thermal Free Energies= -2309.832935

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.763307	-2.192010	0.076822
2	8	0	-0.500808	-2.705841	-1.033608
3	6	0	-1.958295	-1.923273	0.710178
4	1	0	-1.943166	-1.449704	1.682131
5	6	0	-3.262489	-2.238223	0.164266
6	6	0	-4.412439	-1.939180	0.927635

7	6	0	-3.469734	-2.818021	-1.106410
8	6	0	-5.688813	-2.215571	0.463152
9	1	0	-4.283966	-1.471084	1.901488
10	6	0	-4.755911	-3.091339	-1.566198
11	1	0	-2.605959	-3.057101	-1.714497
12	6	0	-5.875809	-2.799115	-0.792022
13	1	0	-6.548408	-1.963604	1.078680
14	1	0	-4.881281	-3.542383	-2.547457
15	1	0	-6.874773	-3.014876	-1.157996
16	6	0	0.293596	1.137213	-1.398209
17	6	0	-1.101156	1.570591	-1.167564
18	6	0	-1.001909	3.020463	-0.987794
19	7	0	0.227191	3.416002	-1.085050
20	7	0	1.037342	2.300996	-1.284901
21	6	0	2.435375	2.421491	-1.146816
22	6	0	2.997797	3.683982	-0.923586
23	6	0	3.262133	1.287566	-1.187379
24	6	0	4.370557	3.803074	-0.736016
25	1	0	2.353992	4.553870	-0.895063
26	6	0	4.632089	1.428815	-0.985775
27	1	0	2.833645	0.313404	-1.380136
28	6	0	5.196919	2.681260	-0.760431
29	1	0	4.795417	4.787388	-0.566054
30	1	0	5.255628	0.538256	-1.009344
31	1	0	6.265850	2.784067	-0.607299
32	6	0	-2.094414	4.020486	-0.797757
33	1	0	-2.437795	4.027731	0.240566
34	1	0	-1.719451	5.013354	-1.049885
35	1	0	-2.954857	3.779910	-1.426656
36	6	0	-2.109925	0.674691	-1.199140
37	1	0	-1.849796	-0.332258	-1.536664
38	6	0	-3.498986	0.920592	-0.807408
39	6	0	-4.552388	0.431862	-1.588952
40	6	0	-3.780976	1.587046	0.391659
41	6	0	-5.867889	0.669032	-1.210699
42	1	0	-4.333033	-0.129523	-2.491727
43	6	0	-5.098963	1.799694	0.780317
44	1	0	-2.955921	1.896827	1.028128
45	6	0	-6.143273	1.354271	-0.028020
46	1	0	-6.680280	0.295563	-1.825511
47	1	0	-5.311017	2.306790	1.716326
48	1	0	-7.172362	1.523027	0.273526
49	8	0	0.715760	0.012805	-1.612024
50	6	0	1.648120	-1.982558	0.328716

51	6	0	2.077472	-1.417736	2.521199
52	6	0	0.554588	-1.267761	2.215946
53	6	0	3.916345	-1.819870	0.695348
54	6	0	3.882416	-2.308421	-0.618129
55	6	0	5.063780	-2.516380	-1.319677
56	1	0	5.046100	-2.886344	-2.338998
57	6	0	6.270012	-2.240535	-0.677969
58	6	0	6.293121	-1.763768	0.636135
59	6	0	5.114696	-1.543454	1.343396
60	1	0	2.295063	-2.279203	3.157887
61	1	0	7.202429	-2.399381	-1.207933
62	1	0	7.244101	-1.557747	1.114769
63	1	0	5.123555	-1.165863	2.359876
64	16	0	2.218993	-2.580228	-1.183648
65	7	0	2.626725	-1.650573	1.184934
66	7	0	0.444173	-1.820513	0.836923
67	6	0	0.096560	0.172337	2.323073
68	6	0	0.821952	1.180584	1.682790
69	6	0	-0.985327	0.514575	3.132195
70	6	0	0.470509	2.514762	1.854319
71	1	0	1.678177	0.921589	1.060082
72	6	0	-1.350302	1.850599	3.291590
73	1	0	-1.540236	-0.264896	3.648293
74	6	0	-0.622604	2.852025	2.653421
75	1	0	1.047323	3.291055	1.361423
76	1	0	-2.197111	2.107068	3.920143
77	1	0	-0.895909	3.894002	2.787269
78	1	0	2.492361	-0.512886	2.966606
79	1	0	-0.038608	-1.899262	2.880884

TS4*RR*

Total Energy= -2310.40182847
Sum of electronic and zero-point Energies= -2309.767752
Sum of electronic and thermal Energies= -2309.730202
Sum of electronic and thermal Enthalpies= -2309.729257
Sum of electronic and thermal Free Energies= -2309.838153

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.196440	0.943939	0.968099
2	6	0	-1.413896	1.571533	-1.248651
3	6	0	0.099435	1.457141	-0.878416

4	6	0	-3.404608	1.226408	0.423099
5	6	0	-3.500551	0.850395	1.768785
6	6	0	-4.743773	0.738966	2.380471
7	1	0	-4.828533	0.443697	3.420372
8	6	0	-5.873938	1.018979	1.618462
9	6	0	-5.765826	1.392272	0.273941
10	6	0	-4.528390	1.498553	-0.347685
11	1	0	-1.696468	0.826830	-1.995710
12	1	0	-6.854015	0.939396	2.075440
13	1	0	-6.664317	1.591717	-0.299636
14	1	0	-4.434842	1.765777	-1.394441
15	16	0	-1.904305	0.556015	2.483470
16	7	0	-2.074048	1.266676	0.023311
17	7	0	0.064919	1.005942	0.541002
18	6	0	0.860852	2.752091	-1.040937
19	6	0	1.830229	2.865378	-2.036452
20	6	0	0.579084	3.846897	-0.221045
21	6	0	2.512219	4.067402	-2.215729
22	1	0	2.057168	2.007729	-2.665887
23	6	0	1.261222	5.045345	-0.398503
24	1	0	-0.169534	3.759458	0.563371
25	6	0	2.227903	5.157280	-1.397752
26	1	0	3.267624	4.149513	-2.990164
27	1	0	1.040766	5.892075	0.243036
28	1	0	2.760027	6.092929	-1.534358
29	1	0	-1.680543	2.578591	-1.575968
30	1	0	0.551346	0.664363	-1.480240
31	6	0	1.151852	0.550568	1.362780
32	8	0	0.840936	0.272671	2.528322
33	6	0	2.371330	0.352926	0.683073
34	1	0	2.460484	0.798385	-0.300161
35	6	0	3.638294	0.107355	1.362476
36	6	0	4.831259	0.401682	0.678194
37	6	0	3.739604	-0.487923	2.634369
38	6	0	6.072952	0.119950	1.235176
39	1	0	4.769257	0.849349	-0.311198
40	6	0	4.984964	-0.768905	3.187166
41	1	0	2.834131	-0.721144	3.182306
42	6	0	6.158209	-0.469918	2.495118
43	1	0	6.976186	0.358219	0.681501
44	1	0	5.040189	-1.228647	4.169646
45	1	0	7.125873	-0.693528	2.932648
46	6	0	-0.615158	-1.688255	-1.046448
47	6	0	0.387846	-1.965397	-0.034369

48	6	0	-0.366897	-2.417439	1.108194
49	7	0	-1.649353	-2.455685	0.877025
50	7	0	-1.823021	-1.995316	-0.419165
51	6	0	-3.134588	-1.833427	-0.910195
52	6	0	-4.211276	-2.019582	-0.030326
53	6	0	-3.386873	-1.486204	-2.245024
54	6	0	-5.513990	-1.859902	-0.482388
55	1	0	-4.008582	-2.282289	0.999808
56	6	0	-4.702894	-1.322835	-2.674421
57	1	0	-2.562215	-1.361718	-2.931649
58	6	0	-5.772996	-1.506928	-1.805881
59	1	0	-6.333746	-2.000985	0.215547
60	1	0	-4.884752	-1.056989	-3.711473
61	1	0	-6.793050	-1.378645	-2.152653
62	6	0	0.176376	-2.881787	2.421216
63	1	0	0.715690	-2.070658	2.916034
64	1	0	-0.647957	-3.203967	3.059513
65	1	0	0.864523	-3.721682	2.283659
66	6	0	1.778809	-1.776000	0.000779
67	1	0	2.215699	-2.096137	0.947209
68	6	0	2.758591	-1.820734	-1.100288
69	6	0	4.062529	-2.229650	-0.776557
70	6	0	2.473437	-1.483704	-2.433982
71	6	0	5.052496	-2.306847	-1.751222
72	1	0	4.297983	-2.484154	0.253606
73	6	0	3.468792	-1.554172	-3.402070
74	1	0	1.464562	-1.190107	-2.701734
75	6	0	4.759728	-1.965453	-3.068125
76	1	0	6.052596	-2.626998	-1.476779
77	1	0	3.233167	-1.293720	-4.429438
78	1	0	5.529552	-2.022757	-3.831250
79	8	0	-0.527733	-1.229101	-2.200982

TS4′*RR*

Total Energy= -2310.381831

Sum of electronic and zero-point Energies= -2309.748198

Sum of electronic and thermal Energies= -2309.710454

Sum of electronic and thermal Enthalpies= -2309.709510

Sum of electronic and thermal Free Energies= -2309.819902

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

1	6	0	-3.330788	-0.149170	0.182230
2	6	0	-3.541871	1.478851	-1.445036
3	6	0	-2.145951	1.598373	-0.746878
4	6	0	-5.440301	-0.179648	-0.715595
5	6	0	-5.515252	-1.235217	0.201568
6	6	0	-6.688501	-1.968691	0.336669
7	1	0	-6.755813	-2.787305	1.044486
8	6	0	-7.771967	-1.620755	-0.464212
9	6	0	-7.686447	-0.565069	-1.378994
10	6	0	-6.517923	0.173710	-1.520246
11	1	0	-3.460806	1.184382	-2.493359
12	1	0	-8.697185	-2.178859	-0.376440
13	1	0	-8.546350	-0.316241	-1.990490
14	1	0	-6.441866	0.992314	-2.227156
15	16	0	-3.988543	-1.457228	1.078670
16	7	0	-4.178614	0.406783	-0.678470
17	7	0	-2.130404	0.429290	0.168489
18	6	0	-1.958895	2.908073	-0.012369
19	6	0	-1.349063	3.972153	-0.678196
20	6	0	-2.429930	3.082694	1.289427
21	6	0	-1.209673	5.204902	-0.045864
22	1	0	-0.983766	3.837989	-1.693489
23	6	0	-2.287282	4.315305	1.920053
24	1	0	-2.896122	2.255916	1.818752
25	6	0	-1.677973	5.377076	1.254212
26	1	0	-0.728754	6.026105	-0.566541
27	1	0	-2.649216	4.444251	2.934538
28	1	0	-1.563387	6.335301	1.749798
29	1	0	-4.115056	2.403481	-1.360102
30	1	0	-1.354383	1.479335	-1.491795
31	6	0	-1.066605	-0.060599	1.019118
32	8	0	-1.399939	-0.969681	1.776611
33	6	0	0.222063	0.476286	0.753367
34	1	0	0.230379	1.435732	0.243792
35	6	0	1.360048	0.255074	1.645589
36	6	0	2.502288	1.050232	1.449704
37	6	0	1.423733	-0.763179	2.614846
38	6	0	3.669746	0.832466	2.173267
39	1	0	2.473964	1.843633	0.706213
40	6	0	2.588506	-0.966807	3.346249
41	1	0	0.558167	-1.391644	2.781143
42	6	0	3.720139	-0.181705	3.125452
43	1	0	4.542052	1.450974	1.982794
44	1	0	2.617089	-1.757371	4.090659

45	1	0	4.630112	-0.359524	3.690030
46	6	0	3.328501	-0.964011	-0.749466
47	6	0	2.113852	-0.327568	-1.220601
48	6	0	2.551752	0.894621	-1.828971
49	7	0	3.847587	1.045511	-1.795737
50	7	0	4.340622	-0.071499	-1.145443
51	6	0	5.722704	-0.163416	-0.912368
52	6	0	6.579991	0.765081	-1.521042
53	6	0	6.264407	-1.151447	-0.076259
54	6	0	7.949979	0.702141	-1.297092
55	1	0	6.156289	1.527377	-2.161622
56	6	0	7.639865	-1.198228	0.131754
57	1	0	5.603335	-1.863699	0.395055
58	6	0	8.494326	-0.279584	-0.471639
59	1	0	8.597325	1.430070	-1.777163
60	1	0	8.043938	-1.967538	0.783200
61	1	0	9.564756	-0.325861	-0.301009
62	6	0	1.683444	1.955477	-2.425667
63	1	0	1.054755	2.425745	-1.657955
64	1	0	2.304706	2.732095	-2.874469
65	1	0	1.019680	1.547310	-3.194705
66	6	0	0.752286	-0.632082	-1.023655
67	1	0	0.105282	-0.029747	-1.662030
68	6	0	0.139186	-1.948293	-0.749962
69	6	0	-1.102131	-2.219367	-1.348037
70	6	0	0.689301	-2.902575	0.116798
71	6	0	-1.773034	-3.412168	-1.104234
72	1	0	-1.535139	-1.488435	-2.029162
73	6	0	0.009096	-4.092491	0.365451
74	1	0	1.654986	-2.708470	0.567214
75	6	0	-1.218665	-4.353690	-0.238709
76	1	0	-2.726729	-3.604474	-1.586622
77	1	0	0.445074	-4.823933	1.039070
78	1	0	-1.738414	-5.285807	-0.040819
79	8	0	3.536898	-2.037645	-0.169910

TS4''*RR*

Total Energy= -2310.3914977

Sum of electronic and zero-point Energies= -2309.758169

Sum of electronic and thermal Energies= -2309.720324

Sum of electronic and thermal Enthalpies= -2309.719380

Sum of electronic and thermal Free Energies= -2309.830820

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.212998	1.772288	-0.515781
2	6	0	-1.302675	3.059934	0.661037
3	6	0	-1.953151	1.693062	0.274964
4	6	0	1.048106	3.880121	-0.175379
5	6	0	2.096942	3.273296	-0.879726
6	6	0	3.261937	3.980663	-1.154572
7	1	0	4.079722	3.515350	-1.693867
8	6	0	3.348300	5.298012	-0.715053
9	6	0	2.294864	5.895743	-0.014017
10	6	0	1.127143	5.196117	0.267769
11	1	0	-1.157342	3.150033	1.739948
12	1	0	4.247771	5.867499	-0.919870
13	1	0	2.388784	6.923134	0.319463
14	1	0	0.308443	5.652213	0.813190
15	16	0	1.725943	1.593487	-1.302701
16	7	0	-0.003502	2.985920	-0.009901
17	7	0	-0.816265	0.950856	-0.330596
18	6	0	-3.119443	1.824459	-0.677623
19	6	0	-4.413378	1.659212	-0.184804
20	6	0	-2.925403	2.149502	-2.021418
21	6	0	-5.510246	1.824548	-1.027202
22	1	0	-4.557399	1.394540	0.860575
23	6	0	-4.021387	2.309792	-2.862943
24	1	0	-1.918391	2.266522	-2.415503
25	6	0	-5.314875	2.150004	-2.366691
26	1	0	-6.514309	1.691716	-0.638105
27	1	0	-3.866206	2.556088	-3.908134
28	1	0	-6.167445	2.273209	-3.026417
29	1	0	-1.880043	3.906582	0.285698
30	1	0	-2.275698	1.179590	1.181866
31	6	0	-0.759149	-0.412626	-0.799398
32	8	0	0.284134	-0.712779	-1.386857
33	6	0	-1.817866	-1.264554	-0.410965
34	1	0	-2.704849	-0.794231	0.000001
35	6	0	-2.023476	-2.577449	-1.024787
36	6	0	-3.214531	-3.269108	-0.730093
37	6	0	-1.071836	-3.227399	-1.832140
38	6	0	-3.445078	-4.551882	-1.209386
39	1	0	-3.967567	-2.783055	-0.113112
40	6	0	-1.314433	-4.509221	-2.319669
41	1	0	-0.143138	-2.724492	-2.063490

42	6	0	-2.492343	-5.183671	-2.009941
43	1	0	-4.372333	-5.059767	-0.961654
44	1	0	-0.563485	-4.989398	-2.940407
45	1	0	-2.669136	-6.185787	-2.387098
46	6	0	1.639283	-1.277696	1.088110
47	6	0	0.493802	-2.159371	1.244803
48	6	0	0.970810	-3.455378	0.838195
49	7	0	2.227939	-3.438017	0.493896
50	7	0	2.649701	-2.123466	0.626710
51	6	0	3.954294	-1.785422	0.223178
52	6	0	4.750234	-2.765388	-0.387005
53	6	0	4.478164	-0.497780	0.416304
54	6	0	6.041369	-2.458935	-0.799338
55	1	0	4.340577	-3.756464	-0.529978
56	6	0	5.772425	-0.211295	-0.008972
57	1	0	3.868956	0.257295	0.891064
58	6	0	6.564604	-1.180379	-0.618132
59	1	0	6.641473	-3.231479	-1.270707
60	1	0	6.164174	0.789883	0.145904
61	1	0	7.572476	-0.945116	-0.943566
62	6	0	0.221969	-4.749513	0.908309
63	1	0	-0.763593	-4.673828	0.441220
64	1	0	0.790035	-5.528908	0.397450
65	1	0	0.080544	-5.049335	1.952080
66	6	0	-0.848304	-1.871570	1.517342
67	1	0	-1.488834	-2.752376	1.482417
68	6	0	-1.410384	-0.823010	2.399648
69	6	0	-2.784656	-0.888823	2.690100
70	6	0	-0.658999	0.216109	2.964485
71	6	0	-3.402500	0.076935	3.474026
72	1	0	-3.372999	-1.704723	2.275729
73	6	0	-1.279936	1.178253	3.761545
74	1	0	0.401641	0.277393	2.752181
75	6	0	-2.649997	1.126504	4.005694
76	1	0	-4.467057	0.010703	3.675305
77	1	0	-0.683874	1.977500	4.192539
78	1	0	-3.127155	1.885325	4.617449
79	8	0	1.777976	-0.060092	1.290284

TS4*RS*

Total Energy= -2310.3967769

Sum of electronic and zero-point Energies= -2309.763496

Sum of electronic and thermal Energies= -2309.726653

Sum of electronic and thermal Enthalpies= -2309.725709
Sum of electronic and thermal Free Energies= -2309.832318

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.888941	-0.098004	-1.436351
2	6	0	1.858294	1.772888	-0.490107
3	6	0	0.318097	1.788956	-0.239954
4	6	0	3.172438	-0.205757	-1.592245
5	6	0	2.795783	-1.363802	-2.284144
6	6	0	3.763304	-2.210432	-2.811881
7	1	0	3.484043	-3.111273	-3.346824
8	6	0	5.101009	-1.867451	-2.633335
9	6	0	5.464899	-0.706890	-1.941641
10	6	0	4.503915	0.144586	-1.409559
11	1	0	2.430948	1.830937	0.437622
12	1	0	5.871381	-2.515841	-3.035362
13	1	0	6.514647	-0.470813	-1.805547
14	1	0	4.773479	1.029278	-0.841649
15	16	0	1.031899	-1.536525	-2.363679
16	7	0	2.050955	0.476161	-1.137862
17	7	0	-0.153111	0.574583	-0.957442
18	6	0	-0.345300	3.056675	-0.723588
19	6	0	-0.658080	4.049907	0.203514
20	6	0	-0.602223	3.267146	-2.079413
21	6	0	-1.218942	5.252420	-0.220637
22	1	0	-0.461639	3.879478	1.259732
23	6	0	-1.168811	4.465800	-2.500907
24	1	0	-0.371751	2.488902	-2.802735
25	6	0	-1.475268	5.460538	-1.573203
26	1	0	-1.459911	6.021470	0.505855
27	1	0	-1.374643	4.623244	-3.554499
28	1	0	-1.917447	6.394070	-1.905460
29	1	0	2.168220	2.571082	-1.170276
30	1	0	0.126697	1.661771	0.827107
31	6	0	-1.500065	0.041926	-1.063043
32	8	0	-1.625158	-0.874430	-1.883831
33	6	0	-2.425397	0.574737	-0.145373
34	1	0	-2.107057	1.437114	0.430037
35	6	0	-3.863009	0.365496	-0.216648
36	6	0	-4.682696	1.060959	0.693937
37	6	0	-4.484502	-0.536977	-1.099609
38	6	0	-6.057323	0.866682	0.725461

39	1	0	-4.223080	1.763793	1.386270
40	6	0	-5.864252	-0.717884	-1.071653
41	1	0	-3.871599	-1.098456	-1.794145
42	6	0	-6.660187	-0.026329	-0.161393
43	1	0	-6.661453	1.416786	1.440845
44	1	0	-6.319658	-1.419774	-1.764470
45	1	0	-7.734325	-0.179608	-0.140986
46	6	0	0.832945	-1.007150	1.560149
47	6	0	-0.484889	-0.565192	1.985290
48	6	0	-0.228438	0.540913	2.871033
49	7	0	1.045541	0.791640	3.012722
50	7	0	1.704488	-0.141633	2.229867
51	6	0	3.110648	-0.099063	2.141354
52	6	0	3.778192	1.071479	2.528557
53	6	0	3.847277	-1.196312	1.676852
54	6	0	5.164670	1.141641	2.442736
55	1	0	3.199556	1.907138	2.903936
56	6	0	5.234146	-1.106857	1.602261
57	1	0	3.331661	-2.096271	1.374086
58	6	0	5.902885	0.055338	1.977319
59	1	0	5.668355	2.054194	2.746134
60	1	0	5.794871	-1.962424	1.238221
61	1	0	6.984327	0.113377	1.912139
62	6	0	-1.249054	1.378685	3.571197
63	1	0	-1.885270	0.768266	4.218518
64	1	0	-0.749341	2.134962	4.178060
65	1	0	-1.903961	1.884674	2.851816
66	6	0	-1.781838	-0.915826	1.582429
67	1	0	-2.556564	-0.378198	2.129074
68	6	0	-2.291058	-2.151007	0.986827
69	6	0	-3.651833	-2.445801	1.186176
70	6	0	-1.513351	-3.045653	0.232513
71	6	0	-4.214206	-3.610096	0.677942
72	1	0	-4.270171	-1.747981	1.745475
73	6	0	-2.083569	-4.205051	-0.280608
74	1	0	-0.464117	-2.828823	0.072547
75	6	0	-3.429252	-4.494819	-0.057748
76	1	0	-5.265387	-3.819310	0.848342
77	1	0	-1.471304	-4.889275	-0.859874
78	1	0	-3.864156	-5.404849	-0.459415
79	8	0	1.214630	-1.883197	0.769864

TS4′*RS*

Total Energy= -2310.3813244
Sum of electronic and zero-point Energies= -2309.747576
Sum of electronic and thermal Energies= -2309.709696
Sum of electronic and thermal Enthalpies= -2309.708752
Sum of electronic and thermal Free Energies= -2309.820231

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.010760	-1.093754	-0.307222
2	6	0	4.169658	0.584606	0.784293
3	6	0	2.757181	1.105773	0.359739
4	6	0	5.108345	-1.812896	0.281532
5	6	0	4.591645	-2.956799	-0.339318
6	6	0	5.359664	-4.110533	-0.443308
7	1	0	4.966215	-5.000852	-0.920802
8	6	0	6.647187	-4.087350	0.084281
9	6	0	7.155554	-2.939202	0.701224
10	6	0	6.393402	-1.781881	0.811030
11	1	0	4.303357	0.582183	1.867423
12	1	0	7.264362	-4.975918	0.015741
13	1	0	8.162503	-2.949373	1.102864
14	1	0	6.779662	-0.887585	1.286920
15	16	0	2.932765	-2.700024	-0.919216
16	7	0	4.167179	-0.787518	0.274675
17	7	0	2.145139	-0.084504	-0.301515
18	6	0	2.814184	2.316382	-0.543066
19	6	0	2.317485	3.535965	-0.083144
20	6	0	3.370175	2.227130	-1.820162
21	6	0	2.380897	4.665088	-0.896971
22	1	0	1.866053	3.596443	0.906130
23	6	0	3.430010	3.354946	-2.632019
24	1	0	3.745908	1.274456	-2.187430
25	6	0	2.936992	4.575220	-2.170281
26	1	0	1.989400	5.610760	-0.537197
27	1	0	3.856900	3.280924	-3.626610
28	1	0	2.980611	5.453031	-2.806376
29	1	0	4.970421	1.157975	0.312934
30	1	0	2.161271	1.343660	1.243718
31	6	0	0.806813	-0.243740	-0.833626
32	8	0	0.577470	-1.350744	-1.326289
33	6	0	-0.068475	0.850340	-0.624444
34	1	0	0.401829	1.786228	-0.353095
35	6	0	-1.305251	0.991877	-1.388609

36	6	0	-1.786175	2.287336	-1.651983
37	6	0	-2.081342	-0.103587	-1.805978
38	6	0	-3.002246	2.486271	-2.288801
39	1	0	-1.187921	3.141601	-1.341734
40	6	0	-3.304875	0.102244	-2.439787
41	1	0	-1.726669	-1.110171	-1.619692
42	6	0	-3.775004	1.389897	-2.677418
43	1	0	-3.353243	3.496040	-2.479617
44	1	0	-3.903218	-0.755816	-2.733226
45	1	0	-4.733661	1.541139	-3.164369
46	6	0	-3.264780	-0.203712	0.894675
47	6	0	-1.882237	-0.561233	1.174960
48	6	0	-1.844514	-1.996299	1.081953
49	7	0	-3.007543	-2.510894	0.792610
50	7	0	-3.876399	-1.442610	0.650862
51	6	0	-5.207392	-1.690277	0.279328
52	6	0	-5.726902	-2.984910	0.414486
53	6	0	-6.014788	-0.672461	-0.248480
54	6	0	-7.036245	-3.252414	0.032534
55	1	0	-5.090318	-3.765409	0.811721
56	6	0	-7.325170	-0.959826	-0.618788
57	1	0	-5.601332	0.319663	-0.365284
58	6	0	-7.847946	-2.243743	-0.482548
59	1	0	-7.425017	-4.260211	0.143514
60	1	0	-7.941716	-0.164617	-1.027486
61	1	0	-8.870900	-2.456329	-0.775345
62	6	0	-0.671053	-2.887160	1.343205
63	1	0	-0.299143	-2.750642	2.364049
64	1	0	-0.971391	-3.928884	1.218410
65	1	0	0.146212	-2.671439	0.650278
66	6	0	-0.746659	0.239369	1.366378
67	1	0	0.135636	-0.351420	1.622903
68	6	0	-0.685243	1.588279	1.986711
69	6	0	0.346885	1.836419	2.904615
70	6	0	-1.572988	2.629354	1.681241
71	6	0	0.506131	3.088892	3.491316
72	1	0	1.023366	1.028190	3.175761
73	6	0	-1.402715	3.884557	2.259328
74	1	0	-2.395123	2.433689	1.003532
75	6	0	-0.364825	4.124108	3.159204
76	1	0	1.305819	3.252834	4.206775
77	1	0	-2.092956	4.684063	2.007824
78	1	0	-0.243538	5.105229	3.607119
79	8	0	-3.860359	0.878988	0.876938

TS4''*RS*

Total Energy= -2310.3893658
Sum of electronic and zero-point Energies= -2309.755506
Sum of electronic and thermal Energies= -2309.717873
Sum of electronic and thermal Enthalpies= -2309.716928
Sum of electronic and thermal Free Energies= -2309.827166

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.313885	-0.199275	-0.585489
2	6	0	3.665601	1.241771	1.187355
3	6	0	2.177005	1.328601	0.722284
4	6	0	5.458476	-0.399649	0.200605
5	6	0	5.462921	-1.327512	-0.848365
6	6	0	6.608092	-2.059202	-1.139499
7	1	0	6.618625	-2.777560	-1.951552
8	6	0	7.738548	-1.839322	-0.358852
9	6	0	7.725210	-0.911057	0.688088
10	6	0	6.583943	-0.175200	0.985828
11	1	0	3.745594	0.934603	2.231457
12	1	0	8.643900	-2.397361	-0.568694
13	1	0	8.621082	-0.759384	1.279647
14	1	0	6.566085	0.545905	1.795395
15	16	0	3.894810	-1.394042	-1.676300
16	7	0	4.209933	0.205292	0.309182
17	7	0	2.131796	0.395317	-0.441737
18	6	0	1.748785	2.728096	0.350010
19	6	0	0.797612	3.390857	1.123230
20	6	0	2.320004	3.370513	-0.750456
21	6	0	0.418644	4.692349	0.799766
22	1	0	0.347256	2.883990	1.973623
23	6	0	1.939498	4.667851	-1.074091
24	1	0	3.055428	2.852055	-1.361643
25	6	0	0.988897	5.330508	-0.298022
26	1	0	-0.326072	5.202486	1.401410
27	1	0	2.381769	5.161431	-1.933023
28	1	0	0.691104	6.342122	-0.553267
29	1	0	4.201544	2.180481	1.027239
30	1	0	1.527600	0.926714	1.504233
31	6	0	0.997823	-0.008468	-1.238048
32	8	0	1.271291	-0.754162	-2.182883

33	6	0	-0.280034	0.391419	-0.759100
34	1	0	-0.280949	1.055029	0.098705
35	6	0	-1.438823	0.545967	-1.636949
36	6	0	-2.598274	1.112453	-1.078233
37	6	0	-1.500625	0.090895	-2.965113
38	6	0	-3.781933	1.196199	-1.801713
39	1	0	-2.570004	1.460815	-0.048375
40	6	0	-2.684581	0.186268	-3.689107
41	1	0	-0.618861	-0.347193	-3.418280
42	6	0	-3.834199	0.724122	-3.111096
43	1	0	-4.668760	1.616330	-1.336028
44	1	0	-2.712322	-0.174726	-4.713181
45	1	0	-4.758878	0.777490	-3.677395
46	6	0	-3.164535	-0.878117	1.078803
47	6	0	-2.145500	-1.554605	0.300722
48	6	0	-2.869509	-2.218274	-0.750286
49	7	0	-4.159934	-2.057913	-0.653561
50	7	0	-4.360005	-1.255480	0.456875
51	6	0	-5.637262	-0.717324	0.685181
52	6	0	-6.571179	-0.707538	-0.359212
53	6	0	-5.995047	-0.203704	1.938470
54	6	0	-7.844455	-0.191710	-0.148012
55	1	0	-6.277695	-1.103466	-1.323425
56	6	0	-7.271644	0.317926	2.127957
57	1	0	-5.272094	-0.212885	2.742228
58	6	0	-8.204561	0.327437	1.094149
59	1	0	-8.558261	-0.191114	-0.966288
60	1	0	-7.538909	0.713815	3.103192
61	1	0	-9.198136	0.733301	1.253343
62	6	0	-2.292706	-3.090097	-1.820117
63	1	0	-1.848553	-3.994450	-1.391000
64	1	0	-3.080981	-3.382907	-2.515702
65	1	0	-1.511986	-2.564417	-2.376946
66	6	0	-0.743051	-1.449499	0.304081
67	1	0	-0.283770	-2.059974	-0.475028
68	6	0	0.152492	-1.305017	1.476253
69	6	0	1.427133	-1.887296	1.392361
70	6	0	-0.184114	-0.595351	2.639211
71	6	0	2.357006	-1.739716	2.417728
72	1	0	1.691347	-2.455234	0.502030
73	6	0	0.745240	-0.456200	3.668260
74	1	0	-1.173725	-0.155225	2.714813
75	6	0	2.019201	-1.015635	3.561490
76	1	0	3.339721	-2.194270	2.325283

77	1	0	0.472982	0.099037	4.560558
78	1	0	2.738674	-0.898233	4.365745
79	8	0	-3.103312	-0.096317	2.042382

TS4*SR*

Total Energy= -2310.38159271
Sum of electronic and zero-point Energies= -2309.747913
Sum of electronic and thermal Energies= -2309.710213
Sum of electronic and thermal Enthalpies= -2309.709269
Sum of electronic and thermal Free Energies= -2309.818962

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.564502	-1.180368	0.789326
2	8	0	-1.816565	-2.236181	0.203163
3	6	0	-2.387490	-0.063919	1.025911
4	1	0	-1.935234	0.779534	1.533183
5	6	0	-3.843158	-0.120671	1.042795
6	6	0	-4.550010	1.038769	1.418278
7	6	0	-4.592781	-1.251937	0.668457
8	6	0	-5.938309	1.073566	1.415342
9	1	0	-3.988101	1.922670	1.714407
10	6	0	-5.984053	-1.214473	0.678637
11	1	0	-4.069649	-2.148981	0.360761
12	6	0	-6.667762	-0.056843	1.044301
13	1	0	-6.454350	1.983836	1.706092
14	1	0	-6.540423	-2.100848	0.387279
15	1	0	-7.752687	-0.033597	1.041294
16	6	0	0.607418	1.075898	-1.372793
17	6	0	-0.731720	1.546396	-1.076274
18	6	0	-0.580606	2.960995	-0.860659
19	7	0	0.632215	3.376175	-1.091180
20	7	0	1.373648	2.244258	-1.393591
21	6	0	2.763887	2.373536	-1.558782
22	6	0	3.315909	3.659163	-1.669929
23	6	0	3.611476	1.255679	-1.597173
24	6	0	4.687909	3.817871	-1.820407
25	1	0	2.656611	4.516817	-1.634265
26	6	0	4.983395	1.438600	-1.751860
27	1	0	3.189725	0.264485	-1.513397
28	6	0	5.534330	2.711380	-1.864841
29	1	0	5.097004	4.819816	-1.907322

30	1	0	5.626560	0.564235	-1.780803
31	1	0	6.604668	2.841170	-1.985263
32	6	0	-1.645941	3.921430	-0.443790
33	1	0	-2.470512	3.948748	-1.162586
34	1	0	-2.058990	3.629988	0.528353
35	1	0	-1.220869	4.922349	-0.354761
36	6	0	-1.977797	0.905093	-1.066555
37	1	0	-2.791207	1.570696	-0.775722
38	6	0	-2.450683	-0.198958	-1.905753
39	6	0	-3.832165	-0.278366	-2.150640
40	6	0	-1.606206	-1.150483	-2.501857
41	6	0	-4.356773	-1.269851	-2.971733
42	1	0	-4.495371	0.451361	-1.693246
43	6	0	-2.135419	-2.138155	-3.323919
44	1	0	-0.539381	-1.099264	-2.313443
45	6	0	-3.508065	-2.203598	-3.561538
46	1	0	-5.426638	-1.311709	-3.149822
47	1	0	-1.470998	-2.865403	-3.780797
48	1	0	-3.914008	-2.977995	-4.205154
49	8	0	1.067132	-0.066497	-1.533460
50	6	0	0.738512	-1.920412	0.853648
51	6	0	1.627732	-1.097430	2.818342
52	6	0	0.275834	-0.376946	2.507000
53	6	0	2.816080	-2.817634	1.247678
54	6	0	2.425033	-3.529521	0.106791
55	6	0	3.270436	-4.482632	-0.449955
56	1	0	2.977795	-5.040258	-1.332553
57	6	0	4.503596	-4.699758	0.158439
58	6	0	4.883270	-3.985324	1.299915
59	6	0	4.044344	-3.030909	1.863207
60	1	0	1.569816	-1.738567	3.700568
61	1	0	5.179778	-5.435577	-0.261841
62	1	0	5.849508	-4.174558	1.753927
63	1	0	4.330709	-2.468740	2.745233
64	16	0	0.791480	-3.081694	-0.414466
65	7	0	1.822888	-1.922459	1.627770
66	7	0	-0.179190	-1.041418	1.242466
67	6	0	0.448965	1.121847	2.417630
68	6	0	1.475778	1.670694	1.646199
69	6	0	-0.365055	1.960250	3.179079
70	6	0	1.688713	3.043984	1.645988
71	1	0	2.109836	1.025583	1.037849
72	6	0	-0.158882	3.338753	3.169397
73	1	0	-1.158886	1.531788	3.786339

74	6	0	0.871439	3.879652	2.406536
75	1	0	2.480391	3.463601	1.032973
76	1	0	-0.796432	3.983796	3.765229
77	1	0	1.038168	4.951952	2.399313
78	1	0	2.445784	-0.385845	2.934220
79	1	0	-0.467837	-0.610654	3.272909

TS4'*SR*

Total Energy= -2310.3808426
Sum of electronic and zero-point Energies= -2309.746199
Sum of electronic and thermal Energies= -2309.708810
Sum of electronic and thermal Enthalpies= -2309.707866
Sum of electronic and thermal Free Energies= -2309.815581

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.130191	-1.199280	-0.605931
2	8	0	-1.491507	-2.319240	-0.228555
3	6	0	0.189851	-0.702076	-0.748622
4	1	0	0.287447	0.357925	-0.944579
5	6	0	1.283641	-1.521422	-1.265472
6	6	0	2.478144	-0.865058	-1.613047
7	6	0	1.241579	-2.921317	-1.378644
8	6	0	3.595028	-1.577488	-2.033949
9	1	0	2.527730	0.218031	-1.522766
10	6	0	2.358419	-3.628911	-1.811245
11	1	0	0.332176	-3.448895	-1.112992
12	6	0	3.543650	-2.966646	-2.130320
13	1	0	4.512489	-1.046088	-2.270711
14	1	0	2.305457	-4.711175	-1.888986
15	1	0	4.415804	-3.527880	-2.450953
16	6	0	3.039982	0.361079	1.075819
17	6	0	2.103870	-0.687062	1.431305
18	6	0	2.903949	-1.879412	1.512802
19	7	0	4.172688	-1.648594	1.315428
20	7	0	4.277021	-0.294375	1.045432
21	6	0	5.488526	0.207665	0.544220
22	6	0	6.448949	-0.686057	0.050388
23	6	0	5.756156	1.583292	0.537707
24	6	0	7.657554	-0.206065	-0.441031
25	1	0	6.226152	-1.745743	0.057318
26	6	0	6.968617	2.044857	0.033676

27	1	0	5.012822	2.269783	0.917595
28	6	0	7.927196	1.161159	-0.456290
29	1	0	8.391686	-0.910147	-0.821021
30	1	0	7.165459	3.112749	0.033464
31	1	0	8.870498	1.531938	-0.843470
32	6	0	2.435547	-3.249602	1.886917
33	1	0	2.068759	-3.270380	2.918155
34	1	0	1.622941	-3.577737	1.233447
35	1	0	3.262858	-3.955183	1.792196
36	6	0	0.700240	-0.682239	1.404036
37	1	0	0.265977	-1.678701	1.504444
38	6	0	-0.191239	0.362979	1.958077
39	6	0	-1.526944	0.013847	2.217393
40	6	0	0.245306	1.641225	2.331065
41	6	0	-2.412591	0.917587	2.792464
42	1	0	-1.861410	-0.992311	1.974955
43	6	0	-0.636078	2.537290	2.931778
44	1	0	1.271901	1.927485	2.130778
45	6	0	-1.967317	2.189344	3.154668
46	1	0	-3.441212	0.621446	2.978977
47	1	0	-0.278603	3.519609	3.226693
48	1	0	-2.648314	2.895812	3.618647
49	8	0	2.870938	1.554934	0.781885
50	6	0	-3.461874	-0.595889	-0.489678
51	6	0	-3.744080	1.377399	-1.642263
52	6	0	-2.284133	0.872201	-1.809511
53	6	0	-5.681530	-0.010989	-0.547968
54	6	0	-5.729353	-1.186187	0.211893
55	6	0	-6.939806	-1.662334	0.702889
56	1	0	-6.983953	-2.574081	1.287956
57	6	0	-8.089027	-0.928920	0.425917
58	6	0	-8.031191	0.249640	-0.326940
59	6	0	-6.826251	0.727604	-0.828604
60	1	0	-4.224879	1.560870	-2.603217
61	1	0	-9.043816	-1.277826	0.802426
62	1	0	-8.942483	0.802283	-0.525759
63	1	0	-6.774921	1.639147	-1.413489
64	16	0	-4.124263	-1.916287	0.391888
65	7	0	-4.374750	0.258828	-0.943678
66	7	0	-2.211538	-0.247527	-0.806271
67	6	0	-1.278172	1.980383	-1.642839
68	6	0	-1.186553	2.683425	-0.441867
69	6	0	-0.443295	2.312029	-2.709816
70	6	0	-0.261661	3.714420	-0.313311

71	1	0	-1.809731	2.403957	0.406044
72	6	0	0.481403	3.344658	-2.578764
73	1	0	-0.507714	1.752468	-3.638917
74	6	0	0.572386	4.046350	-1.379255
75	1	0	-0.181455	4.244947	0.629866
76	1	0	1.132910	3.594448	-3.409333
77	1	0	1.298766	4.844837	-1.270808
78	1	0	-3.796478	2.275337	-1.020808
79	1	0	-2.160274	0.410925	-2.794257

TS4''*SR*

Total Energy= -2310.3786996

Sum of electronic and zero-point Energies= -2309.745301

Sum of electronic and thermal Energies= -2309.707840

Sum of electronic and thermal Enthalpies= -2309.706896

Sum of electronic and thermal Free Energies= -2309.814724

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.152566	-0.123674	-1.168196
2	8	0	1.089086	-1.296265	-1.525243
3	6	0	2.269001	0.613343	-0.690604
4	1	0	2.051101	1.624171	-0.361359
5	6	0	3.630273	0.394055	-1.171289
6	6	0	4.606591	1.360641	-0.872650
7	6	0	4.034305	-0.756607	-1.871931
8	6	0	5.932973	1.187592	-1.251170
9	1	0	4.310863	2.256126	-0.328962
10	6	0	5.360541	-0.920854	-2.254361
11	1	0	3.301530	-1.524185	-2.091556
12	6	0	6.319817	0.042649	-1.946183
13	1	0	6.666274	1.950248	-1.005341
14	1	0	5.650524	-1.819661	-2.791184
15	1	0	7.354635	-0.096406	-2.242478
16	6	0	-0.167692	-1.247198	1.717379
17	6	0	0.920217	-0.301139	1.836533
18	6	0	0.335939	0.859121	2.444258
19	7	0	-0.946835	0.732809	2.661215
20	7	0	-1.274718	-0.536675	2.214669
21	6	0	-2.626921	-0.877358	2.034872
22	6	0	-3.575913	0.138678	1.866673
23	6	0	-3.033817	-2.218227	1.988947

24	6	0	-4.909452	-0.184585	1.633368
25	1	0	-3.254672	1.171601	1.933370
26	6	0	-4.369483	-2.522853	1.747112
27	1	0	-2.297088	-2.998006	2.122111
28	6	0	-5.314626	-1.514745	1.563509
29	1	0	-5.633824	0.612793	1.497454
30	1	0	-4.673315	-3.564823	1.707562
31	1	0	-6.352503	-1.763023	1.367054
32	6	0	1.077525	2.082472	2.875885
33	1	0	1.917977	1.813451	3.523446
34	1	0	1.478701	2.629817	2.013943
35	1	0	0.409707	2.748692	3.422398
36	6	0	2.245083	-0.305851	1.349280
37	1	0	2.812544	0.566116	1.675711
38	6	0	3.124792	-1.457431	1.100496
39	6	0	4.502563	-1.267865	1.301526
40	6	0	2.675888	-2.707926	0.651472
41	6	0	5.408871	-2.294384	1.073329
42	1	0	4.860917	-0.297103	1.633043
43	6	0	3.590085	-3.731594	0.415180
44	1	0	1.615032	-2.861101	0.501130
45	6	0	4.953113	-3.532858	0.624570
46	1	0	6.468874	-2.125675	1.235352
47	1	0	3.232228	-4.695824	0.066941
48	1	0	5.657613	-4.338375	0.440450
49	8	0	-0.241418	-2.412466	1.296702
50	6	0	-1.269656	-0.059965	-1.329132
51	6	0	-1.759633	2.062613	-2.095717
52	6	0	-0.300372	2.032205	-1.540024
53	6	0	-3.482914	0.107337	-1.917794
54	6	0	-3.370378	-1.260077	-1.640974
55	6	0	-4.479448	-2.093197	-1.737238
56	1	0	-4.402751	-3.150354	-1.508046
57	6	0	-5.688356	-1.526672	-2.125915
58	6	0	-5.790064	-0.159232	-2.408068
59	6	0	-4.688649	0.682236	-2.306194
60	1	0	-1.795496	2.178135	-3.181341
61	1	0	-6.567600	-2.156180	-2.205427
62	1	0	-6.745797	0.254707	-2.709874
63	1	0	-4.760105	1.743240	-2.518475
64	16	0	-1.719857	-1.707864	-1.196755
65	7	0	-2.258022	0.737700	-1.734837
66	7	0	-0.117596	0.596462	-1.130596
67	6	0	-0.112504	3.062560	-0.448749

68	6	0	-1.039463	3.169777	0.590286
69	6	0	0.919924	3.995546	-0.548044
70	6	0	-0.945521	4.210449	1.506611
71	1	0	-1.831767	2.431231	0.687882
72	6	0	1.021302	5.033932	0.376521
73	1	0	1.639075	3.917479	-1.359967
74	6	0	0.082716	5.146797	1.398303
75	1	0	-1.668959	4.284194	2.312298
76	1	0	1.824093	5.758318	0.288617
77	1	0	0.153383	5.959758	2.113591
78	1	0	-2.355346	2.843858	-1.623807
79	1	0	0.415373	2.224112	-2.342548

TS4*SS*

Total Energy= -2310.38326496
Sum of electronic and zero-point Energies= -2309.750611
Sum of electronic and thermal Energies= -2309.713076
Sum of electronic and thermal Enthalpies= -2309.712132
Sum of electronic and thermal Free Energies= -2309.821164

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.712126	-1.880080	-0.102245
2	8	0	-0.480916	-2.598861	-1.073671
3	6	0	-1.953977	-1.351662	0.341588
4	1	0	-1.947599	-0.805083	1.277733
5	6	0	-3.202297	-2.051796	0.030262
6	6	0	-4.284545	-1.936509	0.921475
7	6	0	-3.409599	-2.772174	-1.160114
8	6	0	-5.518284	-2.506418	0.639818
9	1	0	-4.146802	-1.376523	1.843237
10	6	0	-4.647320	-3.350106	-1.434073
11	1	0	-2.593538	-2.876183	-1.864493
12	6	0	-5.709654	-3.219800	-0.543877
13	1	0	-6.334974	-2.393034	1.346904
14	1	0	-4.781952	-3.901352	-2.360529
15	1	0	-6.673336	-3.667073	-0.766284
16	6	0	0.203670	1.078043	-1.425754
17	6	0	-1.142214	1.385368	-0.993884
18	6	0	-1.120996	2.801055	-0.710693
19	7	0	0.062100	3.318262	-0.922396
20	7	0	0.895144	2.284112	-1.311648

21	6	0	2.283569	2.490897	-1.340636
22	6	0	2.790994	3.782494	-1.137147
23	6	0	3.175198	1.421509	-1.525234
24	6	0	4.164945	3.993604	-1.114027
25	1	0	2.096815	4.600752	-0.993714
26	6	0	4.547146	1.654806	-1.490342
27	1	0	2.783206	0.428823	-1.700219
28	6	0	5.054880	2.935116	-1.286219
29	1	0	4.541523	4.999780	-0.956775
30	1	0	5.223358	0.814897	-1.624411
31	1	0	6.125701	3.106865	-1.262238
32	6	0	-2.217659	3.737553	-0.308494
33	1	0	-2.478572	3.613674	0.746686
34	1	0	-1.869658	4.761045	-0.460762
35	1	0	-3.124548	3.571271	-0.894851
36	6	0	-2.149029	0.410962	-1.069634
37	1	0	-1.994098	-0.360804	-1.824863
38	6	0	-3.552290	0.719100	-0.732803
39	6	0	-4.577795	0.385850	-1.622916
40	6	0	-3.885865	1.286958	0.502734
41	6	0	-5.905815	0.651915	-1.301731
42	1	0	-4.328873	-0.089235	-2.567374
43	6	0	-5.211588	1.551410	0.825379
44	1	0	-3.092227	1.490726	1.218694
45	6	0	-6.225517	1.239151	-0.079923
46	1	0	-6.692279	0.391119	-2.002928
47	1	0	-5.456377	1.990299	1.787834
48	1	0	-7.261819	1.441017	0.172367
49	8	0	0.676737	0.005745	-1.821399
50	6	0	1.673136	-1.849025	0.297204
51	6	0	1.962988	-1.374157	2.536237
52	6	0	0.495213	-1.048345	2.112247
53	6	0	3.893670	-1.976622	0.868875
54	6	0	3.925622	-2.406985	-0.464019
55	6	0	5.133551	-2.743672	-1.065028
56	1	0	5.168350	-3.075644	-2.096680
57	6	0	6.294630	-2.641681	-0.304259
58	6	0	6.250946	-2.216876	1.028325
59	6	0	5.048496	-1.876999	1.637083
60	1	0	2.030562	-2.249185	3.186882
61	1	0	7.247319	-2.897519	-0.754154
62	1	0	7.170682	-2.149133	1.598455
63	1	0	5.006002	-1.543592	2.668059
64	16	0	2.304729	-2.454104	-1.180326

65	7	0	2.591249	-1.676438	1.250012
66	7	0	0.448591	-1.528640	0.697977
67	6	0	0.185756	0.423477	2.261652
68	6	0	1.029259	1.372449	1.678201
69	6	0	-0.885385	0.842164	3.047924
70	6	0	0.807988	2.727426	1.889120
71	1	0	1.865697	1.053704	1.056049
72	6	0	-1.117688	2.203752	3.247052
73	1	0	-1.537333	0.104820	3.511057
74	6	0	-0.268596	3.144972	2.672453
75	1	0	1.464660	3.455926	1.424742
76	1	0	-1.955970	2.523454	3.858011
77	1	0	-0.444998	4.204152	2.830841
78	1	0	2.442326	-0.517726	3.011383
79	1	0	-0.213578	-1.643463	2.692022

TS4'*SS*

Total Energy= -2310.3759812
Sum of electronic and zero-point Energies= -2309.741956
Sum of electronic and thermal Energies= -2309.704568
Sum of electronic and thermal Enthalpies= -2309.703624
Sum of electronic and thermal Free Energies= -2309.812473

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.502762	-0.295890	-0.945894
2	8	0	-0.191284	-1.464237	-0.698051
3	6	0	0.336417	0.824537	-1.154466
4	1	0	-0.168809	1.775330	-1.284515
5	6	0	1.599183	0.697125	-1.884530
6	6	0	2.103389	1.828464	-2.548548
7	6	0	2.353796	-0.487173	-1.920471
8	6	0	3.318551	1.789032	-3.214290
9	1	0	1.526781	2.750826	-2.527743
10	6	0	3.576413	-0.520711	-2.588730
11	1	0	1.979505	-1.369049	-1.413560
12	6	0	4.068225	0.610660	-3.231722
13	1	0	3.688107	2.678217	-3.716558
14	1	0	4.156393	-1.439446	-2.592270
15	1	0	5.025904	0.577279	-3.742431
16	6	0	3.431706	0.427337	0.637544
17	6	0	2.083433	0.067950	1.066329

18	6	0	2.200875	-1.283592	1.556110
19	7	0	3.422178	-1.736050	1.436364
20	7	0	4.179735	-0.729158	0.867552
21	6	0	5.540930	-0.947298	0.611606
22	6	0	6.192391	-2.028511	1.219427
23	6	0	6.251463	-0.108268	-0.258571
24	6	0	7.538798	-2.260884	0.962834
25	1	0	5.629082	-2.673660	1.881813
26	6	0	7.599970	-0.355328	-0.497514
27	1	0	5.735841	0.715446	-0.734004
28	6	0	8.254639	-1.426599	0.106726
29	1	0	8.031528	-3.101760	1.441665
30	1	0	8.142848	0.298805	-1.173576
31	1	0	9.306016	-1.610352	-0.088501
32	6	0	1.186129	-2.198356	2.168740
33	1	0	0.422224	-2.473096	1.436734
34	1	0	1.695082	-3.102581	2.507960
35	1	0	0.690415	-1.728738	3.022325
36	6	0	1.069077	1.018019	0.903173
37	1	0	1.485978	1.982746	0.609762
38	6	0	-0.128442	1.150341	1.774344
39	6	0	-0.311853	2.376546	2.426660
40	6	0	-1.025367	0.111920	2.056731
41	6	0	-1.318646	2.542671	3.372464
42	1	0	0.362976	3.199380	2.206794
43	6	0	-2.047320	0.283448	2.985651
44	1	0	-0.912983	-0.840490	1.554109
45	6	0	-2.189261	1.494867	3.660195
46	1	0	-1.429096	3.498027	3.876545
47	1	0	-2.726849	-0.538998	3.190824
48	1	0	-2.976080	1.623456	4.396867
49	8	0	3.872268	1.503816	0.228502
50	6	0	-2.807026	-0.999120	-0.710704
51	6	0	-4.079391	0.571538	-1.825589
52	6	0	-2.636342	1.125846	-1.598001
53	6	0	-4.998394	-1.673668	-0.830317
54	6	0	-4.407162	-2.780193	-0.208010
55	6	0	-5.172850	-3.884560	0.147008
56	1	0	-4.720923	-4.745577	0.626386
57	6	0	-6.535931	-3.849200	-0.131022
58	6	0	-7.118420	-2.740358	-0.754876
59	6	0	-6.358772	-1.633225	-1.115217
60	1	0	-4.294658	0.371721	-2.877294
61	1	0	-7.153631	-4.697608	0.140360

62	1	0	-8.182473	-2.741303	-0.962442
63	1	0	-6.802303	-0.769855	-1.598616
64	16	0	-2.655995	-2.566387	-0.015760
65	7	0	-4.046673	-0.691957	-1.087044
66	7	0	-1.930460	-0.029467	-0.959539
67	6	0	-2.642243	2.380163	-0.753247
68	6	0	-3.283976	2.386319	0.486292
69	6	0	-2.087820	3.558943	-1.250634
70	6	0	-3.384847	3.567215	1.211805
71	1	0	-3.704602	1.466694	0.888829
72	6	0	-2.175237	4.739345	-0.514991
73	1	0	-1.593640	3.555655	-2.219467
74	6	0	-2.830329	4.745149	0.712647
75	1	0	-3.886609	3.565487	2.173665
76	1	0	-1.741058	5.652875	-0.907343
77	1	0	-2.907383	5.665434	1.282475
78	1	0	-4.835348	1.239551	-1.411232
79	1	0	-2.145611	1.320559	-2.553976

TS4''*SS*

Total Energy= -2310.3829387
Sum of electronic and zero-point Energies= -2309.748917
Sum of electronic and thermal Energies= -2309.711417
Sum of electronic and thermal Enthalpies= -2309.710473
Sum of electronic and thermal Free Energies= -2309.820260

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.029688	-0.808972	-0.962060
2	8	0	-1.523415	-1.932990	-0.891902
3	6	0	0.345605	-0.440592	-1.000808
4	1	0	0.559600	0.607668	-1.191352
5	6	0	1.359432	-1.361704	-1.525927
6	6	0	2.598438	-0.815975	-1.905417
7	6	0	1.218072	-2.760616	-1.572266
8	6	0	3.664462	-1.627439	-2.277962
9	1	0	2.725427	0.263136	-1.882246
10	6	0	2.283898	-3.568136	-1.959291
11	1	0	0.269433	-3.207025	-1.301063
12	6	0	3.516131	-3.011943	-2.301362
13	1	0	4.615866	-1.172425	-2.539394
14	1	0	2.150096	-4.645862	-1.986636

15	1	0	4.346918	-3.649741	-2.586091
16	6	0	3.019098	0.710914	0.570796
17	6	0	2.259938	-0.398930	1.098639
18	6	0	3.239962	-1.410774	1.382433
19	7	0	4.456047	-1.000782	1.114013
20	7	0	4.344387	0.281294	0.615229
21	6	0	5.467167	0.895372	0.039505
22	6	0	6.605792	0.126118	-0.237484
23	6	0	5.467899	2.264859	-0.260248
24	6	0	7.725651	0.722628	-0.805128
25	1	0	6.591088	-0.930556	-0.002614
26	6	0	6.596572	2.841314	-0.835353
27	1	0	4.586601	2.851882	-0.044209
28	6	0	7.731242	2.082322	-1.110940
29	1	0	8.600337	0.114469	-1.015447
30	1	0	6.586134	3.902918	-1.063806
31	1	0	8.606660	2.542390	-1.557112
32	6	0	3.095687	-2.785714	1.960004
33	1	0	2.765131	-3.497665	1.196358
34	1	0	4.070139	-3.113780	2.326751
35	1	0	2.375414	-2.810107	2.780698
36	6	0	0.851258	-0.292998	1.075345
37	1	0	0.531222	0.747628	1.090105
38	6	0	-0.118119	-1.198090	1.729194
39	6	0	-1.195998	-0.624995	2.419845
40	6	0	-0.065339	-2.592668	1.620406
41	6	0	-2.170878	-1.420592	3.013172
42	1	0	-1.254918	0.457308	2.499913
43	6	0	-1.038208	-3.389953	2.215484
44	1	0	0.723172	-3.050026	1.036198
45	6	0	-2.092314	-2.809147	2.917047
46	1	0	-2.990256	-0.955623	3.553122
47	1	0	-0.978984	-4.469639	2.119079
48	1	0	-2.850811	-3.433037	3.379340
49	8	0	2.623145	1.798904	0.113144
50	6	0	-3.298888	-0.009569	-0.829941
51	6	0	-3.269568	2.161302	-1.602272
52	6	0	-1.837435	1.738937	-1.166071
53	6	0	-5.439669	0.796934	-1.016597
54	6	0	-5.676383	-0.528017	-0.628275
55	6	0	-6.976328	-0.996142	-0.473817
56	1	0	-7.167973	-2.021487	-0.177488
57	6	0	-8.022119	-0.110230	-0.712871
58	6	0	-7.776271	1.211039	-1.102925

59	6	0	-6.480001	1.687028	-1.260934
60	1	0	-3.382256	2.230040	-2.686733
61	1	0	-9.043891	-0.453123	-0.596470
62	1	0	-8.610278	1.878917	-1.286759
63	1	0	-6.281812	2.709452	-1.562587
64	16	0	-4.165907	-1.437033	-0.430555
65	7	0	-4.072119	1.040404	-1.103331
66	7	0	-1.998739	0.267861	-0.924677
67	6	0	-1.371300	2.459443	0.079142
68	6	0	-2.220252	2.576855	1.187411
69	6	0	-0.091347	3.001136	0.134580
70	6	0	-1.782595	3.221866	2.337289
71	1	0	-3.223481	2.155509	1.161734
72	6	0	0.354689	3.631487	1.296176
73	1	0	0.590686	2.892546	-0.702341
74	6	0	-0.489324	3.746469	2.394222
75	1	0	-2.444592	3.306827	3.192842
76	1	0	1.372263	4.003160	1.335829
77	1	0	-0.143923	4.237023	3.298448
78	1	0	-3.571649	3.098040	-1.133209
79	1	0	-1.125532	1.878010	-1.980998

M4*RR*

Total Energy= -2310.42923687
Sum of electronic and zero-point Energies= -2309.792441
Sum of electronic and thermal Energies= -2309.754886
Sum of electronic and thermal Enthalpies= -2309.753942
Sum of electronic and thermal Free Energies= -2309.862656

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.645263	0.832563	-0.835803
2	6	0	1.818867	1.904949	1.205760
3	6	0	0.349329	1.428468	0.998910
4	6	0	3.833677	1.270266	-0.349503
5	6	0	3.948194	0.640663	-1.594919
6	6	0	5.197757	0.430900	-2.168234
7	1	0	5.296847	-0.061258	-3.129091
8	6	0	6.314140	0.875542	-1.468492
9	6	0	6.188758	1.515612	-0.228802
10	6	0	4.944952	1.723775	0.351731
11	1	0	2.253821	1.489426	2.116620

12	1	0	7.299531	0.725150	-1.895020
13	1	0	7.079071	1.850291	0.291734
14	1	0	4.836584	2.202065	1.318839
15	16	0	2.366045	0.193333	-2.250697
16	7	0	2.499584	1.344802	0.035089
17	7	0	0.374508	0.888879	-0.399422
18	6	0	-0.683374	2.513114	1.172392
19	6	0	-1.427670	2.549632	2.351822
20	6	0	-0.898809	3.477846	0.185871
21	6	0	-2.378757	3.548895	2.548203
22	1	0	-1.270073	1.785912	3.108871
23	6	0	-1.858175	4.467029	0.377787
24	1	0	-0.327769	3.446804	-0.738958
25	6	0	-2.598064	4.504319	1.558948
26	1	0	-2.956818	3.570409	3.466091
27	1	0	-2.030661	5.207566	-0.396096
28	1	0	-3.347854	5.274920	1.704862
29	1	0	1.912329	2.993980	1.196436
30	1	0	0.141782	0.579711	1.659955
31	6	0	-0.672110	0.307343	-1.145853
32	8	0	-0.464537	0.075266	-2.319049
33	6	0	-1.942117	-0.063696	-0.408738
34	1	0	-1.817124	0.142534	0.657522
35	6	0	-3.141661	0.694163	-0.936396
36	6	0	-3.934132	1.433926	-0.057594
37	6	0	-3.495140	0.637389	-2.288547
38	6	0	-5.062310	2.108205	-0.518548
39	1	0	-3.659723	1.485950	0.992830
40	6	0	-4.622945	1.310528	-2.749135
41	1	0	-2.878550	0.069827	-2.979382
42	6	0	-5.410351	2.046883	-1.865241
43	1	0	-5.667226	2.682754	0.176142
44	1	0	-4.888021	1.260111	-3.800587
45	1	0	-6.290334	2.570286	-2.225619
46	6	0	0.081030	-1.907729	0.885002
47	6	0	-0.719359	-2.231549	-0.231543
48	6	0	0.159862	-2.822075	-1.167442
49	7	0	1.403854	-2.903881	-0.733002
50	7	0	1.376334	-2.336494	0.526650
51	6	0	2.590611	-1.934208	1.105088
52	6	0	3.783219	-2.101729	0.380645
53	6	0	2.645199	-1.346355	2.380076
54	6	0	4.995865	-1.691377	0.920380
55	1	0	3.732882	-2.550213	-0.603373

56	6	0	3.871366	-0.931086	2.896785
57	1	0	1.729471	-1.229130	2.942642
58	6	0	5.053251	-1.098911	2.180197
59	1	0	5.903526	-1.819282	0.337232
60	1	0	3.895870	-0.478465	3.884305
61	1	0	6.001161	-0.766687	2.590989
62	6	0	-0.181557	-3.290952	-2.546834
63	1	0	-0.492850	-2.441874	-3.165874
64	1	0	0.691076	-3.757354	-3.008087
65	1	0	-1.004270	-4.012078	-2.534566
66	6	0	-2.060936	-1.627195	-0.553445
67	1	0	-2.256574	-1.815361	-1.616711
68	6	0	-3.261840	-2.122834	0.229057
69	6	0	-4.484333	-2.324218	-0.417638
70	6	0	-3.180544	-2.353360	1.606381
71	6	0	-5.604188	-2.755555	0.289974
72	1	0	-4.557633	-2.138752	-1.486730
73	6	0	-4.300511	-2.783230	2.314153
74	1	0	-2.232037	-2.183407	2.109981
75	6	0	-5.514455	-2.987561	1.660176
76	1	0	-6.544783	-2.912506	-0.229109
77	1	0	-4.224668	-2.962769	3.382602
78	1	0	-6.384387	-3.325414	2.214949
79	8	0	-0.198875	-1.327762	1.976893

M4*RS*

Total Energy= -2310.42556020
Sum of electronic and zero-point Energies= -2309.788241
Sum of electronic and thermal Energies= -2309.750777
Sum of electronic and thermal Enthalpies= -2309.749832
Sum of electronic and thermal Free Energies= -2309.860202

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.269022	0.153598	-1.373321
2	6	0	2.016639	1.881917	-0.030540
3	6	0	0.499685	1.641585	0.230861
4	6	0	3.536614	0.383017	-1.543692
5	6	0	3.295149	-0.652964	-2.453767
6	6	0	4.350515	-1.247825	-3.138294
7	1	0	4.176512	-2.055079	-3.840694
8	6	0	5.634323	-0.772383	-2.893990

9	6	0	5.863176	0.271349	-1.988144
10	6	0	4.816424	0.865981	-1.296492
11	1	0	2.605431	1.785940	0.885185
12	1	0	6.472128	-1.220986	-3.415842
13	1	0	6.876302	0.617226	-1.816023
14	1	0	4.983646	1.655548	-0.572256
15	16	0	1.571940	-1.041702	-2.560422
16	7	0	2.346345	0.800487	-0.958868
17	7	0	0.144026	0.607927	-0.791020
18	6	0	-0.344606	2.887711	0.120213
19	6	0	-0.725688	3.538506	1.294243
20	6	0	-0.749433	3.388962	-1.117461
21	6	0	-1.503849	4.692103	1.231730
22	1	0	-0.416179	3.131674	2.254706
23	6	0	-1.533666	4.537567	-1.177365
24	1	0	-0.466274	2.871881	-2.030623
25	6	0	-1.910338	5.190226	-0.004466
26	1	0	-1.798985	5.194753	2.146774
27	1	0	-1.856570	4.919614	-2.140076
28	1	0	-2.524433	6.083336	-0.053511
29	1	0	2.207852	2.845232	-0.510201
30	1	0	0.376699	1.205757	1.224008
31	6	0	-1.071437	-0.100681	-0.957029
32	8	0	-1.146480	-0.886684	-1.874731
33	6	0	-2.170228	0.191596	0.039160
34	1	0	-1.909838	1.110143	0.567048
35	6	0	-3.495068	0.440157	-0.648167
36	6	0	-4.146922	1.653320	-0.407645
37	6	0	-4.091636	-0.492499	-1.504532
38	6	0	-5.375409	1.932506	-1.001479
39	1	0	-3.678757	2.389027	0.244654
40	6	0	-5.317695	-0.210851	-2.100143
41	1	0	-3.593165	-1.435173	-1.701925
42	6	0	-5.964116	0.998432	-1.849818
43	1	0	-5.867183	2.880086	-0.805610
44	1	0	-5.770654	-0.941340	-2.763127
45	1	0	-6.920451	1.211714	-2.316891
46	6	0	0.414920	-1.333318	1.366057
47	6	0	-0.839294	-0.908470	1.872852
48	6	0	-0.539458	-0.135042	3.016416
49	7	0	0.759165	-0.046142	3.264363
50	7	0	1.353118	-0.789882	2.266654
51	6	0	2.748997	-0.744497	2.115109
52	6	0	3.486404	0.182470	2.869168

53	6	0	3.423897	-1.591809	1.221105
54	6	0	4.867032	0.264681	2.719913
55	1	0	2.959636	0.823580	3.564833
56	6	0	4.805018	-1.489011	1.084686
57	1	0	2.856266	-2.306729	0.642609
58	6	0	5.538688	-0.564954	1.824730
59	1	0	5.419799	0.988299	3.311718
60	1	0	5.309686	-2.140179	0.376135
61	1	0	6.614641	-0.491490	1.704258
62	6	0	-1.512335	0.582002	3.902363
63	1	0	-2.238344	-0.109654	4.340375
64	1	0	-0.975622	1.083809	4.709631
65	1	0	-2.078874	1.336369	3.343099
66	6	0	-2.183222	-0.903518	1.188704
67	1	0	-2.891293	-0.472409	1.907122
68	6	0	-2.783650	-2.229925	0.765275
69	6	0	-4.136133	-2.468340	1.032947
70	6	0	-2.051027	-3.211489	0.088869
71	6	0	-4.753704	-3.648821	0.629389
72	1	0	-4.715274	-1.709876	1.554687
73	6	0	-2.669820	-4.392727	-0.316730
74	1	0	-0.997954	-3.035779	-0.110420
75	6	0	-4.019882	-4.615749	-0.052991
76	1	0	-5.804784	-3.811856	0.847060
77	1	0	-2.091079	-5.146981	-0.841832
78	1	0	-4.494872	-5.538543	-0.371925
79	8	0	0.745861	-1.967605	0.327174

M4*SR*

Total Energy= -2310.41524611
Sum of electronic and zero-point Energies= -2309.778439
Sum of electronic and thermal Energies= -2309.740781
Sum of electronic and thermal Enthalpies= -2309.739837
Sum of electronic and thermal Free Energies= -2309.849708

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.020740	1.288709	-0.060059
2	8	0	1.125578	1.850322	-1.125970
3	6	0	2.077865	0.431020	0.585747
4	1	0	1.685932	0.045022	1.527026
5	6	0	3.323673	1.240570	0.900465

6	6	0	3.941296	1.047190	2.139725
7	6	0	3.906291	2.121970	-0.015911
8	6	0	5.116264	1.720492	2.463532
9	1	0	3.496988	0.357215	2.854000
10	6	0	5.077975	2.799725	0.310795
11	1	0	3.442371	2.267608	-0.985541
12	6	0	5.686636	2.602238	1.548509
13	1	0	5.582197	1.559019	3.430455
14	1	0	5.519101	3.482544	-0.408523
15	1	0	6.600142	3.132287	1.798170
16	6	0	-0.079846	-1.554518	-0.807983
17	6	0	1.219468	-1.804483	-0.315761
18	6	0	1.210382	-3.146367	0.116880
19	7	0	0.047712	-3.745794	-0.071274
20	7	0	-0.752299	-2.780824	-0.645191
21	6	0	-2.102842	-3.069592	-0.874149
22	6	0	-2.586395	-4.352688	-0.565108
23	6	0	-2.994221	-2.113757	-1.391491
24	6	0	-3.924343	-4.666627	-0.768153
25	1	0	-1.894449	-5.083833	-0.167973
26	6	0	-4.331520	-2.450644	-1.585863
27	1	0	-2.619872	-1.129580	-1.635257
28	6	0	-4.811701	-3.720669	-1.279447
29	1	0	-4.274873	-5.664968	-0.522901
30	1	0	-5.006361	-1.700225	-1.987876
31	1	0	-5.855779	-3.970057	-1.437222
32	6	0	2.340148	-3.899804	0.748497
33	1	0	2.619074	-3.456075	1.710816
34	1	0	2.043121	-4.936118	0.921136
35	1	0	3.231801	-3.892138	0.113270
36	6	0	2.390913	-0.866131	-0.256466
37	1	0	3.154727	-1.357044	0.361150
38	6	0	3.049025	-0.582374	-1.597252
39	6	0	4.442708	-0.566544	-1.697402
40	6	0	2.289390	-0.360415	-2.751574
41	6	0	5.072562	-0.326794	-2.917474
42	1	0	5.041018	-0.742109	-0.805679
43	6	0	2.916832	-0.117355	-3.969759
44	1	0	1.205289	-0.365450	-2.674922
45	6	0	4.308866	-0.099882	-4.058629
46	1	0	6.156795	-0.323007	-2.975102
47	1	0	2.316907	0.056493	-4.858290
48	1	0	4.793344	0.083878	-5.012746
49	8	0	-0.614780	-0.509704	-1.282514

50	6	0	-1.241385	2.046631	0.089816
51	6	0	-1.840613	1.987628	2.321102
52	6	0	-0.449479	1.295140	2.140980
53	6	0	-3.365938	2.850660	0.370189
54	6	0	-3.182742	3.021456	-1.007800
55	6	0	-4.194536	3.566129	-1.791643
56	1	0	-4.060971	3.700393	-2.859128
57	6	0	-5.379992	3.931181	-1.163468
58	6	0	-5.552945	3.758920	0.215438
59	6	0	-4.548618	3.214925	1.005702
60	1	0	-1.778730	2.913314	2.896141
61	1	0	-6.182981	4.357678	-1.753868
62	1	0	-6.488041	4.054360	0.677754
63	1	0	-4.675699	3.077291	2.073641
64	16	0	-1.576003	2.493874	-1.527858
65	7	0	-2.227106	2.292198	0.942432
66	7	0	-0.173742	1.497829	0.681854
67	6	0	-0.476510	-0.150013	2.579264
68	6	0	-1.291948	-1.078622	1.929122
69	6	0	0.282685	-0.538970	3.682123
70	6	0	-1.344110	-2.390932	2.386184
71	1	0	-1.854722	-0.785604	1.043013
72	6	0	0.233394	-1.856077	4.134829
73	1	0	0.916483	0.188485	4.184042
74	6	0	-0.581395	-2.779833	3.487227
75	1	0	-1.963487	-3.115649	1.867236
76	1	0	0.830060	-2.155668	4.990109
77	1	0	-0.618005	-3.807750	3.833354
78	1	0	-2.564745	1.311095	2.776737
79	1	0	0.314873	1.838831	2.701446

M4*SS*

Total Energy= -2310.41592879
Sum of electronic and zero-point Energies= -2309.780266
Sum of electronic and thermal Energies= -2309.742262
Sum of electronic and thermal Enthalpies= -2309.741318
Sum of electronic and thermal Free Energies= -2309.854287

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.115409	-0.850746	-1.074969
2	8	0	0.175889	-0.506403	-2.198178

3	6	0	-1.491932	-0.773903	-0.464617
4	1	0	-1.377448	-0.545472	0.599234
5	6	0	-2.168508	-2.127012	-0.622441
6	6	0	-2.939529	-2.650047	0.419811
7	6	0	-2.069719	-2.843421	-1.818288
8	6	0	-3.592731	-3.870614	0.272293
9	1	0	-3.040212	-2.082095	1.341249
10	6	0	-2.722207	-4.065564	-1.965889
11	1	0	-1.481313	-2.441092	-2.639029
12	6	0	-3.482424	-4.583238	-0.920422
13	1	0	-4.191578	-4.263156	1.088031
14	1	0	-2.636181	-4.611792	-2.899836
15	1	0	-3.989108	-5.536009	-1.035219
16	6	0	-0.359921	1.962289	-0.390965
17	6	0	-1.638548	1.710493	-0.928066
18	6	0	-2.169251	2.977543	-1.256157
19	7	0	-1.347068	3.971347	-0.967819
20	7	0	-0.234803	3.361506	-0.429083
21	6	0	0.842024	4.153341	-0.008055
22	6	0	0.830655	5.528701	-0.288686
23	6	0	1.926327	3.611979	0.701025
24	6	0	1.879699	6.337858	0.129953
25	1	0	-0.010686	5.940446	-0.830766
26	6	0	2.968971	4.439529	1.107572
27	1	0	1.930620	2.553369	0.918934
28	6	0	2.960163	5.804054	0.830076
29	1	0	1.850223	7.399538	-0.097491
30	1	0	3.799859	4.003582	1.655267
31	1	0	3.777906	6.439739	1.153230
32	6	0	-3.509957	3.273724	-1.855298
33	1	0	-4.314898	3.083608	-1.137330
34	1	0	-3.555089	4.319955	-2.165061
35	1	0	-3.702349	2.637733	-2.725597
36	6	0	-2.304916	0.376074	-1.123457
37	1	0	-2.372072	0.127438	-2.193871
38	6	0	-3.716195	0.343052	-0.555144
39	6	0	-4.771531	-0.203476	-1.285162
40	6	0	-3.965466	0.818257	0.735511
41	6	0	-6.053068	-0.274761	-0.741276
42	1	0	-4.583955	-0.582431	-2.287305
43	6	0	-5.242233	0.745379	1.284466
44	1	0	-3.146947	1.260858	1.299019
45	6	0	-6.291754	0.198558	0.545950
46	1	0	-6.864515	-0.699807	-1.324228

47	1	0	-5.420999	1.120416	2.287690
48	1	0	-7.289055	0.145327	0.971236
49	8	0	0.542315	1.176502	0.034741
50	6	0	2.155185	-1.475479	-0.675138
51	6	0	2.171165	-2.987996	1.066711
52	6	0	0.738415	-2.376826	0.919961
53	6	0	4.304342	-2.095641	-0.188685
54	6	0	4.503647	-1.221086	-1.264720
55	6	0	5.786098	-0.956061	-1.731302
56	1	0	5.948361	-0.278234	-2.561670
57	6	0	6.852899	-1.583251	-1.096054
58	6	0	6.644460	-2.457625	-0.023118
59	6	0	5.365997	-2.728893	0.448646
60	1	0	2.208458	-4.042258	0.785482
61	1	0	7.862344	-1.389933	-1.440823
62	1	0	7.494791	-2.933553	0.451944
63	1	0	5.196273	-3.405167	1.278955
64	16	0	2.972535	-0.583711	-1.889476
65	7	0	2.947398	-2.199053	0.106059
66	7	0	0.869839	-1.564983	-0.329430
67	6	0	0.331728	-1.571639	2.132507
68	6	0	0.967782	-0.365870	2.431457
69	6	0	-0.650340	-2.072021	2.987218
70	6	0	0.606809	0.342325	3.572288
71	1	0	1.704162	0.044968	1.748488
72	6	0	-1.006407	-1.363182	4.133217
73	1	0	-1.141555	-3.012848	2.751815
74	6	0	-0.379763	-0.154186	4.423390
75	1	0	1.089543	1.289402	3.790241
76	1	0	-1.773870	-1.753501	4.793271
77	1	0	-0.661701	0.404290	5.310017
78	1	0	2.562898	-2.853510	2.075447
79	1	0	0.006980	-3.166669	0.734882

TS5*RR*

Total Energy= -2310.42030195

Sum of electronic and zero-point Energies= -2309.784269

Sum of electronic and thermal Energies= -2309.747495

Sum of electronic and thermal Enthalpies= -2309.746551

Sum of electronic and thermal Free Energies= -2309.854491

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

1	6	0	-2.071769	-1.347406	-0.530850
2	6	0	-2.159724	-2.151228	1.624596
3	6	0	-0.770006	-1.499066	1.349623
4	6	0	-4.201845	-2.035393	-0.024068
5	6	0	-4.361498	-1.598150	-1.344746
6	6	0	-5.602619	-1.673621	-1.966290
7	1	0	-5.735357	-1.332920	-2.987044
8	6	0	-6.666132	-2.201917	-1.241103
9	6	0	-6.495414	-2.641221	0.076384
10	6	0	-5.259283	-2.564358	0.707651
11	1	0	-2.660442	-1.714975	2.489363
12	1	0	-7.642067	-2.275409	-1.707476
13	1	0	-7.341347	-3.050098	0.617562
14	1	0	-5.118568	-2.902475	1.728314
15	16	0	-2.845276	-0.969406	-2.018782
16	7	0	-2.887357	-1.846106	0.393210
17	7	0	-0.810004	-1.234025	-0.117721
18	6	0	0.366443	-2.394292	1.777385
19	6	0	1.167264	-2.026365	2.855456
20	6	0	0.593083	-3.611333	1.128246
21	6	0	2.188539	-2.871134	3.289664
22	1	0	0.994001	-1.076588	3.354967
23	6	0	1.613064	-4.450042	1.557709
24	1	0	-0.013450	-3.886135	0.268397
25	6	0	2.411362	-4.081133	2.641490
26	1	0	2.809047	-2.579023	4.130509
27	1	0	1.796930	-5.385798	1.040171
28	1	0	3.210629	-4.736011	2.973481
29	1	0	-2.081257	-3.234585	1.747403
30	1	0	-0.701497	-0.521842	1.837585
31	6	0	0.026977	-0.259345	-0.826889
32	8	0	-0.284548	-0.063987	-2.000253
33	6	0	1.476019	-0.168700	-0.359042
34	1	0	1.496725	-0.053987	0.730687
35	6	0	2.249048	-1.423002	-0.731206
36	6	0	3.308463	-1.834386	0.084092
37	6	0	1.959840	-2.163981	-1.880443
38	6	0	4.058120	-2.960564	-0.236145
39	1	0	3.542785	-1.264604	0.979851
40	6	0	2.703629	-3.300116	-2.195569
41	1	0	1.144316	-1.854609	-2.526328
42	6	0	3.754175	-3.702545	-1.376255
43	1	0	4.872597	-3.266782	0.413342

44	1	0	2.460050	-3.869398	-3.087443
45	1	0	4.332858	-4.586961	-1.623913
46	6	0	0.001247	2.235472	-0.101865
47	6	0	1.278847	2.307331	-0.644731
48	6	0	1.532759	3.690711	-0.799627
49	7	0	0.518697	4.434186	-0.388059
50	7	0	-0.435012	3.540354	0.035082
51	6	0	-1.651952	4.016298	0.559641
52	6	0	-1.754130	5.363708	0.925860
53	6	0	-2.761431	3.173585	0.703119
54	6	0	-2.950921	5.856553	1.432567
55	1	0	-0.891048	6.005361	0.802919
56	6	0	-3.948741	3.683696	1.220329
57	1	0	-2.681650	2.135660	0.409358
58	6	0	-4.056073	5.022207	1.588161
59	1	0	-3.015530	6.903797	1.711795
60	1	0	-4.802872	3.021471	1.325864
61	1	0	-4.987336	5.410774	1.986679
62	6	0	2.766228	4.337451	-1.348279
63	1	0	3.054000	3.883715	-2.301666
64	1	0	2.590806	5.403904	-1.501997
65	1	0	3.612804	4.212791	-0.665339
66	6	0	2.113521	1.108664	-0.992032
67	1	0	2.105276	0.939305	-2.078273
68	6	0	3.559273	1.246461	-0.551079
69	6	0	4.600304	0.874522	-1.401943
70	6	0	3.871664	1.711638	0.729560
71	6	0	5.927557	0.962071	-0.986216
72	1	0	4.364790	0.503100	-2.396498
73	6	0	5.195418	1.797153	1.151337
74	1	0	3.063556	2.020568	1.388711
75	6	0	6.228822	1.422500	0.292648
76	1	0	6.725762	0.670124	-1.661720
77	1	0	5.422562	2.161626	2.148626
78	1	0	7.261701	1.493261	0.618784
79	8	0	-0.691629	1.185494	0.216929

TS5*RS*

Total Energy= -2310.41691581

Sum of electronic and zero-point Energies= -2309.781266

Sum of electronic and thermal Energies= -2309.744300

Sum of electronic and thermal Enthalpies= -2309.743355

Sum of electronic and thermal Free Energies= -2309.853059

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.531702	-1.545309	0.705131
2	6	0	1.952863	-2.629262	-1.280205
3	6	0	0.688661	-1.727655	-1.412453
4	6	0	3.576988	-2.587492	0.786088
5	6	0	3.512512	-2.009416	2.059974
6	6	0	4.557494	-2.173354	2.961507
7	1	0	4.515885	-1.725834	3.948445
8	6	0	5.654843	-2.930443	2.561774
9	6	0	5.708625	-3.507193	1.288399
10	6	0	4.669904	-3.344517	0.378352
11	1	0	2.703691	-2.409727	-2.039638
12	1	0	6.479091	-3.074182	3.251137
13	1	0	6.575429	-4.092309	1.002401
14	1	0	4.706126	-3.786429	-0.611200
15	16	0	2.010088	-1.092503	2.294509
16	7	0	2.436405	-2.272391	0.053375
17	7	0	0.434565	-1.299752	-0.006189
18	6	0	-0.465863	-2.459099	-2.051730
19	6	0	-0.913906	-2.070166	-3.311512
20	6	0	-1.063785	-3.547051	-1.408992
21	6	0	-1.952144	-2.764165	-3.932141
22	1	0	-0.451168	-1.220991	-3.807876
23	6	0	-2.101377	-4.235186	-2.024742
24	1	0	-0.731607	-3.835506	-0.414432
25	6	0	-2.545232	-3.845515	-3.289231
26	1	0	-2.296707	-2.454872	-4.913465
27	1	0	-2.574742	-5.067893	-1.514974
28	1	0	-3.358843	-4.381671	-3.767304
29	1	0	1.696955	-3.691833	-1.307126
30	1	0	0.926658	-0.817199	-1.971694
31	6	0	-0.353373	-0.109642	0.402810
32	8	0	-0.285890	0.148236	1.605806
33	6	0	-1.631716	0.096323	-0.403401
34	1	0	-1.367576	0.053458	-1.466099
35	6	0	-2.662245	-0.982313	-0.140201
36	6	0	-3.594492	-1.255605	-1.144870
37	6	0	-2.750425	-1.674239	1.069749
38	6	0	-4.598820	-2.197055	-0.948229
39	1	0	-3.520877	-0.731205	-2.095133
40	6	0	-3.748427	-2.627717	1.262794

41	1	0	-2.039535	-1.457046	1.860812
42	6	0	-4.676284	-2.890456	0.258384
43	1	0	-5.310909	-2.400932	-1.742244
44	1	0	-3.804703	-3.161416	2.206742
45	1	0	-5.453956	-3.631777	0.413309
46	6	0	0.202601	2.203576	-0.590056
47	6	0	-1.139396	2.526272	-0.453290
48	6	0	-1.198252	3.927471	-0.631856
49	7	0	-0.008473	4.449994	-0.876767
50	7	0	0.863528	3.389225	-0.841923
51	6	0	2.228200	3.599329	-1.123557
52	6	0	2.613884	4.783808	-1.761452
53	6	0	3.197257	2.656269	-0.762364
54	6	0	3.956126	5.016611	-2.036730
55	1	0	1.851846	5.505445	-2.027653
56	6	0	4.535751	2.902667	-1.054961
57	1	0	2.894638	1.747526	-0.259070
58	6	0	4.926423	4.078433	-1.690624
59	1	0	4.242919	5.939237	-2.531958
60	1	0	5.281051	2.166022	-0.770320
61	1	0	5.972603	4.263152	-1.910721
62	6	0	-2.416701	4.790453	-0.553096
63	1	0	-2.862800	4.735295	0.445315
64	1	0	-2.160108	5.828768	-0.770792
65	1	0	-3.178004	4.458862	-1.266651
66	6	0	-2.219706	1.528852	-0.173245
67	1	0	-3.006037	1.619388	-0.936904
68	6	0	-2.919595	1.732731	1.167704
69	6	0	-4.254625	1.345525	1.317498
70	6	0	-2.276505	2.334862	2.251913
71	6	0	-4.927627	1.537671	2.521889
72	1	0	-4.770089	0.880348	0.480144
73	6	0	-2.946711	2.534920	3.455539
74	1	0	-1.240966	2.639763	2.140851
75	6	0	-4.274376	2.134822	3.596901
76	1	0	-5.963795	1.227172	2.616383
77	1	0	-2.430840	3.006953	4.286383
78	1	0	-4.796330	2.293850	4.535455
79	8	0	0.777839	1.036717	-0.515626

TS5*SR*

Total Energy= -2310.41130471

Sum of electronic and zero-point Energies= -2309.776100

Sum of electronic and thermal Energies= -2309.738916
Sum of electronic and thermal Enthalpies= -2309.737972
Sum of electronic and thermal Free Energies= -2309.847942

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.575531	-0.968614	-0.278321
2	8	0	-0.704354	-1.443279	-1.393595
3	6	0	-1.704784	-0.546475	0.640546
4	1	0	-1.264964	0.046546	1.447135
5	6	0	-2.348121	-1.771267	1.267988
6	6	0	-2.809591	-1.673706	2.585507
7	6	0	-2.543739	-2.967363	0.571930
8	6	0	-3.457892	-2.743524	3.195994
9	1	0	-2.668394	-0.742155	3.129854
10	6	0	-3.187331	-4.040548	1.184794
11	1	0	-2.198189	-3.049196	-0.453729
12	6	0	-3.647203	-3.932675	2.495110
13	1	0	-3.812459	-2.648906	4.217439
14	1	0	-3.334505	-4.963617	0.632881
15	1	0	-4.150016	-4.770052	2.968114
16	6	0	-0.675476	1.803114	-0.599838
17	6	0	-2.045986	1.698123	-0.353192
18	6	0	-2.532481	3.023396	-0.376274
19	7	0	-1.577664	3.911474	-0.602583
20	7	0	-0.430336	3.164030	-0.747788
21	6	0	0.821760	3.794247	-0.814702
22	6	0	0.961171	5.104428	-0.342606
23	6	0	1.936378	3.119081	-1.329405
24	6	0	2.207909	5.719812	-0.363817
25	1	0	0.087659	5.613942	0.045231
26	6	0	3.178559	3.745519	-1.332024
27	1	0	1.816512	2.109657	-1.699991
28	6	0	3.327217	5.044515	-0.848062
29	1	0	2.305341	6.734222	0.011118
30	1	0	4.038547	3.212531	-1.726860
31	1	0	4.299280	5.526572	-0.855679
32	6	0	-3.951317	3.458558	-0.187454
33	1	0	-4.328237	3.152539	0.794280
34	1	0	-4.027013	4.544731	-0.265855
35	1	0	-4.603182	3.004131	-0.940395
36	6	0	-2.744317	0.415950	-0.020790
37	1	0	-3.460277	0.611578	0.790629

38	6	0	-3.553555	-0.201192	-1.154575
39	6	0	-4.699807	-0.947178	-0.864968
40	6	0	-3.196585	-0.018912	-2.492346
41	6	0	-5.465701	-1.509636	-1.884042
42	1	0	-4.992981	-1.088867	0.173257
43	6	0	-3.958171	-0.577960	-3.513828
44	1	0	-2.312363	0.567551	-2.722565
45	6	0	-5.095940	-1.326482	-3.213744
46	1	0	-6.353917	-2.083568	-1.637984
47	1	0	-3.666294	-0.425759	-4.548646
48	1	0	-5.692555	-1.757924	-4.011608
49	8	0	0.225415	0.893480	-0.659608
50	6	0	1.687060	-1.784286	-0.240365
51	6	0	2.404901	-1.854616	1.948910
52	6	0	1.011954	-1.148092	1.870678
53	6	0	3.866900	-2.494706	-0.139372
54	6	0	3.618465	-2.564655	-1.516284
55	6	0	4.609858	-2.991884	-2.390978
56	1	0	4.424229	-3.049329	-3.457695
57	6	0	5.845894	-3.344194	-1.856558
58	6	0	6.084175	-3.273802	-0.480068
59	6	0	5.097531	-2.847364	0.402136
60	1	0	2.353371	-2.829270	2.439142
61	1	0	6.634324	-3.679921	-2.520500
62	1	0	7.055443	-3.556970	-0.090115
63	1	0	5.274759	-2.789580	1.470353
64	16	0	1.956347	-2.079904	-1.913239
65	7	0	2.740098	-2.035032	0.535288
66	7	0	0.636248	-1.349462	0.437295
67	6	0	1.073134	0.299927	2.309060
68	6	0	1.864900	1.230678	1.632063
69	6	0	0.368407	0.691881	3.446552
70	6	0	1.936663	2.543398	2.084023
71	1	0	2.387629	0.944837	0.723954
72	6	0	0.442186	2.007113	3.902602
73	1	0	-0.242993	-0.035082	3.976650
74	6	0	1.224708	2.932643	3.219347
75	1	0	2.533330	3.268187	1.536867
76	1	0	-0.114884	2.304400	4.784878
77	1	0	1.277055	3.960199	3.564766
78	1	0	3.147165	-1.225737	2.442029
79	1	0	0.282910	-1.685396	2.483239

TS5*SS*

Total Energy= -2310.41471571
Sum of electronic and zero-point Energies= -2309.779123
Sum of electronic and thermal Energies= -2309.741933
Sum of electronic and thermal Enthalpies= -2309.740989
Sum of electronic and thermal Free Energies= -2309.851788

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.005906	-0.975993	-0.932174
2	8	0	0.236421	-1.015731	-2.125440
3	6	0	-1.395611	-1.023757	-0.334268
4	1	0	-1.354764	-0.584821	0.666900
5	6	0	-1.841387	-2.472519	-0.225076
6	6	0	-2.473264	-2.915652	0.940489
7	6	0	-1.688046	-3.362978	-1.291725
8	6	0	-2.938893	-4.223710	1.043449
9	1	0	-2.624217	-2.216532	1.759455
10	6	0	-2.153521	-4.671797	-1.189329
11	1	0	-1.200191	-3.026025	-2.202091
12	6	0	-2.778127	-5.106233	-0.022322
13	1	0	-3.431646	-4.550927	1.953539
14	1	0	-2.028555	-5.354095	-2.024265
15	1	0	-3.140913	-6.126103	0.054972
16	6	0	-0.664458	1.707277	-0.832284
17	6	0	-1.935228	1.259873	-1.213002
18	6	0	-2.659121	2.430037	-1.542651
19	7	0	-1.944100	3.530791	-1.381021
20	7	0	-0.713031	3.095777	-0.944263
21	6	0	0.248858	4.032663	-0.533832
22	6	0	-0.123798	5.375629	-0.385439
23	6	0	1.573986	3.653959	-0.270162
24	6	0	0.810703	6.317044	0.029335
25	1	0	-1.147210	5.657193	-0.597715
26	6	0	2.492761	4.610593	0.152075
27	1	0	1.860563	2.619340	-0.398317
28	6	0	2.124462	5.944640	0.307871
29	1	0	0.503444	7.352648	0.140800
30	1	0	3.514989	4.303723	0.354466
31	1	0	2.848683	6.682168	0.637804
32	6	0	-4.071348	2.529302	-2.032860
33	1	0	-4.782949	2.250352	-1.248886
34	1	0	-4.280116	3.552569	-2.351635

35	1	0	-4.243782	1.853125	-2.876031
36	6	0	-2.385195	-0.173321	-1.182589
37	1	0	-2.393836	-0.618464	-2.188802
38	6	0	-3.777148	-0.323510	-0.590081
39	6	0	-4.757968	-1.076834	-1.232885
40	6	0	-4.080402	0.267560	0.640771
41	6	0	-6.022317	-1.233689	-0.664836
42	1	0	-4.528133	-1.546364	-2.186380
43	6	0	-5.337985	0.109315	1.213943
44	1	0	-3.321665	0.867981	1.138621
45	6	0	-6.315428	-0.641686	0.560006
46	1	0	-6.777531	-1.818177	-1.181331
47	1	0	-5.559131	0.576317	2.168935
48	1	0	-7.299127	-0.761317	1.003008
49	8	0	0.364069	1.047538	-0.453741
50	6	0	2.311187	-1.377762	-0.466133
51	6	0	2.486397	-2.152940	1.697422
52	6	0	1.022147	-1.677172	1.425642
53	6	0	4.511950	-1.720346	0.078211
54	6	0	4.619885	-1.305075	-1.255160
55	6	0	5.865082	-1.207939	-1.864417
56	1	0	5.957178	-0.886039	-2.895567
57	6	0	6.988684	-1.533082	-1.110037
58	6	0	6.870754	-1.948628	0.220735
59	6	0	5.629081	-2.048700	0.837548
60	1	0	2.562041	-3.237135	1.804690
61	1	0	7.970395	-1.461432	-1.564237
62	1	0	7.762617	-2.197612	0.784566
63	1	0	5.528199	-2.369228	1.868436
64	16	0	3.029181	-0.976673	-1.974065
65	7	0	3.178981	-1.733775	0.477000
66	7	0	1.053659	-1.394066	-0.042633
67	6	0	0.633239	-0.489919	2.279207
68	6	0	1.297277	0.732445	2.158124
69	6	0	-0.369399	-0.639053	3.236209
70	6	0	0.946991	1.799020	2.976823
71	1	0	2.060030	0.863536	1.396589
72	6	0	-0.717845	0.428553	4.062515
73	1	0	-0.877484	-1.594977	3.337582
74	6	0	-0.061685	1.648539	3.929368
75	1	0	1.449996	2.753460	2.858544
76	1	0	-1.500627	0.305118	4.803390
77	1	0	-0.336484	2.485188	4.563422
78	1	0	2.914252	-1.659128	2.570577

79	1	0	0.320406	-2.498040	1.592985

M5*RR*

Total Energy= -2310.42142137
Sum of electronic and zero-point Energies= -2309.784977
Sum of electronic and thermal Energies= -2309.747774
Sum of electronic and thermal Enthalpies= -2309.746830
Sum of electronic and thermal Free Energies= -2309.856041

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.463539	-0.202515	-0.409979
2	6	0	-2.932991	-0.252998	1.848682
3	6	0	-1.391585	-0.381093	1.608786
4	6	0	-4.738173	-0.272755	-0.055058
5	6	0	-4.682688	-0.154903	-1.449924
6	6	0	-5.851818	-0.109273	-2.198029
7	1	0	-5.817546	-0.015814	-3.278026
8	6	0	-7.068712	-0.186154	-1.524021
9	6	0	-7.113887	-0.300667	-0.131815
10	6	0	-5.947189	-0.346198	0.625951
11	1	0	-3.213525	0.693915	2.316229
12	1	0	-7.992450	-0.155505	-2.090689
13	1	0	-8.073266	-0.357023	0.370477
14	1	0	-5.973033	-0.435909	1.706374
15	16	0	-3.007698	-0.035689	-2.040328
16	7	0	-3.455865	-0.303324	0.483258
17	7	0	-1.268159	-0.250629	0.131331
18	6	0	-0.846484	-1.695763	2.121328
19	6	0	0.150014	-1.713737	3.092685
20	6	0	-1.375980	-2.901042	1.650139
21	6	0	0.615545	-2.928790	3.596937
22	1	0	0.562123	-0.776609	3.458335
23	6	0	-0.915602	-4.110127	2.153582
24	1	0	-2.140386	-2.890614	0.875052
25	6	0	0.081577	-4.124918	3.130117
26	1	0	1.393688	-2.936434	4.353517
27	1	0	-1.321742	-5.042898	1.776107
28	1	0	0.444571	-5.070568	3.519939
29	1	0	-3.316166	-1.085337	2.441171
30	1	0	-0.853787	0.456361	2.059291
31	6	0	-0.060654	0.204151	-0.674911

32	8	0	-0.347987	0.351305	-1.894559
33	6	0	1.187897	-0.639200	-0.317041
34	1	0	1.401883	-0.518628	0.753569
35	6	0	1.017460	-2.116288	-0.601915
36	6	0	1.704483	-3.038396	0.194322
37	6	0	0.229464	-2.597195	-1.652638
38	6	0	1.607287	-4.404545	-0.045155
39	1	0	2.317364	-2.676891	1.016643
40	6	0	0.121738	-3.967501	-1.885552
41	1	0	-0.296922	-1.886554	-2.281179
42	6	0	0.809423	-4.876183	-1.085457
43	1	0	2.144083	-5.101411	0.591799
44	1	0	-0.500665	-4.324087	-2.701067
45	1	0	0.725047	-5.942633	-1.270979
46	6	0	1.323114	2.090977	-0.271429
47	6	0	2.413302	1.441134	-0.805720
48	6	0	3.383885	2.463290	-0.961073
49	7	0	2.930201	3.637239	-0.548513
50	7	0	1.646352	3.409622	-0.130848
51	6	0	0.875538	4.469004	0.400586
52	6	0	1.532359	5.588717	0.917316
53	6	0	-0.520965	4.413180	0.393083
54	6	0	0.789182	6.645889	1.429386
55	1	0	2.614871	5.614808	0.903502
56	6	0	-1.248791	5.475370	0.921150
57	1	0	-1.021804	3.550307	-0.025828
58	6	0	-0.603346	6.594667	1.440262
59	1	0	1.305117	7.513577	1.828249
60	1	0	-2.333155	5.428180	0.912828
61	1	0	-1.178728	7.420414	1.845336
62	6	0	4.769884	2.339781	-1.510318
63	1	0	4.760980	1.820317	-2.472986
64	1	0	5.204796	3.331515	-1.646074
65	1	0	5.409147	1.760467	-0.837193
66	6	0	2.389448	-0.029178	-1.105105
67	1	0	2.166044	-0.192620	-2.167888
68	6	0	3.682271	-0.741719	-0.768880
69	6	0	4.201283	-1.704301	-1.635361
70	6	0	4.346074	-0.495646	0.436919
71	6	0	5.357999	-2.408957	-1.309213
72	1	0	3.683156	-1.910529	-2.568637
73	6	0	5.502445	-1.196855	0.767353
74	1	0	3.952232	0.260067	1.113177
75	6	0	6.012133	-2.157165	-0.106148

76	1	0	5.747676	-3.154187	-1.995704
77	1	0	6.008216	-0.993232	1.706256
78	1	0	6.914480	-2.703308	0.149730
79	8	0	0.146085	1.574813	0.068840

M5*RS*

Total Energy= -2310.41803543
Sum of electronic and zero-point Energies= -2309.780877
Sum of electronic and thermal Energies= -2309.743715
Sum of electronic and thermal Enthalpies= -2309.742771
Sum of electronic and thermal Free Energies= -2309.851483

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.161753	0.273264	0.494105
2	6	0	3.146840	0.380920	-1.590939
3	6	0	1.677873	-0.151512	-1.704410
4	6	0	4.379226	0.867814	0.673280
5	6	0	3.967508	0.945027	2.009981
6	6	0	4.866572	1.316548	3.001060
7	1	0	4.555159	1.380267	4.038082
8	6	0	6.177655	1.604284	2.626957
9	6	0	6.578154	1.526023	1.290325
10	6	0	5.683867	1.155433	0.290480
11	1	0	3.280066	1.363931	-2.048022
12	1	0	6.895121	1.894131	3.386464
13	1	0	7.603586	1.757360	1.024131
14	1	0	5.987193	1.092172	-0.748782
15	16	0	2.238358	0.561976	2.194870
16	7	0	3.321087	0.479852	-0.141708
17	7	0	1.188347	-0.107939	-0.301496
18	6	0	1.628711	-1.545963	-2.287568
19	6	0	1.004224	-1.779298	-3.509278
20	6	0	2.253652	-2.601275	-1.616273
21	6	0	1.005556	-3.060027	-4.063290
22	1	0	0.515739	-0.959331	-4.029708
23	6	0	2.253548	-3.875701	-2.165790
24	1	0	2.722793	-2.425623	-0.650195
25	6	0	1.629849	-4.106333	-3.393284
26	1	0	0.517372	-3.235428	-5.016516
27	1	0	2.727939	-4.693892	-1.633926
28	1	0	1.627081	-5.103991	-3.820778

29	1	0	3.861488	-0.324633	-2.017788
30	1	0	1.059926	0.532311	-2.292086
31	6	0	-0.255714	0.006494	0.189056
32	8	0	-0.305348	0.122389	1.441577
33	6	0	-1.132907	-1.052333	-0.515405
34	1	0	-1.021769	-0.899076	-1.597419
35	6	0	-0.734170	-2.478825	-0.211053
36	6	0	-1.028001	-3.463182	-1.158964
37	6	0	-0.129394	-2.860258	0.989738
38	6	0	-0.727298	-4.800058	-0.919459
39	1	0	-1.480839	-3.172044	-2.104676
40	6	0	0.184737	-4.197321	1.224438
41	1	0	0.078634	-2.099505	1.734963
42	6	0	-0.114117	-5.171720	0.275247
43	1	0	-0.952529	-5.548096	-1.673965
44	1	0	0.658729	-4.480005	2.159890
45	1	0	0.129529	-6.212764	0.464187
46	6	0	-1.889306	1.582388	-0.527024
47	6	0	-2.903399	0.662293	-0.393156
48	6	0	-4.087498	1.436647	-0.450264
49	7	0	-3.827033	2.723488	-0.620200
50	7	0	-2.460722	2.816696	-0.654071
51	6	0	-1.838327	4.074542	-0.819607
52	6	0	-2.541146	5.100532	-1.455688
53	6	0	-0.549566	4.300659	-0.329300
54	6	0	-1.948123	6.349727	-1.602835
55	1	0	-3.543320	4.905290	-1.817563
56	6	0	0.033853	5.553146	-0.496675
57	1	0	-0.021570	3.503931	0.178916
58	6	0	-0.657999	6.582407	-1.130577
59	1	0	-2.498548	7.144514	-2.096144
60	1	0	1.034364	5.725543	-0.112726
61	1	0	-0.198690	7.557764	-1.251624
62	6	0	-5.491183	0.940182	-0.321836
63	1	0	-5.646627	0.484274	0.661134
64	1	0	-6.196966	1.762928	-0.446400
65	1	0	-5.705452	0.174258	-1.073662
66	6	0	-2.650877	-0.801754	-0.210523
67	1	0	-3.190917	-1.368074	-0.982083
68	6	0	-3.137515	-1.341756	1.128467
69	6	0	-3.631546	-2.646709	1.205991
70	6	0	-3.125227	-0.561440	2.287375
71	6	0	-4.095061	-3.167795	2.411879
72	1	0	-3.641903	-3.263520	0.310118

73	6	0	-3.591211	-1.077120	3.493701
74	1	0	-2.728166	0.446492	2.232422
75	6	0	-4.077920	-2.381506	3.561269
76	1	0	-4.474426	-4.184351	2.451307
77	1	0	-3.575375	-0.457691	4.385438
78	1	0	-4.444398	-2.780450	4.502137
79	8	0	-0.579045	1.363655	-0.553030

M5*SR*

Total Energy= -2310.41839272

Sum of electronic and zero-point Energies= -2309.781771

Sum of electronic and thermal Energies= -2309.744439

Sum of electronic and thermal Enthalpies= -2309.743495

Sum of electronic and thermal Free Energies= -2309.853179

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.114333	-0.416375	-0.340947
2	8	0	0.563886	-0.875244	-1.425782
3	6	0	-0.179477	-1.379885	0.840641
4	1	0	-0.598729	-0.770430	1.652505
5	6	0	1.068726	-2.047481	1.370703
6	6	0	1.206462	-2.211920	2.753551
7	6	0	2.074456	-2.546696	0.533722
8	6	0	2.316512	-2.856890	3.294287
9	1	0	0.428010	-1.833835	3.414014
10	6	0	3.188525	-3.183977	1.074560
11	1	0	1.962724	-2.426945	-0.538451
12	6	0	3.313779	-3.344198	2.453266
13	1	0	2.402497	-2.975196	4.370032
14	1	0	3.960538	-3.564245	0.412455
15	1	0	4.182400	-3.844681	2.869552
16	6	0	-2.256324	-0.244488	-0.446309
17	6	0	-2.450362	-1.540145	-0.025706
18	6	0	-3.854625	-1.717849	-0.096408
19	7	0	-4.471877	-0.621494	-0.510321
20	7	0	-3.475174	0.290409	-0.737186
21	6	0	-3.775372	1.633470	-1.058009
22	6	0	-4.946692	2.204775	-0.559581
23	6	0	-2.903992	2.379995	-1.853730
24	6	0	-5.240591	3.532150	-0.853617
25	1	0	-5.604507	1.601911	0.055303

26	6	0	-3.205558	3.710241	-2.130382
27	1	0	-2.000783	1.920851	-2.236938
28	6	0	-4.370910	4.292424	-1.634079
29	1	0	-6.151573	3.974876	-0.463610
30	1	0	-2.528113	4.291664	-2.747735
31	1	0	-4.601865	5.328678	-1.857964
32	6	0	-4.619440	-2.959117	0.232018
33	1	0	-4.442346	-3.262881	1.268579
34	1	0	-5.688675	-2.790589	0.094573
35	1	0	-4.306114	-3.788643	-0.409016
36	6	0	-1.323593	-2.385209	0.484030
37	1	0	-1.617213	-2.834833	1.442841
38	6	0	-0.920087	-3.536141	-0.424483
39	6	0	-0.378261	-4.695633	0.137246
40	6	0	-1.087005	-3.479073	-1.809395
41	6	0	-0.002167	-5.771596	-0.663021
42	1	0	-0.242625	-4.748965	1.215472
43	6	0	-0.717098	-4.554035	-2.613298
44	1	0	-1.501033	-2.578584	-2.251292
45	6	0	-0.172993	-5.703916	-2.043568
46	1	0	0.417526	-6.663555	-0.208026
47	1	0	-0.854740	-4.494081	-3.688718
48	1	0	0.112165	-6.542771	-2.670863
49	8	0	-1.130648	0.451704	-0.533771
50	6	0	2.188172	0.949007	-0.353273
51	6	0	2.200878	2.345402	1.476030
52	6	0	1.010753	1.344910	1.560777
53	6	0	4.135725	2.179614	-0.288594
54	6	0	4.292423	1.486543	-1.496048
55	6	0	5.424064	1.683990	-2.275873
56	1	0	5.553016	1.152916	-3.212780
57	6	0	6.385527	2.588062	-1.827309
58	6	0	6.217944	3.276969	-0.623318
59	6	0	5.089156	3.081780	0.166887
60	1	0	2.806055	2.344166	2.382502
61	1	0	7.274022	2.759429	-2.424648
62	1	0	6.978879	3.976354	-0.294986
63	1	0	4.952414	3.609517	1.104408
64	16	0	2.908567	0.416341	-1.832954
65	7	0	2.947003	1.816348	0.334610
66	7	0	1.040407	0.692501	0.222070
67	6	0	-0.310301	1.994533	1.896985
68	6	0	-0.900442	2.905569	1.017041
69	6	0	-0.951402	1.683344	3.094401

70	6	0	-2.122770	3.486809	1.327006
71	1	0	-0.424681	3.118391	0.062993
72	6	0	-2.173233	2.275913	3.413578
73	1	0	-0.497537	0.970916	3.779396
74	6	0	-2.760887	3.173371	2.528163
75	1	0	-2.592637	4.164273	0.619865
76	1	0	-2.666754	2.025921	4.347010
77	1	0	-3.720378	3.622989	2.763806
78	1	0	1.862910	3.363477	1.257059
79	1	0	1.238536	0.570933	2.304455

M5*SS*

Total Energy= -2310.42307809

Sum of electronic and zero-point Energies= -2309.786255

Sum of electronic and thermal Energies= -2309.749039

Sum of electronic and thermal Enthalpies= -2309.748095

Sum of electronic and thermal Free Energies= -2309.857683

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.280973	0.220009	-0.888000
2	8	0	-0.738703	0.421030	-2.048932
3	6	0	0.538392	1.351206	-0.207822
4	1	0	0.913207	0.971114	0.751798
5	6	0	-0.299748	2.579443	0.065582
6	6	0	-0.198873	3.206762	1.312118
7	6	0	-1.140708	3.142915	-0.901478
8	6	0	-0.923188	4.361617	1.596702
9	1	0	0.472785	2.790604	2.060566
10	6	0	-1.869207	4.295998	-0.615649
11	1	0	-1.224286	2.655564	-1.866576
12	6	0	-1.764636	4.909009	0.631313
13	1	0	-0.826775	4.833450	2.569604
14	1	0	-2.522165	4.718558	-1.373430
15	1	0	-2.332216	5.808351	0.848493
16	6	0	1.832343	-0.848138	-1.072377
17	6	0	2.500603	0.342992	-1.248851
18	6	0	3.844117	-0.050937	-1.485867
19	7	0	3.984151	-1.368468	-1.446881
20	7	0	2.731418	-1.861737	-1.199879
21	6	0	2.525011	-3.238938	-0.959732
22	6	0	3.546108	-3.985805	-0.371180

23	6	0	1.309517	-3.839398	-1.294346
24	6	0	3.343788	-5.336803	-0.109418
25	1	0	4.479685	-3.494836	-0.123142
26	6	0	1.117328	-5.189313	-1.016170
27	1	0	0.528460	-3.248607	-1.756908
28	6	0	2.128751	-5.943822	-0.423804
29	1	0	4.138920	-5.914987	0.350543
30	1	0	0.171732	-5.655526	-1.274462
31	1	0	1.972893	-6.996726	-0.213531
32	6	0	5.028251	0.822252	-1.759127
33	1	0	5.302112	1.401388	-0.872122
34	1	0	5.879468	0.207041	-2.056020
35	1	0	4.810992	1.537207	-2.557686
36	6	0	1.791808	1.656008	-1.076560
37	1	0	1.429832	2.039318	-2.040025
38	6	0	2.643619	2.718969	-0.414604
39	6	0	2.718945	4.006955	-0.943075
40	6	0	3.328186	2.437540	0.772934
41	6	0	3.468328	4.995534	-0.306442
42	1	0	2.182056	4.237302	-1.859752
43	6	0	4.075377	3.421266	1.412463
44	1	0	3.279198	1.432119	1.187872
45	6	0	4.148399	4.705697	0.872654
46	1	0	3.520065	5.992311	-0.733503
47	1	0	4.604495	3.186819	2.331026
48	1	0	4.733031	5.473892	1.368728
49	8	0	0.552344	-1.057591	-0.792736
50	6	0	-2.642593	-0.198619	-0.293148
51	6	0	-2.768869	-0.807974	1.921059
52	6	0	-1.339875	-0.298871	1.577195
53	6	0	-4.836021	-0.551166	0.315473
54	6	0	-4.969661	-0.288117	-1.054288
55	6	0	-6.221408	-0.306544	-1.654356
56	1	0	-6.332293	-0.102816	-2.713858
57	6	0	-7.329408	-0.600095	-0.861722
58	6	0	-7.185756	-0.867233	0.502090
59	6	0	-5.935195	-0.844687	1.113211
60	1	0	-3.183964	-0.309659	2.797134
61	1	0	-8.314892	-0.623988	-1.313136
62	1	0	-8.061678	-1.097024	1.098562
63	1	0	-5.816135	-1.046512	2.171998
64	16	0	-3.398840	0.033681	-1.829458
65	7	0	-3.503342	-0.454532	0.704370
66	7	0	-1.391195	-0.189326	0.091854

67	6	0	-0.223328	-1.174927	2.091824
68	6	0	-0.073016	-2.487502	1.637900
69	6	0	0.687607	-0.658333	3.012161
70	6	0	0.986477	-3.266399	2.086078
71	1	0	-0.756243	-2.880713	0.889178
72	6	0	1.743904	-1.442791	3.474198
73	1	0	0.576048	0.365017	3.363434
74	6	0	1.896642	-2.744097	3.006324
75	1	0	1.120877	-4.271102	1.695031
76	1	0	2.450069	-1.031275	4.187851
77	1	0	2.729617	-3.351108	3.346702
78	1	0	-2.792893	-1.893238	2.064746
79	1	0	-1.213134	0.718117	1.969746

TS6*RR*

Total Energy= -2310.41792786

Sum of electronic and zero-point Energies= -2309.783179

Sum of electronic and thermal Energies= -2309.745891

Sum of electronic and thermal Enthalpies= -2309.744947

Sum of electronic and thermal Free Energies= -2309.855353

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.518465	-0.851112	-0.299576
2	6	0	2.275640	-2.300759	1.472155
3	6	0	0.896888	-1.871874	0.872562
4	6	0	4.582599	-1.610787	0.433552
5	6	0	4.972334	-0.703821	-0.565043
6	6	0	6.314339	-0.483669	-0.835566
7	1	0	6.617523	0.214163	-1.608680
8	6	0	7.264621	-1.176009	-0.084094
9	6	0	6.872689	-2.069808	0.913127
10	6	0	5.525859	-2.301671	1.185232
11	1	0	2.392605	-3.384724	1.506473
12	1	0	8.318464	-1.012651	-0.279320
13	1	0	7.626516	-2.596786	1.487846
14	1	0	5.215203	-2.998570	1.956116
15	16	0	3.570533	0.056150	-1.354948
16	7	0	3.202315	-1.697197	0.515818
17	7	0	1.240323	-0.843369	-0.139744
18	6	0	-0.099204	-1.319198	1.866669
19	6	0	-1.418254	-1.768943	1.850887

20	6	0	0.260283	-0.285436	2.735526
21	6	0	-2.375470	-1.183468	2.677957
22	1	0	-1.699259	-2.573894	1.175932
23	6	0	-0.691255	0.299141	3.565804
24	1	0	1.284329	0.081873	2.745747
25	6	0	-2.013151	-0.147939	3.536054
26	1	0	-3.402016	-1.535457	2.644081
27	1	0	-0.404968	1.108478	4.229949
28	1	0	-2.756924	0.313951	4.177838
29	1	0	2.441573	-1.887616	2.472555
30	1	0	0.435474	-2.713341	0.344248
31	6	0	0.084717	-0.045333	-1.380292
32	8	0	0.636709	-0.025175	-2.466774
33	6	0	-0.276472	1.223128	-0.588684
34	1	0	-0.475705	0.914023	0.442479
35	6	0	0.865245	2.208066	-0.595309
36	6	0	1.464079	2.581500	0.609190
37	6	0	1.329072	2.780393	-1.784792
38	6	0	2.516293	3.494468	0.630515
39	1	0	1.088995	2.157247	1.537404
40	6	0	2.376758	3.696592	-1.765485
41	1	0	0.881522	2.484045	-2.727569
42	6	0	2.976744	4.053194	-0.558972
43	1	0	2.971390	3.773188	1.575957
44	1	0	2.729317	4.130381	-2.696270
45	1	0	3.795837	4.765424	-0.546080
46	6	0	-2.176283	-0.611908	-1.143590
47	6	0	-2.593614	0.696986	-1.144415
48	6	0	-4.008168	0.601506	-1.063073
49	7	0	-4.410441	-0.658997	-1.012654
50	7	0	-3.271639	-1.413786	-1.069722
51	6	0	-3.330123	-2.817816	-0.910155
52	6	0	-4.390618	-3.368704	-0.187423
53	6	0	-2.337025	-3.638334	-1.451037
54	6	0	-4.449390	-4.745434	-0.001578
55	1	0	-5.149572	-2.708840	0.215559
56	6	0	-2.403356	-5.013053	-1.241149
57	1	0	-1.528114	-3.203301	-2.024434
58	6	0	-3.454634	-5.572771	-0.519291
59	1	0	-5.274637	-5.171872	0.559580
60	1	0	-1.630345	-5.649961	-1.658781
61	1	0	-3.500696	-6.645400	-0.364439
62	6	0	-5.004553	1.716504	-1.033488
63	1	0	-4.813574	2.431722	-1.838185

64	1	0	-6.012060	1.313237	-1.147792
65	1	0	-4.947186	2.267160	-0.089568
66	6	0	-1.608600	1.829174	-1.121568
67	1	0	-1.439828	2.228038	-2.130754
68	6	0	-2.026909	2.969063	-0.213757
69	6	0	-1.945257	4.294336	-0.637661
70	6	0	-2.448331	2.700463	1.092567
71	6	0	-2.287603	5.336568	0.223533
72	1	0	-1.607302	4.510968	-1.647969
73	6	0	-2.787707	3.737434	1.954790
74	1	0	-2.516957	1.666620	1.426966
75	6	0	-2.710286	5.061333	1.520585
76	1	0	-2.222724	6.363806	-0.121395
77	1	0	-3.113678	3.512851	2.966141
78	1	0	-2.977672	5.872209	2.190604
79	8	0	-0.929224	-1.097814	-1.188124

TS6*RS*

Total Energy= -2310.41118319
Sum of electronic and zero-point Energies= -2309.776795
Sum of electronic and thermal Energies= -2309.740983
Sum of electronic and thermal Enthalpies= -2309.740038
Sum of electronic and thermal Free Energies= -2309.846966

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.248666	0.618027	-0.502970
2	6	0	-2.670681	2.298608	1.011031
3	6	0	-1.340857	1.536958	1.328712
4	6	0	-4.348627	1.547637	-0.855359
5	6	0	-4.276178	0.644786	-1.928182
6	6	0	-5.320328	0.538334	-2.834318
7	1	0	-5.265537	-0.157692	-3.664416
8	6	0	-6.440248	1.350954	-2.654584
9	6	0	-6.504928	2.251102	-1.590373
10	6	0	-5.460673	2.361561	-0.674185
11	1	0	-2.496289	3.317952	0.654772
12	1	0	-7.265936	1.280780	-3.353696
13	1	0	-7.382146	2.877596	-1.469885
14	1	0	-5.506452	3.057762	0.156255
15	16	0	-2.736007	-0.245830	-1.942401
16	7	0	-3.212525	1.476008	-0.067256

17	7	0	-1.166684	0.597195	0.193872
18	6	0	-1.382668	0.770398	2.635285
19	6	0	-0.293282	0.800875	3.505228
20	6	0	-2.494825	-0.011666	2.960193
21	6	0	-0.311371	0.059878	4.686659
22	1	0	0.575698	1.403980	3.252798
23	6	0	-2.519564	-0.744362	4.142059
24	1	0	-3.343356	-0.056686	2.280349
25	6	0	-1.426150	-0.711148	5.007571
26	1	0	0.542441	0.089693	5.355693
27	1	0	-3.387801	-1.348418	4.385206
28	1	0	-1.443953	-1.285178	5.928285
29	1	0	-3.344387	2.323187	1.870003
30	1	0	-0.488582	2.221774	1.332275
31	6	0	0.431409	-0.142766	-0.574702
32	8	0	0.174046	-0.394501	-1.736603
33	6	0	0.758452	-1.182053	0.499078
34	1	0	0.740855	-0.645269	1.452869
35	6	0	-0.253166	-2.296554	0.580797
36	6	0	-0.738525	-2.657692	1.840269
37	6	0	-0.702300	-3.000719	-0.543052
38	6	0	-1.660284	-3.691664	1.982577
39	1	0	-0.401967	-2.108406	2.717693
40	6	0	-1.626749	-4.033015	-0.400810
41	1	0	-0.326924	-2.730927	-1.524189
42	6	0	-2.108152	-4.382596	0.859531
43	1	0	-2.032522	-3.948228	2.969990
44	1	0	-1.969860	-4.568770	-1.280703
45	1	0	-2.829742	-5.186795	0.964644
46	6	0	2.485253	0.811197	-0.104477
47	6	0	3.052481	-0.405151	0.188992
48	6	0	4.430712	-0.111721	0.334669
49	7	0	4.678031	1.176395	0.158820
50	7	0	3.468501	1.750593	-0.122479
51	6	0	3.371953	3.148820	-0.326401
52	6	0	4.342985	3.977088	0.239656
53	6	0	2.337865	3.689393	-1.093646
54	6	0	4.273333	5.350555	0.037256
55	1	0	5.139173	3.531092	0.823129
56	6	0	2.275959	5.068222	-1.274499
57	1	0	1.599465	3.038644	-1.544146
58	6	0	3.238735	5.903926	-0.714706
59	1	0	5.030646	5.991891	0.476478
60	1	0	1.472136	5.487302	-1.871165

61	1	0	3.185989	6.976807	-0.865983
62	6	0	5.526644	-1.080228	0.638567
63	1	0	5.589051	-1.847128	-0.139408
64	1	0	6.483461	-0.559642	0.699739
65	1	0	5.342464	-1.591211	1.588532
66	6	0	2.242674	-1.659011	0.323928
67	1	0	2.497557	-2.165295	1.263974
68	6	0	2.458834	-2.661298	-0.796342
69	6	0	2.422237	-4.028674	-0.512303
70	6	0	2.671783	-2.254687	-2.115774
71	6	0	2.583582	-4.973160	-1.522448
72	1	0	2.253173	-4.353524	0.511885
73	6	0	2.830110	-3.196420	-3.129432
74	1	0	2.702499	-1.194177	-2.346982
75	6	0	2.786438	-4.558250	-2.836407
76	1	0	2.552553	-6.031526	-1.282903
77	1	0	2.991672	-2.865232	-4.150643
78	1	0	2.914698	-5.291348	-3.626488
79	8	0	1.190638	1.094004	-0.329493

TS6*SR*

Total Energy= -2310.41333961
Sum of electronic and zero-point Energies= -2309.778109
Sum of electronic and thermal Energies= -2309.740893
Sum of electronic and thermal Enthalpies= -2309.739949
Sum of electronic and thermal Free Energies= -2309.850045

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.058462	0.575359	-0.503310
2	8	0	-0.445773	0.992470	-1.532239
3	6	0	0.366641	1.422968	0.737810
4	1	0	0.568449	0.710199	1.545775
5	6	0	-0.782396	2.302749	1.165428
6	6	0	-1.089089	2.380278	2.527794
7	6	0	-1.524090	3.076753	0.264902
8	6	0	-2.118473	3.198495	2.987719
9	1	0	-0.507888	1.793923	3.237165
10	6	0	-2.557004	3.890078	0.723910
11	1	0	-1.285369	3.032325	-0.791251
12	6	0	-2.858926	3.954115	2.082939
13	1	0	-2.341044	3.242306	4.049220

14	1	0	-3.127145	4.481826	0.014388
15	1	0	-3.664583	4.591201	2.433918
16	6	0	2.291687	-0.071379	-0.402698
17	6	0	2.701585	1.132672	0.115981
18	6	0	4.112268	1.012537	0.179267
19	7	0	4.523113	-0.169191	-0.253108
20	7	0	3.389811	-0.841314	-0.622324
21	6	0	3.456787	-2.186816	-1.054788
22	6	0	4.501005	-2.990207	-0.595343
23	6	0	2.487649	-2.704319	-1.916091
24	6	0	4.565463	-4.321421	-0.991935
25	1	0	5.240217	-2.562708	0.071241
26	6	0	2.557498	-4.042843	-2.291373
27	1	0	1.688361	-2.069063	-2.276341
28	6	0	3.591218	-4.857160	-1.833285
29	1	0	5.377786	-4.945272	-0.633140
30	1	0	1.802024	-4.445897	-2.958129
31	1	0	3.641156	-5.898118	-2.134732
32	6	0	5.081169	2.045942	0.654133
33	1	0	4.886822	2.311492	1.697834
34	1	0	6.102005	1.669959	0.572277
35	1	0	4.991403	2.960742	0.060780
36	6	0	1.723849	2.184313	0.544708
37	1	0	1.994876	2.552928	1.542417
38	6	0	1.639483	3.390629	-0.373387
39	6	0	1.405551	4.655124	0.172906
40	6	0	1.760040	3.269607	-1.759745
41	6	0	1.286802	5.776031	-0.644320
42	1	0	1.306720	4.757641	1.251276
43	6	0	1.638184	4.387669	-2.580592
44	1	0	1.941401	2.291510	-2.195593
45	6	0	1.401621	5.644141	-2.026083
46	1	0	1.107566	6.750935	-0.201681
47	1	0	1.731580	4.277539	-3.656599
48	1	0	1.312669	6.515463	-2.667280
49	8	0	1.045746	-0.487161	-0.669143
50	6	0	-2.411885	-0.678093	-0.236777
51	6	0	-2.594056	-2.103817	1.550696
52	6	0	-1.296145	-1.242854	1.614444
53	6	0	-4.514890	-1.660484	-0.174523
54	6	0	-4.588633	-0.951129	-1.383396
55	6	0	-5.728898	-1.009861	-2.170093
56	1	0	-5.787510	-0.460705	-3.103792
57	6	0	-6.794508	-1.799262	-1.735957

58	6	0	-6.712927	-2.510696	-0.538664
59	6	0	-5.572849	-2.449647	0.261192
60	1	0	-3.159081	-2.077166	2.482739
61	1	0	-7.692890	-1.858894	-2.339999
62	1	0	-7.550235	-3.121884	-0.219727
63	1	0	-5.507250	-2.996288	1.195661
64	16	0	-3.092690	-0.047083	-1.719149
65	7	0	-3.305619	-1.431246	0.464286
66	7	0	-1.241578	-0.581488	0.290691
67	6	0	-0.038416	-2.016118	1.928604
68	6	0	0.469981	-2.943601	1.015001
69	6	0	0.640987	-1.791337	3.124911
70	6	0	1.643924	-3.633063	1.294927
71	1	0	-0.034795	-3.092450	0.063663
72	6	0	1.816836	-2.484758	3.410087
73	1	0	0.251620	-1.065243	3.834661
74	6	0	2.320317	-3.402904	2.493546
75	1	0	2.048581	-4.329386	0.565243
76	1	0	2.340886	-2.298605	4.341915
77	1	0	3.243784	-3.933230	2.704112
78	1	0	-2.382149	-3.143863	1.275490
79	1	0	-1.429712	-0.453854	2.367853

TS6*SS*

Total Energy= -2310.41597826

Sum of electronic and zero-point Energies= -2309.780735

Sum of electronic and thermal Energies= -2309.743559

Sum of electronic and thermal Enthalpies= -2309.742615

Sum of electronic and thermal Free Energies= -2309.853403

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.131740	-0.341149	-1.199594
2	8	0	0.740571	-0.551673	-2.231578
3	6	0	-0.712994	-1.375203	-0.449691
4	1	0	-0.893833	-0.964344	0.550122
5	6	0	-0.034223	-2.714332	-0.306896
6	6	0	-0.019238	-3.331720	0.947047
7	6	0	0.523051	-3.391522	-1.396829
8	6	0	0.552779	-4.589559	1.120192
9	1	0	-0.479665	-2.824827	1.792806
10	6	0	1.097438	-4.648894	-1.224112

11	1	0	0.517072	-2.921535	-2.373672
12	6	0	1.116565	-5.250831	0.032266
13	1	0	0.553890	-5.052398	2.102039
14	1	0	1.532066	-5.160849	-2.077148
15	1	0	1.564423	-6.231059	0.161259
16	6	0	-1.750439	1.012439	-1.143455
17	6	0	-2.610518	-0.055557	-1.235405
18	6	0	-3.891985	0.548937	-1.325911
19	7	0	-3.810384	1.869630	-1.287205
20	7	0	-2.478188	2.159107	-1.179810
21	6	0	-2.049585	3.493231	-0.982001
22	6	0	-2.940173	4.403965	-0.410736
23	6	0	-0.757067	3.888465	-1.331962
24	6	0	-2.525610	5.709201	-0.171878
25	1	0	-3.938088	4.071760	-0.152183
26	6	0	-0.352056	5.194261	-1.069791
27	1	0	-0.077305	3.180184	-1.788348
28	6	0	-1.227935	6.108946	-0.488787
29	1	0	-3.219244	6.414288	0.274787
30	1	0	0.655764	5.498060	-1.333995
31	1	0	-0.905100	7.125634	-0.291173
32	6	0	-5.220114	-0.126569	-1.454624
33	1	0	-5.464028	-0.685363	-0.545991
34	1	0	-5.997157	0.618637	-1.632399
35	1	0	-5.215532	-0.840158	-2.283346
36	6	0	-2.115892	-1.469713	-1.126205
37	1	0	-1.989710	-1.927958	-2.116499
38	6	0	-3.024434	-2.353212	-0.294439
39	6	0	-3.410125	-3.613188	-0.748273
40	6	0	-3.454372	-1.926793	0.967116
41	6	0	-4.219782	-4.433570	0.037011
42	1	0	-3.071911	-3.955098	-1.723041
43	6	0	-4.260186	-2.743618	1.753386
44	1	0	-3.162485	-0.940921	1.325838
45	6	0	-4.647330	-4.000717	1.288601
46	1	0	-4.516367	-5.410461	-0.331696
47	1	0	-4.591213	-2.398478	2.727968
48	1	0	-5.279506	-4.636771	1.899828
49	8	0	-0.412765	0.999139	-1.040276
50	6	0	2.726624	-0.116383	-0.140289
51	6	0	2.837923	0.459973	2.076912
52	6	0	1.401027	0.030384	1.649717
53	6	0	4.931766	0.166724	0.531339
54	6	0	5.099144	-0.043147	-0.846394

55	6	0	6.361067	-0.013249	-1.419166
56	1	0	6.490830	-0.177924	-2.483445
57	6	0	7.458071	0.243233	-0.595568
58	6	0	7.286287	0.463097	0.771263
59	6	0	6.021054	0.424846	1.355078
60	1	0	3.176657	-0.057888	2.974683
61	1	0	8.452146	0.275841	-1.027154
62	1	0	8.149831	0.667167	1.395049
63	1	0	5.882783	0.589077	2.418218
64	16	0	3.547156	-0.319792	-1.672641
65	7	0	3.598575	0.053757	0.895679
66	7	0	1.481259	-0.076933	0.174289
67	6	0	0.293186	0.954624	2.094813
68	6	0	0.248135	2.276935	1.646532
69	6	0	-0.723408	0.479421	2.922687
70	6	0	-0.798052	3.111655	2.023140
71	1	0	1.013986	2.640512	0.965581
72	6	0	-1.775382	1.313551	3.301016
73	1	0	-0.696624	-0.551853	3.268206
74	6	0	-1.813713	2.629450	2.849348
75	1	0	-0.834477	4.132033	1.651149
76	1	0	-2.563533	0.931543	3.942070
77	1	0	-2.636597	3.278456	3.131747
78	1	0	2.918498	1.543756	2.223558
79	1	0	1.201198	-0.977523	2.038831

P*RR*

Total Energy= -1224.19167281

Sum of electronic and zero-point Energies= -1223.795956

Sum of electronic and thermal Energies= -1223.772856

Sum of electronic and thermal Enthalpies= -1223.771912

Sum of electronic and thermal Free Energies= -1223.851330

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.616710	0.609668	-1.653158
2	8	0	0.776717	0.811172	-2.821989
3	6	0	1.634146	0.944666	-0.564283
4	1	0	2.587330	1.007594	-1.095799
5	6	0	1.278485	2.346060	-0.060245
6	6	0	1.393246	3.409795	-0.962161
7	6	0	0.860318	2.608627	1.245173

8	6	0	1.104463	4.710731	-0.567167
9	1	0	1.712043	3.207950	-1.981675
10	6	0	0.572997	3.914500	1.641161
11	1	0	0.749489	1.802944	1.963432
12	6	0	0.693005	4.967119	0.739744
13	1	0	1.203889	5.523698	-1.278971
14	1	0	0.251901	4.103941	2.660344
15	1	0	0.467735	5.981565	1.052119
16	6	0	-0.693572	-0.313012	0.032687
17	6	0	0.336216	-0.508613	0.909315
18	6	0	-0.297242	-1.063787	2.048587
19	7	0	-1.603716	-1.182664	1.861462
20	7	0	-1.851565	-0.711131	0.607195
21	6	0	-3.164759	-0.746081	0.068829
22	6	0	-4.050078	-1.717115	0.536953
23	6	0	-3.560858	0.179105	-0.896507
24	6	0	-5.342701	-1.760025	0.028253
25	1	0	-3.714090	-2.418529	1.290864
26	6	0	-4.853798	0.110703	-1.407859
27	1	0	-2.873871	0.943775	-1.238176
28	6	0	-5.747908	-0.853233	-0.949254
29	1	0	-6.033361	-2.512834	0.393480
30	1	0	-5.164060	0.827059	-2.161321
31	1	0	-6.755561	-0.895829	-1.348505
32	6	0	0.346183	-1.474626	3.332186
33	1	0	1.118156	-2.228361	3.153159
34	1	0	-0.402019	-1.888509	4.009249
35	1	0	0.825093	-0.619831	3.819210
36	6	0	1.736813	-0.145990	0.532546
37	1	0	2.260981	0.303000	1.384350
38	6	0	2.568611	-1.322009	0.040443
39	6	0	3.945259	-1.336242	0.276790
40	6	0	1.999032	-2.359522	-0.700486
41	6	0	4.739083	-2.368475	-0.214644
42	1	0	4.396862	-0.531776	0.852330
43	6	0	2.792303	-3.391060	-1.197565
44	1	0	0.927011	-2.370012	-0.880883
45	6	0	4.163666	-3.398906	-0.955343
46	1	0	5.806080	-2.369976	-0.016153
47	1	0	2.335492	-4.191614	-1.770602
48	1	0	4.780620	-4.205519	-1.337754
49	8	0	-0.615525	0.130599	-1.249670

P*RS*

Total Energy= -1224.19313804
Sum of electronic and zero-point Energies= -1223.797662
Sum of electronic and thermal Energies= -1223.774564
Sum of electronic and thermal Enthalpies= -1223.773620
Sum of electronic and thermal Free Energies= -1223.852549

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.272499	-1.521300	0.450414
2	8	0	-0.603858	-2.333023	1.262912
3	6	0	-1.132215	-0.971031	-0.685907
4	1	0	-0.695237	-1.430379	-1.584482
5	6	0	-2.576706	-1.397234	-0.581808
6	6	0	-3.231735	-1.842558	-1.730792
7	6	0	-3.299183	-1.284755	0.610198
8	6	0	-4.584628	-2.174206	-1.695514
9	1	0	-2.677884	-1.929954	-2.662366
10	6	0	-4.649158	-1.617396	0.647295
11	1	0	-2.804604	-0.932386	1.510137
12	6	0	-5.295757	-2.062788	-0.504563
13	1	0	-5.078434	-2.521709	-2.597280
14	1	0	-5.198001	-1.527095	1.579192
15	1	0	-6.349005	-2.322613	-0.472351
16	6	0	1.372368	-0.029213	-0.281523
17	6	0	0.518757	0.807381	-0.942712
18	6	0	1.381701	1.750877	-1.553049
19	7	0	2.651312	1.488220	-1.276884
20	7	0	2.645891	0.382016	-0.481663
21	6	0	3.863055	-0.175398	-0.009281
22	6	0	5.012540	-0.024193	-0.784151
23	6	0	3.906287	-0.843301	1.214423
24	6	0	6.214540	-0.551909	-0.326490
25	1	0	4.949260	0.506244	-1.726743
26	6	0	5.114647	-1.379226	1.650151
27	1	0	3.012579	-0.936169	1.819328
28	6	0	6.270042	-1.235203	0.887031
29	1	0	7.110723	-0.433727	-0.926673
30	1	0	5.150539	-1.901073	2.600646
31	1	0	7.209452	-1.649238	1.237355
32	6	0	0.995665	2.918889	-2.400132
33	1	0	0.467767	2.590557	-3.300169
34	1	0	1.886087	3.473601	-2.698528

35	1	0	0.328612	3.589509	-1.851068
36	6	0	-0.957210	0.574068	-0.890553
37	1	0	-1.417359	0.802787	-1.857811
38	6	0	-1.668283	1.379327	0.182845
39	6	0	-2.926881	1.926002	-0.071072
40	6	0	-1.115125	1.518263	1.459056
41	6	0	-3.625262	2.595490	0.930927
42	1	0	-3.368525	1.811413	-1.057919
43	6	0	-1.815021	2.178194	2.465351
44	1	0	-0.127822	1.113189	1.669478
45	6	0	-3.072498	2.718541	2.203370
46	1	0	-4.602644	3.017101	0.718779
47	1	0	-1.375126	2.276100	3.452635
48	1	0	-3.616035	3.236571	2.986791
49	8	0	1.047681	-1.100515	0.488313

P*SR*

Total Energy= -1224.19313804
Sum of electronic and zero-point Energies= -1223.797662
Sum of electronic and thermal Energies= -1223.774564
Sum of electronic and thermal Enthalpies= -1223.773620
Sum of electronic and thermal Free Energies= -1223.852549

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.272499	-1.521300	0.450414
2	8	0	0.603858	-2.333023	1.262912
3	6	0	1.132215	-0.971031	-0.685907
4	1	0	0.695237	-1.430379	-1.584482
5	6	0	2.576706	-1.397234	-0.581808
6	6	0	3.231735	-1.842558	-1.730792
7	6	0	3.299183	-1.284755	0.610198
8	6	0	4.584628	-2.174206	-1.695514
9	1	0	2.677884	-1.929954	-2.662366
10	6	0	4.649158	-1.617396	0.647295
11	1	0	2.804604	-0.932386	1.510137
12	6	0	5.295757	-2.062788	-0.504563
13	1	0	5.078434	-2.521709	-2.597280
14	1	0	5.198001	-1.527095	1.579192
15	1	0	6.349005	-2.322613	-0.472351
16	6	0	-1.372368	-0.029213	-0.281523
17	6	0	-0.518757	0.807381	-0.942712

18	6	0	-1.381701	1.750877	-1.553049
19	7	0	-2.651312	1.488220	-1.276884
20	7	0	-2.645891	0.382016	-0.481663
21	6	0	-3.863055	-0.175398	-0.009281
22	6	0	-5.012540	-0.024193	-0.784151
23	6	0	-3.906287	-0.843301	1.214423
24	6	0	-6.214540	-0.551909	-0.326490
25	1	0	-4.949260	0.506244	-1.726743
26	6	0	-5.114647	-1.379226	1.650151
27	1	0	-3.012579	-0.936169	1.819328
28	6	0	-6.270042	-1.235203	0.887031
29	1	0	-7.110723	-0.433727	-0.926673
30	1	0	-5.150539	-1.901073	2.600646
31	1	0	-7.209452	-1.649238	1.237355
32	6	0	-0.995665	2.918889	-2.400132
33	1	0	-0.467767	2.590557	-3.300169
34	1	0	-1.886087	3.473601	-2.698528
35	1	0	-0.328612	3.589509	-1.851068
36	6	0	0.957210	0.574068	-0.890553
37	1	0	1.417359	0.802787	-1.857811
38	6	0	1.668283	1.379327	0.182845
39	6	0	2.926881	1.926002	-0.071072
40	6	0	1.115125	1.518263	1.459056
41	6	0	3.625262	2.595490	0.930927
42	1	0	3.368525	1.811413	-1.057919
43	6	0	1.815021	2.178194	2.465351
44	1	0	0.127822	1.113189	1.669478
45	6	0	3.072498	2.718541	2.203370
46	1	0	4.602644	3.017101	0.718779
47	1	0	1.375126	2.276100	3.452635
48	1	0	3.616035	3.236571	2.986791
49	8	0	-1.047681	-1.100515	0.488313

PSS

Total Energy= -1224.19167281
Sum of electronic and zero-point Energies= -1223.795956
Sum of electronic and thermal Energies= -1223.772856
Sum of electronic and thermal Enthalpies= -1223.771912
Sum of electronic and thermal Free Energies= -1223.851330

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

1	6	0	0.616710	-0.609668	-1.653158
2	8	0	0.776717	-0.811172	-2.821989
3	6	0	1.634146	-0.944666	-0.564283
4	1	0	2.587330	-1.007594	-1.095799
5	6	0	1.278485	-2.346060	-0.060245
6	6	0	1.393246	-3.409795	-0.962161
7	6	0	0.860318	-2.608627	1.245173
8	6	0	1.104463	-4.710731	-0.567167
9	1	0	1.712043	-3.207950	-1.981675
10	6	0	0.572997	-3.914500	1.641161
11	1	0	0.749489	-1.802944	1.963432
12	6	0	0.693005	-4.967119	0.739744
13	1	0	1.203889	-5.523698	-1.278971
14	1	0	0.251901	-4.103941	2.660344
15	1	0	0.467735	-5.981565	1.052119
16	6	0	-0.693572	0.313012	0.032687
17	6	0	0.336216	0.508613	0.909315
18	6	0	-0.297242	1.063787	2.048587
19	7	0	-1.603716	1.182664	1.861462
20	7	0	-1.851565	0.711131	0.607195
21	6	0	-3.164759	0.746081	0.068829
22	6	0	-4.050078	1.717115	0.536953
23	6	0	-3.560858	-0.179105	-0.896507
24	6	0	-5.342701	1.760025	0.028253
25	1	0	-3.714090	2.418529	1.290864
26	6	0	-4.853798	-0.110703	-1.407859
27	1	0	-2.873871	-0.943775	-1.238176
28	6	0	-5.747908	0.853233	-0.949254
29	1	0	-6.033361	2.512834	0.393480
30	1	0	-5.164060	-0.827059	-2.161321
31	1	0	-6.755561	0.895829	-1.348505
32	6	0	0.346183	1.474626	3.332186
33	1	0	1.118156	2.228361	3.153159
34	1	0	-0.402019	1.888509	4.009249
35	1	0	0.825093	0.619831	3.819210
36	6	0	1.736813	0.145990	0.532546
37	1	0	2.260981	-0.303000	1.384350
38	6	0	2.568611	1.322009	0.040443
39	6	0	3.945259	1.336242	0.276790
40	6	0	1.999032	2.359522	-0.700486
41	6	0	4.739083	2.368475	-0.214644
42	1	0	4.396862	0.531776	0.852330
43	6	0	2.792303	3.391060	-1.197565
44	1	0	0.927011	2.370012	-0.880883

45	6	0	4.163666	3.398906	-0.955343
46	1	0	5.806080	2.369976	-0.016153
47	1	0	2.335492	4.191614	-1.770602
48	1	0	4.780620	4.205519	-1.337754
49	8	0	-0.615525	-0.130599	-1.249670

_Si_-TS4-B

Total Energy= -1469.72538473
Sum of electronic and zero-point Energies= -1469.370473
Sum of electronic and thermal Energies= -1469.348519
Sum of electronic and thermal Enthalpies= -1469.347575
Sum of electronic and thermal Free Energies= -1469.426020

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.570204	-0.502760	-0.161736
2	6	0	-1.950124	1.629113	-0.914779
3	6	0	-0.432863	1.245359	-0.915487
4	6	0	-3.849517	-0.058543	-0.328501
5	6	0	-3.878265	-1.332696	0.261047
6	6	0	-5.081594	-1.929923	0.601027
7	1	0	-5.103366	-2.914890	1.054981
8	6	0	-6.263998	-1.228690	0.356846
9	6	0	-6.231886	0.041084	-0.218721
10	6	0	-5.024864	0.642723	-0.571604
11	1	0	-2.284127	2.021171	-1.876450
12	1	0	-7.213987	-1.678756	0.622344
13	1	0	-7.159957	0.572966	-0.398282
14	1	0	-4.993871	1.627860	-1.024534
15	16	0	-2.241639	-1.993499	0.483611
16	7	0	-2.554176	0.334444	-0.619114
17	7	0	-0.364633	-0.074369	-0.243242
18	6	0	0.440129	2.274447	-0.235373
19	6	0	1.296351	3.085577	-0.979667
20	6	0	0.396398	2.418015	1.154077
21	6	0	2.095931	4.035467	-0.345479
22	1	0	1.342768	2.968459	-2.059256
23	6	0	1.193876	3.364007	1.787942
24	1	0	-0.253236	1.770003	1.736825
25	6	0	2.045602	4.175975	1.038419
26	1	0	2.759774	4.660556	-0.933947
27	1	0	1.157604	3.465258	2.867844

28	1	0	2.670719	4.911852	1.533732
29	1	0	-2.187887	2.348964	-0.122552
30	1	0	-0.089371	1.115385	-1.949177
31	6	0	1.281425	-1.508632	-0.017173
32	8	0	0.704384	-2.523355	0.140413
33	6	0	2.310913	-0.668639	-0.151595
34	1	0	2.113948	0.385422	-0.265679
35	6	0	3.692133	-1.157375	-0.121604
36	6	0	4.734532	-0.224098	-0.238488
37	6	0	4.030810	-2.513448	0.015616
38	6	0	6.064073	-0.630041	-0.220144
39	1	0	4.489193	0.829669	-0.343789
40	6	0	5.361779	-2.914161	0.033873
41	1	0	3.243939	-3.256873	0.109315
42	6	0	6.388677	-1.978254	-0.084106
43	1	0	6.850654	0.112816	-0.313525
44	1	0	5.598176	-3.968591	0.141416
45	1	0	7.425954	-2.296021	-0.070195

M4-B

Total Energy= -383.50046843
Sum of electronic and zero-point Energies= -383.384928
Sum of electronic and thermal Energies= -383.377606
Sum of electronic and thermal Enthalpies= -383.376661
Sum of electronic and thermal Free Energies= -383.417541

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.533216	0.119240	-0.000367
2	8	0	3.473778	-0.567092	-0.002831
3	6	0	1.465913	0.895964	0.002479
4	1	0	1.662563	1.962092	0.005742
5	6	0	0.087984	0.385088	0.001305
6	6	0	-0.974412	1.297100	-0.000420
7	6	0	-0.203923	-0.986862	0.002085
8	6	0	-2.291888	0.849842	-0.001593
9	1	0	-0.762599	2.362290	-0.000858
10	6	0	-1.521071	-1.428430	0.000657
11	1	0	0.605791	-1.712665	0.003978
12	6	0	-2.573733	-0.513899	-0.001191
13	1	0	-3.101370	1.573126	-0.002936
14	1	0	-1.726006	-2.494358	0.001169

15	1	0	-3.601121	-0.862001	-0.002180

TS5-B*RR*

Total Energy= -1224.0988083
Sum of electronic and zero-point Energies= -1223.708609
Sum of electronic and thermal Energies= -1223.684569
Sum of electronic and thermal Enthalpies= -1223.683625
Sum of electronic and thermal Free Energies= -1223.765398

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.351906	-1.133167	1.789852
2	8	0	-0.594825	-1.321190	2.390030
3	6	0	1.498772	-0.716310	1.134917
4	1	0	2.010503	-0.036698	1.821955
5	6	0	2.358178	-1.780217	0.531702
6	6	0	3.741932	-1.713726	0.702474
7	6	0	1.792334	-2.776145	-0.270800
8	6	0	4.558534	-2.659405	0.089526
9	1	0	4.175484	-0.924701	1.310525
10	6	0	2.616776	-3.723562	-0.869695
11	1	0	0.716893	-2.782172	-0.432395
12	6	0	3.997814	-3.668853	-0.689968
13	1	0	5.633890	-2.606833	0.223299
14	1	0	2.178542	-4.501390	-1.486327
15	1	0	4.637011	-4.407138	-1.162733
16	6	0	-1.372043	-0.102469	-0.267791
17	6	0	-0.380153	0.918606	-0.148534
18	6	0	-1.104246	2.138800	0.008079
19	7	0	-2.401322	1.927822	-0.027926
20	7	0	-2.584183	0.566204	-0.173821
21	6	0	-3.889265	0.041595	-0.225947
22	6	0	-4.982165	0.900753	-0.058359
23	6	0	-4.106282	-1.325027	-0.445647
24	6	0	-6.275361	0.393620	-0.112776
25	1	0	-4.800750	1.954360	0.110034
26	6	0	-5.409070	-1.811819	-0.495561
27	1	0	-3.257975	-1.983235	-0.572593
28	6	0	-6.501017	-0.963828	-0.331411
29	1	0	-7.113610	1.071213	0.017770
30	1	0	-5.566876	-2.872228	-0.667591
31	1	0	-7.512440	-1.353939	-0.373356

32	6	0	-0.610805	3.547691	0.125548
33	1	0	-0.190907	3.749887	1.115074
34	1	0	-1.446122	4.230568	-0.038115
35	1	0	0.170838	3.753147	-0.610125
36	6	0	0.974147	0.477466	-0.269495
37	1	0	1.059471	-0.326901	-1.003746
38	6	0	2.129667	1.414643	-0.301585
39	6	0	3.067847	1.303182	-1.331287
40	6	0	2.323703	2.375363	0.697814
41	6	0	4.159805	2.166276	-1.385466
42	1	0	2.934707	0.541681	-2.094360
43	6	0	3.416882	3.231996	0.648318
44	1	0	1.616261	2.440378	1.520596
45	6	0	4.334202	3.132296	-0.398317
46	1	0	4.877490	2.077349	-2.194211
47	1	0	3.557288	3.974585	1.426735
48	1	0	5.188262	3.800455	-0.436359
49	8	0	-1.170422	-1.336701	-0.366954

TS5-B*RS*

Total Energy= -1224.0994853
Sum of electronic and zero-point Energies= -1223.710140
Sum of electronic and thermal Energies= -1223.685797
Sum of electronic and thermal Enthalpies= -1223.684852
Sum of electronic and thermal Free Energies= -1223.767522

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.019455	0.305101	-1.769212
2	8	0	1.051345	1.256703	-2.400224
3	6	0	1.239404	-0.792993	-0.973364
4	1	0	0.425186	-1.510839	-1.005241
5	6	0	2.631467	-1.320599	-0.965176
6	6	0	2.827698	-2.646397	-0.562766
7	6	0	3.739280	-0.525261	-1.278188
8	6	0	4.113348	-3.168845	-0.481362
9	1	0	1.969694	-3.263922	-0.312439
10	6	0	5.023213	-1.055955	-1.196683
11	1	0	3.605854	0.510011	-1.581549
12	6	0	5.215332	-2.376417	-0.798371
13	1	0	4.253599	-4.198797	-0.170136
14	1	0	5.874984	-0.431892	-1.445850

15	1	0	6.217523	-2.786588	-0.735392
16	6	0	-1.484094	0.248462	0.127976
17	6	0	-0.523461	-0.218313	1.073978
18	6	0	-1.241029	-1.109157	1.929429
19	7	0	-2.522331	-1.117554	1.657075
20	7	0	-2.686795	-0.303150	0.550153
21	6	0	-3.958053	-0.184585	-0.043949
22	6	0	-4.992245	-1.030057	0.374115
23	6	0	-4.200779	0.775071	-1.035051
24	6	0	-6.253470	-0.915472	-0.199578
25	1	0	-4.794270	-1.762903	1.145662
26	6	0	-5.468855	0.870218	-1.599848
27	1	0	-3.398872	1.425681	-1.355607
28	6	0	-6.502283	0.031308	-1.190958
29	1	0	-7.047410	-1.576724	0.133654
30	1	0	-5.646275	1.616918	-2.367690
31	1	0	-7.487847	0.115734	-1.636423
32	6	0	-0.690684	-1.903833	3.068760
33	1	0	-0.240512	-1.251717	3.822426
34	1	0	-1.488313	-2.484476	3.534179
35	1	0	0.086500	-2.592848	2.721991
36	6	0	0.877588	-0.055716	0.926851
37	1	0	1.466190	-0.826422	1.432064
38	6	0	1.594670	1.241435	0.891316
39	6	0	2.944997	1.262775	1.267279
40	6	0	0.969522	2.441471	0.520340
41	6	0	3.661603	2.455735	1.268033
42	1	0	3.429474	0.337415	1.567867
43	6	0	1.690283	3.629890	0.522381
44	1	0	-0.070725	2.429303	0.213066
45	6	0	3.035010	3.641401	0.893758
46	1	0	4.704940	2.458476	1.565937
47	1	0	1.199506	4.553870	0.234396
48	1	0	3.590545	4.573607	0.895322
49	8	0	-1.275518	0.870230	-0.940411

TS5-B*SR*

Total Energy= -1224.0994853

Sum of electronic and zero-point Energies= -1223.710140

Sum of electronic and thermal Energies= -1223.685797

Sum of electronic and thermal Enthalpies= -1223.684852

Sum of electronic and thermal Free Energies= -1223.767522

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.019455	0.305101	-1.769212
2	8	0	-1.051345	1.256703	-2.400224
3	6	0	-1.239404	-0.792993	-0.973364
4	1	0	-0.425186	-1.510839	-1.005241
5	6	0	-2.631467	-1.320599	-0.965176
6	6	0	-2.827698	-2.646397	-0.562766
7	6	0	-3.739280	-0.525261	-1.278188
8	6	0	-4.113348	-3.168845	-0.481362
9	1	0	-1.969694	-3.263922	-0.312439
10	6	0	-5.023213	-1.055955	-1.196683
11	1	0	-3.605854	0.510011	-1.581549
12	6	0	-5.215332	-2.376417	-0.798371
13	1	0	-4.253599	-4.198797	-0.170136
14	1	0	-5.874984	-0.431892	-1.445850
15	1	0	-6.217523	-2.786588	-0.735392
16	6	0	1.484094	0.248462	0.127976
17	6	0	0.523461	-0.218313	1.073978
18	6	0	1.241029	-1.109157	1.929429
19	7	0	2.522331	-1.117554	1.657075
20	7	0	2.686795	-0.303150	0.550153
21	6	0	3.958053	-0.184585	-0.043949
22	6	0	4.992245	-1.030057	0.374115
23	6	0	4.200779	0.775071	-1.035051
24	6	0	6.253470	-0.915472	-0.199578
25	1	0	4.794270	-1.762903	1.145662
26	6	0	5.468855	0.870218	-1.599848
27	1	0	3.398872	1.425681	-1.355607
28	6	0	6.502283	0.031308	-1.190958
29	1	0	7.047410	-1.576724	0.133654
30	1	0	5.646275	1.616918	-2.367690
31	1	0	7.487847	0.115734	-1.636423
32	6	0	0.690684	-1.903833	3.068760
33	1	0	0.240512	-1.251717	3.822426
34	1	0	1.488313	-2.484476	3.534179
35	1	0	-0.086500	-2.592848	2.721991
36	6	0	-0.877588	-0.055716	0.926851
37	1	0	-1.466190	-0.826422	1.432064
38	6	0	-1.594670	1.241435	0.891316
39	6	0	-2.944997	1.262775	1.267279
40	6	0	-0.969522	2.441471	0.520340
41	6	0	-3.661603	2.455735	1.268033

42	1	0	-3.429474	0.337415	1.567867
43	6	0	-1.690283	3.629890	0.522381
44	1	0	0.070725	2.429303	0.213066
45	6	0	-3.035010	3.641401	0.893758
46	1	0	-4.704940	2.458476	1.565937
47	1	0	-1.199506	4.553870	0.234396
48	1	0	-3.590545	4.573607	0.895322
49	8	0	1.275518	0.870230	-0.940411

TS5-B*SS*

Total Energy= -1224.09880829
Sum of electronic and zero-point Energies= -1223.708609
Sum of electronic and thermal Energies= -1223.684569
Sum of electronic and thermal Enthalpies= -1223.683625
Sum of electronic and thermal Free Energies= -1223.765398

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.351906	1.133167	1.789852
2	8	0	-0.594825	1.321190	2.390030
3	6	0	1.498772	0.716310	1.134917
4	1	0	2.010503	0.036698	1.821955
5	6	0	2.358178	1.780217	0.531702
6	6	0	3.741932	1.713726	0.702474
7	6	0	1.792334	2.776145	-0.270800
8	6	0	4.558534	2.659405	0.089526
9	1	0	4.175484	0.924701	1.310525
10	6	0	2.616776	3.723562	-0.869695
11	1	0	0.716893	2.782172	-0.432395
12	6	0	3.997814	3.668853	-0.689968
13	1	0	5.633890	2.606833	0.223299
14	1	0	2.178542	4.501390	-1.486327
15	1	0	4.637011	4.407138	-1.162733
16	6	0	-1.372043	0.102469	-0.267791
17	6	0	-0.380153	-0.918606	-0.148534
18	6	0	-1.104246	-2.138800	0.008079
19	7	0	-2.401322	-1.927822	-0.027926
20	7	0	-2.584183	-0.566204	-0.173821
21	6	0	-3.889265	-0.041595	-0.225947
22	6	0	-4.982165	-0.900753	-0.058359
23	6	0	-4.106282	1.325027	-0.445647
24	6	0	-6.275361	-0.393620	-0.112776

25	1	0	-4.800750	-1.954360	0.110034
26	6	0	-5.409070	1.811819	-0.495561
27	1	0	-3.257975	1.983235	-0.572593
28	6	0	-6.501017	0.963828	-0.331411
29	1	0	-7.113610	-1.071213	0.017770
30	1	0	-5.566876	2.872228	-0.667591
31	1	0	-7.512440	1.353939	-0.373356
32	6	0	-0.610805	-3.547691	0.125548
33	1	0	-0.190907	-3.749887	1.115074
34	1	0	-1.446122	-4.230568	-0.038115
35	1	0	0.170838	-3.753147	-0.610125
36	6	0	0.974147	-0.477466	-0.269495
37	1	0	1.059471	0.326901	-1.003746
38	6	0	2.129667	-1.414643	-0.301585
39	6	0	3.067847	-1.303182	-1.331287
40	6	0	2.323703	-2.375363	0.697814
41	6	0	4.159805	-2.166276	-1.385466
42	1	0	2.934707	-0.541681	-2.094360
43	6	0	3.416882	-3.231996	0.648318
44	1	0	1.616261	-2.440378	1.520596
45	6	0	4.334202	-3.132296	-0.398317
46	1	0	4.877490	-2.077349	-2.194211
47	1	0	3.557288	-3.974585	1.426735
48	1	0	5.188262	-3.800455	-0.436359
49	8	0	-1.170422	1.336701	-0.366954

Cat1

Total Energy= -894.5522902
Sum of electronic and zero-point Energies= -894.367601
Sum of electronic and thermal Energies= -894.357108
Sum of electronic and thermal Enthalpies= -894.356164
Sum of electronic and thermal Free Energies= -894.404321

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.535755	-1.070978	0.522392
2	6	0	-0.393088	1.012277	0.634557
3	6	0	-1.379985	-0.139747	1.023736
4	6	0	2.125506	0.599261	0.148117
5	6	0	2.893826	-0.545091	-0.130548
6	6	0	4.207562	-0.434824	-0.554499
7	1	0	4.796579	-1.320371	-0.767941

8	6	0	4.751411	0.842214	-0.714981
9	6	0	3.985217	1.976546	-0.452919
10	6	0	2.664816	1.870336	-0.015702
11	1	0	-0.375877	1.817020	1.371346
12	1	0	5.776778	0.945904	-1.051643
13	1	0	4.419550	2.961408	-0.587691
14	1	0	2.067904	2.750623	0.197836
15	16	0	1.959359	-2.037456	0.131685
16	7	0	0.860828	0.271255	0.601032
17	7	0	-0.680164	-1.406285	0.706796
18	1	0	-0.619926	1.426126	-0.356286
19	1	0	-1.604287	-0.094799	2.068996
20	6	0	-2.675179	-0.029237	0.197988
21	1	0	-3.340157	-0.822251	0.469710
22	1	0	-3.144004	0.912363	0.394185
23	1	0	-2.441284	-0.101039	-0.843663

Cat1-TS1

Total Energy= -1624.9855605
Sum of electronic and zero-point Energies= -1624.531462
Sum of electronic and thermal Energies= -1624.504689
Sum of electronic and thermal Enthalpies= -1624.503745
Sum of electronic and thermal Free Energies= -1624.590196

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.747389	-0.316002	0.267134
2	6	0	-2.384542	1.155500	1.900981
3	6	0	-0.847674	1.144629	1.690047
4	6	0	-4.049647	-0.038504	0.269650
5	6	0	-3.902577	-1.041176	-0.701485
6	6	0	-5.013646	-1.588489	-1.325446
7	1	0	-4.900734	-2.359735	-2.079781
8	6	0	-6.277716	-1.131061	-0.952029
9	6	0	-6.418778	-0.141828	0.022389
10	6	0	-5.306614	0.421136	0.645198
11	1	0	-2.805014	2.161600	1.899352
12	1	0	-7.157818	-1.553416	-1.423780
13	1	0	-7.409753	0.198732	0.302236
14	1	0	-5.412096	1.193854	1.398899
15	16	0	-2.193470	-1.444204	-0.987092
16	7	0	-2.814495	0.387185	0.734482

17	7	0	-0.620666	-0.046923	0.836194
18	1	0	-2.674137	0.633195	2.822017
19	1	0	-0.570969	2.023360	1.091600
20	6	0	0.927316	-0.613828	-0.030692
21	8	0	0.594971	-1.127499	-1.093914
22	6	0	1.581821	-1.430539	1.080980
23	1	0	1.590121	-0.861816	2.012142
24	1	0	0.959256	-2.318600	1.218394
25	6	0	2.985203	-1.806677	0.670769
26	6	0	4.080739	-1.066102	1.120436
27	6	0	3.204179	-2.868613	-0.209898
28	6	0	5.372169	-1.385535	0.707330
29	1	0	3.915952	-0.232001	1.798587
30	6	0	4.493534	-3.191940	-0.623768
31	1	0	2.352373	-3.435394	-0.575135
32	6	0	5.581423	-2.451535	-0.165077
33	1	0	6.214824	-0.803099	1.067072
34	1	0	4.649656	-4.021298	-1.306622
35	1	0	6.587117	-2.703935	-0.485852
36	8	0	1.603371	0.663870	-0.033554
37	6	0	1.191299	1.655329	-0.849849
38	8	0	0.114890	1.683424	-1.397390
39	6	0	2.248155	2.752359	-0.939536
40	6	0	2.489206	3.309938	0.472303
41	1	0	3.230433	4.113633	0.424590
42	1	0	1.567903	3.723690	0.896492
43	1	0	2.863790	2.531295	1.141414
44	6	0	1.743127	3.854545	-1.867818
45	1	0	2.491410	4.649406	-1.936900
46	1	0	1.555971	3.463436	-2.871124
47	1	0	0.810247	4.284104	-1.493734
48	6	0	3.548208	2.140236	-1.482798
49	1	0	3.913340	1.349371	-0.822413
50	1	0	3.395947	1.715912	-2.479912
51	1	0	4.313221	2.919271	-1.557024
52	6	0	-0.047926	1.124472	2.977666
53	1	0	1.021531	1.183243	2.760377
54	1	0	-0.316311	1.985066	3.596363
55	1	0	-0.249696	0.209293	3.541420

Cat1-TS2

Total Energy= -1624.982003

Sum of electronic and zero-point Energies= -1624.527024

Sum of electronic and thermal Energies= -1624.500327
Sum of electronic and thermal Enthalpies= -1624.499383
Sum of electronic and thermal Free Energies= -1624.585506

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.736288	-0.962172	-0.110783
2	6	0	-0.803538	-1.570671	2.108561
3	6	0	0.521042	-0.815448	1.797100
4	6	0	-2.796877	-1.824349	0.419961
5	6	0	-2.969613	-1.517539	-0.935659
6	6	0	-4.182806	-1.769989	-1.565396
7	1	0	-4.325208	-1.533580	-2.613982
8	6	0	-5.206426	-2.336610	-0.811806
9	6	0	-5.023744	-2.641560	0.541357
10	6	0	-3.814670	-2.390025	1.180175
11	1	0	-1.379599	-1.104948	2.909236
12	1	0	-6.160242	-2.543710	-1.283752
13	1	0	-5.838224	-3.083109	1.104700
14	1	0	-3.664553	-2.622689	2.228590
15	16	0	-1.508522	-0.797821	-1.639615
16	7	0	-1.517157	-1.472943	0.836827
17	7	0	0.487921	-0.658404	0.312708
18	1	0	-0.622603	-2.622662	2.348492
19	1	0	0.487148	0.195852	2.212811
20	6	0	1.183736	0.398936	-0.448286
21	8	0	0.910638	0.428572	-1.645701
22	6	0	2.545669	0.787602	0.081348
23	1	0	2.759922	1.736619	-0.418186
24	1	0	2.493980	0.999116	1.152395
25	6	0	3.621484	-0.244490	-0.200991
26	6	0	4.756219	-0.275964	0.617800
27	6	0	3.532380	-1.161041	-1.252204
28	6	0	5.775205	-1.197138	0.396576
29	1	0	4.836925	0.430105	1.441211
30	6	0	4.550265	-2.087927	-1.471894
31	1	0	2.662666	-1.146316	-1.900614
32	6	0	5.673724	-2.111167	-0.650534
33	1	0	6.646002	-1.204275	1.044660
34	1	0	4.461977	-2.795189	-2.290865
35	1	0	6.463325	-2.835429	-0.822899
36	8	0	0.138494	1.733012	0.465519
37	6	0	0.123380	2.906530	-0.076499

38	8	0	1.024855	3.389770	-0.762569
39	6	0	-1.170295	3.701815	0.209412
40	6	0	-2.362003	2.872934	-0.287036
41	1	0	-3.301504	3.402972	-0.094943
42	1	0	-2.288468	2.688681	-1.364487
43	1	0	-2.392168	1.905381	0.222386
44	6	0	-1.130522	5.050983	-0.503205
45	1	0	-2.042194	5.618918	-0.287945
46	1	0	-0.267649	5.637848	-0.178122
47	1	0	-1.050242	4.916666	-1.585297
48	6	0	-1.288027	3.906117	1.725236
49	1	0	-1.295507	2.942104	2.239996
50	1	0	-0.447375	4.495148	2.107406
51	1	0	-2.213514	4.440183	1.966867
52	6	0	1.727792	-1.594697	2.290669
53	1	0	2.659156	-1.050373	2.137144
54	1	0	1.614565	-1.784991	3.361610
55	1	0	1.795960	-2.553370	1.769285

Cat2

Total Energy= -1314.8263886
Sum of electronic and zero-point Energies= -1314.679038
Sum of electronic and thermal Energies= -1314.669003
Sum of electronic and thermal Enthalpies= -1314.668059
Sum of electronic and thermal Free Energies= -1314.715770

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.742875	0.915850	0.282939
2	6	0	1.370468	-1.216466	0.755242
3	6	0	2.542313	-0.208190	0.675678
4	6	0	-1.062700	-0.545796	0.079736
5	6	0	-1.708064	0.688556	-0.104742
6	6	0	-3.079337	0.752944	-0.295536
7	1	0	-3.574378	1.707129	-0.439461
8	6	0	-3.806544	-0.438207	-0.287069
9	6	0	-3.165507	-1.661703	-0.092370
10	6	0	-1.785585	-1.733110	0.090377
11	1	0	1.161423	-1.477862	1.798970
12	1	0	-4.880728	-0.407246	-0.430112
13	1	0	-3.747249	-2.577001	-0.083586
14	1	0	-1.283086	-2.683009	0.236711

15	16	0	-0.559682	2.043611	-0.039715
16	7	0	0.305021	-0.382097	0.222265
17	7	0	1.978339	1.115244	0.587873
18	1	0	1.532782	-2.119524	0.168121
19	1	0	3.263596	-0.307674	1.482563
20	17	0	3.541855	-0.546346	-0.846721

Cat2-TS1

Total Energy= -2045.2562135
Sum of electronic and zero-point Energies= -2044.840371
Sum of electronic and thermal Energies= -2044.813688
Sum of electronic and thermal Enthalpies= -2044.812744
Sum of electronic and thermal Free Energies= -2044.901123

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.621021	-0.752502	0.248051
2	6	0	2.123805	-0.575256	-1.973891
3	6	0	0.731062	-1.202204	-1.730906
4	6	0	3.818653	-0.102464	-0.032474
5	6	0	3.681780	-0.002954	1.358968
6	6	0	4.747882	0.414957	2.144639
7	1	0	4.646452	0.495195	3.221388
8	6	0	5.948182	0.731075	1.512162
9	6	0	6.075255	0.635677	0.123756
10	6	0	5.012612	0.214618	-0.669857
11	1	0	2.030521	0.451033	-2.340889
12	1	0	6.793410	1.055850	2.108384
13	1	0	7.017972	0.890944	-0.347508
14	1	0	5.106133	0.135257	-1.747299
15	16	0	2.040933	-0.419160	1.891220
16	7	0	2.638894	-0.555496	-0.608394
17	7	0	0.497124	-1.125648	-0.314159
18	1	0	2.747028	-1.167966	-2.642313
19	1	0	-0.071157	-0.723239	-2.290183
20	6	0	-1.014845	-0.577088	0.447320
21	8	0	-0.752221	-0.197319	1.591240
22	6	0	-1.953906	-1.751865	0.179245
23	1	0	-1.898838	-2.048379	-0.872125
24	1	0	-1.591688	-2.581416	0.792443
25	6	0	-3.363175	-1.361542	0.551829
26	6	0	-4.312197	-1.079386	-0.432559

27	6	0	-3.718138	-1.211914	1.895196
28	6	0	-5.594475	-0.659856	-0.084320
29	1	0	-4.040832	-1.186653	-1.479869
30	6	0	-4.998071	-0.792410	2.246443
31	1	0	-2.973730	-1.409745	2.660590
32	6	0	-5.940301	-0.514880	1.257113
33	1	0	-6.322894	-0.447415	-0.860790
34	1	0	-5.260581	-0.679999	3.293859
35	1	0	-6.938767	-0.189251	1.531140
36	8	0	-1.402381	0.440197	-0.529571
37	6	0	-0.742843	1.616536	-0.564754
38	8	0	0.451948	1.720612	-0.395428
39	6	0	-1.688502	2.773904	-0.850104
40	6	0	-2.483752	2.479796	-2.130434
41	1	0	-3.165567	3.311821	-2.330696
42	1	0	-1.818813	2.370090	-2.993181
43	1	0	-3.072719	1.566039	-2.021471
44	6	0	-0.884325	4.062833	-0.996705
45	1	0	-1.562181	4.899749	-1.187671
46	1	0	-0.315499	4.274032	-0.087884
47	1	0	-0.177716	3.991406	-1.828241
48	6	0	-2.652813	2.864386	0.345383
49	1	0	-3.228341	1.939840	0.447725
50	1	0	-2.107335	3.038892	1.277975
51	1	0	-3.345613	3.697248	0.191043
52	17	0	0.711028	-2.951380	-2.275918

Cat2-TS2

Total Energy= -2045.255272
Sum of electronic and zero-point Energies= -2044.838297
Sum of electronic and thermal Energies= -2044.811930
Sum of electronic and thermal Enthalpies= -2044.810986
Sum of electronic and thermal Free Energies= -2044.896693

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.488997	-0.831663	-0.130278
2	6	0	-1.997778	-0.166256	2.002006
3	6	0	-0.565474	-0.740547	1.931042
4	6	0	-3.699298	-0.249538	0.011367
5	6	0	-3.558948	-0.470151	-1.364433
6	6	0	-4.641070	-0.299442	-2.219775

7	1	0	-4.539899	-0.467245	-3.286196
8	6	0	-5.855165	0.096603	-1.667229
9	6	0	-5.984714	0.320432	-0.292331
10	6	0	-4.908447	0.147721	0.570521
11	1	0	-1.972831	0.920263	2.109416
12	1	0	-6.712428	0.235819	-2.316195
13	1	0	-6.941013	0.634205	0.110893
14	1	0	-5.002019	0.317143	1.637409
15	16	0	-1.895933	-0.914994	-1.792135
16	7	0	-2.496040	-0.494603	0.667206
17	7	0	-0.346950	-1.021326	0.530062
18	1	0	-2.597424	-0.629352	2.784207
19	1	0	0.197056	-0.059641	2.303492
20	6	0	0.947431	-0.907468	-0.187383
21	8	0	0.845252	-0.939801	-1.409293
22	6	0	2.083235	-1.593792	0.563329
23	1	0	2.105451	-1.264431	1.604393
24	1	0	1.840306	-2.663165	0.554230
25	6	0	3.410946	-1.351019	-0.106268
26	6	0	4.232017	-0.295533	0.296564
27	6	0	3.828796	-2.167323	-1.158239
28	6	0	5.450251	-0.064256	-0.336297
29	1	0	3.896819	0.354375	1.099433
30	6	0	5.046531	-1.938505	-1.794924
31	1	0	3.192267	-2.986901	-1.480383
32	6	0	5.861418	-0.886390	-1.384163
33	1	0	6.078920	0.759442	-0.012100
34	1	0	5.358798	-2.582604	-2.611018
35	1	0	6.812001	-0.708001	-1.876830
36	8	0	1.399394	0.794217	0.402076
37	6	0	0.600114	1.792467	0.209569
38	8	0	-0.623322	1.709111	0.044772
39	6	0	1.305819	3.160785	0.235108
40	6	0	1.927834	3.347992	1.626217
41	1	0	2.444881	4.311863	1.680421
42	1	0	1.158358	3.332253	2.406053
43	1	0	2.648325	2.553001	1.834550
44	6	0	0.304506	4.277809	-0.048192
45	1	0	0.811653	5.248151	-0.028671
46	1	0	-0.158778	4.146463	-1.029594
47	1	0	-0.493558	4.287108	0.698851
48	6	0	2.415683	3.152352	-0.823739
49	1	0	3.121558	2.340218	-0.631717
50	1	0	1.998221	3.013391	-1.826416

51	1	0	2.955657	4.105233	-0.809542
52	17	0	-0.425011	-2.262357	2.910784

Cat3

Total Energy= -954.4628302
Sum of electronic and zero-point Energies= -954.313634
Sum of electronic and thermal Energies= -954.303978
Sum of electronic and thermal Enthalpies= -954.303034
Sum of electronic and thermal Free Energies= -954.349491

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.108868	0.799060	-0.152711
2	6	0	-1.654128	-1.402431	-0.385034
3	6	0	-2.876510	-0.448430	-0.304354
4	6	0	0.795958	-0.549727	-0.038635
5	6	0	1.382349	0.725227	0.043712
6	6	0	2.757193	0.870659	0.133766
7	1	0	3.207103	1.855553	0.199083
8	6	0	3.548712	-0.279756	0.133704
9	6	0	2.965315	-1.543480	0.045043
10	6	0	1.582481	-1.696247	-0.040637
11	1	0	-1.535086	-1.842579	-1.379037
12	1	0	4.626566	-0.184375	0.201409
13	1	0	3.594768	-2.426763	0.042875
14	1	0	1.123873	-2.676866	-0.108103
15	16	0	0.154419	2.011432	0.003613
16	7	0	-0.581175	-0.465688	-0.105316
17	7	0	-2.376974	0.915275	-0.317978
18	1	0	-1.729643	-2.188621	0.368576
19	1	0	-3.605073	-0.617619	-1.099339
20	9	0	-3.533464	-0.677555	0.896739

Cat3-TS1

Total Energy= -1684.8932148
Sum of electronic and zero-point Energies= -1684.476021
Sum of electronic and thermal Energies= -1684.450067
Sum of electronic and thermal Enthalpies= -1684.449123
Sum of electronic and thermal Free Energies= -1684.534147

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-1.680746	-0.759385	0.277319
2	6	0	-2.168023	0.450854	2.162198
3	6	0	-0.704842	-0.051554	2.142883
4	6	0	-3.915649	-0.144909	0.297076
5	6	0	-3.812286	-0.789117	-0.950095
6	6	0	-4.924921	-0.899431	-1.766671
7	1	0	-4.858442	-1.393935	-2.730437
8	6	0	-6.130466	-0.369684	-1.331316
9	6	0	-6.225313	0.272994	-0.088851
10	6	0	-5.114252	0.388445	0.746018
11	1	0	-2.242881	1.538341	2.105770
12	1	0	-7.013863	-0.448663	-1.958869
13	1	0	-7.172364	0.689687	0.236007
14	1	0	-5.171781	0.883242	1.710353
15	16	0	-2.161897	-1.349994	-1.276071
16	7	0	-2.689839	-0.162641	0.949292
17	7	0	-0.530437	-0.764700	0.905755
18	1	0	-2.680882	0.078162	3.059071
19	6	0	0.986421	-0.790354	-0.125073
20	8	0	0.658844	-1.054355	-1.285733
21	6	0	1.874323	-1.700341	0.712924
22	1	0	1.790020	-1.436563	1.763489
23	1	0	1.491907	-2.713313	0.568772
24	6	0	3.316512	-1.583338	0.249756
25	6	0	4.293236	-1.042591	1.087947
26	6	0	3.673836	-1.978902	-1.047571
27	6	0	5.603840	-0.902601	0.644608
28	1	0	4.017160	-0.737066	2.089089
29	6	0	4.981754	-1.828232	-1.494881
30	1	0	2.906877	-2.384142	-1.707730
31	6	0	5.951456	-1.289779	-0.649849
32	1	0	6.356207	-0.480756	1.309265
33	1	0	5.250842	-2.138947	-2.497041
34	1	0	6.981489	-1.179758	-0.990701
35	8	0	1.443014	0.560772	0.159744
36	6	0	0.804742	1.632667	-0.340448
37	8	0	-0.372131	1.645754	-0.620461
38	6	0	1.752944	2.826129	-0.452741
39	6	0	2.916294	2.435090	-1.399932
40	1	0	3.604625	3.283316	-1.505741
41	1	0	3.472231	1.584021	-1.004330
42	1	0	2.533610	2.161934	-2.396074

43	6	0	2.317758	3.145981	0.959464
44	1	0	2.999791	4.006288	0.886200
45	1	0	1.504692	3.398393	1.659992
46	1	0	2.878755	2.304784	1.358638
47	6	0	0.978068	4.021401	-1.007723
48	1	0	0.581529	3.807157	-2.010766
49	1	0	0.127742	4.287442	-0.352949
50	1	0	1.649763	4.890502	-1.075404
51	9	0	-0.488718	-0.905262	3.211637
52	1	0	0.037774	0.761077	2.231803

Cat3-TS2

Total Energy= -1684.8960521
Sum of electronic and zero-point Energies= -1684.476670
Sum of electronic and thermal Energies= -1684.450977
Sum of electronic and thermal Enthalpies= -1684.450033
Sum of electronic and thermal Free Energies= -1684.532528

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.501264	-0.876309	-0.092338
2	6	0	-2.067866	-0.887711	2.131809
3	6	0	-0.575959	-1.239487	1.944672
4	6	0	-3.731453	-0.412330	0.163045
5	6	0	-3.573595	-0.245041	-1.218281
6	6	0	-4.655416	0.119040	-2.011296
7	1	0	-4.541916	0.252046	-3.081508
8	6	0	-5.886846	0.311124	-1.390903
9	6	0	-6.033840	0.144595	-0.009966
10	6	0	-4.957463	-0.222292	0.790007
11	1	0	-2.202759	0.070665	2.633666
12	1	0	-6.744293	0.594898	-1.990475
13	1	0	-7.003939	0.301808	0.448067
14	1	0	-5.063575	-0.357315	1.860682
15	16	0	-1.893121	-0.516068	-1.725260
16	7	0	-2.525207	-0.781459	0.749052
17	7	0	-0.363679	-1.208085	0.508624
18	1	0	-2.580948	-1.690291	2.664022
19	1	0	0.108104	-0.543825	2.430631
20	6	0	0.940608	-0.920317	-0.151652
21	8	0	0.842273	-0.684357	-1.360395
22	6	0	2.040499	-1.817489	0.413974

23	1	0	2.004396	-1.814100	1.506061
24	1	0	1.796928	-2.830556	0.074103
25	6	0	3.399127	-1.402091	-0.083277
26	6	0	4.210339	-0.561770	0.682968
27	6	0	3.855420	-1.821597	-1.333980
28	6	0	5.454725	-0.152683	0.212419
29	1	0	3.848321	-0.216591	1.647045
30	6	0	5.100142	-1.414292	-1.809250
31	1	0	3.226077	-2.468212	-1.938864
32	6	0	5.903433	-0.578710	-1.036877
33	1	0	6.074259	0.499528	0.820440
34	1	0	5.442457	-1.750351	-2.783083
35	1	0	6.873735	-0.260967	-1.405272
36	8	0	1.391329	0.538215	0.735597
37	6	0	0.584283	1.561834	0.697425
38	8	0	-0.624560	1.506724	0.935907
39	6	0	1.261276	2.870597	0.275361
40	6	0	2.580291	3.048254	1.035663
41	1	0	3.069937	3.973880	0.715059
42	1	0	2.408621	3.112671	2.115420
43	1	0	3.252171	2.208930	0.840273
44	6	0	0.332497	4.055834	0.523108
45	1	0	0.806210	4.981554	0.180704
46	1	0	-0.612647	3.927040	-0.009251
47	1	0	0.105733	4.159277	1.588636
48	6	0	1.554671	2.717582	-1.225939
49	1	0	2.164341	1.826891	-1.402749
50	1	0	0.625315	2.611845	-1.795728
51	1	0	2.088349	3.599922	-1.594573
52	9	0	-0.322969	-2.505550	2.416456

Cat4

Total Energy= -1774.3886957
Sum of electronic and zero-point Energies= -1774.252089
Sum of electronic and thermal Energies= -1774.240727
Sum of electronic and thermal Enthalpies= -1774.239782
Sum of electronic and thermal Free Energies= -1774.291023

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.239014	0.961514	-0.053296
2	6	0	0.992931	-1.176766	-0.236289

3	6	0	2.107266	-0.099308	-0.072973
4	6	0	-1.535368	-0.548773	-0.004134
5	6	0	-2.229936	0.671247	-0.010819
6	6	0	-3.616159	0.699092	-0.014677
7	1	0	-4.152881	1.641377	-0.018255
8	6	0	-4.301780	-0.515598	-0.022063
9	6	0	-3.608482	-1.726331	-0.024652
10	6	0	-2.215581	-1.760423	-0.013107
11	1	0	1.099141	-1.997661	0.471426
12	1	0	-5.385801	-0.513780	-0.028047
13	1	0	-4.159522	-2.660279	-0.033407
14	1	0	-1.672597	-2.699100	-0.009589
15	16	0	-1.120834	2.059219	-0.017575
16	7	0	-0.164425	-0.340941	0.033861
17	7	0	1.506743	1.190558	-0.163882
18	1	0	0.963812	-1.555075	-1.262505
19	17	0	3.401853	-0.309593	-1.293792
20	17	0	2.883649	-0.286774	1.575192

Cat4-TS1

Total Energy= -2504.8114066
Sum of electronic and zero-point Energies= -2504.405250
Sum of electronic and thermal Energies= -2504.377574
Sum of electronic and thermal Enthalpies= -2504.376630
Sum of electronic and thermal Free Energies= -2504.466037

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.645258	-0.391637	-0.251432
2	6	0	-2.328357	-0.425533	1.928212
3	6	0	-0.858699	-0.896560	1.769494
4	6	0	-3.934765	-0.134965	-0.125855
5	6	0	-3.707983	0.027833	-1.497747
6	6	0	-4.770671	0.284022	-2.355931
7	1	0	-4.605938	0.414001	-3.419955
8	6	0	-6.049351	0.376042	-1.812303
9	6	0	-6.262581	0.215276	-0.439943
10	6	0	-5.206332	-0.045221	0.427016
11	1	0	-2.361966	0.586234	2.341978
12	1	0	-6.890519	0.578394	-2.465778
13	1	0	-7.267347	0.294189	-0.040234
14	1	0	-5.364634	-0.174117	1.491953

15	16	0	-1.986368	-0.115658	-1.916256
16	7	0	-2.734236	-0.398702	0.529766
17	7	0	-0.520209	-0.593144	0.411040
18	1	0	-2.923165	-1.110193	2.530365
19	6	0	0.911549	-0.506619	-0.438521
20	8	0	0.631071	-0.417517	-1.651642
21	6	0	1.770184	-1.677315	0.060065
22	1	0	1.832939	-1.671223	1.151895
23	1	0	1.261388	-2.593004	-0.254564
24	6	0	3.149876	-1.584781	-0.541321
25	6	0	4.239854	-1.179626	0.231173
26	6	0	3.347215	-1.862260	-1.896446
27	6	0	5.507726	-1.061025	-0.335235
28	1	0	4.089472	-0.956541	1.284697
29	6	0	4.612345	-1.746083	-2.465101
30	1	0	2.492473	-2.149238	-2.500740
31	6	0	5.696537	-1.345645	-1.685509
32	1	0	6.347093	-0.748381	0.278319
33	1	0	4.753725	-1.965792	-3.518860
34	1	0	6.683358	-1.255494	-2.128614
35	8	0	1.546921	0.668625	0.186415
36	6	0	1.012992	1.887004	0.047774
37	8	0	-0.120003	2.104721	-0.323718
38	6	0	2.026925	2.979468	0.378951
39	6	0	2.811793	2.628122	1.648519
40	1	0	3.581037	3.387247	1.820023
41	1	0	2.155325	2.604609	2.524493
42	1	0	3.296112	1.654319	1.550632
43	6	0	1.293172	4.310232	0.548826
44	1	0	1.970689	5.053213	0.979469
45	1	0	0.932554	4.686388	-0.411845
46	1	0	0.430494	4.200170	1.211048
47	6	0	2.991135	3.048065	-0.818781
48	1	0	3.564728	2.121074	-0.910422
49	1	0	2.444687	3.213171	-1.752253
50	1	0	3.689643	3.879122	-0.678222
51	17	0	-0.776807	-2.695165	2.054981
52	17	0	0.208755	-0.098605	2.947796

Cat4-TS2

Total Energy= -2504.8029899

Sum of electronic and zero-point Energies= -2504.396413

Sum of electronic and thermal Energies= -2504.368902

Sum of electronic and thermal Enthalpies= -2504.367957

Sum of electronic and thermal Free Energies= -2504.455540

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.414724	-0.854346	-0.143589
2	6	0	-2.047331	0.054899	1.847600
3	6	0	-0.597074	-0.482614	1.932657
4	6	0	-3.662614	-0.417247	-0.147729
5	6	0	-3.452469	-0.808917	-1.474027
6	6	0	-4.509278	-0.827346	-2.377587
7	1	0	-4.355787	-1.128341	-3.407793
8	6	0	-5.764954	-0.440123	-1.921270
9	6	0	-5.962697	-0.044885	-0.593241
10	6	0	-4.913845	-0.030594	0.318008
11	1	0	-2.028488	1.144099	1.758358
12	1	0	-6.603319	-0.443005	-2.608503
13	1	0	-6.951648	0.255182	-0.265827
14	1	0	-5.059217	0.270075	1.349521
15	16	0	-1.755512	-1.218556	-1.781072
16	7	0	-2.473042	-0.501818	0.573248
17	7	0	-0.278227	-0.852116	0.567962
18	1	0	-2.660437	-0.279567	2.683005
19	6	0	0.998609	-1.005620	-0.158473
20	8	0	0.873616	-1.412343	-1.299860
21	6	0	2.196089	-1.325377	0.714571
22	1	0	2.261654	-0.629494	1.548488
23	1	0	2.002701	-2.327131	1.119790
24	6	0	3.473851	-1.323320	-0.084936
25	6	0	4.259225	-0.171186	-0.154047
26	6	0	3.883530	-2.466720	-0.771961
27	6	0	5.439769	-0.165721	-0.891902
28	1	0	3.923644	0.724036	0.360319
29	6	0	5.063306	-2.463769	-1.512203
30	1	0	3.273093	-3.364590	-0.725849
31	6	0	5.845255	-1.312452	-1.572506
32	1	0	6.043546	0.735543	-0.935935
33	1	0	5.371593	-3.360199	-2.041122
34	1	0	6.765807	-1.308832	-2.147569
35	8	0	1.408655	0.941495	-0.259433
36	6	0	0.515139	1.852312	-0.322376
37	8	0	-0.719733	1.676555	-0.356560
38	6	0	1.032718	3.309186	-0.367500
39	6	0	0.283154	4.116344	0.698138

40	1	0	0.589890	5.167453	0.665455
41	1	0	-0.794202	4.056621	0.529542
42	1	0	0.494961	3.731812	1.701991
43	6	0	0.695516	3.865186	-1.757682
44	1	0	0.991664	4.917575	-1.828884
45	1	0	1.222523	3.309020	-2.539978
46	1	0	-0.378827	3.789214	-1.944296
47	6	0	2.537903	3.382089	-0.121480
48	1	0	2.789933	2.979644	0.865100
49	1	0	3.085219	2.801136	-0.868241
50	1	0	2.876811	4.423021	-0.166390
51	17	0	0.439126	0.750319	2.681009
52	17	0	-0.521997	-1.972270	2.960374

Cat5

Total Energy= -1053.6850257
Sum of electronic and zero-point Energies= -1053.544667
Sum of electronic and thermal Energies= -1053.534184
Sum of electronic and thermal Enthalpies= -1053.533239
Sum of electronic and thermal Free Energies= -1053.582045

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.787250	0.876770	0.000184
2	6	0	1.443180	-1.310637	0.000384
3	6	0	2.606244	-0.276969	-0.000025
4	6	0	-1.063113	-0.548998	0.000067
5	6	0	-1.700474	0.702486	0.000002
6	6	0	-3.083361	0.795138	-0.000084
7	1	0	-3.574502	1.762250	-0.000128
8	6	0	-3.826628	-0.386007	-0.000112
9	6	0	-3.190659	-1.627603	-0.000038
10	6	0	-1.800711	-1.727207	0.000060
11	1	0	1.471849	-1.930254	0.898853
12	1	0	-4.909403	-0.333183	-0.000200
13	1	0	-3.784690	-2.534967	-0.000057
14	1	0	-1.301161	-2.689924	0.000129
15	16	0	-0.526006	2.036417	0.000038
16	7	0	0.312125	-0.405513	0.000166
17	7	0	2.064617	1.045752	0.000248
18	1	0	1.471831	-1.930808	-0.897706
19	9	0	3.409206	-0.466011	-1.079863

20	9	0	3.410195	-0.466134	1.079081

Cat5-TS1

Total Energy= -1784.1135576
Sum of electronic and zero-point Energies= -1783.703268
Sum of electronic and thermal Energies= -1783.676779
Sum of electronic and thermal Enthalpies= -1783.675835
Sum of electronic and thermal Free Energies= -1783.760507

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.623144	-0.562749	0.210483
2	6	0	-2.262890	0.500905	2.141595
3	6	0	-0.727196	0.341125	2.037690
4	6	0	-3.912400	-0.273952	0.256025
5	6	0	-3.737076	-0.930618	-0.968346
6	6	0	-4.833991	-1.223437	-1.768964
7	1	0	-4.707675	-1.728202	-2.720526
8	6	0	-6.098083	-0.852202	-1.317087
9	6	0	-6.261397	-0.199226	-0.092058
10	6	0	-5.168720	0.101364	0.715510
11	1	0	-2.540272	1.553537	2.212566
12	1	0	-6.966512	-1.075686	-1.926411
13	1	0	-7.255601	0.079983	0.238480
14	1	0	-5.287998	0.607027	1.667422
15	16	0	-2.027505	-1.282000	-1.303170
16	7	0	-2.682208	-0.083097	0.877856
17	7	0	-0.479248	-0.410652	0.843611
18	1	0	-2.650867	-0.063496	2.991569
19	6	0	0.950203	-0.724889	0.014793
20	8	0	0.662526	-1.311427	-1.045148
21	6	0	1.842911	-1.405359	1.062571
22	1	0	1.882552	-0.799037	1.970946
23	1	0	1.363557	-2.359072	1.301139
24	6	0	3.225962	-1.618196	0.503098
25	6	0	4.277646	-0.767726	0.850316
26	6	0	3.464162	-2.645534	-0.413564
27	6	0	5.545911	-0.943903	0.300711
28	1	0	4.098052	0.039423	1.556345
29	6	0	4.730200	-2.826006	-0.963415
30	1	0	2.640873	-3.292417	-0.701459
31	6	0	5.775456	-1.975779	-0.606722

32	1	0	6.354727	-0.276693	0.582412
33	1	0	4.901109	-3.628994	-1.673769
34	1	0	6.763128	-2.116106	-1.034540
35	8	0	1.518123	0.632378	-0.086979
36	6	0	0.892896	1.596060	-0.771622
37	8	0	-0.235538	1.512522	-1.206033
38	6	0	1.772819	2.839550	-0.889961
39	6	0	1.985071	3.402796	0.524629
40	1	0	2.623608	4.290020	0.472434
41	1	0	1.031894	3.690756	0.978330
42	1	0	2.463369	2.662118	1.170384
43	6	0	1.067354	3.870002	-1.768761
44	1	0	1.682467	4.771582	-1.844790
45	1	0	0.900068	3.476437	-2.774933
46	1	0	0.096570	4.143494	-1.348073
47	6	0	3.125013	2.445770	-1.500573
48	1	0	3.634147	1.702255	-0.882108
49	1	0	2.995620	2.028184	-2.503878
50	1	0	3.760040	3.333756	-1.580015
51	9	0	-0.217856	-0.283129	3.123229
52	9	0	-0.110778	1.546865	1.989675

Cat5-TS2

Total Energy= -1784.1049398
Sum of electronic and zero-point Energies= -1783.694960
Sum of electronic and thermal Energies= -1783.668951
Sum of electronic and thermal Enthalpies= -1783.668006
Sum of electronic and thermal Free Energies= -1783.750311

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.459156	-0.958239	0.257496
2	6	0	-1.980829	0.364423	2.047280
3	6	0	-0.514828	-0.087380	2.120574
4	6	0	-3.672810	-0.365954	0.190749
5	6	0	-3.528789	-1.039727	-1.027609
6	6	0	-4.612323	-1.175577	-1.889318
7	1	0	-4.508954	-1.699248	-2.833112
8	6	0	-5.818331	-0.598769	-1.514735
9	6	0	-5.950744	0.077007	-0.296126
10	6	0	-4.874597	0.210394	0.574301
11	1	0	-2.021888	1.437861	1.838379

12	1	0	-6.675888	-0.690671	-2.172732
13	1	0	-6.909631	0.516144	-0.024343
14	1	0	-4.970549	0.733068	1.519559
15	16	0	-1.878673	-1.637256	-1.260962
16	7	0	-2.468814	-0.380809	0.890533
17	7	0	-0.301340	-0.887572	0.922923
18	1	0	-2.518722	0.098985	2.966189
19	6	0	0.949396	-1.191519	0.218433
20	8	0	0.823493	-1.863968	-0.783016
21	6	0	2.158698	-1.234032	1.135888
22	1	0	2.139357	-0.400297	1.825878
23	1	0	2.044042	-2.164806	1.716335
24	6	0	3.448015	-1.262114	0.354096
25	6	0	4.291559	-0.133784	0.345266
26	6	0	3.803640	-2.402295	-0.389816
27	6	0	5.483590	-0.154451	-0.376302
28	1	0	4.011952	0.754983	0.913317
29	6	0	4.994360	-2.426767	-1.125116
30	1	0	3.145612	-3.268949	-0.413451
31	6	0	5.833453	-1.297412	-1.113647
32	1	0	6.134202	0.726347	-0.360554
33	1	0	5.262426	-3.317624	-1.704590
34	1	0	6.760686	-1.318913	-1.680478
35	8	0	1.348959	0.676870	-0.343321
36	6	0	0.483827	1.605662	-0.505471
37	8	0	-0.762056	1.473734	-0.462512
38	6	0	1.078409	3.016345	-0.696694
39	6	0	2.359406	2.938353	-1.555989
40	1	0	2.798109	3.941455	-1.654931
41	1	0	3.087277	2.270289	-1.099516
42	1	0	2.124436	2.566861	-2.563953
43	6	0	1.434943	3.516951	0.712509
44	1	0	1.889620	4.511338	0.665208
45	1	0	0.535834	3.584936	1.343135
46	1	0	2.144454	2.835576	1.202977
47	6	0	0.054099	3.945293	-1.347807
48	1	0	-0.209342	3.597857	-2.353416
49	1	0	-0.862682	3.982529	-0.752079
50	1	0	0.471607	4.962246	-1.433500
51	9	0	-0.263542	-0.839514	3.207375
52	9	0	0.322298	0.955433	2.185946