Elecrtonic Supplementray Information for

DFT perspective toward [3 + 2] annulation reaction of enals with α-ketoamides through NHC and Brønsted acid cooperative catalysis: mechanism, stereoselectivity, and role of NHC

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Content

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Part 1: Energy Profiles of Re addition and direct proton transfer pathways

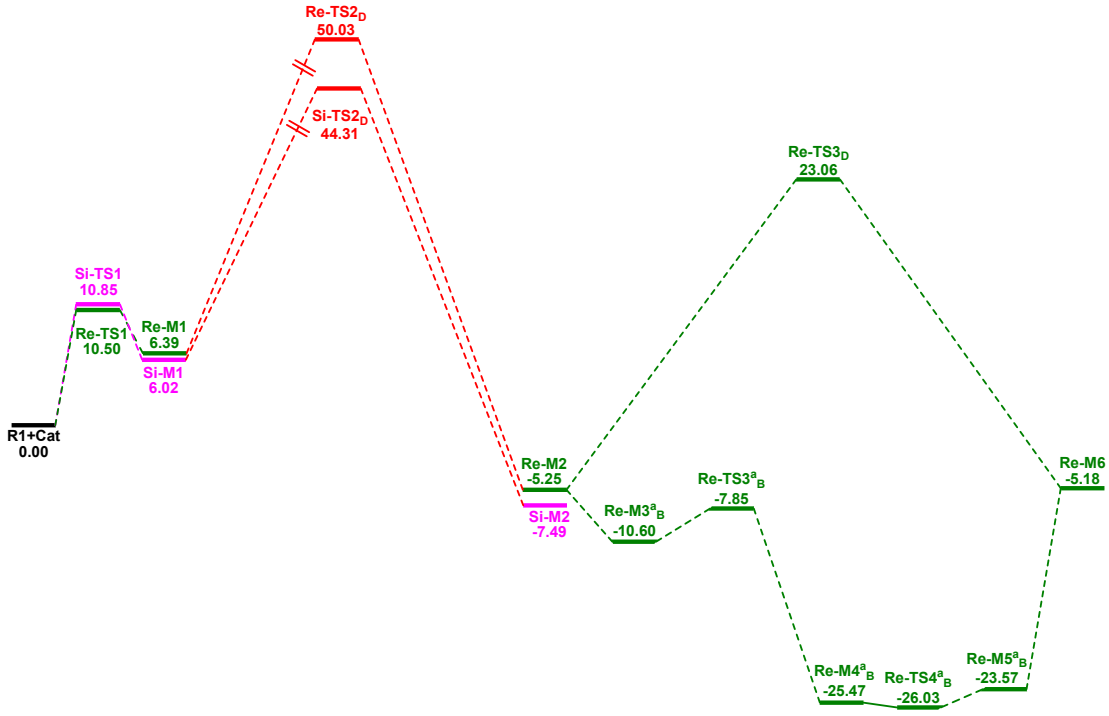


Fig. S1 Energy Profiles of *Re* addition and direct proton transfer pathways

Part 2: Energy Profiles of the other three pathways involved in steps 5~7

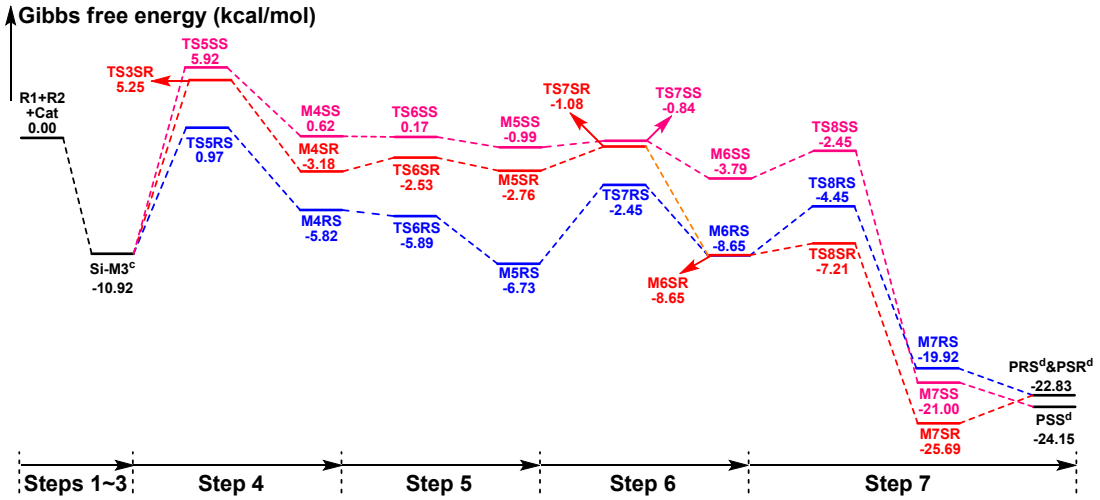


Fig. S2 Energy Profiles of the other three pathways involved in steps 5~7

Part 3: Geometrical patameters of Re/Si-TS2D

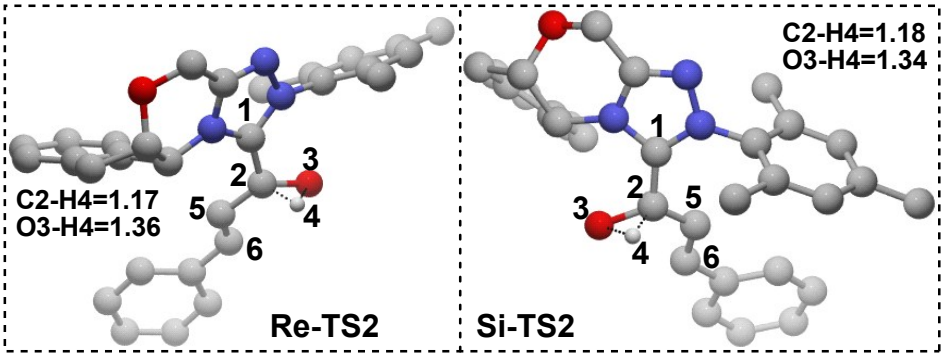


Fig. S3 Geometrical patameters of **Re/Si-TS2$_D$**

Part 4: Comparison of the Gibbs free energies of the stereoselective transition states calculated by M06-2X and ωB97X-D methods using IEF-PCM and SMD salvation models

Table S1 Comparision of the single-point energies of the stereoselective transition states calculated by M06-2X and ωB97X-D methods

	$\Delta\Delta G^{\neq}$	M06-2X/6-311++G(2df, 2pd)		ωB97X-D/6-311++G(2df, 2pd)	
		IEF-PCM	SMD	IEF-PCM	SMD
TS5RR	0.00	0.00	0.00	0.00	0.00
TS5RS	4.28	3.22	1.84	1.59	0.88
TS5SR	8.56	8.77	6.60	7.89	5.80
TS5SS	9.23	8.42	7.40	8.43	7.52

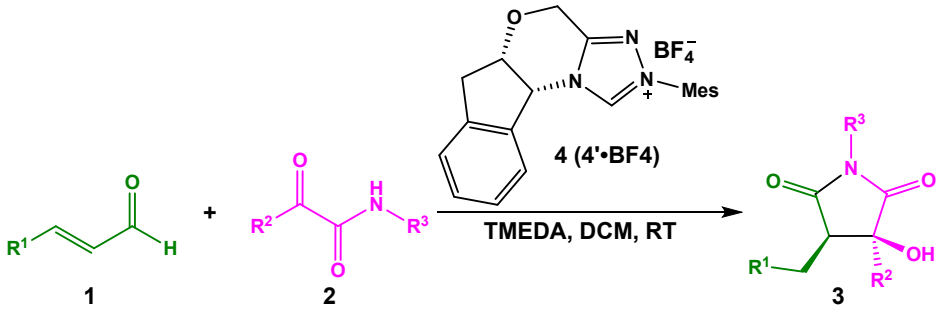
Table S2 Comparision of the Gibbs free energies of the stereoselective transition states calculated by M06-2X and ωB97X-D methods

	M06-2X/6-31G(d, p)	ωB97X-D/6-31G(d, p)	
	SMD	IEF-PCM	SMD
R1	-422.698277	-422.732777	-422.742313
R2	-744.878393	-744.927136	-744.940997
Cat	-1051.613112	-1051.698004	-1051.724838
R1+R2 +Cat	-2219.189782 (0.00)	-2219.357917 (0.00)	-2219.408148 (0.00)
Si-M3	-1474.323170 (-7.39)	-1474.450594 (-12.43)	-1474.479573 (-7.79)
TS5RR	-2219.181230 (5.37)	-2219.370225 (-7.72)	-2219.406862 (0.81)
TS5RS	-2219.178267 (7.23)	-2219.366841 (-5.60)	-2219.404483 (2.30)
TS5SR	-2219.171224 (11.65)	-2219.358884 (-0.61)	-2219.394379 (8.64)
TS5SS	-2219.169246 (12.89)	-2219.355968 (1.22)	-2219.392636 (9.73)

Note: Free energies in parenthesis are the relative Gibbs free energies with respect to the free energies of the **R1+R2+Cat**.

Part 5: Substituent effects

Table S3 Prediction of reaction selectivities using the computational model



Substiuent	Relative Free Energy of TS5			
(R^1/R^2/R^3)	RR	RS	SR	SS
Ph/Ph/Ph	0	2.87	8.56	9.23
4-OMeC_6H_4/Ph/Ph	0	4.22	9.78	11.12
4-FC_6H_4/Ph/Ph	0	2.01	10.51	9.10
Furan/Ph/Ph	0	1.08	9.04	7.79
Me/Ph/Ph	0	4.43	11.72	10.39
Ph/4-MeC_6H_4/Ph	0	3.19	8.80	8.44
Ph/Me/Ph	0	1.34	5.55	4.13
Ph/Ph/4-OMeC_6H_4	0	2.20	9.68	9.07

Part 6: NCI pictures of TS5RS, TS5SR, and TS5SS

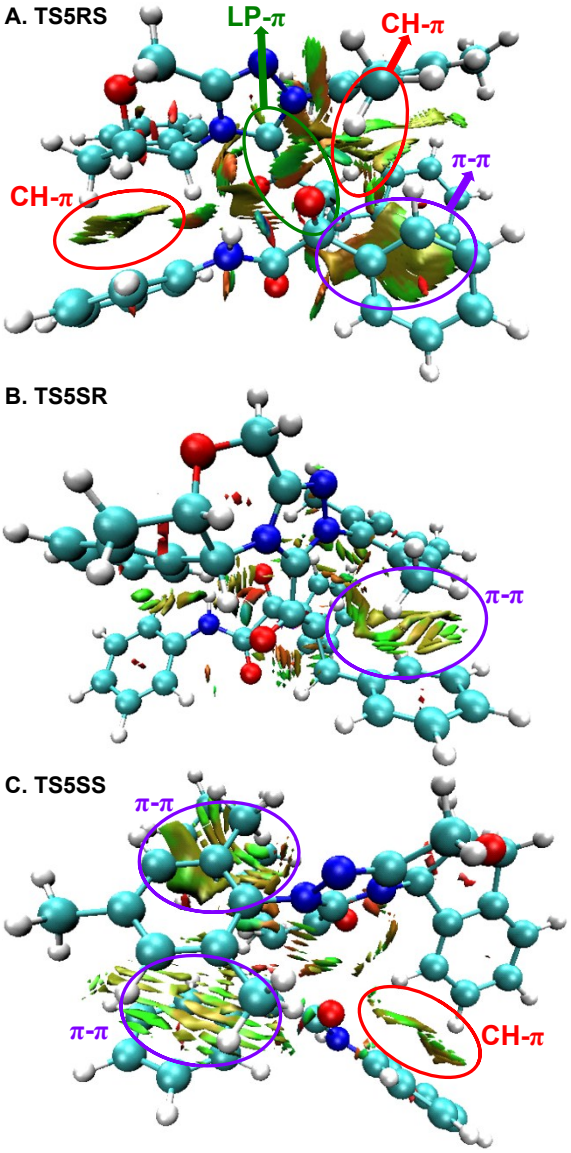


Fig. S4 The interaction analysis of the transition state **TS5RS**, **TS5SR**, and **TS5SS**. (Blue, green, and red represent the strong interaction, weak interaction, and steric effect, respectively)

Part 7: NBO charges of TS5RR, TS5RS, TS5SR, and TS5SS

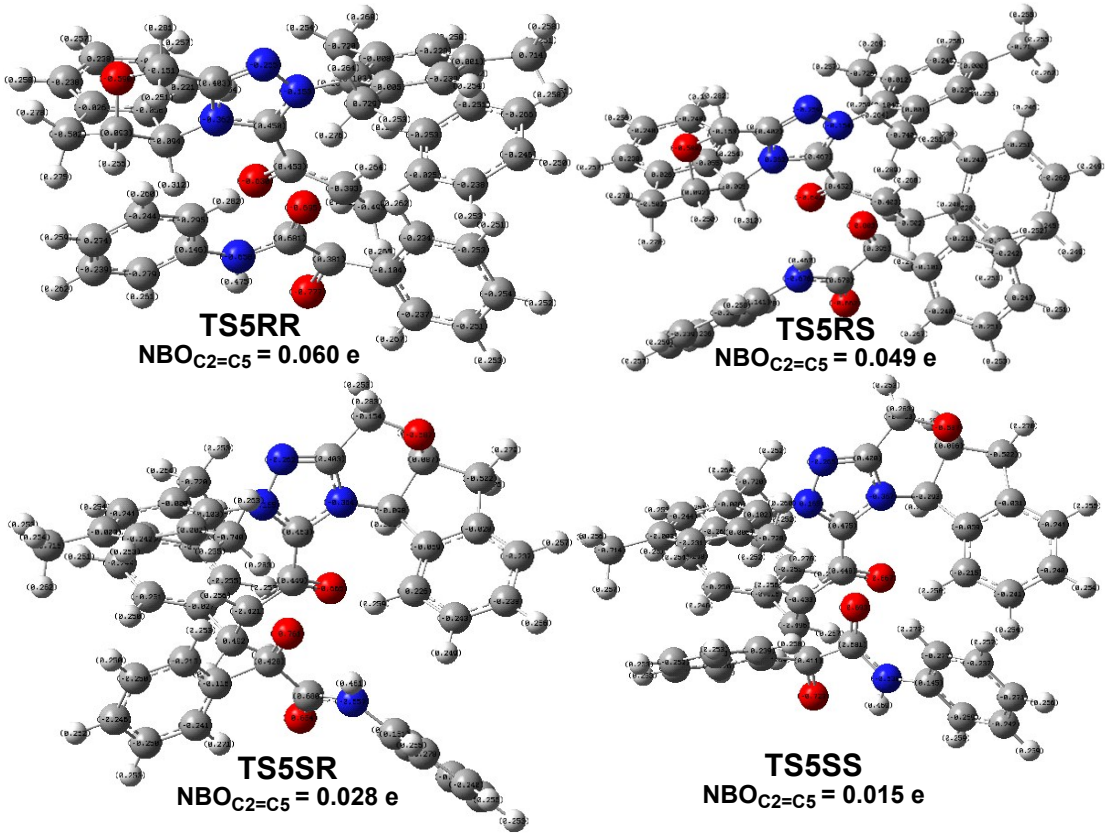
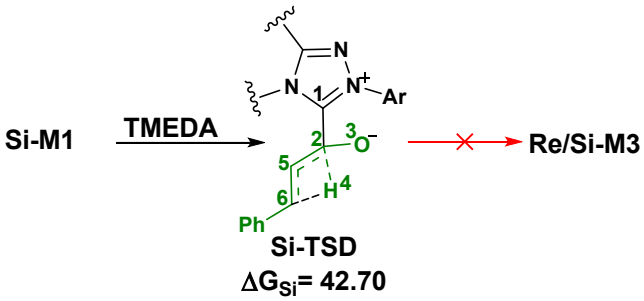


Fig. S5 NBO charge values of **TS5RR**, **TS5RS**, **TS5SR**, and **TS5SS**

Part 8: The direct [1, 3]-proton transfer pathway



Scheme S1 The direct [1, 3]-proton transfer pathway

Part 9: List of the energies and Cartesian coordinates of all the structures involved in the reaction

Cat

Total energy= -1051.92077869
Sum of electronic and zero-point Energies= -1051.537070
Sum of electronic and thermal Energies= -1051.516983
Sum of electronic and thermal Enthalpies= -1051.516039
Sum of electronic and thermal Free Energies= -1051.586771

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.899430	-0.593386	-0.628751
2	6	0	4.235731	-0.376246	-0.291898
3	6	0	5.080005	-1.454838	-0.058228
4	6	0	4.563562	-2.747840	-0.161364
5	6	0	3.224561	-2.956770	-0.494363
6	6	0	2.376877	-1.874663	-0.734914
7	6	0	2.211065	0.735037	-0.858871
8	6	0	3.137447	1.732058	-0.117843
9	6	0	4.531150	1.105984	-0.240110
10	1	0	6.119975	-1.296560	0.211981
11	1	0	5.209076	-3.599791	0.027795
12	1	0	2.838927	-3.968804	-0.563994
13	1	0	1.331396	-2.019051	-0.991578
14	1	0	2.184127	0.974545	-1.927332
15	1	0	3.068505	2.746788	-0.531385
16	1	0	5.016885	1.443609	-1.162439
17	6	0	0.509251	1.497456	0.784127
18	6	0	1.539068	2.297567	1.519015
19	6	0	-0.240888	0.164106	-0.878478
20	1	0	1.361882	2.251823	2.594230
21	1	0	5.159425	1.403254	0.602886
22	7	0	0.849313	0.809546	-0.351251
23	7	0	-0.753454	1.354283	1.044635
24	7	0	-1.180704	0.538972	0.013285
25	8	0	2.818325	1.754011	1.266919
26	1	0	1.494424	3.348792	1.198973
27	6	0	-2.549635	0.121442	-0.007169
28	6	0	-3.425384	0.707340	-0.924359
29	6	0	-2.957554	-0.866261	0.893291
30	6	0	-4.750569	0.272396	-0.925535
31	6	0	-4.292719	-1.266397	0.860199

32	6	0	-5.201888	-0.707198	-0.039449
33	1	0	-5.447717	0.711337	-1.635455
34	1	0	-4.628750	-2.038319	1.548613
35	6	0	-2.942084	1.763296	-1.882265
36	1	0	-2.453675	2.582443	-1.345709
37	1	0	-2.204520	1.349308	-2.575680
38	1	0	-3.774420	2.171755	-2.457947
39	6	0	-6.647057	-1.135347	-0.037966
40	1	0	-7.237161	-0.504324	0.634738
41	1	0	-7.085187	-1.052166	-1.035288
42	1	0	-6.752890	-2.168214	0.301737
43	6	0	-1.970712	-1.481456	1.849326
44	1	0	-1.083666	-1.835150	1.313675
45	1	0	-1.628191	-0.747331	2.584283
46	1	0	-2.419078	-2.323308	2.379490

R1

Total energy= -422.79929385

Sum of electronic and zero-point Energies= -422.654395

Sum of electronic and thermal Energies= -422.645787

Sum of electronic and thermal Enthalpies= -422.644843

Sum of electronic and thermal Free Energies= -422.688939

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.408719	0.384787	0.000016
2	8	0	-3.849311	-0.748928	-0.000024
3	1	0	-4.098872	1.249322	-0.000043
4	6	0	-1.972677	0.719321	0.000009
5	6	0	-1.052789	-0.259621	0.000016
6	1	0	-1.711871	1.773218	-0.000006
7	1	0	-1.430298	-1.282170	0.000028
8	6	0	0.404499	-0.112798	0.000008
9	6	0	1.195136	-1.270076	0.000006
10	6	0	1.040651	1.138128	0.000002
11	6	0	2.583453	-1.184846	-0.000003
12	1	0	0.710292	-2.242441	0.000011
13	6	0	2.425953	1.223363	-0.000006
14	1	0	0.450372	2.048781	0.000005
15	6	0	3.201744	0.062547	-0.000009
16	1	0	3.181071	-2.090276	-0.000005
17	1	0	2.905761	2.196588	-0.000010

18	1	0	4.284523	0.133583	-0.000015

R2

Total energy= -745.04284913

Sum of electronic and zero-point Energies= -744.821596

Sum of electronic and thermal Energies= -744.807943

Sum of electronic and thermal Enthalpies= -744.806999

Sum of electronic and thermal Free Energies= -744.864513

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.153629	0.851768	-0.039278
2	8	0	0.985769	2.056744	-0.006747
3	6	0	-0.101541	-0.050811	-0.162616
4	8	0	-0.032418	-1.232550	-0.462309
5	6	0	2.505474	0.241890	0.002670
6	6	0	2.737701	-1.088498	0.373828
7	6	0	3.587271	1.082705	-0.293002
8	6	0	4.043197	-1.565380	0.440781
9	1	0	1.906041	-1.738229	0.611565
10	6	0	4.885579	0.596242	-0.239125
11	1	0	3.387832	2.113648	-0.566161
12	6	0	5.113394	-0.730117	0.129401
13	1	0	4.224690	-2.593566	0.735131
14	1	0	5.719827	1.246478	-0.479642
15	1	0	6.128417	-1.111671	0.176161
16	7	0	-1.229449	0.655281	0.076586
17	1	0	-1.073003	1.642339	0.249327
18	6	0	-2.565279	0.213093	0.040803
19	6	0	-3.557613	1.172984	0.273053
20	6	0	-2.925561	-1.116701	-0.202774
21	6	0	-4.897353	0.809716	0.260907
22	1	0	-3.272737	2.203835	0.464239
23	6	0	-4.274678	-1.463256	-0.210428
24	1	0	-2.161847	-1.859174	-0.382047
25	6	0	-5.264988	-0.512829	0.018891
26	1	0	-5.655527	1.564742	0.440924
27	1	0	-4.548174	-2.496243	-0.400835
28	1	0	-6.311584	-0.797513	0.009029

TMEDA

Total energy= -347.58486021
Sum of electronic and zero-point Energies= -347.359995
Sum of electronic and thermal Energies= -347.349738
Sum of electronic and thermal Enthalpies= -347.348794
Sum of electronic and thermal Free Energies= -347.395093

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.857513	-0.177816	-0.347497
2	6	0	-0.588589	0.486948	-0.072665
3	6	0	0.588590	-0.486950	-0.072666
4	1	0	-0.637844	1.036254	0.888261
5	1	0	-0.411742	1.226088	-0.862961
6	1	0	0.637846	-1.036256	0.888260
7	1	0	0.411743	-1.226089	-0.862962
8	7	0	1.857513	0.177816	-0.347497
9	6	0	-2.185690	-1.141170	0.693598
10	1	0	-2.231352	-0.675236	1.696041
11	1	0	-3.160057	-1.589263	0.481218
12	1	0	-1.445245	-1.944096	0.722385
13	6	0	-2.918268	0.811214	-0.456828
14	1	0	-3.862160	0.315185	-0.699095
15	1	0	-3.060386	1.382754	0.478970
16	1	0	-2.684428	1.518941	-1.256972
17	6	0	2.918270	-0.811213	-0.456827
18	1	0	3.862161	-0.315183	-0.699094
19	1	0	3.060388	-1.382753	0.478971
20	1	0	2.684432	-1.518940	-1.256972
21	6	0	2.185687	1.141170	0.693599
22	1	0	2.231350	0.675236	1.696041
23	1	0	3.160054	1.589265	0.481219
24	1	0	1.445240	1.944095	0.722385

TMEDA·H

Total energy= -348.03620585
Sum of electronic and zero-point Energies= -347.795968
Sum of electronic and thermal Energies= -347.786207
Sum of electronic and thermal Enthalpies= -347.785262
Sum of electronic and thermal Free Energies= -347.830381

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

1	7	0	-1.855006	-0.169718	-0.300689
2	6	0	-0.524981	0.508533	-0.130057
3	6	0	0.630075	-0.487644	-0.071173
4	1	0	-0.609412	1.111333	0.776927
5	1	0	-0.388639	1.167765	-0.989926
6	1	0	0.641953	-1.011463	0.902165
7	1	0	0.488647	-1.244212	-0.853612
8	7	0	1.889636	0.190044	-0.329969
9	6	0	-2.155238	-1.125892	0.809699
10	1	0	-2.099339	-0.578216	1.750631
11	1	0	-3.157007	-1.524745	0.660924
12	1	0	-1.427976	-1.934938	0.796219
13	6	0	-2.950528	0.838377	-0.446460
14	1	0	-3.881030	0.311807	-0.651035
15	1	0	-3.026059	1.393966	0.487771
16	1	0	-2.702979	1.507028	-1.268961
17	6	0	2.955247	-0.793149	-0.484630
18	1	0	3.891201	-0.278121	-0.712117
19	1	0	3.105499	-1.397730	0.426624
20	1	0	2.721163	-1.465987	-1.313548
21	6	0	2.222339	1.122591	0.741955
22	1	0	2.274843	0.626534	1.727385
23	1	0	3.193905	1.575597	0.533473
24	1	0	1.488273	1.930336	0.798169
25	1	0	-1.816928	-0.708129	-1.172489

Re-TS1

Total energy= -1474.72720409
Sum of electronic and zero-point Energies= -1474.196617
Sum of electronic and thermal Energies= -1474.166906
Sum of electronic and thermal Enthalpies= -1474.165962
Sum of electronic and thermal Free Energies= -1474.258982

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.015310	-1.107302	0.613946
2	6	0	-3.217113	-1.787952	0.412958
3	6	0	-4.042365	-2.079394	1.491082
4	6	0	-3.633275	-1.694799	2.770119
5	6	0	-2.417990	-1.036264	2.963651
6	6	0	-1.589284	-0.731363	1.880408

7	6	0	-1.367117	-0.852649	-0.727206
8	6	0	-1.990672	-1.948260	-1.621028
9	6	0	-3.406194	-2.099179	-1.055128
10	1	0	-4.980702	-2.606676	1.346528
11	1	0	-4.261968	-1.922982	3.625182
12	1	0	-2.112889	-0.756770	3.967093
13	1	0	-0.652606	-0.192885	2.028368
14	1	0	-1.649269	0.137063	-1.103061
15	1	0	-1.962503	-1.685888	-2.686515
16	1	0	-4.075913	-1.370925	-1.527591
17	6	0	0.762014	-2.034506	-1.231986
18	6	0	0.012175	-3.161854	-1.875502
19	6	0	0.995691	-0.046020	-0.268263
20	1	0	0.473993	-4.116155	-1.619121
21	1	0	-3.797205	-3.100549	-1.249892
22	7	0	0.091874	-0.944343	-0.738722
23	7	0	2.046382	-1.886497	-1.103234
24	7	0	2.160733	-0.652993	-0.506233
25	8	0	-1.317987	-3.182268	-1.407326
26	1	0	0.042096	-3.038008	-2.967636
27	6	0	3.463774	-0.135967	-0.196928
28	6	0	4.195381	0.467563	-1.224347
29	6	0	3.942792	-0.266664	1.106519
30	6	0	5.460286	0.955554	-0.910892
31	6	0	5.217032	0.239597	1.371699
32	6	0	5.984683	0.850520	0.381201
33	1	0	6.050764	1.430616	-1.690802
34	1	0	5.617755	0.149151	2.378116
35	6	0	3.616608	0.584663	-2.609112
36	1	0	4.304006	1.112848	-3.271482
37	1	0	3.413002	-0.402896	-3.033613
38	1	0	2.667688	1.131078	-2.588897
39	6	0	7.354146	1.399302	0.688289
40	1	0	8.095538	1.017547	-0.018987
41	1	0	7.360654	2.490736	0.609698
42	1	0	7.671614	1.130803	1.697692
43	6	0	3.103792	-0.913473	2.175133
44	1	0	3.695353	-1.082460	3.076665
45	1	0	2.255577	-0.263083	2.419244
46	1	0	2.708496	-1.875354	1.834124
47	6	0	0.836294	1.667721	0.746318
48	8	0	0.841200	1.459346	1.983289
49	1	0	1.752975	2.055806	0.254541
50	6	0	-0.422255	2.108462	0.048256

51	6	0	-1.583004	2.202480	0.701003
52	1	0	-0.356613	2.254799	-1.031003
53	1	0	-1.572184	1.993250	1.768796
54	6	0	-2.895014	2.396751	0.061905
55	6	0	-4.013091	1.748714	0.606271
56	6	0	-3.056803	3.144270	-1.112240
57	6	0	-5.254919	1.832072	-0.016784
58	1	0	-3.894620	1.158419	1.513043
59	6	0	-4.300200	3.233647	-1.729414
60	1	0	-2.203919	3.670963	-1.531257
61	6	0	-5.402821	2.575118	-1.186541
62	1	0	-6.108129	1.316409	0.413228
63	1	0	-4.410749	3.823409	-2.634172
64	1	0	-6.372323	2.647201	-1.668985

Si-TS1

Total energy= -1474.72901318

Sum of electronic and zero-point Energies= -1474.197929

Sum of electronic and thermal Energies= -1474.168476

Sum of electronic and thermal Enthalpies= -1474.167532

Sum of electronic and thermal Free Energies= -1474.258415

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.883818	-0.870100	0.175683
2	6	0	5.244048	-0.911612	-0.139111
3	6	0	6.173970	-1.283323	0.822555
4	6	0	5.721958	-1.603694	2.103731
5	6	0	4.363200	-1.548450	2.413289
6	6	0	3.421690	-1.181279	1.448633
7	6	0	3.105000	-0.479506	-1.065252
8	6	0	4.175047	0.234975	-1.926366
9	6	0	5.469162	-0.504204	-1.577785
10	1	0	7.233840	-1.311080	0.587441
11	1	0	6.436275	-1.889207	2.869646
12	1	0	4.031395	-1.791435	3.417649
13	1	0	2.363849	-1.137299	1.706992
14	1	0	2.732927	-1.365998	-1.590756
15	1	0	3.924698	0.225791	-2.994858
16	1	0	5.587206	-1.380803	-2.224555
17	6	0	1.998547	1.754741	-1.080361
18	6	0	3.202751	2.378239	-1.716240

19	6	0	0.757513	0.070268	-0.323861
20	1	0	3.392522	3.362100	-1.285653
21	1	0	6.335033	0.145923	-1.723175
22	7	0	1.968485	0.406017	-0.835120
23	7	0	0.871632	2.308340	-0.746590
24	7	0	0.127362	1.247450	-0.281942
25	8	0	4.335962	1.573292	-1.474944
26	1	0	3.026114	2.493366	-2.795423
27	6	0	-1.194098	1.477187	0.231539
28	6	0	-2.274309	1.414366	-0.652368
29	6	0	-1.339662	1.713830	1.597270
30	6	0	-3.548983	1.585540	-0.122868
31	6	0	-2.639048	1.879062	2.082875
32	6	0	-3.749058	1.811345	1.241890
33	1	0	-4.410195	1.508653	-0.783523
34	1	0	-2.783620	2.056506	3.145820
35	6	0	-2.057542	1.103633	-2.107455
36	1	0	-1.658634	0.088780	-2.219580
37	1	0	-2.997154	1.162690	-2.659380
38	1	0	-1.337476	1.792298	-2.559337
39	6	0	-5.147809	1.970694	1.778217
40	1	0	-5.157113	1.985681	2.869977
41	1	0	-5.599811	2.901425	1.421418
42	1	0	-5.782975	1.147044	1.436770
43	6	0	-0.139537	1.753193	2.504192
44	1	0	0.302354	0.752784	2.564144
45	1	0	0.619456	2.443259	2.123155
46	1	0	-0.427173	2.074495	3.506997
47	6	0	0.159465	-1.634053	0.633153
48	8	0	0.132553	-1.406078	1.860136
49	1	0	1.017023	-2.190671	0.197836
50	6	0	-1.103074	-1.827589	-0.157378
51	6	0	-2.299868	-1.668955	0.413845
52	1	0	-0.977345	-2.085278	-1.208188
53	1	0	-2.300794	-1.399492	1.469811
54	6	0	-3.615398	-1.751428	-0.236625
55	6	0	-4.763204	-1.523075	0.534521
56	6	0	-3.777241	-2.001386	-1.606790
57	6	0	-6.030472	-1.536128	-0.039494
58	1	0	-4.650240	-1.317478	1.596330
59	6	0	-5.042239	-2.012893	-2.183453
60	1	0	-2.907507	-2.184376	-2.231175
61	6	0	-6.174799	-1.778298	-1.403998
62	1	0	-6.905042	-1.353948	0.577914

63	1	0	-5.146230	-2.204682	-3.246896
64	1	0	-7.160831	-1.786017	-1.857294

Re-M1

Total energy= -1474.73649094
Sum of electronic and zero-point Energies= -1474.203656
Sum of electronic and thermal Energies= -1474.174093
Sum of electronic and thermal Enthalpies= -1474.173149
Sum of electronic and thermal Free Energies= -1474.265527

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.054907	-1.430978	0.471131
2	6	0	-3.175975	-2.204975	0.163701
3	6	0	-4.067097	-2.568293	1.164305
4	6	0	-3.808111	-2.156323	2.473044
5	6	0	-2.674138	-1.400064	2.771540
6	6	0	-1.776878	-1.022375	1.768735
7	6	0	-1.305962	-1.132665	-0.810015
8	6	0	-1.758090	-2.283421	-1.740324
9	6	0	-3.205955	-2.534033	-1.311591
10	1	0	-4.940424	-3.172111	0.936175
11	1	0	-4.490403	-2.439132	3.268755
12	1	0	-2.483860	-1.103242	3.798383
13	1	0	-0.888734	-0.420961	1.981466
14	1	0	-1.617500	-0.168717	-1.223414
15	1	0	-1.639003	-2.036016	-2.803011
16	1	0	-3.880151	-1.864383	-1.857114
17	6	0	0.943880	-2.160934	-1.130212
18	6	0	0.331416	-3.367667	-1.774820
19	6	0	0.994424	-0.140836	-0.275179
20	1	0	0.833950	-4.271517	-1.428018
21	1	0	-3.497158	-3.564065	-1.530158
22	7	0	0.161767	-1.113345	-0.712405
23	7	0	2.207056	-1.902030	-0.968946
24	7	0	2.217073	-0.643029	-0.437952
25	8	0	-1.028565	-3.462785	-1.428249
26	1	0	0.458418	-3.289651	-2.864204
27	6	0	3.464304	-0.003081	-0.116740
28	6	0	4.088750	0.755725	-1.108852
29	6	0	3.988464	-0.180985	1.164308
30	6	0	5.300621	1.358890	-0.782525

31	6	0	5.205127	0.442817	1.440770
32	6	0	5.871927	1.209860	0.484386
33	1	0	5.808431	1.960727	-1.532008
34	1	0	5.639051	0.328165	2.430818
35	6	0	3.453095	0.922568	-2.463200
36	1	0	3.255291	-0.048294	-2.927324
37	1	0	2.495297	1.449204	-2.382660
38	1	0	4.101461	1.498242	-3.124928
39	6	0	7.198643	1.849624	0.801640
40	1	0	8.022868	1.214431	0.461252
41	1	0	7.300139	2.815963	0.302262
42	1	0	7.317502	2.000375	1.876648
43	6	0	3.241603	-0.989727	2.187954
44	1	0	2.264261	-0.520564	2.358101
45	1	0	3.076105	-2.011374	1.830357
46	1	0	3.799855	-1.036351	3.124319
47	6	0	0.701749	1.182625	0.475216
48	8	0	0.656638	0.919820	1.779899
49	1	0	1.557078	1.828891	0.144186
50	6	0	-0.541487	1.808996	-0.147548
51	6	0	-1.622144	2.058663	0.592633
52	1	0	-0.512277	2.033335	-1.216712
53	1	0	-1.560725	1.773114	1.641340
54	6	0	-2.900383	2.602491	0.105813
55	6	0	-4.081398	2.272690	0.784052
56	6	0	-2.987347	3.421690	-1.028267
57	6	0	-5.315581	2.730884	0.332693
58	1	0	-4.023466	1.636020	1.663599
59	6	0	-4.219973	3.882509	-1.478123
60	1	0	-2.078552	3.713200	-1.547035
61	6	0	-5.389440	3.537275	-0.801242
62	1	0	-6.220232	2.459645	0.867863
63	1	0	-4.267956	4.520995	-2.354846
64	1	0	-6.349953	3.900922	-1.151875

Si-M1

Total energy= -1474.73852026
Sum of electronic and zero-point Energies= -1474.205819
Sum of electronic and thermal Energies= -1474.176426
Sum of electronic and thermal Enthalpies= -1474.175482
Sum of electronic and thermal Free Energies= -1474.266111

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	3.876612	-0.893006	0.287735
2	6	0	5.236524	-0.948592	-0.026398
3	6	0	6.167055	-1.265346	0.954000
4	6	0	5.714231	-1.516323	2.250142
5	6	0	4.354557	-1.450908	2.554648
6	6	0	3.409253	-1.140889	1.573289
7	6	0	3.100056	-0.577085	-0.975033
8	6	0	4.167678	0.085739	-1.881098
9	6	0	5.462023	-0.628605	-1.486530
10	1	0	7.226942	-1.303942	0.720753
11	1	0	6.429240	-1.755564	3.031190
12	1	0	4.024128	-1.641140	3.570987
13	1	0	2.344606	-1.081346	1.819389
14	1	0	2.723082	-1.488863	-1.449952
15	1	0	3.916510	0.008218	-2.946516
16	1	0	5.582408	-1.542407	-2.078927
17	6	0	1.985347	1.654738	-1.167946
18	6	0	3.198537	2.234610	-1.828262
19	6	0	0.740798	0.068714	-0.297120
20	1	0	3.377620	3.245506	-1.460468
21	1	0	6.325535	0.014272	-1.672055
22	7	0	1.961884	0.332880	-0.805816
23	7	0	0.848891	2.228642	-0.909233
24	7	0	0.085733	1.228932	-0.369878
25	8	0	4.324963	1.449179	-1.514516
26	1	0	3.034934	2.276065	-2.914497
27	6	0	-1.249436	1.513667	0.086687
28	6	0	-2.305295	1.378978	-0.818906
29	6	0	-1.419309	1.906941	1.412898
30	6	0	-3.590591	1.597524	-0.335950
31	6	0	-2.730037	2.115734	1.848333
32	6	0	-3.821120	1.949601	0.997061
33	1	0	-4.435458	1.464710	-1.008349
34	1	0	-2.897487	2.407953	2.882002
35	6	0	-2.063241	0.959549	-2.242397
36	1	0	-1.285234	1.567976	-2.712751
37	1	0	-1.737770	-0.085858	-2.280608
38	1	0	-2.978887	1.049595	-2.828968
39	6	0	-5.233118	2.131419	1.488375
40	1	0	-5.738770	2.934034	0.943376
41	1	0	-5.809075	1.214052	1.326224
42	1	0	-5.258219	2.371322	2.553111

43	6	0	-0.236696	2.068233	2.325980
44	1	0	0.258124	1.095018	2.423118
45	1	0	0.479169	2.787337	1.914558
46	1	0	-0.555462	2.422561	3.307886
47	6	0	0.288908	-1.228174	0.435308
48	8	0	0.252805	-0.975797	1.738721
49	1	0	1.065749	-1.970654	0.108540
50	6	0	-1.017057	-1.671211	-0.223060
51	6	0	-2.170641	-1.551865	0.434998
52	1	0	-0.958433	-2.042799	-1.246984
53	1	0	-2.092644	-1.156767	1.447733
54	6	0	-3.524982	-1.810915	-0.076148
55	6	0	-4.621902	-1.498050	0.738745
56	6	0	-3.777129	-2.310053	-1.361973
57	6	0	-5.926719	-1.671390	0.287570
58	1	0	-4.438957	-1.096355	1.732628
59	6	0	-5.080018	-2.482963	-1.816009
60	1	0	-2.946332	-2.564623	-2.013892
61	6	0	-6.161239	-2.163085	-0.994862
62	1	0	-6.760782	-1.421437	0.936576
63	1	0	-5.253681	-2.870645	-2.815136
64	1	0	-7.176849	-2.298384	-1.352563

Re-TS2$_D$

Total energy= -1474.66295670
Sum of electronic and zero-point Energies= -1474.134622
Sum of electronic and thermal Energies= -1474.104996
Sum of electronic and thermal Enthalpies= -1474.104052
Sum of electronic and thermal Free Energies= -1474.195976

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.163743	-1.822698	0.311479
2	6	0	-3.133357	-2.822814	0.202120
3	6	0	-4.193194	-2.873616	1.096321
4	6	0	-4.261345	-1.920732	2.114179
5	6	0	-3.274477	-0.943800	2.241030
6	6	0	-2.210306	-0.887374	1.337517
7	6	0	-1.159103	-1.998030	-0.815003
8	6	0	-1.305211	-3.503680	-1.139465
9	6	0	-2.798213	-3.762729	-0.933784
10	1	0	-4.946335	-3.651756	1.016988

11	1	0	-5.080584	-1.951659	2.825212
12	1	0	-3.328832	-0.223043	3.050140
13	1	0	-1.437921	-0.129572	1.444676
14	1	0	-1.432076	-1.402760	-1.695416
15	1	0	-0.931620	-3.755208	-2.140155
16	1	0	-3.353252	-3.509285	-1.843682
17	6	0	1.147733	-2.649257	-0.156410
18	6	0	0.777628	-4.102412	-0.200471
19	6	0	0.883143	-0.488346	-0.541255
20	1	0	1.205569	-4.628766	0.653663
21	1	0	-2.981507	-4.813819	-0.700756
22	7	0	0.225618	-1.689356	-0.490307
23	7	0	2.315325	-2.140128	0.057993
24	7	0	2.148474	-0.788788	-0.167663
25	8	0	-0.621388	-4.259141	-0.149531
26	1	0	1.187807	-4.537052	-1.123301
27	6	0	3.235341	0.091591	0.141180
28	6	0	4.443630	-0.092152	-0.532703
29	6	0	3.063139	1.066666	1.131015
30	6	0	5.512793	0.733940	-0.180847
31	6	0	4.159266	1.865513	1.443373
32	6	0	5.391463	1.712888	0.802701
33	1	0	6.461116	0.610644	-0.698173
34	1	0	4.047429	2.630491	2.208359
35	6	0	4.593907	-1.122697	-1.620920
36	1	0	4.684278	-2.129559	-1.204866
37	1	0	3.722500	-1.122818	-2.282317
38	1	0	5.482909	-0.913194	-2.218527
39	6	0	6.553566	2.600659	1.167525
40	1	0	7.450568	2.328933	0.607366
41	1	0	6.324768	3.649340	0.955242
42	1	0	6.781876	2.527547	2.234736
43	6	0	1.738017	1.268103	1.814849
44	1	0	1.048419	1.770600	1.126741
45	1	0	1.293526	0.315923	2.123110
46	1	0	1.858195	1.892072	2.702506
47	6	0	0.443410	0.767423	-1.095827
48	8	0	1.450498	1.767606	-1.224099
49	1	0	0.939870	0.917217	-2.148540
50	6	0	-0.930195	1.238073	-0.868888
51	6	0	-1.216689	2.551061	-0.842646
52	1	0	-1.723789	0.509328	-0.740788
53	1	0	-0.392478	3.238977	-1.012800
54	6	0	-2.544110	3.140145	-0.625610

55	6	0	-2.717095	4.515571	-0.838422
56	6	0	-3.657137	2.395611	-0.200243
57	6	0	-3.953514	5.125984	-0.651713
58	1	0	-1.863942	5.108347	-1.157799
59	6	0	-4.892991	3.003965	-0.015688
60	1	0	-3.552721	1.333411	0.005881
61	6	0	-5.050236	4.371770	-0.242153
62	1	0	-4.060036	6.192266	-0.826288
63	1	0	-5.738892	2.408526	0.314425
64	1	0	-6.016382	4.843286	-0.094196

Si-TS2$_D$

Total energy= -1474.67065532

Sum of electronic and zero-point Energies= -1474.142694

Sum of electronic and thermal Energies= -1474.112870

Sum of electronic and thermal Enthalpies= -1474.111926

Sum of electronic and thermal Free Energies= -1474.205098

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.170453	-1.207968	-0.015146
2	6	0	4.497581	-1.530903	0.268961
3	6	0	4.797902	-2.645686	1.042756
4	6	0	3.748941	-3.427129	1.527611
5	6	0	2.423994	-3.107593	1.226016
6	6	0	2.120655	-1.995966	0.438728
7	6	0	3.129285	0.021958	-0.895678
8	6	0	4.529975	0.652933	-0.678845
9	6	0	5.433606	-0.550718	-0.399617
10	1	0	5.828712	-2.901044	1.270282
11	1	0	3.966160	-4.295916	2.141113
12	1	0	1.621303	-3.734655	1.600680
13	1	0	1.093511	-1.771585	0.164946
14	1	0	2.967969	-0.263153	-1.936778
15	1	0	4.845302	1.259934	-1.537003
16	1	0	5.819231	-0.960023	-1.339776
17	6	0	2.322328	2.145339	0.157260
18	6	0	3.731287	2.584780	0.395062
19	6	0	0.723846	0.844242	-0.620632
20	1	0	3.793682	3.143427	1.329303
21	1	0	6.285267	-0.252632	0.216292
22	7	0	2.077263	0.987038	-0.541242

23	7	0	1.228356	2.734142	0.520319
24	7	0	0.233376	1.924123	0.030221
25	8	0	4.552155	1.445248	0.502003
26	1	0	4.062197	3.231383	-0.430699
27	6	0	-1.141334	2.268080	0.228476
28	6	0	-1.836868	2.875843	-0.816641
29	6	0	-1.736407	1.935988	1.450388
30	6	0	-3.191827	3.144134	-0.616105
31	6	0	-3.088938	2.225651	1.605416
32	6	0	-3.831990	2.821472	0.580226
33	1	0	-3.757355	3.614654	-1.416306
34	1	0	-3.579140	1.972665	2.542495
35	6	0	-1.144100	3.201005	-2.111999
36	1	0	-0.229589	3.774366	-1.933637
37	1	0	-0.859402	2.279643	-2.631612
38	1	0	-1.797235	3.779893	-2.766324
39	6	0	-5.303387	3.085812	0.767936
40	1	0	-5.499564	3.534495	1.745092
41	1	0	-5.688257	3.754678	-0.004139
42	1	0	-5.870141	2.150628	0.717284
43	6	0	-0.937882	1.241663	2.520190
44	1	0	-0.555352	0.282377	2.151624
45	1	0	-0.073660	1.840981	2.820132
46	1	0	-1.553688	1.049198	3.399689
47	6	0	0.015055	-0.164107	-1.367716
48	8	0	0.840693	-1.068762	-2.117153
49	1	0	0.142416	0.000230	-2.528810
50	6	0	-1.243928	-0.691744	-0.829939
51	6	0	-1.649390	-1.947438	-1.086650
52	1	0	-1.849312	-0.034030	-0.213270
53	1	0	-0.999034	-2.567448	-1.698766
54	6	0	-2.894055	-2.557690	-0.602085
55	6	0	-3.112157	-3.925519	-0.824364
56	6	0	-3.891349	-1.836990	0.077411
57	6	0	-4.270743	-4.555111	-0.379792
58	1	0	-2.353962	-4.497888	-1.352534
59	6	0	-5.048030	-2.464912	0.522166
60	1	0	-3.767009	-0.771831	0.254958
61	6	0	-5.245834	-3.827927	0.297922
62	1	0	-4.412197	-5.615607	-0.564701
63	1	0	-5.804831	-1.886652	1.043787
64	1	0	-6.151902	-4.314104	0.644882

Re-M02$_B$

Total energy= -1822.84236911
Sum of electronic and zero-point Energies= -1822.068447
Sum of electronic and thermal Energies= -1822.028213
Sum of electronic and thermal Enthalpies= -1822.027269
Sum of electronic and thermal Free Energies= -1822.142644

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.907631	-1.360168	0.711945
2	6	0	-4.225415	-1.822684	0.710814
3	6	0	-5.027213	-1.642299	1.829424
4	6	0	-4.484476	-1.010086	2.949474
5	6	0	-3.159204	-0.575394	2.951836
6	6	0	-2.351551	-0.745959	1.825245
7	6	0	-2.303174	-1.630686	-0.647905
8	6	0	-3.164930	-2.801331	-1.177656
9	6	0	-4.550378	-2.497376	-0.602716
10	1	0	-6.052024	-2.000445	1.840006
11	1	0	-5.096140	-0.870110	3.835027
12	1	0	-2.748266	-0.105991	3.839689
13	1	0	-1.315864	-0.414733	1.830558
14	1	0	-2.405404	-0.762719	-1.305005
15	1	0	-3.137379	-2.880241	-2.271432
16	1	0	-5.095553	-1.824186	-1.273163
17	6	0	-0.464288	-3.315693	-0.780131
18	6	0	-1.455510	-4.412312	-1.032316
19	6	0	0.229127	-1.264529	-0.500844
20	1	0	-1.164247	-5.306997	-0.481317
21	1	0	-5.129460	-3.417175	-0.495504
22	7	0	-0.880353	-2.014930	-0.641879
23	7	0	0.833841	-3.403367	-0.723999
24	7	0	1.244988	-2.120051	-0.552383
25	8	0	-2.728619	-4.015584	-0.585136
26	1	0	-1.463236	-4.643363	-2.106662
27	6	0	2.639512	-1.791631	-0.412951
28	6	0	3.347080	-1.414012	-1.556323
29	6	0	3.202881	-1.870233	0.861087
30	6	0	4.689037	-1.079233	-1.385519
31	6	0	4.553990	-1.544726	0.972934
32	6	0	5.304073	-1.134685	-0.131330
33	1	0	5.269371	-0.776485	-2.253461
34	1	0	5.026234	-1.598191	1.950824

35	6	0	2.683837	-1.384368	-2.907811
36	1	0	2.350182	-2.384839	-3.199740
37	1	0	1.802180	-0.733527	-2.912739
38	1	0	3.376101	-1.016591	-3.666287
39	6	0	6.745786	-0.730235	0.028818
40	1	0	7.327002	-0.979430	-0.861440
41	1	0	6.821973	0.351526	0.181550
42	1	0	7.200868	-1.220321	0.891782
43	6	0	2.371422	-2.276102	2.047171
44	1	0	1.539301	-1.574401	2.174066
45	1	0	1.951711	-3.277288	1.910256
46	1	0	2.974536	-2.275967	2.956269
47	6	0	0.416476	0.227230	-0.303288
48	8	0	0.620049	0.428112	1.060245
49	1	0	1.325479	0.479474	-0.868919
50	6	0	-0.726171	1.014625	-0.890698
51	6	0	-1.533094	1.765936	-0.139616
52	1	0	-0.856382	0.937737	-1.970715
53	1	0	-1.355422	1.781564	0.934177
54	6	0	-2.687840	2.537872	-0.625348
55	6	0	-3.734750	2.808564	0.264814
56	6	0	-2.790254	2.992690	-1.946562
57	6	0	-4.865242	3.500302	-0.157746
58	1	0	-3.661547	2.455280	1.290377
59	6	0	-3.918097	3.688816	-2.367237
60	1	0	-1.976397	2.815157	-2.644105
61	6	0	-4.959861	3.942400	-1.475509
62	1	0	-5.671280	3.695641	0.542120
63	1	0	-3.981951	4.042128	-3.391367
64	1	0	-5.837725	4.488545	-1.805056
65	7	0	2.200013	2.283043	2.038644
66	6	0	2.796930	3.439933	1.361519
67	6	0	3.240234	3.136989	-0.063607
68	1	0	3.662738	3.811432	1.933092
69	1	0	2.058640	4.246464	1.354093
70	1	0	3.745196	4.038774	-0.459425
71	1	0	3.986833	2.333796	-0.063251
72	7	0	2.142995	2.726425	-0.933305
73	6	0	3.228456	1.333520	2.467092
74	1	0	3.922518	1.788497	3.190085
75	1	0	2.749258	0.467853	2.932774
76	1	0	3.794558	0.978522	1.603529
77	6	0	1.393265	2.703239	3.185201
78	1	0	0.938149	1.822219	3.645384

79	1	0	1.996760	3.224905	3.943117
80	1	0	0.596997	3.370561	2.845863
81	6	0	2.668824	2.298490	-2.222571
82	1	0	1.847247	1.945932	-2.855214
83	1	0	3.189453	3.110130	-2.760278
84	1	0	3.375540	1.473989	-2.077946
85	6	0	1.175440	3.800827	-1.122472
86	1	0	1.655579	4.736319	-1.461400
87	1	0	0.441436	3.497221	-1.872767
88	1	0	0.626761	3.999001	-0.198298
89	1	0	1.210120	1.246130	1.217116

Si-M02$_B$

Total energy= -1822.84191351

Sum of electronic and zero-point Energies= -1822.066694

Sum of electronic and thermal Energies= -1822.026113

Sum of electronic and thermal Enthalpies= -1822.025169

Sum of electronic and thermal Free Energies= -1822.139335

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.331483	-0.480299	-1.042795
2	6	0	4.718484	-0.547797	-0.874419
3	6	0	5.566619	-0.254001	-1.933232
4	6	0	5.008350	0.072148	-3.171019
5	6	0	3.625455	0.086423	-3.344878
6	6	0	2.768411	-0.186922	-2.276688
7	6	0	2.683298	-0.767258	0.300792
8	6	0	3.753846	-1.648507	0.983970
9	6	0	5.065598	-1.010089	0.524127
10	1	0	6.644013	-0.302373	-1.808103
11	1	0	5.658139	0.294830	-4.011150
12	1	0	3.207695	0.315348	-4.319854
13	1	0	1.692456	-0.152813	-2.405467
14	1	0	2.504182	0.156739	0.866751
15	1	0	3.629493	-1.712343	2.072277
16	1	0	5.333248	-0.172885	1.179484
17	6	0	1.324089	-2.861068	0.362925
18	6	0	2.545538	-3.678100	0.669227
19	6	0	0.162469	-1.017453	0.185501
20	1	0	2.565082	-4.578383	0.054453
21	1	0	5.880176	-1.736931	0.553127

22	7	0	1.415387	-1.500007	0.272504
23	7	0	0.083334	-3.248798	0.291202
24	7	0	-0.627404	-2.087933	0.172769
25	8	0	3.714793	-2.943807	0.396022
26	1	0	2.497127	-3.974440	1.726477
27	6	0	-2.051227	-2.140688	-0.035827
28	6	0	-2.862126	-2.549441	1.023424
29	6	0	-2.539345	-1.783900	-1.296712
30	6	0	-4.238383	-2.573968	0.792411
31	6	0	-3.919836	-1.817411	-1.469089
32	6	0	-4.781337	-2.203301	-0.438318
33	1	0	-4.898622	-2.882070	1.598685
34	1	0	-4.335266	-1.532824	-2.432472
35	6	0	-2.279789	-2.946302	2.353578
36	1	0	-1.759592	-3.905383	2.278884
37	1	0	-1.553223	-2.209506	2.710791
38	1	0	-3.068242	-3.039998	3.101191
39	6	0	-6.270492	-2.175725	-0.653925
40	1	0	-6.620223	-1.138957	-0.704183
41	1	0	-6.539554	-2.658229	-1.596964
42	1	0	-6.801269	-2.676437	0.157752
43	6	0	-1.613428	-1.369397	-2.409252
44	1	0	-1.176013	-0.382699	-2.215587
45	1	0	-0.791558	-2.083025	-2.526874
46	1	0	-2.157196	-1.316401	-3.353244
47	6	0	-0.144334	0.470014	0.224948
48	8	0	0.460067	1.064559	-0.881300
49	1	0	0.366937	0.801815	1.147304
50	6	0	-1.610230	0.780043	0.360601
51	6	0	-2.244657	1.610169	-0.469341
52	1	0	-2.118569	0.322940	1.207267
53	1	0	-1.665397	2.070325	-1.268036
54	6	0	-3.673035	1.960050	-0.399438
55	6	0	-4.138636	3.077601	-1.101804
56	6	0	-4.593440	1.198615	0.335192
57	6	0	-5.481184	3.442738	-1.054517
58	1	0	-3.437305	3.667170	-1.686216
59	6	0	-5.933534	1.564012	0.385089
60	1	0	-4.263181	0.301722	0.852347
61	6	0	-6.382748	2.688967	-0.307951
62	1	0	-5.821972	4.315129	-1.602826
63	1	0	-6.632161	0.965367	0.961888
64	1	0	-7.430321	2.969583	-0.271511
65	7	0	2.163064	2.976217	-0.188407

66	6	0	2.940243	3.166408	1.047370
67	6	0	2.137363	3.073601	2.339142
68	1	0	3.430964	4.153670	1.016624
69	1	0	3.739855	2.415967	1.049044
70	1	0	2.751315	3.489375	3.156092
71	1	0	1.253378	3.713234	2.271628
72	7	0	1.704273	1.712141	2.659105
73	6	0	1.114397	3.994631	-0.333888
74	1	0	1.517271	5.011312	-0.216012
75	1	0	0.671178	3.902810	-1.327718
76	1	0	0.320322	3.833340	0.398808
77	6	0	3.076369	3.046721	-1.336550
78	1	0	2.522812	2.835987	-2.255073
79	1	0	3.540068	4.041287	-1.418259
80	1	0	3.861636	2.293211	-1.229979
81	6	0	0.507824	1.724480	3.496680
82	1	0	0.198193	0.695108	3.704125
83	1	0	0.674020	2.233133	4.460294
84	1	0	-0.307131	2.231709	2.971390
85	6	0	2.765082	0.971273	3.332034
86	1	0	3.015336	1.407666	4.313408
87	1	0	2.449102	-0.065331	3.486801
88	1	0	3.675853	0.967146	2.725096
89	1	0	1.184519	1.690125	-0.544655

Re-TS2$_B$

Total energy= -1822.80877566

Sum of electronic and zero-point Energies= -1822.036993

Sum of electronic and thermal Energies= -1821.996986

Sum of electronic and thermal Enthalpies= -1821.996041

Sum of electronic and thermal Free Energies= -1822.108847

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.850793	-1.645418	0.715957
2	6	0	-4.093052	-2.282917	0.725363
3	6	0	-4.870302	-2.285019	1.876083
4	6	0	-4.381093	-1.646915	3.016568
5	6	0	-3.137940	-1.015314	3.000839
6	6	0	-2.356323	-1.002187	1.843040
7	6	0	-2.252554	-1.770478	-0.670758
8	6	0	-2.995891	-2.999305	-1.257026

9	6	0	-4.384721	-2.901629	-0.622003
10	1	0	-5.834084	-2.784926	1.892292
11	1	0	-4.971519	-1.648031	3.927214
12	1	0	-2.771249	-0.529017	3.899078
13	1	0	-1.391380	-0.500008	1.838182
14	1	0	-2.487277	-0.891311	-1.274911
15	1	0	-3.000343	-2.993727	-2.354272
16	1	0	-5.030016	-2.252936	-1.224259
17	6	0	-0.254457	-3.238966	-0.830967
18	6	0	-1.105551	-4.394647	-1.252422
19	6	0	0.213056	-1.136674	-0.347915
20	1	0	-0.714801	-5.316605	-0.821380
21	1	0	-4.849222	-3.888536	-0.564943
22	7	0	-0.797115	-1.984764	-0.698687
23	7	0	1.015221	-3.237313	-0.570171
24	7	0	1.297097	-1.933580	-0.273852
25	8	0	-2.417768	-4.203899	-0.779128
26	1	0	-1.089401	-4.478391	-2.348704
27	6	0	2.670270	-1.542874	-0.134901
28	6	0	3.424318	-1.445227	-1.310462
29	6	0	3.223944	-1.391996	1.138635
30	6	0	4.764204	-1.079518	-1.188900
31	6	0	4.571782	-1.031322	1.206144
32	6	0	5.348072	-0.850385	0.059743
33	1	0	5.368788	-0.988302	-2.088114
34	1	0	5.028806	-0.904068	2.184602
35	6	0	2.820547	-1.786958	-2.647899
36	1	0	2.709411	-2.871243	-2.743320
37	1	0	1.825726	-1.347686	-2.771380
38	1	0	3.456904	-1.436177	-3.462565
39	6	0	6.784647	-0.411868	0.165721
40	1	0	7.384869	-0.825379	-0.647549
41	1	0	6.854618	0.679434	0.106795
42	1	0	7.223225	-0.721471	1.116454
43	6	0	2.420788	-1.670436	2.379351
44	1	0	1.525262	-1.046239	2.403797
45	1	0	2.105425	-2.718690	2.396203
46	1	0	3.018613	-1.477505	3.272159
47	6	0	0.165280	0.302336	-0.108504
48	8	0	0.459041	0.573928	1.246981
49	1	0	1.239204	1.155640	-0.830507
50	6	0	-1.031199	0.983680	-0.628290
51	6	0	-1.738005	1.907679	0.046658
52	1	0	-1.256003	0.787003	-1.678799

53	1	0	-1.493778	2.063518	1.096451
54	6	0	-2.822907	2.730202	-0.501634
55	6	0	-3.675606	3.410887	0.380275
56	6	0	-3.047793	2.878485	-1.880026
57	6	0	-4.724389	4.192681	-0.091977
58	1	0	-3.511983	3.313353	1.450334
59	6	0	-4.097381	3.657685	-2.352692
60	1	0	-2.387879	2.391403	-2.592707
61	6	0	-4.943159	4.318067	-1.462146
62	1	0	-5.372501	4.705735	0.611768
63	1	0	-4.250633	3.759013	-3.422753
64	1	0	-5.758618	4.930262	-1.833021
65	7	0	2.063058	2.708339	1.730673
66	6	0	2.999689	3.197618	0.713863
67	6	0	3.170333	2.242174	-0.458252
68	1	0	3.995927	3.366797	1.148648
69	1	0	2.657283	4.168904	0.349711
70	1	0	3.956413	2.639153	-1.110971
71	1	0	3.483271	1.246456	-0.121042
72	7	0	1.944023	2.040859	-1.291559
73	6	0	2.760091	1.883740	2.722787
74	1	0	3.475107	2.479995	3.308774
75	1	0	2.030120	1.433728	3.400472
76	1	0	3.299842	1.079039	2.218496
77	6	0	1.358300	3.805301	2.397113
78	1	0	0.650353	3.389790	3.117965
79	1	0	2.050570	4.474319	2.929502
80	1	0	0.798514	4.390650	1.663213
81	6	0	2.330435	1.556630	-2.634323
82	1	0	1.449732	1.140065	-3.128823
83	1	0	2.729143	2.385054	-3.226060
84	1	0	3.094521	0.787838	-2.527330
85	6	0	1.097441	3.247811	-1.423283
86	1	0	1.687922	4.080062	-1.818335
87	1	0	0.280539	3.021127	-2.109491
88	1	0	0.671332	3.502675	-0.453541
89	1	0	0.972591	1.424689	1.302467

Si-TS2$_B$

Total energy= -1822.81674893
Sum of electronic and zero-point Energies= -1822.045447
Sum of electronic and thermal Energies= -1822.005180
Sum of electronic and thermal Enthalpies= -1822.004236

Sum of electronic and thermal Free Energies= -1822.117947

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.506577	-0.254047	1.084330
2	6	0	-4.891692	-0.232038	0.896873
3	6	0	-5.739322	0.072206	1.953623
4	6	0	-5.182839	0.335447	3.206008
5	6	0	-3.801698	0.285662	3.393850
6	6	0	-2.945938	-0.007688	2.330462
7	6	0	-2.848369	-0.535579	-0.255190
8	6	0	-3.971974	-1.273331	-1.020019
9	6	0	-5.245031	-0.584265	-0.530728
10	1	0	-6.815603	0.089177	1.811510
11	1	0	-5.831297	0.567404	4.044769
12	1	0	-3.385450	0.474949	4.377965
13	1	0	-1.871124	-0.026561	2.467108
14	1	0	-2.591839	0.408764	-0.755749
15	1	0	-3.829863	-1.252208	-2.109036
16	1	0	-5.446510	0.310865	-1.131748
17	6	0	-1.646670	-2.702045	-0.551849
18	6	0	-2.924356	-3.394598	-0.925434
19	6	0	-0.342579	-0.969279	-0.150036
20	1	0	-3.002776	-4.353426	-0.411403
21	1	0	-6.104995	-1.251768	-0.618691
22	7	0	-1.644758	-1.360192	-0.262273
23	7	0	-0.446919	-3.189762	-0.572620
24	7	0	0.360014	-2.109515	-0.293150
25	8	0	-4.035226	-2.613763	-0.554139
26	1	0	-2.913252	-3.576280	-2.009511
27	6	0	1.743738	-2.312236	0.018592
28	6	0	2.609149	-2.713223	-1.000196
29	6	0	2.166230	-2.068414	1.331617
30	6	0	3.961176	-2.845488	-0.678712
31	6	0	3.526159	-2.205977	1.597010
32	6	0	4.436620	-2.582935	0.606241
33	1	0	4.657448	-3.151100	-1.455532
34	1	0	3.886346	-2.012327	2.604470
35	6	0	2.101396	-2.991532	-2.389478
36	1	0	1.588820	-3.957258	-2.429039
37	1	0	1.376990	-2.235470	-2.707853
38	1	0	2.926162	-3.008786	-3.103309
39	6	0	5.906179	-2.668238	0.923780

40	1	0	6.320245	-1.664449	1.066098
41	1	0	6.077049	-3.224904	1.848796
42	1	0	6.460642	-3.154025	0.118667
43	6	0	1.201907	-1.652860	2.412042
44	1	0	0.952077	-0.588762	2.324689
45	1	0	0.269945	-2.224194	2.358267
46	1	0	1.647040	-1.814725	3.394945
47	6	0	0.101037	0.405393	-0.056087
48	8	0	-0.650132	1.123543	0.886764
49	1	0	-0.201888	1.007540	-1.403367
50	6	0	1.548587	0.664272	-0.015611
51	6	0	2.118676	1.651622	0.694387
52	1	0	2.163398	0.052565	-0.672113
53	1	0	1.479245	2.272451	1.318365
54	6	0	3.555439	1.963330	0.697923
55	6	0	3.994242	3.166410	1.268320
56	6	0	4.522615	1.093716	0.165589
57	6	0	5.344811	3.501767	1.293340
58	1	0	3.260736	3.846202	1.694194
59	6	0	5.870771	1.431133	0.185598
60	1	0	4.221575	0.135289	-0.250208
61	6	0	6.290429	2.637055	0.748449
62	1	0	5.658779	4.440430	1.739373
63	1	0	6.600666	0.745516	-0.234683
64	1	0	7.344320	2.894775	0.766950
65	7	0	-2.036663	3.047327	-0.404397
66	6	0	-2.044528	3.239529	-1.857209
67	6	0	-0.714692	2.950086	-2.539817
68	1	0	-2.310816	4.280409	-2.103305
69	1	0	-2.836272	2.615192	-2.282336
70	1	0	-0.776455	3.285997	-3.582115
71	1	0	0.092486	3.511848	-2.063881
72	7	0	-0.293643	1.523428	-2.545941
73	6	0	-1.243347	4.083920	0.269569
74	1	0	-1.613599	5.091725	0.031793
75	1	0	-1.303450	3.929817	1.349146
76	1	0	-0.192041	4.009108	-0.017014
77	6	0	-3.407970	3.059129	0.116926
78	1	0	-3.393507	2.825558	1.184977
79	1	0	-3.891273	4.035952	-0.032094
80	1	0	-4.003629	2.295019	-0.390868
81	6	0	1.078974	1.416526	-3.088432
82	1	0	1.392513	0.371768	-3.050518
83	1	0	1.102236	1.765466	-4.124811

84	1	0	1.752752	2.015115	-2.474562
85	6	0	-1.204434	0.653077	-3.314854
86	1	0	-1.210766	0.945135	-4.369052
87	1	0	-0.856119	-0.379282	-3.226516
88	1	0	-2.217689	0.719663	-2.919291
89	1	0	-1.211319	1.775571	0.388937

Re-M03$_B$

Total energy= -1822.82053809
Sum of electronic and zero-point Energies= -1822.043378
Sum of electronic and thermal Energies= -1822.002537
Sum of electronic and thermal Enthalpies= -1822.001593
Sum of electronic and thermal Free Energies= -1822.117385

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.628384	-0.636661	0.555247
2	6	0	-5.011896	-0.721124	0.373659
3	6	0	-5.877232	-0.524926	1.441679
4	6	0	-5.341748	-0.249648	2.700205
5	6	0	-3.961515	-0.175226	2.881056
6	6	0	-3.088802	-0.363476	1.807833
7	6	0	-2.948781	-0.859641	-0.786800
8	6	0	-4.030605	-1.623548	-1.595140
9	6	0	-5.344020	-1.046952	-1.063894
10	1	0	-6.951667	-0.598894	1.302259
11	1	0	-6.004838	-0.101966	3.546623
12	1	0	-3.557755	0.029756	3.867205
13	1	0	-2.016215	-0.304235	1.960261
14	1	0	-2.785070	0.093766	-1.296721
15	1	0	-3.892031	-1.497612	-2.677054
16	1	0	-5.613074	-0.144125	-1.623336
17	6	0	-1.663772	-2.971806	-1.005358
18	6	0	-2.826420	-3.630871	-1.674633
19	6	0	-0.492907	-1.286356	-0.151082
20	1	0	-2.873141	-4.680442	-1.384620
21	1	0	-6.153588	-1.771551	-1.176815
22	7	0	-1.696033	-1.612460	-0.763213
23	7	0	-0.568530	-3.523845	-0.616888
24	7	0	0.168974	-2.490043	-0.056360
25	8	0	-4.021197	-3.001968	-1.265348
26	1	0	-2.708844	-3.565574	-2.766388

27	6	0	1.590101	-2.653405	0.018315
28	6	0	2.327714	-2.567559	-1.166380
29	6	0	2.183284	-2.952027	1.248981
30	6	0	3.713731	-2.732655	-1.088140
31	6	0	3.564347	-3.131783	1.276151
32	6	0	4.346228	-3.009555	0.123557
33	1	0	4.304583	-2.667569	-1.999079
34	1	0	4.046134	-3.365785	2.223063
35	6	0	1.641797	-2.385787	-2.496920
36	1	0	1.204406	-3.333331	-2.826936
37	1	0	0.824726	-1.659206	-2.443856
38	1	0	2.352036	-2.056308	-3.258880
39	6	0	5.843724	-3.157239	0.202180
40	1	0	6.283066	-3.288098	-0.788722
41	1	0	6.294583	-2.268032	0.655792
42	1	0	6.122648	-4.014571	0.819960
43	6	0	1.344771	-3.067343	2.491092
44	1	0	0.887340	-2.100298	2.718169
45	1	0	0.537034	-3.790953	2.349521
46	1	0	1.952533	-3.383812	3.340613
47	6	0	-0.049725	-0.066982	0.332062
48	8	0	0.920193	-0.122783	1.317813
49	1	0	1.691893	2.035343	-0.609080
50	6	0	-0.578994	1.200714	-0.031681
51	6	0	-0.218456	2.379592	0.557207
52	1	0	-1.247834	1.227301	-0.887478
53	1	0	0.439317	2.339243	1.423905
54	6	0	-0.649831	3.714950	0.145467
55	6	0	-0.035699	4.839862	0.723974
56	6	0	-1.632389	3.943154	-0.836212
57	6	0	-0.367795	6.130779	0.327303
58	1	0	0.716860	4.691472	1.495272
59	6	0	-1.960311	5.233240	-1.234507
60	1	0	-2.154072	3.104834	-1.289089
61	6	0	-1.328301	6.336954	-0.660809
62	1	0	0.126010	6.978411	0.792352
63	1	0	-2.721758	5.379486	-1.994414
64	1	0	-1.588592	7.342481	-0.973534
65	7	0	3.202969	1.514330	1.273445
66	6	0	3.808278	2.558875	0.446086
67	6	0	3.713943	2.228199	-1.032708
68	1	0	4.866927	2.720189	0.701515
69	1	0	3.281583	3.500464	0.640799
70	1	0	4.212563	2.983887	-1.641274

71	1	0	4.163854	1.260156	-1.256924
72	7	0	2.269351	2.172027	-1.458501
73	6	0	4.031200	0.302588	1.322536
74	1	0	5.041181	0.516937	1.703286
75	1	0	3.549899	-0.426729	1.978048
76	1	0	4.109862	-0.162801	0.336030
77	6	0	2.983792	2.010233	2.636560
78	1	0	2.453969	1.247989	3.212575
79	1	0	3.931899	2.244980	3.142097
80	1	0	2.369859	2.913714	2.607748
81	6	0	1.991471	1.010157	-2.348231
82	1	0	0.927822	1.000557	-2.586784
83	1	0	2.586682	1.116464	-3.256083
84	1	0	2.264285	0.099322	-1.813159
85	6	0	1.811743	3.452965	-2.072987
86	1	0	2.350930	3.594147	-3.009800
87	1	0	0.737767	3.389226	-2.248327
88	1	0	2.016331	4.269776	-1.380496
89	1	0	1.639558	0.513794	1.108650

Si-M03$_B$

Total energy= -1822.82897667

Sum of electronic and zero-point Energies= -1822.052775

Sum of electronic and thermal Energies= -1822.012555

Sum of electronic and thermal Enthalpies= -1822.011611

Sum of electronic and thermal Free Energies= -1822.125803

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.838824	0.188284	-0.840404
2	6	0	5.203448	0.459127	-0.723489
3	6	0	5.988423	0.616729	-1.858214
4	6	0	5.389309	0.485399	-3.111804
5	6	0	4.028138	0.200188	-3.223600
6	6	0	3.236198	0.052393	-2.083876
7	6	0	3.233777	0.088003	0.546522
8	6	0	4.468522	-0.240464	1.421346
9	6	0	5.606452	0.516414	0.732629
10	1	0	7.051510	0.821374	-1.772830
11	1	0	5.990135	0.594488	-4.009190
12	1	0	3.580896	0.089536	-4.206147
13	1	0	2.175151	-0.161643	-2.166490

14	1	0	2.807938	1.047651	0.853026
15	1	0	4.317953	0.032341	2.474409
16	1	0	5.646917	1.549700	1.095460
17	6	0	2.464159	-2.168584	1.273056
18	6	0	3.797396	-2.442774	1.899019
19	6	0	0.879044	-0.927028	0.332148
20	1	0	4.081087	-3.482903	1.735055
21	1	0	6.567678	0.042448	0.943953
22	7	0	2.208207	-0.938232	0.714274
23	7	0	1.436246	-2.946408	1.255583
24	7	0	0.444870	-2.192349	0.651374
25	8	0	4.782328	-1.621647	1.316949
26	1	0	3.729048	-2.262312	2.982003
27	6	0	-0.784926	-2.810794	0.282587
28	6	0	-1.714486	-3.098947	1.287417
29	6	0	-1.038144	-3.072914	-1.070245
30	6	0	-2.945152	-3.632454	0.905223
31	6	0	-2.286017	-3.595597	-1.404658
32	6	0	-3.253533	-3.871108	-0.435609
33	1	0	-3.683185	-3.855882	1.671763
34	1	0	-2.507032	-3.797758	-2.450121
35	6	0	-1.389988	-2.822819	2.730527
36	1	0	-0.614844	-3.504567	3.092412
37	1	0	-0.999754	-1.807817	2.856632
38	1	0	-2.276025	-2.939503	3.356553
39	6	0	-4.610123	-4.388206	-0.838477
40	1	0	-5.236876	-3.569592	-1.208330
41	1	0	-4.528195	-5.124995	-1.641305
42	1	0	-5.125789	-4.850699	0.005501
43	6	0	-0.018147	-2.762209	-2.131486
44	1	0	-0.054120	-1.699919	-2.399563
45	1	0	0.996524	-2.980189	-1.786165
46	1	0	-0.214361	-3.346408	-3.032153
47	6	0	0.166206	0.127048	-0.223519
48	8	0	0.889998	1.233015	-0.646229
49	1	0	-1.710166	2.063219	0.774179
50	6	0	-1.240366	0.121175	-0.405974
51	6	0	-1.957018	1.091299	-1.050946
52	1	0	-1.787435	-0.685670	0.072333
53	1	0	-1.420925	1.887219	-1.564620
54	6	0	-3.419557	1.117395	-1.138365
55	6	0	-4.064050	2.285161	-1.582341
56	6	0	-4.229916	0.028885	-0.761209
57	6	0	-5.451726	2.378910	-1.616173

58	1	0	-3.460158	3.131632	-1.901896
59	6	0	-5.615568	0.126312	-0.792097
60	1	0	-3.775249	-0.910267	-0.452961
61	6	0	-6.238294	1.302368	-1.211946
62	1	0	-5.918901	3.296671	-1.960090
63	1	0	-6.215973	-0.728056	-0.493926
64	1	0	-7.320517	1.372829	-1.235047
65	7	0	0.276589	3.809964	0.301434
66	6	0	-0.364270	4.412500	1.471702
67	6	0	-1.786903	3.922875	1.695058
68	1	0	-0.405208	5.510096	1.388703
69	1	0	0.243388	4.187618	2.352343
70	1	0	-2.164200	4.300710	2.648812
71	1	0	-2.465454	4.251892	0.904473
72	7	0	-1.888552	2.427197	1.734256
73	6	0	-0.266043	4.354020	-0.947460
74	1	0	-0.073135	5.433261	-1.035077
75	1	0	0.199910	3.839561	-1.791741
76	1	0	-1.344163	4.187495	-1.002692
77	6	0	1.724970	4.047149	0.349292
78	1	0	2.200265	3.550223	-0.500314
79	1	0	1.964412	5.119829	0.312844
80	1	0	2.133695	3.627796	1.272563
81	6	0	-3.275475	1.994680	2.075636
82	1	0	-3.338593	0.914166	1.942241
83	1	0	-3.481931	2.266376	3.111184
84	1	0	-3.974014	2.485638	1.397388
85	6	0	-0.887866	1.782378	2.630854
86	1	0	-0.968462	2.221045	3.626387
87	1	0	-1.106844	0.716012	2.666959
88	1	0	0.107891	1.934611	2.215306
89	1	0	0.533211	2.031820	-0.192768

Si-M02^{T}

Total energy= -1822.34201477
Sum of electronic and zero-point Energies= -1821.582972
Sum of electronic and thermal Energies= -1821.541651
Sum of electronic and thermal Enthalpies= -1821.540707
Sum of electronic and thermal Free Energies= -1821.657488

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

1	6	0	3.539285	0.471568	0.522740
2	6	0	4.902334	0.621256	0.260759
3	6	0	5.844380	0.100763	1.138590
4	6	0	5.398094	-0.564282	2.281986
5	6	0	4.033042	-0.703280	2.537185
6	6	0	3.079266	-0.188287	1.654646
7	6	0	2.756032	1.032292	-0.645416
8	6	0	3.763363	2.012531	-1.291214
9	6	0	5.117545	1.344376	-1.048938
10	1	0	6.906809	0.213435	0.942952
11	1	0	6.120865	-0.972608	2.981681
12	1	0	3.706586	-1.222336	3.433316
13	1	0	2.005465	-0.305418	1.828662
14	1	0	2.502687	0.211334	-1.328110
15	1	0	3.539864	2.212550	-2.346895
16	1	0	5.338169	0.638126	-1.858753
17	6	0	1.413434	3.118539	-0.320516
18	6	0	2.590768	3.970791	-0.687017
19	6	0	0.285076	1.253930	-0.073087
20	1	0	2.653765	4.832342	-0.020941
21	1	0	5.915893	2.089841	-1.022193
22	7	0	1.514944	1.752014	-0.325047
23	7	0	0.196352	3.499448	-0.066672
24	7	0	-0.489538	2.327596	0.088405
25	8	0	3.779668	3.230385	-0.555672
26	1	0	2.459085	4.331349	-1.717465
27	6	0	-1.911276	2.322798	0.300871
28	6	0	-2.730047	2.423515	-0.827254
29	6	0	-2.396229	2.121419	1.590562
30	6	0	-4.096898	2.250687	-0.638428
31	6	0	-3.773661	1.941078	1.724166
32	6	0	-4.627775	1.966035	0.622145
33	1	0	-4.758666	2.291296	-1.500343
34	1	0	-4.183160	1.749587	2.713106
35	6	0	-2.144429	2.667122	-2.192627
36	1	0	-1.611588	3.621912	-2.230103
37	1	0	-1.425033	1.884797	-2.459853
38	1	0	-2.929897	2.678732	-2.950083
39	6	0	-6.085337	1.621966	0.764519
40	1	0	-6.706057	2.225715	0.097791
41	1	0	-6.234343	0.568727	0.495847
42	1	0	-6.433424	1.762829	1.790091
43	6	0	-1.458659	2.035902	2.761873
44	1	0	-0.829476	1.144726	2.640688

45	1	0	-0.807355	2.914731	2.806013
46	1	0	-2.017682	1.971369	3.697152
47	6	0	-0.067197	-0.231529	0.174556
48	8	0	0.032805	-0.466381	1.489195
49	1	0	0.691365	-0.763675	-0.455940
50	6	0	-1.417393	-0.537583	-0.467267
51	6	0	-2.421572	-1.024367	0.263170
52	1	0	-1.513284	-0.363217	-1.540585
53	1	0	-2.205880	-1.186021	1.318339
54	6	0	-3.781156	-1.346192	-0.199818
55	6	0	-4.640867	-2.056847	0.647711
56	6	0	-4.271273	-0.949892	-1.453606
57	6	0	-5.937094	-2.381608	0.253991
58	1	0	-4.279193	-2.363818	1.625770
59	6	0	-5.564976	-1.268408	-1.848183
60	1	0	-3.637780	-0.365914	-2.115592
61	6	0	-6.404451	-1.990671	-0.997969
62	1	0	-6.581503	-2.939624	0.926383
63	1	0	-5.924637	-0.947347	-2.821108
64	1	0	-7.414697	-2.238546	-1.307584
65	7	0	2.870574	-2.157217	-1.556950
66	6	0	1.852322	-3.170250	-1.289279
67	6	0	1.516710	-3.313530	0.194519
68	1	0	2.166448	-4.143598	-1.715317
69	1	0	0.930209	-2.872112	-1.802400
70	1	0	2.317672	-3.864706	0.726595
71	1	0	1.452177	-2.315020	0.642199
72	7	0	0.225412	-3.966484	0.380869
73	6	0	4.138242	-2.503419	-0.926229
74	1	0	4.482165	-3.513241	-1.218027
75	1	0	4.903197	-1.781642	-1.227063
76	1	0	4.049538	-2.456869	0.162471
77	6	0	3.050765	-2.013358	-2.993745
78	1	0	3.782814	-1.225097	-3.197747
79	1	0	3.407007	-2.943962	-3.471826
80	1	0	2.101126	-1.732428	-3.458948
81	6	0	-0.246354	-3.765684	1.742884
82	1	0	-1.247400	-4.197286	1.849598
83	1	0	0.412237	-4.250064	2.490003
84	1	0	-0.290543	-2.690075	1.939341
85	6	0	0.289980	-5.382928	0.065288
86	1	0	1.018063	-5.922155	0.701748
87	1	0	-0.693479	-5.837931	0.214781
88	1	0	0.573913	-5.534931	-0.979483

Si-TS2^{T}

Total energy= -1822.30670780
Sum of electronic and zero-point Energies= -1821.552109
Sum of electronic and thermal Energies= -1821.511431
Sum of electronic and thermal Enthalpies= -1821.510487
Sum of electronic and thermal Free Energies= -1821.625200

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.661489	-0.581964	1.285145
2	6	0	5.022946	-0.848081	1.433980
3	6	0	5.604245	-0.847370	2.696146
4	6	0	4.800011	-0.576203	3.803872
5	6	0	3.433002	-0.339043	3.650080
6	6	0	2.844792	-0.353629	2.384350
7	6	0	3.285476	-0.665735	-0.180534
8	6	0	4.657811	-0.525045	-0.890935
9	6	0	5.651063	-1.147672	0.092416
10	1	0	6.664374	-1.049159	2.819412
11	1	0	5.240068	-0.559535	4.796268
12	1	0	2.819582	-0.151892	4.526059
13	1	0	1.772349	-0.258517	2.242403
14	1	0	2.823541	-1.633048	-0.387559
15	1	0	4.659350	-0.989721	-1.886683
16	1	0	5.722402	-2.228652	-0.071801
17	6	0	2.781663	1.493780	-1.336481
18	6	0	4.180784	1.567488	-1.857060
19	6	0	1.020686	0.536637	-0.388054
20	1	0	4.518416	2.604144	-1.879928
21	1	0	6.645243	-0.715803	-0.044701
22	7	0	2.367745	0.376860	-0.651464
23	7	0	1.844455	2.367670	-1.485313
24	7	0	0.744548	1.796362	-0.859247
25	8	0	5.032067	0.843105	-1.001299
26	1	0	4.215343	1.160321	-2.878746
27	6	0	-0.355804	2.636381	-0.512287
28	6	0	-1.136878	3.177741	-1.538479
29	6	0	-0.628318	2.888356	0.841360
30	6	0	-2.239669	3.956153	-1.182567
31	6	0	-1.746633	3.661793	1.144942
32	6	0	-2.570420	4.194325	0.150849

33	1	0	-2.859956	4.376538	-1.970634
34	1	0	-1.978075	3.857646	2.189560
35	6	0	-0.798071	2.932328	-2.983882
36	1	0	0.061908	3.535171	-3.289926
37	1	0	-0.524179	1.887376	-3.149684
38	1	0	-1.644579	3.182538	-3.625872
39	6	0	-3.799563	4.983990	0.520171
40	1	0	-4.161121	5.574827	-0.324079
41	1	0	-4.607387	4.313172	0.831606
42	1	0	-3.597938	5.659899	1.355120
43	6	0	0.232607	2.327158	1.941128
44	1	0	-0.035512	1.283404	2.141378
45	1	0	1.293858	2.352911	1.675075
46	1	0	0.091231	2.898632	2.860584
47	6	0	0.154284	-0.523686	0.044780
48	8	0	0.674757	-1.550492	0.707748
49	1	0	0.032001	-0.982622	-1.246880
50	6	0	-1.272639	-0.162954	0.237479
51	6	0	-2.069897	-0.840364	1.080030
52	1	0	-1.690823	0.611076	-0.402704
53	1	0	-1.613169	-1.645370	1.652635
54	6	0	-3.505934	-0.602784	1.264764
55	6	0	-4.286265	-1.564658	1.923139
56	6	0	-4.145808	0.565276	0.814821
57	6	0	-5.652829	-1.382099	2.110093
58	1	0	-3.805353	-2.468522	2.287530
59	6	0	-5.512310	0.745249	0.995866
60	1	0	-3.564142	1.350133	0.336056
61	6	0	-6.275858	-0.226936	1.642511
62	1	0	-6.232653	-2.144841	2.621315
63	1	0	-5.984640	1.655693	0.638089
64	1	0	-7.341477	-0.080422	1.787256
65	7	0	-0.094628	-1.815524	-2.336988
66	6	0	-1.343549	-2.587613	-2.180513
67	6	0	-1.302101	-3.519152	-0.971048
68	1	0	-1.534143	-3.135649	-3.115294
69	1	0	-2.152313	-1.864157	-2.029859
70	1	0	-0.757463	-4.449564	-1.230804
71	1	0	-0.746900	-3.012142	-0.170220
72	7	0	-2.645262	-3.820939	-0.493715
73	6	0	1.106334	-2.659965	-2.354994
74	1	0	1.035592	-3.428613	-3.135609
75	1	0	1.973288	-2.025934	-2.559516
76	1	0	1.227029	-3.116641	-1.372305

77	6	0	-0.161111	-0.948399	-3.516213
78	1	0	0.708404	-0.284137	-3.522350
79	1	0	-0.170474	-1.537149	-4.441504
80	1	0	-1.072571	-0.348299	-3.465756
81	6	0	-2.564885	-4.578049	0.743816
82	1	0	-3.570873	-4.748189	1.139271
83	1	0	-2.078129	-5.561787	0.607603
84	1	0	-1.990244	-4.013613	1.484005
85	6	0	-3.414666	-4.562944	-1.480222
86	1	0	-2.929514	-5.517321	-1.760240
87	1	0	-4.405272	-4.788791	-1.076046
88	1	0	-3.551575	-3.969178	-2.387848

Si-M03^{T}

Total energy= -1822.36777713

Sum of electronic and zero-point Energies= -1821.609013

Sum of electronic and thermal Energies= -1821.567000

Sum of electronic and thermal Enthalpies= -1821.566056

Sum of electronic and thermal Free Energies= -1821.688462

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.597007	-0.902236	0.923570
2	6	0	4.888578	-1.429398	0.976598
3	6	0	5.434847	-1.830593	2.189041
4	6	0	4.672488	-1.686096	3.349221
5	6	0	3.385020	-1.151644	3.292294
6	6	0	2.831015	-0.759046	2.072777
7	6	0	3.249715	-0.573400	-0.515045
8	6	0	4.646420	-0.442865	-1.170418
9	6	0	5.499586	-1.458651	-0.406246
10	1	0	6.441217	-2.236384	2.237307
11	1	0	5.087711	-1.986728	4.306123
12	1	0	2.808107	-1.042212	4.205130
13	1	0	1.824428	-0.356359	2.018100
14	1	0	2.704540	-1.404089	-0.969658
15	1	0	4.612140	-0.611199	-2.255161
16	1	0	5.401929	-2.450816	-0.861349
17	6	0	3.053993	1.844482	-1.057947
18	6	0	4.478456	1.874540	-1.515959
19	6	0	1.134275	0.898319	-0.420431
20	1	0	4.940060	2.823652	-1.241230

21	1	0	6.554034	-1.173843	-0.431796
22	7	0	2.475121	0.646708	-0.712602
23	7	0	2.234070	2.835812	-1.007515
24	7	0	1.030932	2.269134	-0.605360
25	8	0	5.204001	0.835497	-0.898018
26	1	0	4.511479	1.769156	-2.610743
27	6	0	-0.035740	3.127017	-0.218848
28	6	0	-0.815886	3.712175	-1.222582
29	6	0	-0.290762	3.339267	1.140863
30	6	0	-1.883964	4.519687	-0.836813
31	6	0	-1.377687	4.144501	1.482117
32	6	0	-2.185294	4.737624	0.510219
33	1	0	-2.503065	4.979188	-1.603854
34	1	0	-1.595146	4.316455	2.533796
35	6	0	-0.513907	3.428945	-2.669293
36	1	0	0.494235	3.761576	-2.932322
37	1	0	-0.555932	2.351257	-2.862304
38	1	0	-1.231948	3.927997	-3.322197
39	6	0	-3.378542	5.569944	0.904174
40	1	0	-3.568277	6.359573	0.173489
41	1	0	-4.278936	4.948761	0.960203
42	1	0	-3.234033	6.030321	1.884090
43	6	0	0.556077	2.678870	2.193854
44	1	0	0.280078	1.622442	2.294364
45	1	0	1.617002	2.713635	1.928557
46	1	0	0.418459	3.163314	3.162132
47	6	0	0.170225	-0.021892	-0.075883
48	8	0	0.571902	-1.337605	0.100145
49	1	0	0.160253	-1.848639	-0.660614
50	6	0	-1.218017	0.293574	0.087104
51	6	0	-2.170859	-0.586645	0.479557
52	1	0	-1.526044	1.300653	-0.175869
53	1	0	-1.885909	-1.610079	0.717256
54	6	0	-3.597506	-0.275815	0.584777
55	6	0	-4.517421	-1.331847	0.715254
56	6	0	-4.104740	1.037293	0.564964
57	6	0	-5.884582	-1.087666	0.799967
58	1	0	-4.131769	-2.350427	0.740722
59	6	0	-5.471261	1.275990	0.646905
60	1	0	-3.422596	1.882772	0.505104
61	6	0	-6.372961	0.217048	0.762079
62	1	0	-6.573950	-1.921961	0.895620
63	1	0	-5.837000	2.298819	0.630840
64	1	0	-7.439045	0.408771	0.829564

65	7	0	-0.543579	-2.590440	-2.036582
66	6	0	-1.772619	-3.279988	-1.631760
67	6	0	-1.534228	-4.183800	-0.421220
68	1	0	-2.186968	-3.846636	-2.483517
69	1	0	-2.503618	-2.515495	-1.345653
70	1	0	-1.112856	-5.158501	-0.735826
71	1	0	-0.790007	-3.696026	0.221737
72	7	0	-2.745911	-4.374664	0.365296
73	6	0	0.447501	-3.524825	-2.567222
74	1	0	0.061633	-4.074266	-3.441024
75	1	0	1.339587	-2.971058	-2.870913
76	1	0	0.736348	-4.245476	-1.798753
77	6	0	-0.840171	-1.545498	-3.014678
78	1	0	0.079803	-1.005963	-3.256762
79	1	0	-1.261780	-1.961092	-3.943896
80	1	0	-1.553881	-0.841961	-2.578686
81	6	0	-2.446813	-5.125483	1.574334
82	1	0	-3.351054	-5.217141	2.181925
83	1	0	-2.070085	-6.141762	1.358281
84	1	0	-1.689465	-4.595319	2.158230
85	6	0	-3.785712	-5.041909	-0.403794
86	1	0	-3.459544	-6.027584	-0.783936
87	1	0	-4.664855	-5.191219	0.229083
88	1	0	-4.086118	-4.424961	-1.254457

Re-M2

Total energy= -1474.75081461
Sum of electronic and zero-point Energies= -1474.219395
Sum of electronic and thermal Energies= -1474.188770
Sum of electronic and thermal Enthalpies= -1474.187826
Sum of electronic and thermal Free Energies= -1474.284083

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.180524	-1.771910	0.327423
2	6	0	-3.179961	-2.708998	0.053496
3	6	0	-4.200226	-2.935006	0.968214
4	6	0	-4.199391	-2.220602	2.167451
5	6	0	-3.187043	-1.303572	2.447879
6	6	0	-2.163933	-1.070348	1.527279
7	6	0	-1.227918	-1.704732	-0.853154
8	6	0	-1.449551	-3.078155	-1.535197

9	6	0	-2.930112	-3.371534	-1.282213
10	1	0	-4.975537	-3.667226	0.763155
11	1	0	-4.986079	-2.390836	2.895492
12	1	0	-3.190079	-0.768419	3.391705
13	1	0	-1.370235	-0.364785	1.750892
14	1	0	-1.534998	-0.927550	-1.563526
15	1	0	-1.174696	-3.057224	-2.597951
16	1	0	-3.542155	-2.921116	-2.071672
17	6	0	1.097110	-2.534413	-0.567883
18	6	0	0.686362	-3.895950	-1.040710
19	6	0	0.852350	-0.360548	-0.125685
20	1	0	1.206851	-4.663145	-0.466728
21	1	0	-3.114573	-4.448269	-1.280969
22	7	0	0.179016	-1.507811	-0.539087
23	7	0	2.278802	-2.158870	-0.225231
24	7	0	2.146852	-0.806505	0.064403
25	8	0	-0.700799	-4.076005	-0.861283
26	1	0	0.954699	-4.006102	-2.101836
27	6	0	3.337644	-0.016874	0.095021
28	6	0	3.740723	0.654685	-1.062521
29	6	0	4.072615	0.037821	1.282174
30	6	0	4.908107	1.417720	-1.001824
31	6	0	5.240340	0.796995	1.293967
32	6	0	5.670785	1.496361	0.163634
33	1	0	5.232858	1.954493	-1.890352
34	1	0	5.822281	0.855158	2.211000
35	6	0	2.933759	0.556326	-2.330995
36	1	0	2.682166	-0.485976	-2.551297
37	1	0	1.987587	1.104201	-2.250811
38	1	0	3.491844	0.964163	-3.175531
39	6	0	6.948508	2.295399	0.197402
40	1	0	7.811772	1.654831	-0.010721
41	1	0	6.937985	3.090347	-0.551693
42	1	0	7.104576	2.747685	1.179735
43	6	0	3.574699	-0.678562	2.506980
44	1	0	2.601497	-0.276090	2.806320
45	1	0	3.435697	-1.745156	2.309449
46	1	0	4.272581	-0.561933	3.337908
47	6	0	0.402000	0.922254	0.104930
48	8	0	1.311898	1.784334	0.713960
49	1	0	1.747745	2.321269	0.037112
50	6	0	-0.916315	1.424462	-0.137340
51	6	0	-1.316081	2.694410	0.105728
52	1	0	-1.647713	0.735312	-0.544894

53	1	0	-0.587086	3.412317	0.472963
54	6	0	-2.675177	3.191985	-0.111289
55	6	0	-2.900532	4.576091	-0.195951
56	6	0	-3.790191	2.342178	-0.230201
57	6	0	-4.173362	5.089670	-0.419763
58	1	0	-2.055970	5.252777	-0.093237
59	6	0	-5.060907	2.855470	-0.460588
60	1	0	-3.663738	1.268655	-0.112420
61	6	0	-5.262548	4.232220	-0.560954
62	1	0	-4.315270	6.164307	-0.485588
63	1	0	-5.903936	2.176241	-0.546380
64	1	0	-6.256941	4.630674	-0.734000

Si-M2

Total energy= -1474.75655116

Sum of electronic and zero-point Energies= -1474.224828

Sum of electronic and thermal Energies= -1474.194513

Sum of electronic and thermal Enthalpies= -1474.193569

Sum of electronic and thermal Free Energies= -1474.287644

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.553528	-1.125939	0.218856
2	6	0	4.940250	-1.289000	0.219827
3	6	0	5.565428	-1.985159	1.246619
4	6	0	4.783197	-2.504597	2.279146
5	6	0	3.399092	-2.329469	2.279881
6	6	0	2.768775	-1.640316	1.242342
7	6	0	3.143133	-0.356885	-1.021914
8	6	0	4.453756	0.372058	-1.406590
9	6	0	5.548896	-0.611894	-0.987752
10	1	0	6.644220	-2.110579	1.254785
11	1	0	5.257698	-3.041842	3.094265
12	1	0	2.806225	-2.732925	3.094515
13	1	0	1.690852	-1.510556	1.234900
14	1	0	2.860301	-1.045331	-1.821769
15	1	0	4.478341	0.645755	-2.469599
16	1	0	5.738110	-1.331126	-1.792588
17	6	0	2.284029	1.943440	-0.630126
18	6	0	3.648016	2.511592	-0.868950
19	6	0	0.700998	0.373103	-0.635271
20	1	0	3.822336	3.357291	-0.203005

21	1	0	6.481299	-0.083278	-0.776032
22	7	0	2.059228	0.602358	-0.835704
23	7	0	1.218821	2.588419	-0.303975
24	7	0	0.220300	1.623991	-0.291546
25	8	0	4.627476	1.532464	-0.605258
26	1	0	3.719557	2.859786	-1.910161
27	6	0	-1.051199	1.953239	0.257138
28	6	0	-1.944215	2.691821	-0.530815
29	6	0	-1.384164	1.505331	1.539426
30	6	0	-3.205890	2.962652	-0.010140
31	6	0	-2.665061	1.791456	2.017034
32	6	0	-3.586631	2.511922	1.258398
33	1	0	-3.915668	3.526908	-0.610924
34	1	0	-2.946412	1.441416	3.007299
35	6	0	-1.543465	3.135052	-1.911948
36	1	0	-0.670650	3.792841	-1.874263
37	1	0	-1.268104	2.271555	-2.526449
38	1	0	-2.362190	3.663927	-2.402525
39	6	0	-4.970016	2.800672	1.781762
40	1	0	-5.140807	3.878270	1.862844
41	1	0	-5.731500	2.400950	1.105250
42	1	0	-5.121821	2.356277	2.767306
43	6	0	-0.412763	0.695656	2.353999
44	1	0	-0.421688	-0.350388	2.025419
45	1	0	0.609912	1.066451	2.237841
46	1	0	-0.679222	0.723335	3.412102
47	6	0	0.018775	-0.814135	-0.780419
48	8	0	0.786346	-1.954625	-1.019860
49	1	0	0.505579	-2.320059	-1.870909
50	6	0	-1.398459	-0.967662	-0.666440
51	6	0	-2.058889	-2.149603	-0.706023
52	1	0	-1.978913	-0.054476	-0.588324
53	1	0	-1.493064	-3.072771	-0.811962
54	6	0	-3.512700	-2.289510	-0.610966
55	6	0	-4.109677	-3.526283	-0.906988
56	6	0	-4.360187	-1.235944	-0.218938
57	6	0	-5.487795	-3.701564	-0.837757
58	1	0	-3.474855	-4.358261	-1.201425
59	6	0	-5.736711	-1.410640	-0.154582
60	1	0	-3.937152	-0.273597	0.060032
61	6	0	-6.313149	-2.642670	-0.466064
62	1	0	-5.918592	-4.669738	-1.075499
63	1	0	-6.365674	-0.579911	0.152297
64	1	0	-7.388548	-2.776372	-0.410367

Re-TS3^{D}

Total energy= -1474.70316974

Sum of electronic and zero-point Energies= -1474.175906

Sum of electronic and thermal Energies= -1474.146470

Sum of electronic and thermal Enthalpies= -1474.145526

Sum of electronic and thermal Free Energies= -1474.238960

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.052921	0.965693	0.546824
2	6	0	-4.362842	1.412584	0.358471
3	6	0	-5.200937	1.606572	1.448447
4	6	0	-4.712423	1.339762	2.727764
5	6	0	-3.406374	0.885833	2.909730
6	6	0	-2.557752	0.698182	1.817732
7	6	0	-2.369893	0.884540	-0.806196
8	6	0	-3.563306	0.777276	-1.789066
9	6	0	-4.653074	1.610941	-1.111643
10	1	0	-6.222121	1.947371	1.306760
11	1	0	-5.357818	1.478813	3.589189
12	1	0	-3.043499	0.675787	3.910395
13	1	0	-1.542707	0.344014	1.971388
14	1	0	-1.809608	1.796156	-1.022225
15	1	0	-3.297731	1.116128	-2.798214
16	1	0	-4.553565	2.664123	-1.396411
17	6	0	-1.849000	-1.422470	-1.610614
18	6	0	-3.114402	-1.451829	-2.408721
19	6	0	-0.288086	-0.513681	-0.361647
20	1	0	-3.545008	-2.453095	-2.387085
21	1	0	-5.643413	1.266469	-1.417496
22	7	0	-1.475188	-0.265456	-0.975157
23	7	0	-0.981697	-2.368003	-1.430353
24	7	0	-0.011419	-1.798276	-0.645176
25	8	0	-4.042607	-0.559158	-1.834873
26	1	0	-2.896464	-1.178773	-3.450919
27	6	0	1.113401	-2.582648	-0.223772
28	6	0	2.397626	-2.229057	-0.640736
29	6	0	0.856624	-3.683401	0.602462
30	6	0	3.451231	-3.043935	-0.221907
31	6	0	1.942645	-4.462805	0.989484
32	6	0	3.244734	-4.162932	0.581595

33	1	0	4.460995	-2.789734	-0.534330
34	1	0	1.768866	-5.318647	1.637346
35	6	0	2.667210	-1.004874	-1.472899
36	1	0	1.875670	-0.825709	-2.205889
37	1	0	2.734396	-0.120571	-0.827875
38	1	0	3.613879	-1.110872	-2.005699
39	6	0	4.394640	-5.043667	0.996086
40	1	0	5.350531	-4.529240	0.879264
41	1	0	4.293977	-5.355436	2.038731
42	1	0	4.425121	-5.951096	0.384480
43	6	0	-0.535579	-3.996760	1.084217
44	1	0	-1.033003	-3.095084	1.456107
45	1	0	-1.154801	-4.401359	0.279243
46	1	0	-0.498290	-4.727898	1.893233
47	6	0	0.490858	0.395261	0.426749
48	8	0	1.254209	-0.091440	1.401290
49	1	0	2.005451	0.896481	1.341324
50	6	0	0.705416	1.709740	0.095656
51	6	0	1.755558	2.272956	0.935000
52	1	0	0.322887	2.169428	-0.812314
53	1	0	1.439143	2.500809	1.959531
54	6	0	2.664787	3.275895	0.366531
55	6	0	3.259006	4.263535	1.172922
56	6	0	3.006069	3.273849	-0.999095
57	6	0	4.136367	5.203436	0.644467
58	1	0	3.015831	4.290003	2.232560
59	6	0	3.875615	4.220836	-1.531204
60	1	0	2.588103	2.505256	-1.645320
61	6	0	4.449248	5.194328	-0.714992
62	1	0	4.574324	5.953405	1.297281
63	1	0	4.115007	4.192360	-2.590706
64	1	0	5.132475	5.928898	-1.128755

Si-TS3^{D}

Total energy= -1474.70873361
Sum of electronic and zero-point Energies= -1474.181352
Sum of electronic and thermal Energies= -1474.151817
Sum of electronic and thermal Enthalpies= -1474.150872
Sum of electronic and thermal Free Energies= -1474.243676

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

1	6	0	-3.516423	1.005124	0.344244
2	6	0	-4.846289	1.280767	0.019441
3	6	0	-5.738242	1.691353	1.001527
4	6	0	-5.282206	1.810208	2.314748
5	6	0	-3.953868	1.527392	2.635000
6	6	0	-3.052970	1.127413	1.646981
7	6	0	-2.776164	0.613299	-0.919808
8	6	0	-3.924721	0.142999	-1.844501
9	6	0	-5.088182	1.056801	-1.456009
10	1	0	-6.774397	1.903518	0.755214
11	1	0	-5.968367	2.121376	3.096106
12	1	0	-3.615926	1.622742	3.661771
13	1	0	-2.012026	0.933680	1.883728
14	1	0	-2.253118	1.470430	-1.346897
15	1	0	-3.651461	0.181280	-2.906529
16	1	0	-5.033091	1.997356	-2.015064
17	6	0	-2.056494	-1.773554	-1.087569
18	6	0	-3.338596	-2.139511	-1.769983
19	6	0	-0.522235	-0.424756	-0.275568
20	1	0	-3.693440	-3.104794	-1.407302
21	1	0	-6.044369	0.579129	-1.681263
22	7	0	-1.794341	-0.468256	-0.760558
23	7	0	-1.055228	-2.550130	-0.812301
24	7	0	-0.105728	-1.705587	-0.297628
25	8	0	-4.323028	-1.175438	-1.488262
26	1	0	-3.155025	-2.213672	-2.851675
27	6	0	1.154053	-2.228635	0.139566
28	6	0	2.132182	-2.485883	-0.825561
29	6	0	1.346694	-2.447048	1.503479
30	6	0	3.352691	-2.984688	-0.380459
31	6	0	2.587923	-2.945433	1.900919
32	6	0	3.597025	-3.217009	0.977229
33	1	0	4.134692	-3.190659	-1.107297
34	1	0	2.767769	-3.125088	2.957629
35	6	0	1.866396	-2.191859	-2.277293
36	1	0	1.006143	-2.759847	-2.643170
37	1	0	1.640466	-1.128631	-2.417637
38	1	0	2.735363	-2.442131	-2.887141
39	6	0	4.937950	-3.737998	1.424768
40	1	0	5.713917	-2.981001	1.276082
41	1	0	4.926234	-4.007145	2.482540
42	1	0	5.226998	-4.619805	0.846802
43	6	0	0.263550	-2.120649	2.495064
44	1	0	0.130152	-1.034982	2.566330

45	1	0	-0.694773	-2.552434	2.191686
46	1	0	0.519249	-2.498951	3.485697
47	6	0	0.182877	0.748652	0.142914
48	8	0	-0.494142	1.900216	0.202434
49	1	0	0.560255	2.556617	0.086162
50	6	0	1.546580	0.867237	0.294537
51	6	0	1.911200	2.260263	0.502370
52	1	0	2.254610	0.069491	0.093539
53	1	0	1.647058	2.653144	1.491272
54	6	0	3.202428	2.750038	0.003627
55	6	0	3.848702	3.844680	0.606228
56	6	0	3.827099	2.175981	-1.118898
57	6	0	5.053713	4.336593	0.118080
58	1	0	3.389685	4.310182	1.475259
59	6	0	5.039201	2.659678	-1.601113
60	1	0	3.341902	1.345136	-1.625658
61	6	0	5.662841	3.745678	-0.989058
62	1	0	5.525154	5.183657	0.608464
63	1	0	5.495745	2.190902	-2.468467
64	1	0	6.604755	4.127303	-1.369562

Re-M04$_B$

Total energy= -1822.82249938

Sum of electronic and zero-point Energies= -1822.047159

Sum of electronic and thermal Energies= -1822.005684

Sum of electronic and thermal Enthalpies= -1822.004740

Sum of electronic and thermal Free Energies= -1822.122987

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.433405	-2.568970	0.341504
2	6	0	-3.519534	-3.374601	-0.008917
3	6	0	-4.414864	-3.804995	0.961158
4	6	0	-4.198909	-3.432315	2.288741
5	6	0	-3.097753	-2.651146	2.638517
6	6	0	-2.201333	-2.210035	1.663882
7	6	0	-1.642411	-2.234603	-0.909970
8	6	0	-2.045953	-3.378610	-1.874691
9	6	0	-3.496807	-3.678453	-1.489260
10	1	0	-5.257673	-4.435752	0.695198
11	1	0	-4.885336	-3.768721	3.059061
12	1	0	-2.931604	-2.387730	3.677779

13	1	0	-1.336876	-1.613390	1.939331
14	1	0	-1.976668	-1.289510	-1.356810
15	1	0	-1.913344	-3.093496	-2.926767
16	1	0	-4.176973	-3.022923	-2.044354
17	6	0	0.634275	-3.191983	-1.174844
18	6	0	0.074378	-4.368001	-1.915545
19	6	0	0.602356	-1.200187	-0.178120
20	1	0	0.610338	-5.274396	-1.632414
21	1	0	-3.750669	-4.713410	-1.729267
22	7	0	-0.196340	-2.180594	-0.748997
23	7	0	1.871525	-2.957453	-0.908890
24	7	0	1.868296	-1.725713	-0.280286
25	8	0	-1.285951	-4.539434	-1.588205
26	1	0	0.195827	-4.208721	-2.996892
27	6	0	3.106969	-1.249591	0.249719
28	6	0	4.098056	-0.847845	-0.648905
29	6	0	3.305286	-1.248761	1.633946
30	6	0	5.318553	-0.419331	-0.125725
31	6	0	4.536023	-0.803131	2.111372
32	6	0	5.553559	-0.387832	1.249417
33	1	0	6.099261	-0.093518	-0.809423
34	1	0	4.706951	-0.785815	3.185297
35	6	0	3.843068	-0.861358	-2.132422
36	1	0	3.829781	-1.884808	-2.518907
37	1	0	2.867610	-0.420981	-2.363484
38	1	0	4.615697	-0.300648	-2.661969
39	6	0	6.887841	0.055143	1.792638
40	1	0	7.565167	-0.798556	1.898607
41	1	0	7.366956	0.774872	1.124848
42	1	0	6.780358	0.514349	2.777997
43	6	0	2.213601	-1.687328	2.570643
44	1	0	1.447454	-0.908448	2.650636
45	1	0	1.724855	-2.598004	2.210622
46	1	0	2.615356	-1.879382	3.567212
47	6	0	0.270968	0.040994	0.355217
48	8	0	1.327235	0.791134	0.842021
49	1	0	1.330754	1.647721	0.352839
50	6	0	-1.024145	0.606948	0.466365
51	6	0	-1.257985	1.835946	1.021854
52	1	0	-1.867388	0.051136	0.072045
53	1	0	-0.424161	2.353031	1.493050
54	6	0	-2.538638	2.537332	1.045211
55	6	0	-2.586168	3.840257	1.575955
56	6	0	-3.725060	2.017630	0.490766

57	6	0	-3.749808	4.598952	1.531820
58	1	0	-1.683475	4.260312	2.013945
59	6	0	-4.887272	2.780412	0.444617
60	1	0	-3.745722	1.005094	0.095097
61	6	0	-4.907897	4.078443	0.955667
62	1	0	-3.751660	5.603306	1.944038
63	1	0	-5.786236	2.356012	0.008158
64	1	0	-5.815930	4.670228	0.914549
65	7	0	-0.868146	3.147548	-1.751443
66	6	0	0.469783	3.519706	-2.327262
67	6	0	1.342666	4.202981	-1.286067
68	1	0	0.280435	4.164542	-3.188097
69	1	0	0.936236	2.596536	-2.677326
70	1	0	2.131773	4.769376	-1.802091
71	1	0	0.748480	4.933302	-0.727542
72	7	0	1.911690	3.238018	-0.341451
73	6	0	-1.809421	4.307961	-1.722467
74	1	0	-1.997633	4.612278	-2.752853
75	1	0	-2.734399	3.994992	-1.237207
76	1	0	-1.360681	5.126389	-1.162247
77	6	0	-1.485343	1.997640	-2.469912
78	1	0	-2.448346	1.784537	-2.002867
79	1	0	-1.623516	2.273098	-3.515596
80	1	0	-0.820226	1.138427	-2.381163
81	6	0	2.225005	3.877944	0.940626
82	1	0	2.616350	3.123296	1.627263
83	1	0	2.973236	4.676275	0.829709
84	1	0	1.314685	4.302056	1.372016
85	6	0	3.124601	2.619225	-0.891973
86	1	0	3.921479	3.363066	-1.040472
87	1	0	3.477839	1.842355	-0.208521
88	1	0	2.908329	2.145776	-1.853377
89	1	0	-0.721825	2.818981	-0.774017

Re-TS3$_B$

Total energy= -1822.81091534
Sum of electronic and zero-point Energies= -1822.042014
Sum of electronic and thermal Energies= -1822.001011
Sum of electronic and thermal Enthalpies= -1822.000067
Sum of electronic and thermal Free Energies= -1822.118602

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

1	6	0	-2.502149	-2.412790	0.233205
2	6	0	-3.605991	-3.166154	-0.174236
3	6	0	-4.618747	-3.465220	0.726811
4	6	0	-4.502737	-3.014636	2.042888
5	6	0	-3.384259	-2.289715	2.452635
6	6	0	-2.368027	-1.981660	1.547250
7	6	0	-1.583623	-2.213359	-0.957746
8	6	0	-1.961412	-3.406199	-1.870411
9	6	0	-3.461598	-3.576896	-1.622031
10	1	0	-5.476593	-4.055567	0.419733
11	1	0	-5.283498	-3.245783	2.760235
12	1	0	-3.299272	-1.965202	3.484160
13	1	0	-1.491622	-1.427349	1.870584
14	1	0	-1.800707	-1.280191	-1.492164
15	1	0	-1.695895	-3.226102	-2.919777
16	1	0	-4.031426	-2.917704	-2.286097
17	6	0	0.641841	-3.319969	-0.924622
18	6	0	0.070745	-4.544252	-1.574905
19	6	0	0.662245	-1.246738	-0.169413
20	1	0	0.495193	-5.439070	-1.118359
21	1	0	-3.767069	-4.606788	-1.818761
22	7	0	-0.151021	-2.229396	-0.663561
23	7	0	1.876703	-3.099777	-0.610044
24	7	0	1.889369	-1.812740	-0.135642
25	8	0	-1.324981	-4.580743	-1.396308
26	1	0	0.331918	-4.534563	-2.642568
27	6	0	3.133336	-1.304735	0.377426
28	6	0	4.128910	-0.964874	-0.537153
29	6	0	3.299593	-1.207270	1.759638
30	6	0	5.344988	-0.512843	-0.023842
31	6	0	4.529584	-0.747500	2.224368
32	6	0	5.562869	-0.401602	1.350351
33	1	0	6.136671	-0.235051	-0.715542
34	1	0	4.684542	-0.656155	3.296762
35	6	0	3.879512	-1.051365	-2.018794
36	1	0	3.740961	-2.088335	-2.338211
37	1	0	2.971551	-0.501787	-2.290129
38	1	0	4.717152	-0.626311	-2.574303
39	6	0	6.894345	0.058725	1.884524
40	1	0	7.525886	-0.799886	2.134309
41	1	0	7.429535	0.661271	1.147582
42	1	0	6.770725	0.650682	2.794406
43	6	0	2.172920	-1.538233	2.699379

44	1	0	1.407406	-0.754760	2.658589
45	1	0	1.695756	-2.487388	2.436317
46	1	0	2.535160	-1.607690	3.726124
47	6	0	0.366687	0.101549	0.208913
48	8	0	1.463933	0.829534	0.570889
49	1	0	1.478953	1.708404	0.077645
50	6	0	-0.887972	0.655176	0.261214
51	6	0	-1.114902	2.022881	0.590500
52	1	0	-1.744039	0.046580	-0.000848
53	1	0	-0.304158	2.489831	1.155109
54	6	0	-2.464830	2.522087	0.938686
55	6	0	-2.580742	3.739791	1.629353
56	6	0	-3.651775	1.889861	0.533107
57	6	0	-3.821517	4.306266	1.896137
58	1	0	-1.674456	4.247422	1.952490
59	6	0	-4.894804	2.457412	0.801207
60	1	0	-3.616253	0.942151	0.000634
61	6	0	-4.990214	3.670049	1.480227
62	1	0	-3.876438	5.248853	2.432415
63	1	0	-5.795359	1.944792	0.476604
64	1	0	-5.960242	4.110603	1.684696
65	7	0	-0.947605	3.189364	-1.856825
66	6	0	0.404300	3.526722	-2.362402
67	6	0	1.293120	4.155944	-1.291272
68	1	0	0.292931	4.203526	-3.217940
69	1	0	0.856882	2.602512	-2.730608
70	1	0	1.982295	4.874250	-1.760400
71	1	0	0.675321	4.724761	-0.589064
72	7	0	2.051325	3.161548	-0.521157
73	6	0	-1.814424	4.380771	-1.760408
74	1	0	-1.955044	4.822145	-2.752933
75	1	0	-2.778376	4.082609	-1.344654
76	1	0	-1.363024	5.117538	-1.095087
77	6	0	-1.592391	2.152001	-2.679184
78	1	0	-2.571843	1.928453	-2.249216
79	1	0	-1.717299	2.496322	-3.711183
80	1	0	-0.975342	1.251156	-2.662238
81	6	0	2.520256	3.738984	0.743650
82	1	0	3.068250	2.975350	1.301159
83	1	0	3.181346	4.601796	0.576704
84	1	0	1.661930	4.059001	1.340061
85	6	0	3.200495	2.656891	-1.281809
86	1	0	3.930065	3.454845	-1.483820
87	1	0	3.686788	1.861747	-0.709002

88	1	0	2.872952	2.235280	-2.234758
89	1	0	-0.917003	2.645877	-0.674118

Re-M05$_B$

Total energy= -1822.84509122
Sum of electronic and zero-point Energies= -1822.072039
Sum of electronic and thermal Energies= -1822.030941
Sum of electronic and thermal Enthalpies= -1822.029997
Sum of electronic and thermal Free Energies= -1822.146682

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.559525	-1.052115	0.619293
2	6	0	-4.913329	-1.025746	0.270727
3	6	0	-5.889870	-1.099439	1.252810
4	6	0	-5.496346	-1.223817	2.586833
5	6	0	-4.147020	-1.292618	2.926312
6	6	0	-3.161946	-1.209861	1.939386
7	6	0	-2.742226	-0.910178	-0.653166
8	6	0	-3.710891	-1.488437	-1.710223
9	6	0	-5.071511	-0.977767	-1.233068
10	1	0	-6.942434	-1.085275	0.987282
11	1	0	-6.249515	-1.293156	3.364774
12	1	0	-3.856390	-1.422165	3.963219
13	1	0	-2.114113	-1.296001	2.214029
14	1	0	-2.504213	0.138780	-0.866644
15	1	0	-3.443852	-1.205217	-2.735289
16	1	0	-5.237931	0.043417	-1.593041
17	6	0	-1.378554	-2.915172	-1.213133
18	6	0	-2.546778	-3.552021	-1.908008
19	6	0	-0.235713	-1.277673	-0.323939
20	1	0	-2.636340	-4.598546	-1.613939
21	1	0	-5.877237	-1.612462	-1.607370
22	7	0	-1.480395	-1.654306	-0.688358
23	7	0	-0.153459	-3.350781	-1.151255
24	7	0	0.544272	-2.324180	-0.592191
25	8	0	-3.746073	-2.902913	-1.566553
26	1	0	-2.358602	-3.504840	-2.989788
27	6	0	1.935910	-2.511798	-0.269230
28	6	0	2.863011	-2.486903	-1.312302
29	6	0	2.268768	-2.785591	1.058281
30	6	0	4.188122	-2.767296	-0.987411

31	6	0	3.612392	-3.046604	1.331914
32	6	0	4.579050	-3.049034	0.324894
33	1	0	4.935064	-2.756775	-1.777156
34	1	0	3.904313	-3.267441	2.355264
35	6	0	2.435284	-2.135125	-2.709652
36	1	0	1.703186	-2.851443	-3.093125
37	1	0	1.970142	-1.143774	-2.712307
38	1	0	3.293309	-2.122498	-3.382614
39	6	0	6.026840	-3.302628	0.651968
40	1	0	6.533074	-3.814828	-0.168933
41	1	0	6.548230	-2.354757	0.822671
42	1	0	6.128321	-3.905787	1.556399
43	6	0	1.223664	-2.809198	2.143592
44	1	0	0.816276	-1.807951	2.325912
45	1	0	0.387558	-3.462663	1.875078
46	1	0	1.653572	-3.171198	3.078207
47	6	0	0.240716	0.059111	0.083884
48	8	0	1.398515	0.360604	-0.522468
49	1	0	2.024794	0.947980	0.069612
50	6	0	-0.496105	0.841433	0.889873
51	6	0	-0.174465	2.275148	1.189737
52	1	0	-1.421372	0.449293	1.296012
53	1	0	-0.256991	2.463842	2.265307
54	6	0	-1.109171	3.199443	0.433790
55	6	0	-1.866007	4.169202	1.088254
56	6	0	-1.172512	3.114036	-0.961267
57	6	0	-2.667168	5.050859	0.362376
58	1	0	-1.820388	4.243694	2.171498
59	6	0	-1.968940	3.993259	-1.687848
60	1	0	-0.567083	2.368244	-1.472932
61	6	0	-2.718473	4.966834	-1.025977
62	1	0	-3.248287	5.804814	0.883892
63	1	0	-2.002176	3.924393	-2.770973
64	1	0	-3.338525	5.654419	-1.591964
65	7	0	2.141808	3.791254	-0.716072
66	6	0	3.511785	3.508747	-0.295724
67	6	0	3.578475	2.819488	1.062539
68	1	0	4.116190	4.432764	-0.258978
69	1	0	3.977271	2.867673	-1.050992
70	1	0	4.589596	2.916508	1.486936
71	1	0	2.890851	3.312465	1.757860
72	7	0	3.206672	1.394643	0.999714
73	6	0	1.640487	5.004123	-0.081226
74	1	0	2.257762	5.885648	-0.330153

75	1	0	0.613414	5.189196	-0.406974
76	1	0	1.627316	4.893502	1.007660
77	6	0	2.064413	3.924276	-2.164597
78	1	0	1.035099	4.155430	-2.452034
79	1	0	2.718380	4.725938	-2.551530
80	1	0	2.353398	2.981211	-2.637154
81	6	0	2.886900	0.881677	2.336525
82	1	0	2.620319	-0.176289	2.255085
83	1	0	3.744213	0.973241	3.018738
84	1	0	2.040581	1.432571	2.754221
85	6	0	4.281764	0.577790	0.421455
86	1	0	5.185322	0.607165	1.047184
87	1	0	3.931558	-0.453252	0.342416
88	1	0	4.531869	0.929058	-0.581008
89	1	0	0.846462	2.508707	0.868909

Re-TS4$_B$

Total energy= -1822.84185239
Sum of electronic and zero-point Energies= -1822.071854
Sum of electronic and thermal Energies= -1822.030824
Sum of electronic and thermal Enthalpies= -1822.029880
Sum of electronic and thermal Free Energies= -1822.147569

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.526055	-1.165198	0.606845
2	6	0	-4.878553	-1.175031	0.252814
3	6	0	-5.855958	-1.301772	1.228848
4	6	0	-5.463256	-1.442454	2.561563
5	6	0	-4.113519	-1.474170	2.905485
6	6	0	-3.127956	-1.337677	1.924870
7	6	0	-2.707714	-0.970211	-0.657671
8	6	0	-3.652814	-1.556314	-1.730884
9	6	0	-5.030922	-1.097598	-1.250612
10	1	0	-6.907598	-1.314830	0.959437
11	1	0	-6.216698	-1.552272	3.334514
12	1	0	-3.822954	-1.615488	3.940940
13	1	0	-2.077779	-1.389355	2.199728
14	1	0	-2.502008	0.090398	-0.844990
15	1	0	-3.389342	-1.244084	-2.748688
16	1	0	-5.225662	-0.073509	-1.587471
17	6	0	-1.283110	-2.923018	-1.237771

18	6	0	-2.424505	-3.578541	-1.959506
19	6	0	-0.193727	-1.265099	-0.310387
20	1	0	-2.485236	-4.633964	-1.691054
21	1	0	-5.815563	-1.746878	-1.644172
22	7	0	-1.423214	-1.671837	-0.697947
23	7	0	-0.049292	-3.328547	-1.164755
24	7	0	0.613967	-2.289344	-0.583585
25	8	0	-3.647009	-2.974311	-1.617286
26	1	0	-2.227826	-3.500274	-3.038093
27	6	0	2.006878	-2.447807	-0.256602
28	6	0	2.935975	-2.402547	-1.298702
29	6	0	2.344875	-2.715706	1.069164
30	6	0	4.263892	-2.665196	-0.975570
31	6	0	3.694399	-2.954342	1.343913
32	6	0	4.659355	-2.947464	0.336954
33	1	0	5.011839	-2.636320	-1.764276
34	1	0	3.989611	-3.168205	2.367722
35	6	0	2.501819	-2.031985	-2.688854
36	1	0	1.785287	-2.755402	-3.088084
37	1	0	2.013674	-1.051888	-2.663068
38	1	0	3.359227	-1.984581	-3.361185
39	6	0	6.108824	-3.213705	0.647397
40	1	0	6.481111	-4.059930	0.063278
41	1	0	6.723725	-2.345492	0.391859
42	1	0	6.254143	-3.436555	1.705768
43	6	0	1.299898	-2.752411	2.154574
44	1	0	0.869053	-1.758877	2.326453
45	1	0	0.478766	-3.425791	1.888587
46	1	0	1.735741	-3.098556	3.092572
47	6	0	0.258463	0.090222	0.108070
48	8	0	1.407473	0.415103	-0.441756
49	1	0	2.221874	1.107484	0.257408
50	6	0	-0.544877	0.824069	0.910109
51	6	0	-0.287092	2.263015	1.244788
52	1	0	-1.469787	0.393962	1.274115
53	1	0	-0.398596	2.436970	2.321004
54	6	0	-1.215082	3.191172	0.485511
55	6	0	-1.931018	4.197009	1.133072
56	6	0	-1.306807	3.084470	-0.906228
57	6	0	-2.717732	5.090372	0.405744
58	1	0	-1.865170	4.289357	2.214188
59	6	0	-2.087827	3.975503	-1.635392
60	1	0	-0.736222	2.309377	-1.413662
61	6	0	-2.795473	4.984432	-0.980023

62	1	0	-3.267504	5.870044	0.923641
63	1	0	-2.142113	3.887775	-2.716533
64	1	0	-3.404167	5.680536	-1.548020
65	7	0	1.984667	3.829753	-0.723054
66	6	0	3.367372	3.565390	-0.343497
67	6	0	3.478446	2.882238	1.013877
68	1	0	3.966767	4.492540	-0.318782
69	1	0	3.820041	2.929186	-1.110388
70	1	0	4.486884	2.999310	1.427688
71	1	0	2.777137	3.335270	1.720268
72	7	0	3.171170	1.428594	0.954062
73	6	0	1.485708	5.040902	-0.083995
74	1	0	2.089546	5.927002	-0.348688
75	1	0	0.450426	5.213598	-0.389777
76	1	0	1.494106	4.934349	1.005683
77	6	0	1.859565	3.939418	-2.170250
78	1	0	0.818820	4.153953	-2.425717
79	1	0	2.491567	4.741778	-2.590310
80	1	0	2.143005	2.991486	-2.636224
81	6	0	2.864275	0.894747	2.297535
82	1	0	2.662697	-0.174759	2.203778
83	1	0	3.713885	1.047310	2.970139
84	1	0	1.983678	1.400241	2.697311
85	6	0	4.280595	0.651197	0.360765
86	1	0	5.173204	0.722909	0.990087
87	1	0	3.958816	-0.387295	0.282189
88	1	0	4.503215	1.024123	-0.638997
89	1	0	0.733552	2.533223	0.953377

Re-M06$_B$

Total energy= -1822.84105306

Sum of electronic and zero-point Energies= -1822.068778

Sum of electronic and thermal Energies= -1822.028204

Sum of electronic and thermal Enthalpies= -1822.027259

Sum of electronic and thermal Free Energies= -1822.143646

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.673882	-0.759419	0.649838
2	6	0	-5.030784	-0.627497	0.342287
3	6	0	-5.983298	-0.675745	1.349451
4	6	0	-5.562425	-0.881154	2.665226

5	6	0	-4.211808	-1.052055	2.962031
6	6	0	-3.250708	-0.993980	1.950367
7	6	0	-2.878780	-0.634842	-0.637990
8	6	0	-3.914663	-1.099338	-1.687169
9	6	0	-5.222147	-0.509533	-1.153879
10	1	0	-7.039536	-0.580497	1.117167
11	1	0	-6.297181	-0.932506	3.462106
12	1	0	-3.903236	-1.241241	3.984642
13	1	0	-2.201121	-1.150238	2.184867
14	1	0	-2.563921	0.399167	-0.822845
15	1	0	-3.653959	-0.795769	-2.708117
16	1	0	-5.321295	0.534632	-1.470035
17	6	0	-1.691175	-2.719501	-1.283781
18	6	0	-2.911965	-3.229813	-1.992140
19	6	0	-0.406856	-1.213704	-0.340064
20	1	0	-3.076735	-4.280503	-1.750118
21	1	0	-6.081842	-1.068135	-1.529630
22	7	0	-1.680065	-1.471685	-0.718260
23	7	0	-0.511699	-3.264488	-1.237533
24	7	0	0.273518	-2.319097	-0.646916
25	8	0	-4.054899	-2.511548	-1.598524
26	1	0	-2.736888	-3.141443	-3.073745
27	6	0	1.639293	-2.652573	-0.338624
28	6	0	2.565911	-2.671280	-1.383405
29	6	0	1.943788	-3.021320	0.970507
30	6	0	3.852501	-3.108455	-1.082251
31	6	0	3.254545	-3.434287	1.225436
32	6	0	4.212028	-3.498104	0.213056
33	1	0	4.596758	-3.137081	-1.874532
34	1	0	3.523828	-3.727739	2.236613
35	6	0	2.175986	-2.184452	-2.750463
36	1	0	1.388562	-2.807047	-3.185098
37	1	0	1.792486	-1.161992	-2.667617
38	1	0	3.034511	-2.190242	-3.423149
39	6	0	5.618932	-3.951512	0.502174
40	1	0	5.900545	-4.783682	-0.148782
41	1	0	6.331375	-3.140962	0.320878
42	1	0	5.726481	-4.275282	1.538876
43	6	0	0.901878	-2.979067	2.059067
44	1	0	0.575033	-1.951469	2.258745
45	1	0	0.014598	-3.555993	1.779204
46	1	0	1.300663	-3.392976	2.985995
47	6	0	0.217087	0.072041	0.097807
48	8	0	1.409042	0.239500	-0.400206

49	1	0	2.398745	0.919694	0.380937
50	6	0	-0.516007	0.906650	0.876095
51	6	0	-0.071388	2.298883	1.217173
52	1	0	-1.504640	0.612418	1.203280
53	1	0	-0.243805	2.515985	2.277532
54	6	0	-0.773213	3.339112	0.366155
55	6	0	-1.448317	4.418591	0.932981
56	6	0	-0.693229	3.246052	-1.027976
57	6	0	-2.025941	5.398699	0.124979
58	1	0	-1.514414	4.500095	2.014982
59	6	0	-1.265350	4.222936	-1.836008
60	1	0	-0.148343	2.413241	-1.468085
61	6	0	-1.933033	5.305688	-1.260388
62	1	0	-2.546587	6.235042	0.581102
63	1	0	-1.186633	4.145626	-2.916526
64	1	0	-2.378392	6.069126	-1.890197
65	7	0	2.620523	3.611387	-0.522737
66	6	0	3.919195	3.173381	-0.028648
67	6	0	3.803195	2.392935	1.272597
68	1	0	4.600780	4.025234	0.141430
69	1	0	4.394635	2.550999	-0.793048
70	1	0	4.775807	2.306857	1.767969
71	1	0	3.120776	2.900986	1.959766
72	7	0	3.280914	1.009635	1.075759
73	6	0	2.191921	4.833210	0.147930
74	1	0	2.915075	5.655403	0.004909
75	1	0	1.220307	5.143131	-0.244523
76	1	0	2.074288	4.663400	1.223101
77	6	0	2.653952	3.818323	-1.964864
78	1	0	1.669058	4.151026	-2.302062
79	1	0	3.398126	4.576186	-2.266136
80	1	0	2.891519	2.876290	-2.466922
81	6	0	2.798062	0.437155	2.355091
82	1	0	2.462029	-0.583322	2.163904
83	1	0	3.610216	0.430824	3.085677
84	1	0	1.965612	1.038838	2.722641
85	6	0	4.288843	0.102074	0.477080
86	1	0	5.121756	-0.031992	1.171914
87	1	0	3.797337	-0.850030	0.279647
88	1	0	4.649015	0.518039	-0.462558
89	1	0	1.000245	2.405429	1.015422

Si-M04$_B$

Total energy= -1822.82932872
Sum of electronic and zero-point Energies= -1822.053220
Sum of electronic and thermal Energies= -1822.012157
Sum of electronic and thermal Enthalpies= -1822.011213
Sum of electronic and thermal Free Energies= -1822.127308

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.888349	-0.583086	0.911606
2	6	0	5.244795	-0.906798	0.838622
3	6	0	5.941139	-1.279641	1.980978
4	6	0	5.262925	-1.313044	3.200002
5	6	0	3.909941	-0.980134	3.270210
6	6	0	3.206324	-0.615631	2.120969
7	6	0	3.385992	-0.244177	-0.478002
8	6	0	4.689983	0.136472	-1.221680
9	6	0	5.743949	-0.770205	-0.581762
10	1	0	6.997619	-1.525994	1.930373
11	1	0	5.795330	-1.592102	4.103697
12	1	0	3.399100	-1.003454	4.227390
13	1	0	2.152179	-0.360926	2.174597
14	1	0	2.940530	-1.123733	-0.947911
15	1	0	4.595884	0.016427	-2.309113
16	1	0	5.765631	-1.740766	-1.089947
17	6	0	2.778319	2.134350	-0.889511
18	6	0	4.147754	2.409626	-1.428575
19	6	0	1.089816	0.884509	-0.154869
20	1	0	4.472479	3.405679	-1.126688
21	1	0	6.736466	-0.321002	-0.661807
22	7	0	2.417636	0.850629	-0.549746
23	7	0	1.814524	2.977022	-0.743005
24	7	0	0.764771	2.217477	-0.258062
25	8	0	5.063149	1.470950	-0.913354
26	1	0	4.120571	2.363182	-2.527379
27	6	0	-0.539616	2.785411	-0.193819
28	6	0	-1.265678	2.929598	-1.379073
29	6	0	-1.062888	3.132172	1.057176
30	6	0	-2.583225	3.383977	-1.282802
31	6	0	-2.377470	3.588629	1.105722
32	6	0	-3.156514	3.702873	-0.051345
33	1	0	-3.171144	3.492018	-2.191127
34	1	0	-2.810559	3.851705	2.068214
35	6	0	-0.630917	2.622739	-2.710110

36	1	0	0.060182	3.422174	-2.994045
37	1	0	-0.045344	1.698197	-2.673801
38	1	0	-1.387841	2.530367	-3.491512
39	6	0	-4.591827	4.149654	0.046543
40	1	0	-5.019330	4.335819	-0.940398
41	1	0	-5.198297	3.383406	0.540608
42	1	0	-4.677163	5.064472	0.638732
43	6	0	-0.232617	2.951089	2.298169
44	1	0	-0.031767	1.887502	2.475429
45	1	0	0.734994	3.449701	2.195282
46	1	0	-0.746815	3.353265	3.172175
47	6	0	0.317652	-0.198596	0.249045
48	8	0	0.937316	-1.442991	0.227336
49	1	0	0.408066	-2.007724	-0.380291
50	6	0	-1.023379	-0.150200	0.714168
51	6	0	-1.701674	-1.235839	1.197651
52	1	0	-1.552272	0.794012	0.633611
53	1	0	-1.163016	-2.173640	1.316642
54	6	0	-3.107086	-1.237596	1.609137
55	6	0	-3.742380	-2.468055	1.854326
56	6	0	-3.884475	-0.068981	1.724493
57	6	0	-5.097273	-2.536027	2.162838
58	1	0	-3.157451	-3.383527	1.799879
59	6	0	-5.238185	-0.139325	2.030209
60	1	0	-3.427206	0.907021	1.576603
61	6	0	-5.858165	-1.371377	2.243409
62	1	0	-5.559378	-3.502254	2.340523
63	1	0	-5.814309	0.777933	2.109730
64	1	0	-6.915442	-1.419960	2.481047
65	7	0	-2.609991	-1.627395	-1.732010
66	6	0	-2.570846	-3.009297	-2.309597
67	6	0	-1.160076	-3.508853	-2.576961
68	1	0	-3.133836	-2.982733	-3.245914
69	1	0	-3.110364	-3.648585	-1.607221
70	1	0	-1.253285	-4.546085	-2.938392
71	1	0	-0.711212	-2.934008	-3.392007
72	7	0	-0.271630	-3.430621	-1.416332
73	6	0	-1.831893	-0.631106	-2.519913
74	1	0	-2.195954	-0.629766	-3.548691
75	1	0	-1.983325	0.346521	-2.060521
76	1	0	-0.774810	-0.893505	-2.476596
77	6	0	-4.020067	-1.174603	-1.544966
78	1	0	-4.007729	-0.198811	-1.059622
79	1	0	-4.493634	-1.109910	-2.525116

80	1	0	-4.538332	-1.891738	-0.907565
81	6	0	1.098544	-3.748842	-1.841004
82	1	0	1.766370	-3.693172	-0.977835
83	1	0	1.166328	-4.757601	-2.274225
84	1	0	1.429231	-3.020124	-2.586172
85	6	0	-0.684972	-4.359745	-0.360165
86	1	0	-0.683447	-5.402595	-0.711055
87	1	0	0.004285	-4.268706	0.483173
88	1	0	-1.686988	-4.112270	-0.000746
89	1	0	-2.171430	-1.647816	-0.786473

Si-TS3$_B$

Total energy= -1822.81819181

Sum of electronic and zero-point Energies= -1512.301800

Sum of electronic and thermal Energies= -1512.271158

Sum of electronic and thermal Enthalpies= -1512.270214

Sum of electronic and thermal Free Energies= -1512.365528

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.759794	-0.644611	0.888658
2	6	0	5.119475	-0.956498	0.948428
3	6	0	5.671373	-1.473978	2.113287
4	6	0	4.844383	-1.665468	3.220408
5	6	0	3.487824	-1.346770	3.158111
6	6	0	2.928993	-0.837256	1.985302
7	6	0	3.434129	-0.139067	-0.502276
8	6	0	4.814184	0.324542	-1.029955
9	6	0	5.792211	-0.649523	-0.369604
10	1	0	6.729345	-1.712669	2.165463
11	1	0	5.261179	-2.059500	4.141703
12	1	0	2.859418	-1.496123	4.030055
13	1	0	1.871453	-0.595166	1.943371
14	1	0	3.038580	-0.941180	-1.127756
15	1	0	4.857250	0.329411	-2.126548
16	1	0	5.894571	-1.553003	-0.980716
17	6	0	2.856559	2.278813	-0.743897
18	6	0	4.282791	2.610167	-1.058992
19	6	0	1.127447	0.980361	-0.326733
20	1	0	4.548876	3.564859	-0.604418
21	1	0	6.778664	-0.191741	-0.268452
22	7	0	2.472643	0.973843	-0.552628

23	7	0	1.854517	3.094454	-0.654766
24	7	0	0.780046	2.283445	-0.399778
25	8	0	5.124386	1.615610	-0.526899
26	1	0	4.404545	2.689146	-2.148828
27	6	0	-0.539187	2.835350	-0.332866
28	6	0	-1.307663	2.848416	-1.497435
29	6	0	-1.010917	3.279915	0.905605
30	6	0	-2.624464	3.298394	-1.388388
31	6	0	-2.326692	3.730795	0.962328
32	6	0	-3.149276	3.734060	-0.170124
33	1	0	-3.249980	3.313599	-2.277064
34	1	0	-2.725291	4.076805	1.912859
35	6	0	-0.722313	2.399571	-2.809774
36	1	0	0.094507	3.061561	-3.113241
37	1	0	-0.308709	1.388101	-2.736941
38	1	0	-1.481249	2.405398	-3.593927
39	6	0	-4.580353	4.190108	-0.059603
40	1	0	-5.053724	4.257228	-1.040662
41	1	0	-5.159261	3.490730	0.551889
42	1	0	-4.640958	5.169802	0.421565
43	6	0	-0.130192	3.208669	2.123493
44	1	0	0.113312	2.166148	2.361215
45	1	0	0.814171	3.734486	1.957625
46	1	0	-0.629097	3.647747	2.988022
47	6	0	0.307241	-0.166347	-0.073480
48	8	0	0.924757	-1.365442	-0.325904
49	1	0	0.298131	-1.991528	-0.792194
50	6	0	-0.954396	-0.112476	0.461449
51	6	0	-1.732439	-1.272561	0.747356
52	1	0	-1.398030	0.862517	0.625781
53	1	0	-1.136602	-2.165726	0.950458
54	6	0	-2.972895	-1.174603	1.551020
55	6	0	-3.468659	-2.321166	2.191547
56	6	0	-3.738472	0.000711	1.639654
57	6	0	-4.671756	-2.299108	2.889396
58	1	0	-2.892583	-3.242642	2.141941
59	6	0	-4.939868	0.023459	2.340868
60	1	0	-3.406882	0.909899	1.141338
61	6	0	-5.417790	-1.124739	2.970023
62	1	0	-5.025593	-3.203274	3.375738
63	1	0	-5.509432	0.947021	2.391330
64	1	0	-6.355929	-1.104300	3.514329
65	7	0	-2.812547	-1.842052	-1.685745
66	6	0	-2.667433	-3.241144	-2.147256

67	6	0	-1.264851	-3.636465	-2.581068
68	1	0	-3.336104	-3.397486	-3.003805
69	1	0	-3.029358	-3.878027	-1.334664
70	1	0	-1.316005	-4.688167	-2.907979
71	1	0	-0.969035	-3.053287	-3.458074
72	7	0	-0.227451	-3.472775	-1.558180
73	6	0	-2.207969	-0.847931	-2.586742
74	1	0	-2.645853	-0.907908	-3.589463
75	1	0	-2.392596	0.144523	-2.166759
76	1	0	-1.129695	-1.012098	-2.637751
77	6	0	-4.239290	-1.539158	-1.453810
78	1	0	-4.326747	-0.531958	-1.043655
79	1	0	-4.797574	-1.609040	-2.393193
80	1	0	-4.639433	-2.249549	-0.728171
81	6	0	1.086249	-3.723870	-2.165984
82	1	0	1.863293	-3.597614	-1.408486
83	1	0	1.153189	-4.741059	-2.578720
84	1	0	1.259049	-3.002727	-2.968936
85	6	0	-0.426204	-4.397939	-0.438010
86	1	0	-0.374408	-5.446433	-0.767775
87	1	0	0.351271	-4.221661	0.309500
88	1	0	-1.395690	-4.226733	0.033627
89	1	0	-2.246040	-1.634057	-0.545154

Si-M05$_B$

Total energy= -1822.85333621
Sum of electronic and zero-point Energies= -1822.080207
Sum of electronic and thermal Energies= -1822.039105
Sum of electronic and thermal Enthalpies= -1822.038161
Sum of electronic and thermal Free Energies= -1822.155725

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.725710	-0.193971	0.604535
2	6	0	5.111010	-0.351312	0.536567
3	6	0	5.796208	-0.976094	1.571371
4	6	0	5.076818	-1.433968	2.675127
5	6	0	3.693204	-1.267603	2.741936
6	6	0	3.001063	-0.648550	1.700183
7	6	0	3.244998	0.442929	-0.680933
8	6	0	4.519566	1.125526	-1.238014
9	6	0	5.652604	0.218009	-0.754082

10	1	0	6.874070	-1.097573	1.525917
11	1	0	5.598856	-1.917854	3.494067
12	1	0	3.148840	-1.620555	3.611666
13	1	0	1.924398	-0.521970	1.762613
14	1	0	2.870049	-0.309887	-1.378404
15	1	0	4.479731	1.247080	-2.327313
16	1	0	5.837062	-0.574445	-1.487155
17	6	0	2.365575	2.792924	-0.689467
18	6	0	3.727853	3.326765	-1.013026
19	6	0	0.866527	1.266889	-0.264701
20	1	0	3.902097	4.253369	-0.465131
21	1	0	6.574658	0.790820	-0.632923
22	7	0	2.174334	1.445797	-0.532792
23	7	0	1.249106	3.447607	-0.548466
24	7	0	0.321702	2.482823	-0.293972
25	8	0	4.697779	2.388560	-0.614145
26	1	0	3.789051	3.533142	-2.090601
27	6	0	-1.077175	2.821623	-0.227081
28	6	0	-1.869901	2.529098	-1.337627
29	6	0	-1.560280	3.432094	0.933041
30	6	0	-3.224635	2.855324	-1.251567
31	6	0	-2.919749	3.727606	0.970415
32	6	0	-3.764807	3.442415	-0.107074
33	1	0	-3.870404	2.635395	-2.097814
34	1	0	-3.331669	4.190363	1.863541
35	6	0	-1.293128	1.859061	-2.556187
36	1	0	-0.366111	2.344440	-2.876578
37	1	0	-1.064948	0.805523	-2.353320
38	1	0	-2.003368	1.894042	-3.383029
39	6	0	-5.233722	3.761668	-0.016666
40	1	0	-5.752684	3.510875	-0.943754
41	1	0	-5.697737	3.199471	0.799483
42	1	0	-5.389587	4.824346	0.188520
43	6	0	-0.641949	3.749406	2.082876
44	1	0	-0.062135	2.871800	2.388052
45	1	0	0.074247	4.527635	1.803095
46	1	0	-1.213561	4.097897	2.943535
47	6	0	0.200099	-0.023625	-0.012856
48	8	0	0.699835	-0.977593	-0.809395
49	1	0	0.552740	-1.978850	-0.528100
50	6	0	-0.735233	-0.105453	0.946145
51	6	0	-1.471561	-1.355792	1.302345
52	1	0	-0.977673	0.799036	1.496930
53	1	0	-1.138365	-1.717744	2.283996

54	6	0	-2.976538	-1.181355	1.314284
55	6	0	-3.776533	-2.063426	2.045285
56	6	0	-3.595939	-0.198795	0.539989
57	6	0	-5.164499	-1.978343	1.986776
58	1	0	-3.305235	-2.830470	2.655307
59	6	0	-4.985463	-0.109040	0.479660
60	1	0	-2.988430	0.499984	-0.029081
61	6	0	-5.775008	-1.002494	1.199225
62	1	0	-5.771981	-2.673745	2.557552
63	1	0	-5.446593	0.659554	-0.135093
64	1	0	-6.857227	-0.937066	1.152703
65	7	0	-2.014553	-3.230303	-1.309019
66	6	0	-1.214910	-4.370951	-1.729186
67	6	0	0.287343	-4.110431	-1.734136
68	1	0	-1.493436	-4.716679	-2.742889
69	1	0	-1.434487	-5.200828	-1.049054
70	1	0	0.791549	-5.070726	-1.927128
71	1	0	0.563135	-3.434930	-2.551518
72	7	0	0.812306	-3.516558	-0.488935
73	6	0	-1.960105	-2.136265	-2.267700
74	1	0	-2.367144	-2.424245	-3.253784
75	1	0	-2.549931	-1.298383	-1.880285
76	1	0	-0.932427	-1.789664	-2.397645
77	6	0	-3.398084	-3.635384	-1.093088
78	1	0	-3.986997	-2.771792	-0.770676
79	1	0	-3.855822	-4.053557	-2.007584
80	1	0	-3.443705	-4.393015	-0.304787
81	6	0	2.280470	-3.487093	-0.559765
82	1	0	2.680337	-2.991545	0.328254
83	1	0	2.697007	-4.501550	-0.626049
84	1	0	2.587277	-2.922899	-1.444722
85	6	0	0.387087	-4.253214	0.705742
86	1	0	0.706714	-5.304328	0.659795
87	1	0	0.837027	-3.786120	1.585716
88	1	0	-0.699008	-4.209559	0.804610
89	1	0	-1.250852	-2.137167	0.565578

Si-TS4$_B$

Total energy= -1822.85186630
Sum of electronic and zero-point Energies= -1822.081756
Sum of electronic and thermal Energies= -1822.040857
Sum of electronic and thermal Enthalpies= -1822.039913
Sum of electronic and thermal Free Energies= -1822.157193

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.708434	0.143263	0.638956
2	6	0	-5.095882	0.280526	0.572888
3	6	0	-5.788356	0.900054	1.606271
4	6	0	-5.073491	1.373736	2.706200
5	6	0	-3.687144	1.228208	2.770549
6	6	0	-2.987541	0.614575	1.730481
7	6	0	-3.219220	-0.486203	-0.646453
8	6	0	-4.483319	-1.185700	-1.204425
9	6	0	-5.631126	-0.299235	-0.715887
10	1	0	-6.867980	1.005934	1.562344
11	1	0	-5.600778	1.853986	3.523982
12	1	0	-3.146809	1.593463	3.637815
13	1	0	-1.908832	0.502274	1.789093
14	1	0	-2.849858	0.274906	-1.337958
15	1	0	-4.443733	-1.302050	-2.294409
16	1	0	-5.832679	0.489989	-1.448120
17	6	0	-2.300329	-2.820368	-0.677632
18	6	0	-3.655617	-3.375716	-0.995077
19	6	0	-0.829324	-1.265494	-0.245085
20	1	0	-3.812280	-4.307319	-0.450364
21	1	0	-6.542491	-0.888433	-0.591726
22	7	0	-2.135000	-1.472069	-0.503973
23	7	0	-1.169457	-3.453248	-0.558791
24	7	0	-0.259724	-2.470140	-0.299465
25	8	0	-4.639412	-2.455283	-0.586882
26	1	0	-3.720864	-3.578583	-2.073139
27	6	0	1.145843	-2.781162	-0.248639
28	6	0	1.926548	-2.453582	-1.358356
29	6	0	1.649808	-3.398706	0.898474
30	6	0	3.288202	-2.752801	-1.285074
31	6	0	3.015194	-3.668199	0.923365
32	6	0	3.847357	-3.349022	-0.154234
33	1	0	3.924553	-2.504646	-2.130584
34	1	0	3.442108	-4.135792	1.806971
35	6	0	1.327155	-1.782380	-2.565144
36	1	0	0.478875	-2.353410	-2.956006
37	1	0	0.966256	-0.777294	-2.317610
38	1	0	2.071024	-1.686813	-3.357121
39	6	0	5.322685	-3.642597	-0.079224
40	1	0	5.835086	-3.338689	-0.994070

41	1	0	5.777102	-3.110788	0.762176
42	1	0	5.499817	-4.710636	0.075304
43	6	0	0.745387	-3.747537	2.050148
44	1	0	0.150336	-2.884213	2.366553
45	1	0	0.042940	-4.536596	1.765892
46	1	0	1.328662	-4.093577	2.904005
47	6	0	-0.197293	0.051679	0.008915
48	8	0	-0.708635	0.994813	-0.759235
49	1	0	-0.653210	2.205172	-0.527139
50	6	0	0.737718	0.116673	0.978155
51	6	0	1.452482	1.372338	1.358878
52	1	0	0.995731	-0.795653	1.508002
53	1	0	1.115735	1.723080	2.343959
54	6	0	2.961963	1.236741	1.368751
55	6	0	3.741137	2.143990	2.091957
56	6	0	3.606544	0.264092	0.602317
57	6	0	5.130828	2.094825	2.032341
58	1	0	3.251149	2.903370	2.697047
59	6	0	4.997952	0.210766	0.539540
60	1	0	3.014592	-0.454658	0.042191
61	6	0	5.765598	1.129734	1.250626
62	1	0	5.720766	2.810179	2.597001
63	1	0	5.477820	-0.550699	-0.069864
64	1	0	6.849123	1.092230	1.202667
65	7	0	1.899222	3.210986	-1.331503
66	6	0	1.072865	4.299252	-1.828050
67	6	0	-0.416264	3.979248	-1.850006
68	1	0	1.355819	4.601512	-2.853878
69	1	0	1.244841	5.172840	-1.190239
70	1	0	-0.965045	4.897787	-2.093128
71	1	0	-0.651883	3.240291	-2.622001
72	7	0	-0.946002	3.429936	-0.574042
73	6	0	1.914812	2.071155	-2.238468
74	1	0	2.340474	2.329598	-3.224671
75	1	0	2.522995	1.276827	-1.792668
76	1	0	0.904931	1.678396	-2.373571
77	6	0	3.259104	3.678874	-1.089956
78	1	0	3.869026	2.851656	-0.715994
79	1	0	3.729209	4.078791	-2.005954
80	1	0	3.250418	4.467643	-0.331333
81	6	0	-2.421915	3.376715	-0.647756
82	1	0	-2.808255	2.887243	0.248206
83	1	0	-2.836742	4.386324	-0.727633
84	1	0	-2.709205	2.795621	-1.526393

85	6	0	-0.526808	4.200725	0.610926
86	1	0	-0.879468	5.234992	0.534077
87	1	0	-0.962318	3.735363	1.497783
88	1	0	0.559470	4.183385	0.695054
89	1	0	1.211954	2.151703	0.627182

Si-M06$_B$

Total energy= -1822.85241504
Sum of electronic and zero-point Energies= -1822.078748
Sum of electronic and thermal Energies= -1822.037681
Sum of electronic and thermal Enthalpies= -1822.036737
Sum of electronic and thermal Free Energies= -1822.153609

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.669908	0.091673	0.653680
2	6	0	-5.058339	0.224874	0.602417
3	6	0	-5.740303	0.856704	1.635716
4	6	0	-5.013693	1.346065	2.720853
5	6	0	-3.626275	1.203208	2.771014
6	6	0	-2.936803	0.578132	1.730831
7	6	0	-3.193656	-0.546122	-0.632195
8	6	0	-4.460455	-1.254154	-1.171026
9	6	0	-5.607644	-0.371824	-0.672862
10	1	0	-6.820587	0.960140	1.602981
11	1	0	-5.532477	1.835885	3.538436
12	1	0	-3.077110	1.579880	3.627916
13	1	0	-1.857576	0.466856	1.778071
14	1	0	-2.831273	0.213492	-1.328959
15	1	0	-4.433965	-1.374715	-2.261091
16	1	0	-5.827147	0.408678	-1.409393
17	6	0	-2.260960	-2.874703	-0.669620
18	6	0	-3.617228	-3.439026	-0.967207
19	6	0	-0.797491	-1.305498	-0.254783
20	1	0	-3.761636	-4.370171	-0.418332
21	1	0	-6.512519	-0.966673	-0.528926
22	7	0	-2.104264	-1.525415	-0.497334
23	7	0	-1.123510	-3.498083	-0.567248
24	7	0	-0.218842	-2.505587	-0.318909
25	8	0	-4.601306	-2.523179	-0.547792
26	1	0	-3.696970	-3.644804	-2.043782
27	6	0	1.188874	-2.803727	-0.277422

28	6	0	1.969461	-2.432334	-1.373321
29	6	0	1.698051	-3.448578	0.852373
30	6	0	3.334064	-2.719191	-1.305392
31	6	0	3.065983	-3.705226	0.872440
32	6	0	3.897178	-3.344487	-0.192533
33	1	0	3.969806	-2.438357	-2.141110
34	1	0	3.495915	-4.194356	1.742916
35	6	0	1.369128	-1.725277	-2.559122
36	1	0	0.514630	-2.278716	-2.961485
37	1	0	1.016333	-0.724852	-2.282053
38	1	0	2.110414	-1.614474	-3.351642
39	6	0	5.375577	-3.623903	-0.122969
40	1	0	5.882154	-3.311174	-1.038065
41	1	0	5.827615	-3.090497	0.718717
42	1	0	5.563985	-4.690565	0.027339
43	6	0	0.796377	-3.833919	1.994500
44	1	0	0.192569	-2.983056	2.327636
45	1	0	0.102369	-4.623761	1.692465
46	1	0	1.382698	-4.191964	2.841384
47	6	0	-0.187104	0.029678	-0.006516
48	8	0	-0.723389	0.967790	-0.739485
49	1	0	-0.715290	2.383516	-0.530535
50	6	0	0.760075	0.090351	0.957942
51	6	0	1.445173	1.358759	1.354407
52	1	0	1.047469	-0.824747	1.467418
53	1	0	1.104486	1.692616	2.344632
54	6	0	2.958284	1.263617	1.364046
55	6	0	3.714726	2.163858	2.119882
56	6	0	3.629085	0.327494	0.574249
57	6	0	5.105729	2.143045	2.071262
58	1	0	3.205545	2.894071	2.744835
59	6	0	5.021617	0.302155	0.522432
60	1	0	3.053289	-0.386806	-0.008319
61	6	0	5.765729	1.213380	1.267985
62	1	0	5.677332	2.851911	2.662458
63	1	0	5.520720	-0.433081	-0.103465
64	1	0	6.850190	1.196899	1.230044
65	7	0	1.792328	3.334545	-1.296779
66	6	0	0.947020	4.390175	-1.828307
67	6	0	-0.528197	4.016731	-1.880431
68	1	0	1.240767	4.687667	-2.852177
69	1	0	1.073965	5.277678	-1.199161
70	1	0	-1.114794	4.907939	-2.125906
71	1	0	-0.724523	3.261359	-2.645835

72	7	0	-1.056922	3.450328	-0.604051
73	6	0	1.855278	2.176622	-2.180350
74	1	0	2.273000	2.431998	-3.170452
75	1	0	2.494683	1.418885	-1.715665
76	1	0	0.862862	1.737615	-2.303314
77	6	0	3.133901	3.844389	-1.037036
78	1	0	3.756024	3.041031	-0.633368
79	1	0	3.613007	4.237183	-1.951088
80	1	0	3.088381	4.648551	-0.296216
81	6	0	-2.533302	3.326346	-0.688780
82	1	0	-2.894774	2.803598	0.197887
83	1	0	-2.982095	4.320036	-0.752554
84	1	0	-2.782676	2.748192	-1.579497
85	6	0	-0.669133	4.221721	0.598211
86	1	0	-1.044741	5.244483	0.512822
87	1	0	-1.113012	3.737697	1.469828
88	1	0	0.415956	4.218667	0.691414
89	1	0	1.178143	2.142793	0.635439

Re-M3

Total energy= -1474.75499713
Sum of electronic and zero-point Energies= -1474.221699
Sum of electronic and thermal Energies= -1474.192016
Sum of electronic and thermal Enthalpies= -1474.191071
Sum of electronic and thermal Free Energies= -1474.283966

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.765437	0.975148	0.155953
2	6	0	3.977329	1.646663	0.329433
3	6	0	4.966040	1.108325	1.142446
4	6	0	4.720027	-0.104755	1.787822
5	6	0	3.500606	-0.761881	1.627043
6	6	0	2.506854	-0.225417	0.807347
7	6	0	1.898837	1.776825	-0.800405
8	6	0	2.484866	3.203579	-0.659655
9	6	0	3.977717	2.946363	-0.443057
10	1	0	5.908495	1.628079	1.285643
11	1	0	5.481501	-0.535085	2.430344
12	1	0	3.318638	-1.701068	2.139200
13	1	0	1.562849	-0.746015	0.674342
14	1	0	2.005609	1.439226	-1.836362

15	1	0	2.254850	3.834646	-1.527211
16	1	0	4.484565	2.837244	-1.408148
17	6	0	-0.129699	2.806530	0.188184
18	6	0	0.619589	4.069969	0.480739
19	6	0	-0.480491	0.819216	-0.688796
20	1	0	0.312154	4.467513	1.448468
21	1	0	4.437497	3.779213	0.093382
22	7	0	0.467565	1.772988	-0.484013
23	7	0	-1.375782	2.547999	0.438318
24	7	0	-1.582254	1.313389	-0.108416
25	8	0	2.001380	3.808003	0.530376
26	1	0	0.385364	4.810639	-0.297243
27	6	0	-2.858155	0.692503	0.153456
28	6	0	-3.974070	1.169607	-0.526050
29	6	0	-2.922920	-0.285162	1.147856
30	6	0	-5.213687	0.631145	-0.177578
31	6	0	-4.181057	-0.790497	1.460535
32	6	0	-5.335818	-0.343097	0.811935
33	1	0	-6.102233	0.981546	-0.696764
34	1	0	-4.264251	-1.554358	2.230230
35	6	0	-3.829294	2.194850	-1.617579
36	1	0	-3.436866	3.138745	-1.228268
37	1	0	-3.130944	1.834673	-2.379950
38	1	0	-4.791561	2.389141	-2.093594
39	6	0	-6.680088	-0.918763	1.176417
40	1	0	-7.487111	-0.406169	0.649318
41	1	0	-6.729721	-1.981778	0.921696
42	1	0	-6.863868	-0.832983	2.251235
43	6	0	-1.675647	-0.794642	1.816539
44	1	0	-1.091552	-1.392707	1.106565
45	1	0	-1.040022	0.025397	2.167476
46	1	0	-1.925730	-1.423627	2.672581
47	6	0	-0.476250	-0.498227	-1.425722
48	8	0	-1.623849	-1.035366	-1.529321
49	1	0	1.576739	-2.447039	-3.205394
50	6	0	0.729472	-0.975523	-1.869427
51	6	0	0.805214	-2.368551	-2.431854
52	1	0	1.665013	-0.485589	-1.650376
53	1	0	-0.161254	-2.617139	-2.881585
54	6	0	1.106105	-3.342678	-1.308894
55	6	0	0.116757	-3.599895	-0.349204
56	6	0	2.363494	-3.924537	-1.149610
57	6	0	0.384363	-4.419882	0.741316
58	1	0	-0.855702	-3.127889	-0.477429

59	6	0	2.633871	-4.749152	-0.056085
60	1	0	3.140154	-3.728050	-1.884763
61	6	0	1.646763	-4.998794	0.892307
62	1	0	-0.391310	-4.609467	1.477891
63	1	0	3.618165	-5.194813	0.053547
64	1	0	1.856581	-5.639636	1.743033

Si-M3

Total energy= -1474.76453327

Sum of electronic and zero-point Energies= -1474.231291

Sum of electronic and thermal Energies= -1474.201529

Sum of electronic and thermal Enthalpies= -1474.200585

Sum of electronic and thermal Free Energies= -1474.293112

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.802046	-0.920696	0.010697
2	6	0	-4.042366	-1.557107	0.086068
3	6	0	-5.089129	-0.966701	0.782058
4	6	0	-4.873690	0.266421	1.400976
5	6	0	-3.631716	0.895826	1.321929
6	6	0	-2.578716	0.306834	0.619215
7	6	0	-1.872635	-1.750426	-0.847143
8	6	0	-2.513258	-3.157251	-0.789255
9	6	0	-4.011563	-2.866421	-0.669714
10	1	0	-6.055310	-1.457592	0.851874
11	1	0	-5.680792	0.738343	1.952352
12	1	0	-3.479794	1.857693	1.801686
13	1	0	-1.613101	0.802346	0.557033
14	1	0	-1.818839	-1.349453	-1.862693
15	1	0	-2.243575	-3.776136	-1.653965
16	1	0	-4.453754	-2.756526	-1.665842
17	6	0	0.054050	-2.903664	0.265475
18	6	0	-0.763824	-4.145334	0.448598
19	6	0	0.471343	-0.871498	-0.438350
20	1	0	-0.547734	-4.598592	1.416690
21	1	0	-4.521092	-3.686614	-0.158915
22	7	0	-0.486709	-1.817954	-0.365719
23	7	0	1.296439	-2.691805	0.586901
24	7	0	1.542527	-1.422933	0.138185
25	8	0	-2.131406	-3.812474	0.415460
26	1	0	-0.510081	-4.863725	-0.343945

27	6	0	2.867541	-0.876415	0.240370
28	6	0	3.639533	-0.797429	-0.919669
29	6	0	3.317853	-0.466290	1.496555
30	6	0	4.923706	-0.269704	-0.791308
31	6	0	4.609086	0.050945	1.571278
32	6	0	5.421208	0.160287	0.439885
33	1	0	5.550826	-0.197480	-1.676134
34	1	0	4.987861	0.381402	2.535271
35	6	0	3.101137	-1.258774	-2.247795
36	1	0	2.706870	-2.277680	-2.178757
37	1	0	2.285173	-0.612474	-2.589635
38	1	0	3.888134	-1.245355	-3.003166
39	6	0	6.801142	0.755209	0.548787
40	1	0	6.745978	1.848012	0.581217
41	1	0	7.301122	0.424860	1.462461
42	1	0	7.420506	0.477344	-0.306312
43	6	0	2.429007	-0.571464	2.707063
44	1	0	1.465272	-0.082081	2.529003
45	1	0	2.220708	-1.616952	2.952037
46	1	0	2.899723	-0.099580	3.570454
47	6	0	0.311740	0.443440	-1.155691
48	8	0	-0.409753	0.369412	-2.208267
49	1	0	1.745971	3.449187	-1.039380
50	6	0	0.933330	1.511917	-0.577186
51	6	0	0.820497	2.882451	-1.189585
52	1	0	1.484631	1.387908	0.348966
53	1	0	0.678942	2.757657	-2.269765
54	6	0	-0.349460	3.674451	-0.638397
55	6	0	-1.650788	3.201628	-0.850769
56	6	0	-0.173171	4.845342	0.098592
57	6	0	-2.746478	3.884898	-0.334014
58	1	0	-1.776513	2.281112	-1.418426
59	6	0	-1.270683	5.533141	0.618235
60	1	0	0.832222	5.222349	0.270200
61	6	0	-2.560121	5.055258	0.404216
62	1	0	-3.748766	3.500351	-0.501173
63	1	0	-1.115393	6.442868	1.190806
64	1	0	-3.414900	5.588907	0.808208

TS5RR

Total energy= -2219.82864625
Sum of electronic and zero-point Energies= -2219.071659
Sum of electronic and thermal Energies= -2219.028941

Sum of electronic and thermal Enthalpies= -2219.027996
Sum of electronic and thermal Free Energies= -2219.145497

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.461879	1.972568	-0.769242
2	6	0	-4.848703	2.079834	-0.897421
3	6	0	-5.422113	3.261791	-1.346735
4	6	0	-4.589219	4.339792	-1.649986
5	6	0	-3.206252	4.231986	-1.506141
6	6	0	-2.627267	3.039712	-1.069066
7	6	0	-3.129897	0.570388	-0.292231
8	6	0	-4.444820	0.140451	0.400172
9	6	0	-5.518268	0.793983	-0.469113
10	1	0	-6.499868	3.351250	-1.444752
11	1	0	-5.021827	5.274066	-1.993448
12	1	0	-2.573071	5.081536	-1.739926
13	1	0	-1.550204	2.948001	-0.977870
14	1	0	-2.881600	-0.086667	-1.128785
15	1	0	-4.540699	-0.944776	0.498549
16	1	0	-5.740852	0.151099	-1.328760
17	6	0	-2.204400	0.474868	2.020624
18	6	0	-3.577078	0.288746	2.590272
19	6	0	-0.683269	0.562497	0.459993
20	1	0	-3.674962	0.852437	3.518683
21	1	0	-6.439857	0.941656	0.098219
22	7	0	-2.013791	0.497805	0.668082
23	7	0	-1.072040	0.575014	2.657776
24	7	0	-0.135254	0.637009	1.675921
25	8	0	-4.535828	0.764040	1.678831
26	1	0	-3.723935	-0.780585	2.801666
27	6	0	1.247296	0.865694	2.004772
28	6	0	1.864028	2.010609	1.487178
29	6	0	1.916633	-0.072177	2.801867
30	6	0	3.233015	2.153364	1.708774
31	6	0	3.282974	0.125406	2.990004
32	6	0	3.960879	1.211742	2.432963
33	1	0	3.743674	3.012180	1.281788
34	1	0	3.834508	-0.598781	3.585153
35	6	0	1.114799	3.058380	0.704147
36	1	0	1.019154	2.778324	-0.351272
37	1	0	0.112105	3.229696	1.107961
38	1	0	1.661640	4.002427	0.736282

39	6	0	5.447632	1.354904	2.620164
40	1	0	5.710319	1.367941	3.681951
41	1	0	5.970495	0.510243	2.161006
42	1	0	5.817099	2.271393	2.156164
43	6	0	1.215482	-1.232936	3.456702
44	1	0	0.668432	-0.893848	4.341357
45	1	0	0.505068	-1.705989	2.778296
46	1	0	1.949251	-1.977101	3.773348
47	6	0	-0.040655	0.501364	-0.916470
48	8	0	-0.781166	0.811121	-1.855003
49	1	0	2.347979	-0.369904	-2.870574
50	6	0	1.280385	-0.021055	-1.028905
51	6	0	2.079258	0.475343	-2.224685
52	1	0	1.836377	-0.112117	-0.103052
53	1	0	1.435933	1.126367	-2.824496
54	6	0	3.322931	1.219015	-1.794087
55	6	0	3.406571	2.610270	-1.888269
56	6	0	4.415979	0.518315	-1.270153
57	6	0	4.546872	3.291194	-1.462638
58	1	0	2.571384	3.165958	-2.308638
59	6	0	5.555898	1.193976	-0.845396
60	1	0	4.368685	-0.566484	-1.199436
61	6	0	5.625230	2.584441	-0.936787
62	1	0	4.593088	4.372891	-1.547727
63	1	0	6.397220	0.633687	-0.447355
64	1	0	6.516505	3.110589	-0.608192
65	6	0	0.912330	-1.910879	-1.519922
66	8	0	0.517074	-1.935096	-2.722391
67	6	0	-0.169773	-2.231054	-0.463485
68	8	0	0.022935	-2.294597	0.748304
69	6	0	2.304290	-2.446591	-1.206666
70	6	0	2.869344	-2.499464	0.075173
71	6	0	3.067700	-2.868310	-2.297484
72	6	0	4.171112	-2.957756	0.249886
73	1	0	2.290826	-2.171867	0.931176
74	6	0	4.374707	-3.319962	-2.121791
75	1	0	2.612090	-2.828747	-3.281359
76	6	0	4.932040	-3.364662	-0.846994
77	1	0	4.597383	-2.987005	1.248577
78	1	0	4.956747	-3.635357	-2.982345
79	1	0	5.950336	-3.713607	-0.706551
80	7	0	-1.379865	-2.382565	-1.061328
81	1	0	-1.305427	-2.286161	-2.074694
82	6	0	-2.603881	-2.744997	-0.482100

83	6	0	-3.712315	-2.852223	-1.335151
84	6	0	-2.762450	-3.002559	0.887512
85	6	0	-4.952498	-3.228820	-0.834917
86	1	0	-3.589537	-2.646674	-2.395038
87	6	0	-4.013191	-3.388190	1.370731
88	1	0	-1.913012	-2.919451	1.550927
89	6	0	-5.111555	-3.505054	0.523406
90	1	0	-5.796423	-3.309380	-1.512424
91	1	0	-4.121957	-3.600157	2.430258
92	1	0	-6.077933	-3.805352	0.913246

TS5RS

Total energy= -2219.81967162

Sum of electronic and zero-point Energies= -2219.064229

Sum of electronic and thermal Energies= -2219.021740

Sum of electronic and thermal Enthalpies= -2219.020795

Sum of electronic and thermal Free Energies= -2219.138670

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.668042	-1.397858	1.039239
2	6	0	-5.051514	-1.245425	0.915037
3	6	0	-5.903462	-1.830705	1.841522
4	6	0	-5.351342	-2.579791	2.882431
5	6	0	-3.969936	-2.734426	2.994594
6	6	0	-3.110115	-2.133684	2.073229
7	6	0	-3.004006	-0.615333	-0.074382
8	6	0	-4.112676	-0.568990	-1.146823
9	6	0	-5.382205	-0.419944	-0.309996
10	1	0	-6.979963	-1.720842	1.750477
11	1	0	-6.005144	-3.051986	3.608782
12	1	0	-3.558254	-3.323387	3.807685
13	1	0	-2.033374	-2.226962	2.169145
14	1	0	-2.738198	0.382745	0.272329
15	1	0	-3.959259	0.225682	-1.887934
16	1	0	-5.528512	0.637631	-0.054093
17	6	0	-1.816352	-1.998712	-1.771748
18	6	0	-3.074114	-2.148612	-2.573989
19	6	0	-0.512435	-1.133280	-0.253931
20	1	0	-3.177537	-3.176816	-2.923123
21	1	0	-6.258856	-0.769800	-0.859439
22	7	0	-1.794977	-1.214730	-0.653809

23	7	0	-0.627999	-2.457124	-2.045772
24	7	0	0.172618	-1.915440	-1.089238
25	8	0	-4.196455	-1.839253	-1.786130
26	1	0	-3.003444	-1.485031	-3.447818
27	6	0	1.550276	-2.325690	-1.003046
28	6	0	2.401186	-2.056952	-2.082202
29	6	0	1.962134	-3.013502	0.144480
30	6	0	3.733035	-2.447442	-1.946626
31	6	0	3.303569	-3.386274	0.218136
32	6	0	4.205999	-3.093890	-0.804153
33	1	0	4.420248	-2.235281	-2.761780
34	1	0	3.649627	-3.915609	1.103145
35	6	0	1.919689	-1.372197	-3.332791
36	1	0	2.771043	-1.123191	-3.969416
37	1	0	1.246158	-2.024152	-3.895652
38	1	0	1.381365	-0.454742	-3.076138
39	6	0	5.662341	-3.448787	-0.666624
40	1	0	5.794148	-4.364262	-0.085156
41	1	0	6.132179	-3.583431	-1.643116
42	1	0	6.195476	-2.644792	-0.147800
43	6	0	1.022930	-3.340881	1.277636
44	1	0	0.871576	-2.478195	1.938115
45	1	0	0.041181	-3.660872	0.915325
46	1	0	1.438893	-4.147325	1.883410
47	6	0	-0.048941	-0.250778	0.888982
48	8	0	-0.885615	-0.053917	1.779868
49	1	0	1.323308	0.618115	2.854742
50	6	0	1.217448	0.371585	0.736525
51	6	0	1.820905	1.028976	1.965883
52	1	0	1.916243	-0.147099	0.087985
53	1	0	1.606745	2.102070	1.968918
54	6	0	3.310639	0.790700	2.056814
55	6	0	4.221399	1.845542	2.108927
56	6	0	3.806471	-0.516988	2.081372
57	6	0	5.593243	1.601792	2.168603
58	1	0	3.852221	2.866586	2.077791
59	6	0	5.172846	-0.768143	2.143812
60	1	0	3.106057	-1.347665	2.045485
61	6	0	6.074797	0.295512	2.184799
62	1	0	6.286264	2.437535	2.195138
63	1	0	5.532741	-1.793382	2.166050
64	1	0	7.142682	0.105890	2.229485
65	6	0	0.799401	1.672371	-0.763633
66	8	0	0.487979	0.998551	-1.795532

67	6	0	-0.372766	2.412057	-0.075994
68	8	0	-0.300243	3.058960	0.959662
69	6	0	2.139826	2.381489	-0.764679
70	6	0	2.348808	3.665399	-0.256392
71	6	0	3.204326	1.716585	-1.386166
72	6	0	3.602371	4.269990	-0.371308
73	1	0	1.536072	4.194353	0.226855
74	6	0	4.454805	2.310681	-1.481439
75	1	0	3.033069	0.722306	-1.791325
76	6	0	4.657998	3.595397	-0.974164
77	1	0	3.749640	5.271622	0.021289
78	1	0	5.273146	1.776150	-1.954038
79	1	0	5.633964	4.064400	-1.052354
80	7	0	-1.520277	2.224972	-0.791916
81	1	0	-1.351104	1.748554	-1.675114
82	6	0	-2.799677	2.724393	-0.496439
83	6	0	-3.692024	2.939778	-1.552758
84	6	0	-3.219699	2.935111	0.822614
85	6	0	-4.992002	3.361485	-1.294286
86	1	0	-3.357681	2.778991	-2.574184
87	6	0	-4.520493	3.367634	1.065602
88	1	0	-2.527765	2.752427	1.634969
89	6	0	-5.412336	3.582182	0.016310
90	1	0	-5.675026	3.524068	-2.121805
91	1	0	-4.839992	3.528851	2.090266
92	1	0	-6.424676	3.916100	0.217238

TS5SR

Total energy= -2219.80976445
Sum of electronic and zero-point Energies= -2219.053639
Sum of electronic and thermal Energies= -2219.010166
Sum of electronic and thermal Enthalpies= -2219.009222
Sum of electronic and thermal Free Energies= -2219.131858

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.240497	-1.929986	0.013951
2	6	0	4.419638	-2.662283	0.161080
3	6	0	5.624501	-2.138190	-0.285899
4	6	0	5.621517	-0.883790	-0.898620
5	6	0	4.432939	-0.173479	-1.065318
6	6	0	3.220533	-0.689831	-0.602332

7	6	0	2.100890	-2.719686	0.612025
8	6	0	2.627955	-4.170497	0.540345
9	6	0	4.128319	-4.002770	0.798420
10	1	0	6.548015	-2.699718	-0.181341
11	1	0	6.552525	-0.462997	-1.264904
12	1	0	4.455748	0.791138	-1.561659
13	1	0	2.288932	-0.147558	-0.748017
14	1	0	1.906136	-2.417921	1.641328
15	1	0	2.120162	-4.840365	1.245633
16	1	0	4.324763	-3.986783	1.875987
17	6	0	0.390510	-3.572418	-0.969977
18	6	0	1.158826	-4.844785	-1.166862
19	6	0	-0.116741	-1.624777	-0.099303
20	1	0	1.137681	-5.128370	-2.219827
21	1	0	4.687851	-4.831727	0.359199
22	7	0	0.825482	-2.599972	-0.117793
23	7	0	-0.766939	-3.266200	-1.479808
24	7	0	-1.071822	-2.061313	-0.930552
25	8	0	2.498853	-4.665303	-0.786303
26	1	0	0.677888	-5.638811	-0.577662
27	6	0	-2.376472	-1.520473	-1.222674
28	6	0	-2.582457	-0.934248	-2.470948
29	6	0	-3.382734	-1.694196	-0.268574
30	6	0	-3.852527	-0.414552	-2.717127
31	6	0	-4.627239	-1.139314	-0.558898
32	6	0	-4.870817	-0.477276	-1.764666
33	1	0	-4.043823	0.065140	-3.674368
34	1	0	-5.422700	-1.230226	0.176553
35	6	0	-1.479190	-0.868313	-3.491540
36	1	0	-0.610772	-0.347121	-3.074806
37	1	0	-1.168775	-1.873591	-3.791609
38	1	0	-1.817696	-0.333221	-4.381165
39	6	0	-6.199521	0.180131	-2.028038
40	1	0	-6.470545	0.118279	-3.084602
41	1	0	-6.995227	-0.276633	-1.435795
42	1	0	-6.150535	1.241490	-1.761252
43	6	0	-3.123920	-2.443037	1.009321
44	1	0	-2.658359	-3.412652	0.804879
45	1	0	-2.461362	-1.877447	1.673799
46	1	0	-4.057598	-2.609434	1.547892
47	6	0	-0.079929	-0.439406	0.870719
48	8	0	0.844924	-0.500211	1.697468
49	1	0	-0.505039	1.443346	2.638059
50	6	0	-1.046768	0.584504	0.755595

51	6	0	-1.404913	1.313113	2.035815
52	1	0	-1.876476	0.402933	0.082286
53	1	0	-1.794643	2.307896	1.803040
54	6	0	-2.450354	0.533777	2.802242
55	6	0	-3.797087	0.600906	2.429953
56	6	0	-2.086992	-0.317586	3.849647
57	6	0	-4.757740	-0.161899	3.088501
58	1	0	-4.086984	1.253922	1.608605
59	6	0	-3.045234	-1.085985	4.508986
60	1	0	-1.040736	-0.380075	4.138129
61	6	0	-4.383925	-1.010088	4.130635
62	1	0	-5.800092	-0.095147	2.789623
63	1	0	-2.746719	-1.740438	5.322473
64	1	0	-5.132177	-1.604241	4.645770
65	6	0	-0.077835	1.861054	-0.713243
66	8	0	0.331751	1.137289	-1.657283
67	6	0	1.011016	2.464825	0.208162
68	8	0	0.818816	2.973725	1.303071
69	6	0	-1.301494	2.725395	-0.932361
70	6	0	-1.656686	3.824396	-0.139613
71	6	0	-2.099363	2.405615	-2.035806
72	6	0	-2.807432	4.555845	-0.431438
73	1	0	-1.031898	4.107015	0.699078
74	6	0	-3.252038	3.127854	-2.318126
75	1	0	-1.791138	1.581682	-2.667742
76	6	0	-3.614480	4.205968	-1.511054
77	1	0	-3.071524	5.405582	0.190287
78	1	0	-3.864132	2.855330	-3.173191
79	1	0	-4.512233	4.775622	-1.729670
80	7	0	2.221805	2.425540	-0.415588
81	1	0	2.183357	2.042250	-1.354334
82	6	0	3.425299	2.990502	0.040865
83	6	0	4.354387	3.422452	-0.912452
84	6	0	3.724391	3.101339	1.402080
85	6	0	5.574520	3.952400	-0.510350
86	1	0	4.110736	3.343475	-1.968843
87	6	0	4.945163	3.646082	1.790771
88	1	0	3.005565	2.759145	2.134249
89	6	0	5.875079	4.071172	0.845143
90	1	0	6.287392	4.281031	-1.259837
91	1	0	5.172524	3.728722	2.848977
92	1	0	6.824931	4.489277	1.161126

TS5SS

Total energy= -2219.81310735
Sum of electronic and zero-point Energies= -2219.056362
Sum of electronic and thermal Energies= -2219.013443
Sum of electronic and thermal Enthalpies= -2219.012499
Sum of electronic and thermal Free Energies= -2219.130779

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.496934	-1.723549	0.114533
2	6	0	4.617519	-2.558797	0.101852
3	6	0	5.883773	-2.040349	0.334502
4	6	0	6.011319	-0.672175	0.574818
5	6	0	4.891350	0.159172	0.574993
6	6	0	3.615392	-0.360684	0.345512
7	6	0	2.263773	-2.578319	-0.080487
8	6	0	2.828446	-3.825455	-0.797865
9	6	0	4.216201	-3.988202	-0.179180
10	1	0	6.757424	-2.685191	0.321149
11	1	0	6.993652	-0.246542	0.754915
12	1	0	5.013062	1.221458	0.757727
13	1	0	2.739997	0.280980	0.336832
14	1	0	1.834919	-2.847560	0.885972
15	1	0	2.178937	-4.703656	-0.689597
16	1	0	4.150754	-4.573188	0.744863
17	6	0	0.906439	-2.441195	-2.158960
18	6	0	1.819613	-3.392070	-2.873310
19	6	0	0.099040	-1.245411	-0.512663
20	1	0	2.045916	-3.008757	-3.869764
21	1	0	4.885034	-4.509684	-0.867756
22	7	0	1.152958	-2.016543	-0.882262
23	7	0	-0.233696	-1.992298	-2.595512
24	7	0	-0.727705	-1.261676	-1.561744
25	8	0	3.028382	-3.528220	-2.173081
26	1	0	1.303943	-4.357278	-2.976443
27	6	0	-2.077918	-0.770983	-1.675973
28	6	0	-2.314401	0.352112	-2.468786
29	6	0	-3.085170	-1.500673	-1.039299
30	6	0	-3.630970	0.799283	-2.545404
31	6	0	-4.381006	-0.994157	-1.128317
32	6	0	-4.666252	0.160482	-1.859626
33	1	0	-3.851096	1.678850	-3.143967
34	1	0	-5.183266	-1.520520	-0.617248

35	6	0	-1.198357	1.011292	-3.231669
36	1	0	-0.354787	1.227581	-2.570084
37	1	0	-0.845491	0.353745	-4.032835
38	1	0	-1.545913	1.945487	-3.676449
39	6	0	-6.063235	0.718412	-1.919674
40	1	0	-6.790202	0.024575	-1.493060
41	1	0	-6.115328	1.658234	-1.359900
42	1	0	-6.354566	0.936665	-2.950659
43	6	0	-2.780153	-2.766613	-0.284534
44	1	0	-2.151407	-3.435402	-0.881238
45	1	0	-2.260770	-2.555024	0.657471
46	1	0	-3.703991	-3.289426	-0.032708
47	6	0	-0.055055	-0.655465	0.884711
48	8	0	0.883816	-0.942413	1.645184
49	1	0	-0.714487	-0.116415	3.277434
50	6	0	-1.186803	0.134585	1.214857
51	6	0	-1.608172	0.041322	2.668345
52	1	0	-1.999793	0.142441	0.500246
53	1	0	-2.044425	0.988879	2.996560
54	6	0	-2.587455	-1.093015	2.856871
55	6	0	-3.901943	-0.970970	2.390471
56	6	0	-2.192389	-2.307556	3.423133
57	6	0	-4.795734	-2.032762	2.486255
58	1	0	-4.217471	-0.037641	1.926694
59	6	0	-3.084305	-3.375635	3.518717
60	1	0	-1.172299	-2.416098	3.783089
61	6	0	-4.388983	-3.242018	3.050761
62	1	0	-5.811426	-1.918710	2.118205
63	1	0	-2.758508	-4.312263	3.961303
64	1	0	-5.084979	-4.071501	3.125606
65	6	0	-0.667469	2.201469	1.145918
66	8	0	-0.652371	2.599535	2.335493
67	6	0	0.698389	2.091264	0.429556
68	8	0	0.874653	1.564785	-0.667842
69	6	0	-1.803545	2.688520	0.262246
70	6	0	-1.583561	3.296793	-0.974703
71	6	0	-3.097707	2.695967	0.795289
72	6	0	-2.639467	3.889570	-1.667891
73	1	0	-0.586178	3.317745	-1.400778
74	6	0	-4.153774	3.265834	0.095725
75	1	0	-3.262659	2.272417	1.781319
76	6	0	-3.926553	3.870438	-1.141754
77	1	0	-2.449784	4.368905	-2.624098
78	1	0	-5.151653	3.259495	0.524513

79	1	0	-4.747457	4.329378	-1.684588
80	7	0	1.655109	2.716502	1.152996
81	1	0	1.315500	3.013213	2.065143
82	6	0	2.963791	3.060441	0.774481
83	6	0	3.402565	3.015124	-0.554418
84	6	0	3.829967	3.513566	1.776509
85	6	0	4.697518	3.424541	-0.860126
86	1	0	2.735573	2.657398	-1.326160
87	6	0	5.120561	3.916776	1.455220
88	1	0	3.484438	3.546820	2.805660
89	6	0	5.563270	3.874224	0.133824
90	1	0	5.030918	3.386397	-1.892377
91	1	0	5.781330	4.264781	2.242591
92	1	0	6.571140	4.187213	-0.116736

M4RR

Total energy= -2219.83137321

Sum of electronic and zero-point Energies= -2219.073636

Sum of electronic and thermal Energies= -2219.030672

Sum of electronic and thermal Enthalpies= -2219.029728

Sum of electronic and thermal Free Energies= -2219.148707

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.101398	-2.162958	-0.891409
2	6	0	4.486352	-2.321239	-0.989574
3	6	0	5.022476	-3.480189	-1.533643
4	6	0	4.155203	-4.487120	-1.959833
5	6	0	2.774810	-4.332959	-1.840269
6	6	0	2.233292	-3.162093	-1.307224
7	6	0	2.814840	-0.798045	-0.288035
8	6	0	4.126415	-0.506658	0.486649
9	6	0	5.197978	-1.120448	-0.411751
10	1	0	6.098018	-3.609150	-1.608049
11	1	0	4.559151	-5.404261	-2.376233
12	1	0	2.113134	-5.129463	-2.164070
13	1	0	1.159277	-3.038477	-1.226698
14	1	0	2.632581	-0.039503	-1.056877
15	1	0	4.271953	0.554469	0.701724
16	1	0	5.479305	-0.403086	-1.191686
17	6	0	1.812845	-0.869048	2.002555
18	6	0	3.175049	-0.803677	2.622727

19	6	0	0.353820	-0.734227	0.397558
20	1	0	3.215793	-1.443404	3.504584
21	1	0	6.090704	-1.370420	0.165553
22	7	0	1.674469	-0.766433	0.645292
23	7	0	0.651889	-0.969003	2.588160
24	7	0	-0.246446	-0.888299	1.573530
25	8	0	4.131759	-1.257746	1.697045
26	1	0	3.371363	0.236919	2.920073
27	6	0	-1.641570	-1.164119	1.799170
28	6	0	-2.172450	-2.321559	1.215871
29	6	0	-2.383040	-0.297902	2.610035
30	6	0	-3.524052	-2.577086	1.434279
31	6	0	-3.734289	-0.594876	2.773933
32	6	0	-4.320957	-1.719791	2.190882
33	1	0	-3.966050	-3.462214	0.986358
34	1	0	-4.343168	0.071912	3.379424
35	6	0	-1.334695	-3.283585	0.411390
36	1	0	-1.169062	-2.920286	-0.608324
37	1	0	-0.359387	-3.458451	0.877404
38	1	0	-1.848891	-4.242459	0.329865
39	6	0	-5.781734	-2.016723	2.400769
40	1	0	-6.376675	-1.100838	2.358606
41	1	0	-6.153294	-2.707777	1.640851
42	1	0	-5.945803	-2.471583	3.382940
43	6	0	-1.755706	0.885974	3.295242
44	1	0	-1.215774	0.561087	4.190355
45	1	0	-1.042053	1.393769	2.642650
46	1	0	-2.528631	1.592934	3.603663
47	6	0	-0.277947	-0.435136	-0.952898
48	8	0	0.229454	-0.961441	-1.922524
49	1	0	-2.794200	1.332264	-2.369343
50	6	0	-1.339164	0.600984	-0.989173
51	6	0	-2.299988	0.378818	-2.160133
52	1	0	-1.857014	0.650327	-0.027827
53	1	0	-1.698123	0.130630	-3.036514
54	6	0	-3.340933	-0.677564	-1.889746
55	6	0	-3.160512	-2.000665	-2.301831
56	6	0	-4.523095	-0.339383	-1.222445
57	6	0	-4.140484	-2.962481	-2.060053
58	1	0	-2.248385	-2.270591	-2.830050
59	6	0	-5.511133	-1.291934	-0.993810
60	1	0	-4.668004	0.687758	-0.893058
61	6	0	-5.323444	-2.607839	-1.415058
62	1	0	-3.986291	-3.985126	-2.391423

63	1	0	-6.429328	-1.008342	-0.487493
64	1	0	-6.094523	-3.352500	-1.241035
65	6	0	-0.577254	2.032078	-1.258769
66	8	0	-0.023694	2.064396	-2.457239
67	6	0	0.495065	2.189892	-0.126339
68	8	0	0.286162	2.045963	1.080600
69	6	0	-1.658616	3.113401	-1.010207
70	6	0	-2.380537	3.231955	0.181943
71	6	0	-1.922292	4.002315	-2.051033
72	6	0	-3.348283	4.223378	0.324576
73	1	0	-2.176505	2.556854	1.007816
74	6	0	-2.890757	4.994775	-1.910050
75	1	0	-1.348502	3.880622	-2.963610
76	6	0	-3.607586	5.108210	-0.721456
77	1	0	-3.900587	4.305854	1.256115
78	1	0	-3.087262	5.679812	-2.729721
79	1	0	-4.363806	5.878891	-0.608639
80	7	0	1.686386	2.458420	-0.699596
81	1	0	1.538572	2.439638	-1.729154
82	6	0	2.932167	2.647232	-0.097797
83	6	0	4.065303	2.644250	-0.923909
84	6	0	3.084276	2.821318	1.285452
85	6	0	5.333343	2.795924	-0.374750
86	1	0	3.940792	2.514189	-1.995420
87	6	0	4.363130	2.973497	1.819140
88	1	0	2.208534	2.829334	1.920250
89	6	0	5.491538	2.955876	1.001911
90	1	0	6.201139	2.786310	-1.026506
91	1	0	4.473598	3.107763	2.891032
92	1	0	6.481164	3.070989	1.430393

M4RS

Total energy= -2219.83107876
Sum of electronic and zero-point Energies= -2219.073178
Sum of electronic and thermal Energies= -2219.029989
Sum of electronic and thermal Enthalpies= -2219.029045
Sum of electronic and thermal Free Energies= -2219.149493

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.267856	-1.940166	-0.547147
2	6	0	4.652818	-1.802332	-0.419352

3	6	0	5.504451	-2.616297	-1.152744
4	6	0	4.950692	-3.577879	-2.000769
5	6	0	3.568107	-3.720420	-2.109967
6	6	0	2.708216	-2.894174	-1.383271
7	6	0	2.604453	-0.902227	0.333841
8	6	0	3.690119	-0.639455	1.399295
9	6	0	4.985586	-0.727769	0.592521
10	1	0	6.581718	-2.519914	-1.056109
11	1	0	5.603714	-4.228278	-2.573932
12	1	0	3.155372	-4.479661	-2.766077
13	1	0	1.631302	-2.992458	-1.470345
14	1	0	2.384120	0.012021	-0.224426
15	1	0	3.542891	0.309691	1.930664
16	1	0	5.183576	0.236224	0.106066
17	6	0	1.314020	-1.782902	2.286017
18	6	0	2.560140	-1.838688	3.120552
19	6	0	0.101727	-1.126442	0.612281
20	1	0	2.618664	-2.784997	3.660195
21	1	0	5.832665	-0.973796	1.236591
22	7	0	1.370303	-1.309883	1.003677
23	7	0	0.083501	-2.005268	2.653683
24	7	0	-0.660192	-1.615167	1.580132
25	8	0	3.707049	-1.733538	2.311495
26	1	0	2.509682	-1.018520	3.850495
27	6	0	-2.092787	-1.666205	1.556138
28	6	0	-2.796748	-0.839911	2.443753
29	6	0	-2.708222	-2.460295	0.586076
30	6	0	-4.177819	-0.786488	2.286516
31	6	0	-4.097316	-2.369797	0.479415
32	6	0	-4.840762	-1.528024	1.301766
33	1	0	-4.753872	-0.138481	2.943001
34	1	0	-4.600955	-2.960922	-0.280196
35	6	0	-2.082959	-0.031855	3.493744
36	1	0	-2.774691	0.676025	3.955596
37	1	0	-1.681820	-0.681353	4.276810
38	1	0	-1.251511	0.516688	3.035301
39	6	0	-6.334718	-1.419930	1.149790
40	1	0	-6.632724	-0.376852	1.007484
41	1	0	-6.685249	-1.995870	0.290794
42	1	0	-6.845472	-1.787479	2.044978
43	6	0	-1.934266	-3.387198	-0.318339
44	1	0	-1.633146	-2.886784	-1.244092
45	1	0	-1.035826	-3.776418	0.168088
46	1	0	-2.563721	-4.232944	-0.601804

47	6	0	-0.319819	-0.561287	-0.730494
48	8	0	0.226520	-1.021153	-1.710110
49	1	0	-1.079722	0.722091	-2.856745
50	6	0	-1.263777	0.601879	-0.711241
51	6	0	-1.846573	0.886291	-2.097838
52	1	0	-2.073611	0.375196	-0.006553
53	1	0	-2.131014	1.940888	-2.142726
54	6	0	-3.061743	0.025219	-2.348645
55	6	0	-4.314433	0.437792	-1.881472
56	6	0	-2.962890	-1.207891	-2.998224
57	6	0	-5.442229	-0.355370	-2.066877
58	1	0	-4.397595	1.394203	-1.368178
59	6	0	-4.088620	-2.011326	-3.175858
60	1	0	-1.994881	-1.534857	-3.371576
61	6	0	-5.332515	-1.585232	-2.715258
62	1	0	-6.408721	-0.013429	-1.708753
63	1	0	-3.994195	-2.966811	-3.683339
64	1	0	-6.211525	-2.205659	-2.861969
65	6	0	-0.476380	1.748126	0.076454
66	8	0	-0.089716	1.243531	1.272747
67	6	0	0.770242	2.168074	-0.762016
68	8	0	0.787647	2.309144	-1.980891
69	6	0	-1.443885	2.942726	0.197068
70	6	0	-1.488885	4.021387	-0.689503
71	6	0	-2.351300	2.907176	1.258957
72	6	0	-2.422214	5.043911	-0.512138
73	1	0	-0.796888	4.061100	-1.525453
74	6	0	-3.289164	3.919611	1.431162
75	1	0	-2.299245	2.070879	1.948226
76	6	0	-3.326094	4.996060	0.545181
77	1	0	-2.441124	5.879238	-1.205566
78	1	0	-3.989004	3.873500	2.260496
79	1	0	-4.053658	5.790356	0.679463
80	7	0	1.831334	2.331339	0.072739
81	1	0	1.536239	2.086198	1.027700
82	6	0	3.182590	2.539737	-0.228928
83	6	0	4.040908	2.878259	0.826651
84	6	0	3.707166	2.361518	-1.515885
85	6	0	5.403602	3.031603	0.602187
86	1	0	3.626036	3.022590	1.820552
87	6	0	5.075096	2.522799	-1.725408
88	1	0	3.042666	2.104183	-2.329956
89	6	0	5.930377	2.854648	-0.677081
90	1	0	6.054233	3.292863	1.430643

91	1	0	5.474616	2.381223	-2.724763
92	1	0	6.993739	2.975773	-0.853608

M4SR

Total energy= -2219.82801271
Sum of electronic and zero-point Energies= -2219.069519
Sum of electronic and thermal Energies= -2219.026459
Sum of electronic and thermal Enthalpies= -2219.025514
Sum of electronic and thermal Free Energies= -2219.145815

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.046104	-2.250501	0.073702
2	6	0	4.165348	-3.080074	0.161215
3	6	0	5.433175	-2.563696	-0.069101
4	6	0	5.555233	-1.212440	-0.397672
5	6	0	4.427487	-0.398515	-0.506741
6	6	0	3.149735	-0.910828	-0.270646
7	6	0	1.819221	-3.057657	0.431090
8	6	0	2.265678	-4.508447	0.133004
9	6	0	3.751782	-4.494421	0.500150
10	1	0	6.310952	-3.200183	-0.010229
11	1	0	6.538679	-0.792727	-0.584684
12	1	0	4.544907	0.646084	-0.778020
13	1	0	2.264694	-0.286813	-0.388548
14	1	0	1.567065	-2.948268	1.486577
15	1	0	1.673430	-5.250313	0.683525
16	1	0	3.875598	-4.702538	1.568492
17	6	0	0.154967	-3.523782	-1.356600
18	6	0	0.861073	-4.793195	-1.726514
19	6	0	-0.267233	-1.701090	-0.226923
20	1	0	0.881078	-4.900135	-2.811693
21	1	0	4.290948	-5.260425	-0.061811
22	7	0	0.605762	-2.728700	-0.342119
23	7	0	-0.953440	-3.060128	-1.858657
24	7	0	-1.205547	-1.934028	-1.145502
25	8	0	2.187114	-4.757953	-1.262768
26	1	0	0.309250	-5.641440	-1.296858
27	6	0	-2.411314	-1.199619	-1.428925
28	6	0	-2.434460	-0.389202	-2.565852
29	6	0	-3.503232	-1.389474	-0.581496
30	6	0	-3.597109	0.346053	-2.780055

31	6	0	-4.638846	-0.621364	-0.837965
32	6	0	-4.691002	0.266115	-1.914274
33	1	0	-3.644158	1.010000	-3.640000
34	1	0	-5.498703	-0.723458	-0.180589
35	6	0	-1.257013	-0.328379	-3.497674
36	1	0	-0.368626	-0.027547	-2.931281
37	1	0	-1.076175	-1.305515	-3.955650
38	1	0	-1.441541	0.395393	-4.294482
39	6	0	-5.901308	1.130704	-2.150011
40	1	0	-6.224957	1.077499	-3.192937
41	1	0	-6.735621	0.832369	-1.512420
42	1	0	-5.665376	2.177808	-1.934237
43	6	0	-3.450605	-2.385396	0.545593
44	1	0	-3.082111	-3.353073	0.191055
45	1	0	-2.797008	-2.047681	1.358277
46	1	0	-4.443726	-2.525980	0.973020
47	6	0	-0.155991	-0.635044	0.855886
48	8	0	0.666315	-0.861850	1.717091
49	1	0	-0.485496	1.029977	2.911641
50	6	0	-0.992173	0.629052	0.851278
51	6	0	-1.374392	1.037770	2.280909
52	1	0	-1.901743	0.470607	0.265826
53	1	0	-1.737855	2.067283	2.248432
54	6	0	-2.450620	0.148144	2.852393
55	6	0	-3.791087	0.359142	2.510674
56	6	0	-2.135998	-0.912757	3.706206
57	6	0	-4.793724	-0.463244	3.015084
58	1	0	-4.044022	1.181120	1.843863
59	6	0	-3.137470	-1.743961	4.207885
60	1	0	-1.097080	-1.083690	3.977400
61	6	0	-4.468567	-1.520151	3.865402
62	1	0	-5.830056	-0.280009	2.746334
63	1	0	-2.877156	-2.562796	4.871575
64	1	0	-5.248779	-2.163159	4.260150
65	6	0	-0.120475	1.588691	-0.038479
66	8	0	0.365329	0.825290	-1.059792
67	6	0	1.044398	2.240465	0.767833
68	8	0	0.957408	2.687147	1.907485
69	6	0	-1.005901	2.767899	-0.507786
70	6	0	-1.419451	3.811417	0.330056
71	6	0	-1.431383	2.769447	-1.835539
72	6	0	-2.274055	4.804249	-0.144794
73	1	0	-1.045796	3.862415	1.347796
74	6	0	-2.286409	3.760550	-2.312047

75	1	0	-1.061155	1.982767	-2.480873
76	6	0	-2.720942	4.777088	-1.464592
77	1	0	-2.585885	5.606013	0.517938
78	1	0	-2.610414	3.741251	-3.349200
79	1	0	-3.388970	5.550002	-1.832095
80	7	0	2.146558	2.325178	-0.025095
81	1	0	1.963209	1.875941	-0.926961
82	6	0	3.343673	3.011285	0.203240
83	6	0	4.163873	3.276761	-0.902885
84	6	0	3.754447	3.422243	1.477523
85	6	0	5.376046	3.934801	-0.738951
86	1	0	3.837396	2.964262	-1.891372
87	6	0	4.968580	4.088763	1.623747
88	1	0	3.123154	3.216459	2.330305
89	6	0	5.786680	4.348143	0.527567
90	1	0	5.998057	4.130815	-1.606731
91	1	0	5.278726	4.403154	2.615640
92	1	0	6.732171	4.863932	0.656824

M4SS

Total energy= -2219.82085465
Sum of electronic and zero-point Energies= -2219.063129
Sum of electronic and thermal Energies= -2219.019865
Sum of electronic and thermal Enthalpies= -2219.018921
Sum of electronic and thermal Free Energies= -2219.139242

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.467968	-1.572859	-0.572941
2	6	0	-4.658879	-2.284014	-0.741297
3	6	0	-5.851798	-1.608087	-0.952537
4	6	0	-5.835840	-0.212297	-0.973014
5	6	0	-4.649265	0.492566	-0.775890
6	6	0	-3.443801	-0.186410	-0.578893
7	6	0	-2.339167	-2.568431	-0.409793
8	6	0	-3.074237	-3.820188	0.121668
9	6	0	-4.409716	-3.770426	-0.623062
10	1	0	-6.782592	-2.152695	-1.079434
11	1	0	-6.762267	0.332092	-1.126080
12	1	0	-4.661986	1.577942	-0.767892
13	1	0	-2.522037	0.360382	-0.399987
14	1	0	-1.861844	-2.785754	-1.365302

15	1	0	-2.501560	-4.743072	-0.034877
16	1	0	-4.307904	-4.241016	-1.607080
17	6	0	-1.223972	-2.659520	1.804338
18	6	0	-2.221258	-3.660520	2.306213
19	6	0	-0.188724	-1.370368	0.371414
20	1	0	-2.515632	-3.406677	3.325376
21	1	0	-5.181702	-4.304497	-0.064912
22	7	0	-1.270421	-2.172073	0.530049
23	7	0	-0.177528	-2.213923	2.438976
24	7	0	0.453388	-1.417700	1.541532
25	8	0	-3.370894	-3.651090	1.500641
26	1	0	-1.743812	-4.650925	2.313205
27	6	0	1.732517	-0.868344	1.915133
28	6	0	1.797027	0.210494	2.794176
29	6	0	2.862443	-1.549577	1.440972
30	6	0	3.075166	0.695987	3.090581
31	6	0	4.105215	-1.009992	1.748862
32	6	0	4.226886	0.133407	2.547514
33	1	0	3.160398	1.550722	3.758290
34	1	0	4.998641	-1.502150	1.372330
35	6	0	0.589927	0.853077	3.423809
36	1	0	0.470150	1.874716	3.054530
37	1	0	-0.331766	0.318831	3.197975
38	1	0	0.723233	0.889495	4.508246
39	6	0	5.578716	0.741460	2.809391
40	1	0	5.575651	1.336972	3.724645
41	1	0	6.350827	-0.026764	2.893690
42	1	0	5.857259	1.402209	1.981530
43	6	0	2.718881	-2.841060	0.682240
44	1	0	3.695235	-3.300236	0.528726
45	1	0	2.086471	-3.540343	1.239307
46	1	0	2.272955	-2.693767	-0.306814
47	6	0	0.164938	-0.717651	-0.972655
48	8	0	-0.566184	-1.042663	-1.889105
49	1	0	1.327252	-0.047000	-3.242178
50	6	0	1.279187	0.253192	-1.135947
51	6	0	2.058425	-0.011190	-2.433374
52	1	0	1.934023	0.247539	-0.265304
53	1	0	2.682300	0.871031	-2.610619
54	6	0	2.922347	-1.243290	-2.405025
55	6	0	4.196225	-1.196130	-1.828424
56	6	0	2.475828	-2.453787	-2.943490
57	6	0	5.005379	-2.328173	-1.791418
58	1	0	4.551918	-0.257056	-1.408874

59	6	0	3.279398	-3.592768	-2.899409
60	1	0	1.490676	-2.497271	-3.401549
61	6	0	4.546921	-3.532576	-2.325205
62	1	0	5.994915	-2.271189	-1.346997
63	1	0	2.918396	-4.525028	-3.323094
64	1	0	5.176355	-4.416405	-2.298790
65	6	0	0.661164	1.769899	-1.340927
66	8	0	0.208759	1.992494	-2.558093
67	6	0	-0.466921	1.932788	-0.282765
68	8	0	-0.507607	1.330085	0.794687
69	6	0	1.824389	2.708008	-0.917077
70	6	0	2.354828	2.718270	0.374244
71	6	0	2.361365	3.563087	-1.876900
72	6	0	3.418661	3.554671	0.699442
73	1	0	1.927834	2.062268	1.125991
74	6	0	3.427233	4.403062	-1.556381
75	1	0	1.918087	3.536985	-2.867447
76	6	0	3.961293	4.399560	-0.269074
77	1	0	3.823271	3.544921	1.708480
78	1	0	3.844139	5.062328	-2.312402
79	1	0	4.793528	5.051094	-0.020727
80	7	0	-1.396224	2.795068	-0.745367
81	1	0	-1.192289	2.991265	-1.733194
82	6	0	-2.599692	3.212882	-0.168866
83	6	0	-2.981178	2.871890	1.135413
84	6	0	-3.453277	3.996677	-0.957310
85	6	0	-4.214720	3.300408	1.619588
86	1	0	-2.320841	2.268165	1.742892
87	6	0	-4.679545	4.416399	-0.458617
88	1	0	-3.149941	4.262301	-1.965878
89	6	0	-5.071892	4.065789	0.833120
90	1	0	-4.507272	3.025383	2.628244
91	1	0	-5.331065	5.018650	-1.083788
92	1	0	-6.031137	4.390843	1.221443

TS6RR

Total energy= -2219.83046947
Sum of electronic and zero-point Energies= -2219.075323
Sum of electronic and thermal Energies= -2219.032878
Sum of electronic and thermal Enthalpies= -2219.031934
Sum of electronic and thermal Free Energies= -2219.149266

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	3.114522	-2.158583	-0.844065
2	6	0	4.500031	-2.321508	-0.924330
3	6	0	5.039282	-3.486148	-1.453095
4	6	0	4.174472	-4.493626	-1.882914
5	6	0	2.793152	-4.334255	-1.782564
6	6	0	2.248875	-3.157987	-1.264458
7	6	0	2.823923	-0.788419	-0.254818
8	6	0	4.128474	-0.489835	0.529312
9	6	0	5.208109	-1.117254	-0.349857
10	1	0	6.115252	-3.618647	-1.513334
11	1	0	4.580755	-5.414891	-2.287760
12	1	0	2.133020	-5.130770	-2.109436
13	1	0	1.174161	-3.031706	-1.198500
14	1	0	2.647136	-0.034402	-1.029190
15	1	0	4.273728	0.573807	0.731751
16	1	0	5.501117	-0.409392	-1.134044
17	6	0	1.798595	-0.841969	2.026727
18	6	0	3.154184	-0.757017	2.658374
19	6	0	0.356674	-0.732505	0.406647
20	1	0	3.190270	-1.377885	3.553697
21	1	0	6.093210	-1.363982	0.240506
22	7	0	1.674438	-0.751883	0.667791
23	7	0	0.631980	-0.949850	2.600631
24	7	0	-0.255667	-0.884260	1.576773
25	8	0	4.120691	-1.224844	1.749863
26	1	0	3.341577	0.291091	2.934689
27	6	0	-1.651291	-1.169904	1.786338
28	6	0	-2.169871	-2.326136	1.189162
29	6	0	-2.406937	-0.312618	2.594498
30	6	0	-3.523293	-2.588252	1.387552
31	6	0	-3.758854	-0.616672	2.738318
32	6	0	-4.333583	-1.739511	2.139375
33	1	0	-3.955258	-3.472742	0.928707
34	1	0	-4.377958	0.042733	3.341486
35	6	0	-1.318320	-3.283295	0.393178
36	1	0	-1.144342	-2.920288	-0.625184
37	1	0	-0.347012	-3.453116	0.869168
38	1	0	-1.826561	-4.244878	0.306857
39	6	0	-5.795531	-2.043833	2.328950
40	1	0	-6.394488	-1.130990	2.277422
41	1	0	-6.152979	-2.737759	1.564934
42	1	0	-5.970771	-2.498210	3.309400

43	6	0	-1.794358	0.868668	3.297208
44	1	0	-1.261207	0.538172	4.194287
45	1	0	-1.077817	1.387975	2.656444
46	1	0	-2.575618	1.566654	3.605249
47	6	0	-0.260200	-0.429250	-0.949371
48	8	0	0.252015	-0.948650	-1.916525
49	1	0	-2.772845	1.337055	-2.388923
50	6	0	-1.334165	0.608544	-0.990604
51	6	0	-2.275838	0.385132	-2.179000
52	1	0	-1.875374	0.617629	-0.040132
53	1	0	-1.662086	0.144922	-3.049488
54	6	0	-3.314484	-0.678606	-1.928475
55	6	0	-3.123904	-1.997449	-2.348918
56	6	0	-4.503667	-0.350104	-1.269007
57	6	0	-4.101949	-2.965311	-2.122939
58	1	0	-2.206134	-2.259921	-2.871040
59	6	0	-5.489757	-1.308428	-1.057137
60	1	0	-4.655818	0.673788	-0.932833
61	6	0	-5.292077	-2.620395	-1.486158
62	1	0	-3.940281	-3.984792	-2.460245
63	1	0	-6.413802	-1.032586	-0.557345
64	1	0	-6.061337	-3.369618	-1.324404
65	6	0	-0.602835	2.026075	-1.188433
66	8	0	0.010168	2.094262	-2.385118
67	6	0	0.485616	2.182299	-0.065875
68	8	0	0.276073	2.063696	1.147077
69	6	0	-1.672347	3.108793	-0.958279
70	6	0	-2.436733	3.182444	0.211041
71	6	0	-1.885546	4.048419	-1.966001
72	6	0	-3.398243	4.177756	0.363944
73	1	0	-2.270791	2.468234	1.012139
74	6	0	-2.847706	5.045565	-1.813613
75	1	0	-1.281590	3.967320	-2.863126
76	6	0	-3.608084	5.112850	-0.648945
77	1	0	-3.984064	4.224000	1.277164
78	1	0	-3.004863	5.770432	-2.606858
79	1	0	-4.359704	5.886843	-0.529119
80	7	0	1.639956	2.403539	-0.705625
81	1	0	1.267767	2.340238	-1.779470
82	6	0	2.901916	2.617178	-0.159150
83	6	0	4.010183	2.572909	-1.019264
84	6	0	3.105816	2.859882	1.209103
85	6	0	5.296247	2.749394	-0.521319
86	1	0	3.846061	2.391788	-2.077831

87	6	0	4.400755	3.038178	1.692668
88	1	0	2.251581	2.900253	1.871967
89	6	0	5.501393	2.978132	0.839937
90	1	0	6.142164	2.706697	-1.200461
91	1	0	4.547557	3.225383	2.752306
92	1	0	6.504949	3.112918	1.228711

TS4RS

Total energy= -2219.82575709

Sum of electronic and zero-point Energies= -2219.072327

Sum of electronic and thermal Energies= -2219.029262

Sum of electronic and thermal Enthalpies= -2219.028318

Sum of electronic and thermal Free Energies= -2219.149619

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.253949	-2.070717	0.247539
2	6	0	-4.624098	-2.102038	-0.023949
3	6	0	-5.460736	-2.944805	0.694477
4	6	0	-4.904854	-3.766537	1.676247
5	6	0	-3.533892	-3.744516	1.929660
6	6	0	-2.692253	-2.888476	1.217450
7	6	0	-2.609211	-1.039058	-0.656970
8	6	0	-3.609142	-0.965278	-1.834233
9	6	0	-4.964131	-1.152232	-1.150354
10	1	0	-6.525815	-2.975585	0.485953
11	1	0	-5.544281	-4.437062	2.241362
12	1	0	-3.115843	-4.399194	2.687138
13	1	0	-1.627367	-2.863740	1.421756
14	1	0	-2.511333	-0.065028	-0.162131
15	1	0	-3.507423	-0.040768	-2.417142
16	1	0	-5.323757	-0.191983	-0.763041
17	6	0	-1.063244	-1.897514	-2.430428
18	6	0	-2.209285	-2.107086	-3.374029
19	6	0	-0.076005	-1.126960	-0.659932
20	1	0	-2.115032	-3.070477	-3.876813
21	1	0	-5.701902	-1.544508	-1.853444
22	7	0	-1.283396	-1.387728	-1.180946
23	7	0	0.211961	-2.036771	-2.666979
24	7	0	0.812705	-1.561022	-1.542505
25	8	0	-3.426201	-2.103315	-2.669298
26	1	0	-2.179161	-1.308713	-4.128778

27	6	0	2.239412	-1.599452	-1.366409
28	6	0	3.015721	-0.672621	-2.071388
29	6	0	2.756614	-2.508104	-0.441448
30	6	0	4.379487	-0.661976	-1.792141
31	6	0	4.132127	-2.464026	-0.215258
32	6	0	4.949683	-1.541261	-0.864737
33	1	0	5.011669	0.061461	-2.301767
34	1	0	4.565686	-3.150612	0.505711
35	6	0	2.387575	0.291141	-3.042026
36	1	0	3.110590	1.053623	-3.336983
37	1	0	2.050767	-0.234659	-3.941167
38	1	0	1.515006	0.785245	-2.596627
39	6	0	6.426267	-1.482919	-0.577714
40	1	0	6.727402	-0.463025	-0.321108
41	1	0	6.692031	-2.137688	0.254661
42	1	0	7.005652	-1.786049	-1.455014
43	6	0	1.874578	-3.488190	0.289034
44	1	0	1.164500	-3.971414	-0.388710
45	1	0	2.483569	-4.260369	0.761466
46	1	0	1.302860	-2.996840	1.084256
47	6	0	0.168797	-0.414276	0.653782
48	8	0	-0.535960	-0.715144	1.589223
49	1	0	0.908751	0.980205	2.766469
50	6	0	1.176987	0.708255	0.645421
51	6	0	1.730801	0.999373	2.047406
52	1	0	1.997044	0.400287	-0.009141
53	1	0	2.125101	2.018763	2.053264
54	6	0	2.811376	0.014803	2.427087
55	6	0	4.158332	0.314623	2.200203
56	6	0	2.489183	-1.226416	2.985549
57	6	0	5.158233	-0.600176	2.521075
58	1	0	4.426157	1.284958	1.787795
59	6	0	3.485667	-2.149001	3.297593
60	1	0	1.446779	-1.461305	3.188804
61	6	0	4.824493	-1.837066	3.068370
62	1	0	6.199653	-0.344115	2.350577
63	1	0	3.216030	-3.107078	3.732191
64	1	0	5.603006	-2.551270	3.318895
65	6	0	0.447178	1.875719	-0.094370
66	8	0	-0.235311	1.350573	-1.191232
67	6	0	-0.647749	2.485769	0.857371
68	8	0	-0.389291	3.029163	1.931780
69	6	0	1.414431	2.975416	-0.534237
70	6	0	0.859833	4.163948	-1.023053

71	6	0	2.801719	2.827366	-0.571368
72	6	0	1.665903	5.178708	-1.523746
73	1	0	-0.220805	4.284134	-1.012871
74	6	0	3.615357	3.842497	-1.076968
75	1	0	3.273921	1.915793	-0.214662
76	6	0	3.051947	5.021499	-1.551837
77	1	0	1.214742	6.093987	-1.894256
78	1	0	4.692262	3.705451	-1.096510
79	1	0	3.684827	5.812585	-1.941055
80	7	0	-1.820885	2.287489	0.238815
81	1	0	-1.367893	1.760906	-0.756854
82	6	0	-3.097637	2.600918	0.691351
83	6	0	-4.170581	2.394231	-0.191181
84	6	0	-3.367897	3.086727	1.981173
85	6	0	-5.477698	2.655052	0.202486
86	1	0	-3.957122	2.043056	-1.198195
87	6	0	-4.681750	3.344223	2.362313
88	1	0	-2.543224	3.253492	2.661712
89	6	0	-5.743717	3.130438	1.485833
90	1	0	-6.290189	2.490343	-0.499386
91	1	0	-4.875670	3.718107	3.363511
92	1	0	-6.763021	3.335045	1.795804

TS6SR

Total energy= -2219.82230350
Sum of electronic and zero-point Energies= -2219.068145
Sum of electronic and thermal Energies= -2219.025331
Sum of electronic and thermal Enthalpies= -2219.024387
Sum of electronic and thermal Free Energies= -2219.144249

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.434897	-1.701647	0.162896
2	6	0	4.599430	-2.463887	0.292957
3	6	0	5.843995	-1.850590	0.295299
4	6	0	5.905342	-0.463928	0.159448
5	6	0	4.742195	0.292370	0.018987
6	6	0	3.486354	-0.321258	0.020139
7	6	0	2.246931	-2.634236	0.276648
8	6	0	2.845545	-4.001889	-0.129272
9	6	0	4.270386	-3.933137	0.417705
10	1	0	6.751229	-2.439927	0.389467

11	1	0	6.869848	0.034108	0.154409
12	1	0	4.812390	1.369257	-0.091857
13	1	0	2.582704	0.272003	-0.097016
14	1	0	1.881066	-2.673263	1.304272
15	1	0	2.255940	-4.846206	0.249881
16	1	0	4.288275	-4.259129	1.463311
17	6	0	0.787343	-3.086667	-1.686986
18	6	0	1.700123	-4.172092	-2.172012
19	6	0	0.020317	-1.512079	-0.385702
20	1	0	1.850460	-4.071872	-3.248088
21	1	0	4.932557	-4.585046	-0.156337
22	7	0	1.071471	-2.344731	-0.575845
23	7	0	-0.380206	-2.776009	-2.174996
24	7	0	-0.845990	-1.804150	-1.355695
25	8	0	2.951152	-4.071100	-1.543904
26	1	0	1.224522	-5.142383	-1.971214
27	6	0	-2.198517	-1.344805	-1.546159
28	6	0	-2.478844	-0.522164	-2.638057
29	6	0	-3.167764	-1.825890	-0.661965
30	6	0	-3.795183	-0.083754	-2.762681
31	6	0	-4.464896	-1.341590	-0.824913
32	6	0	-4.788066	-0.453784	-1.853141
33	1	0	-4.048346	0.577293	-3.588239
34	1	0	-5.237244	-1.674354	-0.136048
35	6	0	-1.411417	-0.133436	-3.622338
36	1	0	-0.585554	0.350849	-3.092477
37	1	0	-1.026430	-1.014509	-4.143952
38	1	0	-1.815860	0.557216	-4.364928
39	6	0	-6.179100	0.107211	-1.985051
40	1	0	-6.516065	0.083152	-3.024434
41	1	0	-6.893138	-0.448444	-1.374287
42	1	0	-6.194947	1.152443	-1.659108
43	6	0	-2.825049	-2.834348	0.402844
44	1	0	-2.253735	-3.666712	-0.020999
45	1	0	-2.235756	-2.395386	1.216554
46	1	0	-3.735749	-3.231833	0.851820
47	6	0	-0.064610	-0.537852	0.781784
48	8	0	0.816805	-0.650975	1.604836
49	1	0	-0.593215	0.948531	2.927109
50	6	0	-1.133984	0.530222	0.878752
51	6	0	-1.502695	0.793499	2.345582
52	1	0	-2.028190	0.211907	0.336737
53	1	0	-2.075320	1.723179	2.382393
54	6	0	-2.335934	-0.330704	2.909328

55	6	0	-3.701108	-0.404658	2.609707
56	6	0	-1.765165	-1.338329	3.691080
57	6	0	-4.478294	-1.458171	3.080404
58	1	0	-4.152121	0.374072	1.997569
59	6	0	-2.540307	-2.398934	4.160059
60	1	0	-0.706079	-1.287777	3.930990
61	6	0	-3.897806	-2.461552	3.856289
62	1	0	-5.537239	-1.497849	2.842545
63	1	0	-2.083036	-3.173643	4.767920
64	1	0	-4.501888	-3.285055	4.223602
65	6	0	-0.563820	1.723236	0.043496
66	8	0	-0.013016	1.175454	-1.108742
67	6	0	0.603146	2.474834	0.775320
68	8	0	0.536326	2.914220	1.927438
69	6	0	-1.689052	2.724859	-0.246769
70	6	0	-2.159409	3.645076	0.698524
71	6	0	-2.286401	2.697044	-1.507486
72	6	0	-3.228275	4.486010	0.394086
73	1	0	-1.665120	3.719175	1.661646
74	6	0	-3.357396	3.533632	-1.810887
75	1	0	-1.884437	2.014350	-2.245434
76	6	0	-3.839187	4.426951	-0.856632
77	1	0	-3.581012	5.194669	1.137374
78	1	0	-3.812258	3.490464	-2.796731
79	1	0	-4.674380	5.080305	-1.089370
80	7	0	1.584485	2.560008	-0.130558
81	1	0	1.055609	1.870003	-0.980335
82	6	0	2.828887	3.160673	0.009120
83	6	0	3.568173	3.410192	-1.158470
84	6	0	3.393956	3.486217	1.252648
85	6	0	4.844645	3.953584	-1.087398
86	1	0	3.124567	3.158986	-2.117553
87	6	0	4.674989	4.028177	1.310447
88	1	0	2.821850	3.299615	2.152622
89	6	0	5.410913	4.261398	0.149945
90	1	0	5.401296	4.134354	-2.002099
91	1	0	5.105254	4.265991	2.279070
92	1	0	6.409387	4.682025	0.208399

TS6SS

Total energy= -2219.81791808
Sum of electronic and zero-point Energies= -2219.063727
Sum of electronic and thermal Energies= -2219.020858

Sum of electronic and thermal Enthalpies= -2219.019914
Sum of electronic and thermal Free Energies= -2219.139956

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.524794	-1.517679	0.506116
2	6	0	4.716831	-2.226633	0.675806
3	6	0	5.916403	-1.548465	0.836152
4	6	0	5.905113	-0.153107	0.804167
5	6	0	4.716914	0.548649	0.604659
6	6	0	3.505212	-0.131657	0.458106
7	6	0	2.390354	-2.515323	0.408266
8	6	0	3.109398	-3.789992	-0.090203
9	6	0	4.462030	-3.715531	0.620171
10	1	0	6.847669	-2.092002	0.964185
11	1	0	6.836124	0.393350	0.917312
12	1	0	4.731871	1.632425	0.555801
13	1	0	2.583347	0.415846	0.279755
14	1	0	1.935561	-2.694710	1.382976
15	1	0	2.538842	-4.704217	0.116037
16	1	0	4.382695	-4.148859	1.623195
17	6	0	1.215450	-2.702616	-1.768541
18	6	0	2.202091	-3.721226	-2.255688
19	6	0	0.218277	-1.351526	-0.367609
20	1	0	2.468556	-3.507736	-3.291630
21	1	0	5.219263	-4.272603	0.064215
22	7	0	1.298928	-2.155834	-0.521292
23	7	0	0.147083	-2.290391	-2.390187
24	7	0	-0.460861	-1.456457	-1.513019
25	8	0	3.371850	-3.675117	-1.481432
26	1	0	1.728220	-4.712119	-2.209414
27	6	0	-1.757182	-0.939900	-1.877368
28	6	0	-1.858856	0.083587	-2.817129
29	6	0	-2.864228	-1.614535	-1.343383
30	6	0	-3.152097	0.525642	-3.116703
31	6	0	-4.122915	-1.114732	-1.654311
32	6	0	-4.282065	-0.024115	-2.517659
33	1	0	-3.267571	1.335049	-3.834227
34	1	0	-4.999217	-1.601078	-1.232908
35	6	0	-0.677612	0.709616	-3.507679
36	1	0	-0.569238	1.751289	-3.196359
37	1	0	0.257752	0.204410	-3.272123
38	1	0	-0.834370	0.682303	-4.589255

39	6	0	-5.650924	0.539268	-2.790128
40	1	0	-5.679811	1.069101	-3.744544
41	1	0	-6.409062	-0.247307	-2.802529
42	1	0	-5.924853	1.251171	-2.004030
43	6	0	-2.681422	-2.866877	-0.528900
44	1	0	-3.645399	-3.338175	-0.338361
45	1	0	-2.045666	-3.578321	-1.066474
46	1	0	-2.221058	-2.669945	0.444533
47	6	0	-0.076567	-0.626559	0.952203
48	8	0	0.735030	-0.838634	1.828762
49	1	0	-1.161805	-0.014180	3.261435
50	6	0	-1.241152	0.296862	1.147620
51	6	0	-1.936805	0.032493	2.494778
52	1	0	-1.945631	0.204125	0.320105
53	1	0	-2.541954	0.919305	2.709893
54	6	0	-2.811421	-1.192507	2.515698
55	6	0	-4.095770	-1.144517	1.962682
56	6	0	-2.366133	-2.392977	3.075066
57	6	0	-4.917547	-2.267535	1.971432
58	1	0	-4.449512	-0.212444	1.525950
59	6	0	-3.182999	-3.523784	3.076486
60	1	0	-1.372374	-2.437277	3.514411
61	6	0	-4.461079	-3.463053	2.527026
62	1	0	-5.915087	-2.210998	1.545532
63	1	0	-2.823299	-4.449251	3.515650
64	1	0	-5.100256	-4.340140	2.534795
65	6	0	-0.710728	1.808985	1.216597
66	8	0	-0.192475	2.147479	2.418939
67	6	0	0.427102	1.970492	0.163104
68	8	0	0.431692	1.390759	-0.934690
69	6	0	-1.901581	2.695474	0.805647
70	6	0	-2.473667	2.615326	-0.465508
71	6	0	-2.429939	3.594027	1.730917
72	6	0	-3.567031	3.405953	-0.805048
73	1	0	-2.047596	1.930219	-1.190187
74	6	0	-3.527095	4.387107	1.395062
75	1	0	-1.958828	3.648963	2.706645
76	6	0	-4.100849	4.294489	0.128777
77	1	0	-3.999980	3.327639	-1.799199
78	1	0	-3.935785	5.080229	2.124562
79	1	0	-4.956122	4.910818	-0.130482
80	7	0	1.344405	2.750259	0.735442
81	1	0	0.900234	2.727805	1.813271
82	6	0	2.552081	3.203783	0.215156

83	6	0	2.950772	2.965299	-1.110008
84	6	0	3.400040	3.934262	1.061642
85	6	0	4.180557	3.439919	-1.557709
86	1	0	2.297084	2.400248	-1.762095
87	6	0	4.624890	4.401702	0.600978
88	1	0	3.084522	4.121911	2.083634
89	6	0	5.026560	4.154224	-0.711980
90	1	0	4.480736	3.243078	-2.582709
91	1	0	5.269187	4.962100	1.271546
92	1	0	5.983923	4.517182	-1.070698

M5RR

Total energy= -2219.82837182

Sum of electronic and zero-point Energies= -2219.070264

Sum of electronic and thermal Energies= -2219.027228

Sum of electronic and thermal Enthalpies= -2219.026284

Sum of electronic and thermal Free Energies= -2219.145728

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.905767	-1.954488	-0.620042
2	6	0	-4.271879	-1.991114	-0.912208
3	6	0	-5.014596	-3.130236	-0.637092
4	6	0	-4.368056	-4.236125	-0.080708
5	6	0	-3.001157	-4.198822	0.190596
6	6	0	-2.252897	-3.049239	-0.073733
7	6	0	-2.391615	-0.568319	-0.954857
8	6	0	-3.391328	-0.101939	-2.031318
9	6	0	-4.713507	-0.682450	-1.527520
10	1	0	-6.076030	-3.166286	-0.863010
11	1	0	-4.933390	-5.137185	0.134204
12	1	0	-2.512323	-5.070317	0.613435
13	1	0	-1.192797	-3.011160	0.153261
14	1	0	-2.400936	0.084215	-0.076540
15	1	0	-3.396869	0.986337	-2.173107
16	1	0	-5.139205	-0.018194	-0.765024
17	6	0	-0.752984	-0.512346	-2.835388
18	6	0	-1.867647	-0.395832	-3.834708
19	6	0	0.143843	-0.404463	-0.857370
20	1	0	-1.682580	-1.054423	-4.684306
21	1	0	-5.433180	-0.791495	-2.341461
22	7	0	-1.030436	-0.506886	-1.496692

23	7	0	0.534146	-0.498556	-3.048076
24	7	0	1.078076	-0.443695	-1.802091
25	8	0	-3.095306	-0.764970	-3.257597
26	1	0	-1.886954	0.643670	-4.192818
27	6	0	2.493328	-0.602132	-1.590565
28	6	0	2.939429	-1.781778	-0.982735
29	6	0	3.347510	0.421645	-2.012968
30	6	0	4.307048	-1.878287	-0.729392
31	6	0	4.700086	0.276171	-1.717603
32	6	0	5.192902	-0.856401	-1.064284
33	1	0	4.683868	-2.776774	-0.248924
34	1	0	5.386383	1.066937	-2.010537
35	6	0	2.027772	-2.933872	-0.642327
36	1	0	1.667817	-2.866252	0.388236
37	1	0	1.160791	-2.984572	-1.307570
38	1	0	2.578279	-3.871568	-0.738282
39	6	0	6.662418	-0.986121	-0.764526
40	1	0	6.842001	-1.764310	-0.019573
41	1	0	7.220092	-1.245156	-1.670055
42	1	0	7.067251	-0.043754	-0.386427
43	6	0	2.837186	1.603346	-2.788394
44	1	0	2.854272	1.380328	-3.860282
45	1	0	1.810447	1.859015	-2.521394
46	1	0	3.464540	2.478650	-2.611602
47	6	0	0.379821	-0.351585	0.649478
48	8	0	-0.002417	-1.321837	1.260444
49	1	0	1.914078	1.255726	3.193016
50	6	0	1.203461	0.781517	1.239516
51	6	0	1.646557	0.349772	2.649779
52	1	0	2.095244	0.884505	0.601473
53	1	0	0.801540	-0.119552	3.159558
54	6	0	2.837907	-0.578780	2.614753
55	6	0	2.708628	-1.960780	2.769334
56	6	0	4.117258	-0.042847	2.427002
57	6	0	3.831590	-2.787828	2.743620
58	1	0	1.719759	-2.386660	2.918484
59	6	0	5.240466	-0.862875	2.409645
60	1	0	4.226349	1.033218	2.307446
61	6	0	5.100856	-2.240985	2.570492
62	1	0	3.713258	-3.859898	2.870322
63	1	0	6.226356	-0.426874	2.277396
64	1	0	5.976413	-2.883249	2.561551
65	6	0	0.537457	2.208498	1.254399
66	8	0	1.372845	3.034841	2.024087

67	6	0	-0.844644	2.180496	1.968438
68	8	0	-1.008069	3.082894	2.824601
69	6	0	0.416763	2.834479	-0.147186
70	6	0	1.409389	3.731098	-0.559901
71	6	0	-0.669180	2.612604	-1.001861
72	6	0	1.322851	4.382442	-1.787091
73	1	0	2.238313	3.933945	0.107706
74	6	0	-0.744565	3.247494	-2.241970
75	1	0	-1.488240	1.987886	-0.661773
76	6	0	0.250171	4.136799	-2.640364
77	1	0	2.101219	5.081026	-2.079137
78	1	0	-1.605957	3.075688	-2.881590
79	1	0	0.181371	4.642437	-3.598137
80	7	0	-1.634204	1.203008	1.579678
81	1	0	0.722926	3.449501	2.638146
82	6	0	-2.965071	1.148285	2.012490
83	6	0	-3.559695	-0.120668	2.132860
84	6	0	-3.778896	2.277894	2.217749
85	6	0	-4.912950	-0.260456	2.424184
86	1	0	-2.932036	-0.996688	1.988237
87	6	0	-5.130305	2.131360	2.513308
88	1	0	-3.333620	3.262989	2.142145
89	6	0	-5.710962	0.866584	2.613321
90	1	0	-5.342734	-1.255412	2.502362
91	1	0	-5.740091	3.018235	2.663190
92	1	0	-6.767101	0.762651	2.840237

Total energy= -1969.84394663
Sum of electronic and zero-point Energies= -1969.183390
Sum of electronic and thermal Energies= -1969.142224
Sum of electronic and thermal Enthalpies= -1969.141280
Sum of electronic and thermal Free Energies= -1969.259413

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.678312	-0.283105	0.681680
2	6	0	-6.021294	-0.384240	0.326689
3	6	0	-7.010722	0.001526	1.226899
4	6	0	-6.630627	0.492527	2.474339
5	6	0	-5.281287	0.597208	2.822014
6	6	0	-4.289614	0.208338	1.924354

7	6	0	-3.787903	-0.753341	-0.448606
8	6	0	-4.755967	-0.837489	-1.683150
9	6	0	-6.169298	-0.932621	-1.070402
10	1	0	-8.060320	-0.069132	0.958185
11	1	0	-7.391149	0.803406	3.183419
12	1	0	-5.003857	0.984031	3.796814
13	1	0	-3.238410	0.275397	2.191116
14	1	0	-4.512377	-1.705539	-2.296329
15	1	0	-6.882647	-0.376715	-1.685156
16	1	0	-3.314328	-1.719340	-0.244556
17	1	0	-6.500941	-1.976141	-1.045412
18	6	0	-2.968639	1.371188	-1.384747
19	6	0	-1.421044	0.177800	-0.394013
20	7	0	-1.886996	2.084612	-1.492413
21	7	0	-2.723679	0.205259	-0.719954
22	7	0	-0.933362	1.328504	-0.857543
23	6	0	-4.330865	1.520128	-1.979829
24	1	0	-5.066854	1.806260	-1.217366
25	1	0	-4.321576	2.269141	-2.771056
26	8	0	-4.632460	0.267357	-2.572201
27	6	0	0.419853	1.810746	-0.778928
28	6	0	1.348772	1.323541	-1.696134
29	6	0	0.729902	2.726049	0.229559
30	6	0	2.654839	1.798444	-1.581244
31	6	0	2.049627	3.158587	0.309944
32	6	0	3.021945	2.701979	-0.583971
33	1	0	3.406816	1.432086	-2.275302
34	1	0	2.330752	3.856183	1.094898
35	6	0	0.954387	0.303577	-2.729235
36	1	0	0.515852	-0.584240	-2.255575
37	1	0	0.208577	0.714198	-3.418465
38	1	0	1.826046	-0.004749	-3.309474
39	6	0	4.447822	3.165183	-0.439192
40	1	0	4.507242	4.257163	-0.422125
41	1	0	4.862540	2.799431	0.506702
42	1	0	5.071204	2.801300	-1.259774
43	6	0	-0.324946	3.193819	1.196426
44	1	0	-1.141234	3.701765	0.674376
45	1	0	-0.762766	2.349087	1.740383
46	1	0	0.101658	3.882705	1.926501
47	6	0	3.087599	-1.337729	0.798048
48	6	0	1.674121	-1.505016	0.309435
49	1	0	3.299248	-2.093227	1.564173
50	6	0	0.636371	-0.779177	0.704956

51	1	0	1.498099	-2.291097	-0.420976
52	1	0	0.749197	0.017478	1.438245
53	6	0	-0.751225	-1.076343	0.171553
54	8	0	-0.818836	-2.000369	-0.825160
55	1	0	-1.380400	-1.336079	1.053794
56	6	0	4.101601	-1.499999	-0.323757
57	6	0	4.219835	-2.742181	-0.951588
58	6	0	4.918022	-0.450155	-0.737739
59	6	0	5.133460	-2.926729	-1.984543
60	1	0	3.596632	-3.572187	-0.627617
61	6	0	5.834560	-0.634031	-1.771705
62	1	0	4.830023	0.522151	-0.263534
63	6	0	5.943786	-1.871052	-2.399774
64	1	0	5.216345	-3.897583	-2.462529
65	1	0	6.463401	0.194492	-2.083541
66	1	0	6.658776	-2.015010	-3.203137
67	8	0	3.182510	-0.037670	1.401227
68	6	0	4.207617	0.263950	2.199338
69	8	0	4.387588	1.385594	2.607078
70	8	0	4.977925	-0.786610	2.480624
71	6	0	6.102709	-0.500375	3.320455
72	1	0	5.765230	-0.093562	4.274424
73	1	0	6.609008	-1.451924	3.464429
74	1	0	6.762208	0.216969	2.829562
75	8	0	-3.020598	-2.557089	2.363040
76	1	0	-2.786701	-3.098277	1.572735
77	1	0	-3.947386	-2.325362	2.241838
78	8	0	-2.216330	-3.802684	0.118992
79	1	0	-2.840628	-4.075663	-0.560873
80	1	0	-1.587907	-3.080328	-0.331022

M5RS

Total energy= -1969.84597035
Sum of electronic and zero-point Energies= -1969.184645
Sum of electronic and thermal Energies= -1969.143402
Sum of electronic and thermal Enthalpies= -1969.142458
Sum of electronic and thermal Free Energies= -1969.260419

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.385381	2.546314	-0.211695
2	6	0	-2.025594	3.682587	-0.705763

3	6	0	-3.125273	4.213469	-0.039233
4	6	0	-3.563310	3.600145	1.133198
5	6	0	-2.906335	2.475250	1.636872
6	6	0	-1.807793	1.936911	0.965908
7	6	0	-0.246955	2.153271	-1.131518
8	6	0	-0.016669	3.425192	-2.017066
9	6	0	-1.365562	4.169038	-1.971383
10	1	0	-3.625391	5.099078	-0.419670
11	1	0	-4.414402	4.009208	1.668820
12	1	0	-3.240844	2.018150	2.563664
13	1	0	-1.295900	1.065429	1.362123
14	1	0	0.259061	3.132830	-3.031015
15	1	0	-1.202540	5.249604	-1.993141
16	1	0	-0.480853	1.289995	-1.759620
17	1	0	-1.967547	3.907019	-2.848345
18	6	0	1.809876	2.785006	0.069407
19	6	0	1.578116	0.629369	-0.226507
20	7	0	2.898777	2.270317	0.561619
21	7	0	0.981868	1.815656	-0.421840
22	7	0	2.728089	0.920439	0.376506
23	6	0	1.400373	4.195212	-0.200207
24	1	0	0.562545	4.488467	0.444831
25	1	0	2.236009	4.875228	-0.038634
26	8	0	1.061836	4.248407	-1.576496
27	6	0	3.807555	0.007080	0.636850
28	6	0	3.972266	-0.502611	1.923521
29	6	0	4.644681	-0.312065	-0.437284
30	6	0	5.041647	-1.375294	2.128298
31	6	0	5.699582	-1.185852	-0.181002
32	6	0	5.911235	-1.725160	1.092693
33	1	0	5.196030	-1.793248	3.119411
34	1	0	6.369135	-1.455750	-0.993525
35	6	0	3.021389	-0.130696	3.028391
36	1	0	2.939710	0.955357	3.128098
37	1	0	2.018463	-0.519478	2.823692
38	1	0	3.357451	-0.543462	3.980247
39	6	0	7.032048	-2.703504	1.326530
40	1	0	7.308464	-2.743836	2.381832
41	1	0	6.725148	-3.708932	1.021004
42	1	0	7.915940	-2.436033	0.743256
43	6	0	4.398412	0.274155	-1.801831
44	1	0	3.392504	0.024903	-2.160054
45	1	0	4.478242	1.365855	-1.771788
46	1	0	5.132515	-0.102020	-2.516505

47	6	0	-2.760968	-1.223591	-0.244156
48	6	0	-1.373435	-1.088185	-0.795114
49	1	0	-3.357691	-0.379744	-0.605902
50	6	0	-0.259669	-0.972397	-0.080814
51	1	0	-1.291088	-1.046368	-1.879611
52	1	0	-0.276454	-1.030628	1.006513
53	6	0	1.077452	-0.708230	-0.760136
54	8	0	1.036703	-0.598432	-2.114157
55	1	0	1.797621	-1.463115	-0.382862
56	6	0	-3.437858	-2.521819	-0.631861
57	6	0	-4.696866	-2.517959	-1.228424
58	6	0	-2.798319	-3.736598	-0.374509
59	6	0	-5.313221	-3.719717	-1.572460
60	1	0	-5.195844	-1.571452	-1.418044
61	6	0	-3.417094	-4.936422	-0.707225
62	1	0	-1.811854	-3.732423	0.081821
63	6	0	-4.674989	-4.928877	-1.309972
64	1	0	-6.291945	-3.710613	-2.041490
65	1	0	-2.916571	-5.877777	-0.504734
66	1	0	-5.155071	-5.865252	-1.575925
67	8	0	-2.666451	-1.131074	1.196593
68	6	0	-3.683685	-0.648977	1.909658
69	8	0	-3.608863	-0.503813	3.105340
70	8	0	-4.749862	-0.348677	1.166899
71	6	0	-5.852719	0.206853	1.891495
72	1	0	-5.573668	1.175881	2.310670
73	1	0	-6.651346	0.323643	1.162484
74	1	0	-6.154486	-0.467088	2.693759
75	8	0	3.158317	-3.436234	-0.157788
76	1	0	3.009180	-3.130613	-1.081510
77	1	0	3.839917	-2.841931	0.175559
78	8	0	2.607400	-2.477617	-2.657904
79	1	0	3.362256	-2.095827	-3.116751
80	1	0	1.931924	-1.701823	-2.530528

M5SR

Total energy= -2219.82561245
Sum of electronic and zero-point Energies= -2219.068962
Sum of electronic and thermal Energies= -2219.026110
Sum of electronic and thermal Enthalpies= -2219.025166
Sum of electronic and thermal Free Energies= -2219.144620

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	3.452655	-0.632645	-0.549927
2	6	0	4.820428	-0.803196	-0.329748
3	6	0	5.737151	-0.190024	-1.170450
4	6	0	5.260173	0.572631	-2.240410
5	6	0	3.892256	0.703857	-2.471491
6	6	0	2.968569	0.094066	-1.621174
7	6	0	2.699722	-1.374333	0.533390
8	6	0	3.701334	-2.489922	0.888783
9	6	0	5.041371	-1.747841	0.832857
10	1	0	6.804537	-0.316961	-1.015394
11	1	0	5.965833	1.053510	-2.910785
12	1	0	3.537647	1.292159	-3.311394
13	1	0	1.901632	0.195689	-1.788380
14	1	0	2.484937	-0.731290	1.392885
15	1	0	3.481976	-2.984990	1.842272
16	1	0	5.200221	-1.198593	1.768623
17	6	0	1.360674	-3.202198	-0.483820
18	6	0	2.533770	-4.137958	-0.398241
19	6	0	0.210861	-1.424510	0.042367
20	1	0	2.641057	-4.698136	-1.327876
21	1	0	5.870245	-2.443955	0.688048
22	7	0	1.438127	-1.963570	0.087304
23	7	0	0.150261	-3.447441	-0.901803
24	7	0	-0.552938	-2.328136	-0.568432
25	8	0	3.733303	-3.436934	-0.177833
26	1	0	2.328283	-4.846037	0.417301
27	6	0	-1.947568	-2.204540	-0.905522
28	6	0	-2.266695	-1.945483	-2.242654
29	6	0	-2.901752	-2.324846	0.108456
30	6	0	-3.611272	-1.735311	-2.540796
31	6	0	-4.232131	-2.103890	-0.248643
32	6	0	-4.600978	-1.787359	-1.555930
33	1	0	-3.889933	-1.518621	-3.569081
34	1	0	-4.995093	-2.182271	0.521365
35	6	0	-1.222214	-1.936953	-3.325139
36	1	0	-0.269303	-1.547099	-2.964429
37	1	0	-1.054863	-2.953348	-3.695563
38	1	0	-1.552677	-1.319319	-4.162151
39	6	0	-6.037432	-1.488714	-1.895008
40	1	0	-6.257810	-1.729122	-2.937140
41	1	0	-6.719907	-2.051332	-1.254286
42	1	0	-6.246661	-0.423659	-1.747929

43	6	0	-2.537003	-2.654224	1.532209
44	1	0	-1.637394	-3.272517	1.590157
45	1	0	-2.366401	-1.744747	2.119054
46	1	0	-3.358036	-3.194480	2.007348
47	6	0	-0.276750	-0.299309	0.968489
48	8	0	-0.012538	-0.526588	2.127279
49	1	0	-0.832046	1.885343	2.246786
50	6	0	-1.228307	0.755779	0.462012
51	6	0	-1.701132	1.615954	1.643021
52	1	0	-2.094892	0.207060	0.060042
53	1	0	-2.133206	2.539035	1.246734
54	6	0	-2.742614	0.895429	2.469051
55	6	0	-3.999168	0.626947	1.915383
56	6	0	-2.475355	0.454294	3.766737
57	6	0	-4.962094	-0.074157	2.635748
58	1	0	-4.219092	0.967594	0.904156
59	6	0	-3.436965	-0.247007	4.492198
60	1	0	-1.497316	0.646154	4.198206
61	6	0	-4.681302	-0.517450	3.927213
62	1	0	-5.932981	-0.270843	2.190152
63	1	0	-3.211552	-0.586492	5.498445
64	1	0	-5.429683	-1.065806	4.490473
65	6	0	-0.664771	1.530201	-0.748446
66	8	0	-0.507915	0.550784	-1.785672
67	6	0	0.753536	2.105587	-0.512631
68	8	0	1.228718	2.740576	-1.481936
69	6	0	-1.682475	2.566422	-1.206808
70	6	0	-1.519838	3.931924	-0.969932
71	6	0	-2.850096	2.118745	-1.832451
72	6	0	-2.513312	4.834281	-1.345545
73	1	0	-0.607968	4.289858	-0.502740
74	6	0	-3.843432	3.019299	-2.206153
75	1	0	-2.969922	1.055655	-2.032005
76	6	0	-3.677296	4.381556	-1.961762
77	1	0	-2.374307	5.894448	-1.158559
78	1	0	-4.746039	2.658429	-2.690089
79	1	0	-4.449465	5.086249	-2.253909
80	7	0	1.269934	1.725021	0.642959
81	1	0	-0.020320	1.016245	-2.484970
82	6	0	2.576889	2.019871	1.028718
83	6	0	3.554324	2.698211	0.271083
84	6	0	2.951614	1.551614	2.305170
85	6	0	4.844908	2.855341	0.768232
86	1	0	3.287759	3.064649	-0.710494

87	6	0	4.244577	1.707989	2.790380
88	1	0	2.188015	1.054880	2.900037
89	6	0	5.207329	2.359813	2.020047
90	1	0	5.584820	3.367501	0.158285
91	1	0	4.499509	1.327780	3.776100
92	1	0	6.219031	2.485925	2.392632

M5SS

Total energy= -2219.82791412
Sum of electronic and zero-point Energies= -2219.068558
Sum of electronic and thermal Energies= -2219.026049
Sum of electronic and thermal Enthalpies= -2219.025105
Sum of electronic and thermal Free Energies= -2219.141803

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.737871	0.930511	-0.603449
2	6	0	5.026289	1.460681	-0.487939
3	6	0	6.105467	0.832047	-1.094274
4	6	0	5.880948	-0.342769	-1.812385
5	6	0	4.593485	-0.863786	-1.932348
6	6	0	3.504596	-0.221457	-1.341847
7	6	0	2.771672	1.850060	0.117537
8	6	0	3.697902	2.619346	1.093602
9	6	0	5.013012	2.732008	0.326481
10	1	0	7.106565	1.241737	-0.999267
11	1	0	6.715398	-0.855762	-2.279982
12	1	0	4.427543	-1.783104	-2.484453
13	1	0	2.506691	-0.625608	-1.452676
14	1	0	2.297601	2.543482	-0.580198
15	1	0	3.270692	3.581829	1.403127
16	1	0	4.998833	3.616229	-0.319985
17	6	0	1.664600	1.218639	2.266105
18	6	0	2.844738	1.678868	3.065109
19	6	0	0.446426	0.788100	0.510264
20	1	0	3.077367	0.938784	3.832966
21	1	0	5.851804	2.827189	1.019483
22	7	0	1.666767	1.229582	0.897465
23	7	0	0.516603	0.822803	2.737467
24	7	0	-0.233738	0.566019	1.636476
25	8	0	3.964128	1.811789	2.230891
26	1	0	2.590606	2.629144	3.555747

27	6	0	-1.646271	0.318223	1.803940
28	6	0	-2.483503	1.434173	1.689647
29	6	0	-2.100566	-0.964352	2.109633
30	6	0	-3.854602	1.205183	1.756546
31	6	0	-3.483355	-1.132520	2.184186
32	6	0	-4.368874	-0.076755	1.975580
33	1	0	-4.534196	2.046317	1.639360
34	1	0	-3.874306	-2.126175	2.384942
35	6	0	-1.911502	2.815832	1.513578
36	1	0	-1.142615	3.013905	2.267420
37	1	0	-1.461044	2.949396	0.523254
38	1	0	-2.695985	3.565881	1.613629
39	6	0	-5.857020	-0.302741	2.018145
40	1	0	-6.348693	0.188351	1.173644
41	1	0	-6.092378	-1.368592	1.980315
42	1	0	-6.287966	0.110986	2.935330
43	6	0	-1.153503	-2.098747	2.376457
44	1	0	-0.519371	-2.272556	1.503375
45	1	0	-0.507372	-1.865137	3.229573
46	1	0	-1.711206	-3.010213	2.598865
47	6	0	0.032540	0.674503	-0.948445
48	8	0	0.834895	1.115752	-1.744161
49	1	0	-1.072335	1.153148	-3.276897
50	6	0	-1.336107	0.167816	-1.378974
51	6	0	-1.843185	1.096855	-2.506208
52	1	0	-2.020060	0.237053	-0.532997
53	1	0	-2.710782	0.624687	-2.969476
54	6	0	-2.216546	2.473249	-2.015572
55	6	0	-3.477357	2.695292	-1.450261
56	6	0	-1.327026	3.547388	-2.111267
57	6	0	-3.843649	3.958665	-0.996551
58	1	0	-4.178811	1.867170	-1.370109
59	6	0	-1.687892	4.813424	-1.650353
60	1	0	-0.349163	3.386359	-2.557874
61	6	0	-2.947206	5.022519	-1.093540
62	1	0	-4.828651	4.113909	-0.566289
63	1	0	-0.987417	5.638338	-1.736590
64	1	0	-3.231576	6.008903	-0.741372
65	6	0	-1.313940	-1.336829	-1.856731
66	8	0	-1.530971	-1.388182	-3.247946
67	6	0	0.045208	-2.045970	-1.593139
68	8	0	0.419353	-2.805008	-2.515116
69	6	0	-2.447570	-2.108893	-1.161670
70	6	0	-2.239854	-3.319489	-0.499781

71	6	0	-3.757647	-1.627112	-1.269081
72	6	0	-3.310931	-4.018927	0.058151
73	1	0	-1.236386	-3.724235	-0.407524
74	6	0	-4.827903	-2.322326	-0.718908
75	1	0	-3.947638	-0.697097	-1.797993
76	6	0	-4.607018	-3.524484	-0.047733
77	1	0	-3.126193	-4.956933	0.573048
78	1	0	-5.834640	-1.926509	-0.814266
79	1	0	-5.439235	-4.070003	0.386804
80	7	0	0.579599	-1.782941	-0.412231
81	1	0	-0.880475	-2.065759	-3.530810
82	6	0	1.727809	-2.443265	0.045346
83	6	0	2.192421	-2.071386	1.322765
84	6	0	2.465309	-3.428037	-0.644963
85	6	0	3.343225	-2.617488	1.874516
86	1	0	1.615010	-1.348025	1.889841
87	6	0	3.613818	-3.978113	-0.079725
88	1	0	2.135656	-3.741872	-1.624500
89	6	0	4.071403	-3.577134	1.172740
90	1	0	3.670354	-2.294539	2.858876
91	1	0	4.162930	-4.732079	-0.637592
92	1	0	4.973320	-4.006467	1.596558

TS7RR

Total energy= -2219.82661532

Sum of electronic and zero-point Energies=	-2219.068438
Sum of electronic and thermal Energies=	-2219.026428
Sum of electronic and thermal Enthalpies=	-2219.025484
Sum of electronic and thermal Free Energies=	-2219.140921

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.149898	-0.955148	-1.287513
2	6	0	-4.506993	-0.786662	-1.565309
3	6	0	-5.303078	-1.889730	-1.840856
4	6	0	-4.713710	-3.155418	-1.855712
5	6	0	-3.350640	-3.310510	-1.604722
6	6	0	-2.550367	-2.204851	-1.312402
7	6	0	-2.565000	0.398617	-0.945921
8	6	0	-3.514950	1.364815	-1.683356
9	6	0	-4.874326	0.680018	-1.517999
10	1	0	-6.360307	-1.769758	-2.057605

11	1	0	-5.320539	-4.026792	-2.080641
12	1	0	-2.907459	-4.300680	-1.634956
13	1	0	-1.493950	-2.322870	-1.088429
14	1	0	-2.601133	0.581786	0.127350
15	1	0	-3.474829	2.387308	-1.285476
16	1	0	-5.304213	0.946174	-0.545088
17	6	0	-0.882284	1.236280	-2.561374
18	6	0	-1.954482	1.915177	-3.362652
19	6	0	-0.007358	0.234524	-0.829324
20	1	0	-1.760162	1.781006	-4.427309
21	1	0	-5.566850	0.992832	-2.302468
22	7	0	-1.178359	0.605641	-1.381510
23	7	0	0.397151	1.222639	-2.794748
24	7	0	0.925272	0.581509	-1.717451
25	8	0	-3.213501	1.362055	-3.072542
26	1	0	-1.927545	2.989775	-3.130905
27	6	0	2.327244	0.246128	-1.704862
28	6	0	2.700924	-1.084046	-1.919961
29	6	0	3.246294	1.288624	-1.535670
30	6	0	4.067309	-1.366064	-1.877572
31	6	0	4.593750	0.945401	-1.493130
32	6	0	5.019626	-0.376269	-1.651037
33	1	0	4.389238	-2.393976	-2.021920
34	1	0	5.329892	1.731224	-1.342630
35	6	0	1.723375	-2.186863	-2.232380
36	1	0	1.515753	-2.784229	-1.341110
37	1	0	0.771545	-1.805788	-2.611219
38	1	0	2.151123	-2.842750	-2.993673
39	6	0	6.486863	-0.711908	-1.621006
40	1	0	6.640560	-1.781796	-1.465645
41	1	0	6.964917	-0.431711	-2.565202
42	1	0	6.995912	-0.168512	-0.820774
43	6	0	2.800700	2.722303	-1.453506
44	1	0	2.714036	3.144159	-2.460325
45	1	0	1.827360	2.827080	-0.970071
46	1	0	3.524969	3.318340	-0.895568
47	6	0	0.331820	-0.573254	0.442121
48	8	0	0.172672	-1.773225	0.322412
49	1	0	2.142671	-0.599048	3.304634
50	6	0	1.277888	0.063847	1.471714
51	6	0	1.798748	-1.065314	2.380982
52	1	0	2.125461	0.480958	0.907182
53	1	0	0.965857	-1.730146	2.627341
54	6	0	2.941254	-1.847494	1.773477

55	6	0	2.760303	-3.114995	1.213213
56	6	0	4.232165	-1.308393	1.798892
57	6	0	3.841384	-3.825723	0.694334
58	1	0	1.761935	-3.541169	1.186749
59	6	0	5.315871	-2.018628	1.291514
60	1	0	4.385999	-0.324739	2.238229
61	6	0	5.123371	-3.282459	0.736136
62	1	0	3.682301	-4.810631	0.265069
63	1	0	6.312312	-1.588599	1.334625
64	1	0	5.967699	-3.840517	0.341964
65	6	0	0.646690	1.233103	2.297545
66	8	0	1.426536	1.460837	3.447320
67	6	0	-0.748746	0.779061	2.777054
68	8	0	-1.085013	1.124224	3.929315
69	6	0	0.566115	2.548934	1.510569
70	6	0	1.611059	3.470583	1.640464
71	6	0	-0.526582	2.891951	0.709060
72	6	0	1.573053	4.690985	0.973216
73	1	0	2.445181	3.225617	2.288303
74	6	0	-0.556422	4.105707	0.021897
75	1	0	-1.379153	2.222676	0.661494
76	6	0	0.494773	5.009519	0.149658
77	1	0	2.391186	5.394715	1.092314
78	1	0	-1.419038	4.357578	-0.588146
79	1	0	0.466366	5.959074	-0.374902
80	7	0	-1.365532	0.035397	1.882424
81	1	0	0.747346	1.537250	4.148803
82	6	0	-2.647932	-0.474715	2.146572
83	6	0	-2.902239	-1.827826	1.886265
84	6	0	-3.714817	0.346576	2.545415
85	6	0	-4.189242	-2.343909	2.002292
86	1	0	-2.072953	-2.453217	1.569051
87	6	0	-4.999191	-0.176385	2.666814
88	1	0	-3.517339	1.393214	2.757123
89	6	0	-5.245177	-1.521794	2.391258
90	1	0	-4.368604	-3.391712	1.779590
91	1	0	-5.814510	0.471676	2.975431
92	1	0	-6.249186	-1.924014	2.480576

TS7RS

Total energy= -2219.82660590
Sum of electronic and zero-point Energies= -2219.069015
Sum of electronic and thermal Energies= -2219.026410

Sum of electronic and thermal Enthalpies= -2219.025466
Sum of electronic and thermal Free Energies= -2219.144130

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.529819	-1.015195	-0.006926
2	6	0	-4.887299	-1.024131	-0.330315
3	6	0	-5.795895	-1.669831	0.496452
4	6	0	-5.320157	-2.312975	1.641234
5	6	0	-3.961365	-2.301678	1.954582
6	6	0	-3.046795	-1.644424	1.129569
7	6	0	-2.777926	-0.249417	-1.073407
8	6	0	-3.733751	-0.334264	-2.286598
9	6	0	-5.115727	-0.282763	-1.627717
10	1	0	-6.853386	-1.689199	0.250656
11	1	0	-6.016007	-2.832223	2.292673
12	1	0	-3.610854	-2.805069	2.849831
13	1	0	-1.989288	-1.616004	1.385574
14	1	0	-2.629443	0.800100	-0.816638
15	1	0	-3.549774	0.464557	-3.015924
16	1	0	-5.395937	0.760098	-1.437017
17	6	0	-1.294772	-1.664420	-2.478609
18	6	0	-2.373435	-1.813874	-3.507943
19	6	0	-0.318556	-0.859559	-0.701537
20	1	0	-2.351211	-2.823410	-3.919194
21	1	0	-5.870883	-0.732158	-2.276159
22	7	0	-1.471054	-0.843769	-1.393627
23	7	0	-0.114139	-2.208204	-2.474811
24	7	0	0.477197	-1.707320	-1.356858
25	8	0	-3.630809	-1.604989	-2.913533
26	1	0	-2.192111	-1.094554	-4.319221
27	6	0	1.774501	-2.189644	-0.949998
28	6	0	2.906635	-1.735429	-1.635220
29	6	0	1.826419	-3.130782	0.082926
30	6	0	4.142902	-2.193475	-1.187661
31	6	0	3.091570	-3.558123	0.485031
32	6	0	4.255059	-3.092211	-0.125297
33	1	0	5.043057	-1.836553	-1.682374
34	1	0	3.165467	-4.280007	1.294470
35	6	0	2.803034	-0.823308	-2.828484
36	1	0	2.565531	-1.406255	-3.724623
37	1	0	2.018048	-0.071784	-2.711404
38	1	0	3.755655	-0.317153	-2.999004

39	6	0	5.605890	-3.586110	0.318810
40	1	0	6.361841	-2.804482	0.211163
41	1	0	5.583563	-3.902362	1.364025
42	1	0	5.919673	-4.442924	-0.286490
43	6	0	0.583339	-3.685839	0.726649
44	1	0	0.213300	-3.005759	1.497791
45	1	0	-0.215875	-3.830528	-0.006701
46	1	0	0.800832	-4.651067	1.186908
47	6	0	0.246064	-0.109054	0.540898
48	8	0	0.242377	-0.726144	1.591285
49	1	0	2.353611	2.475563	1.210999
50	6	0	1.267544	0.957423	0.133079
51	6	0	1.965663	1.471452	1.400816
52	1	0	2.020428	0.457739	-0.493568
53	1	0	1.225803	1.546210	2.202080
54	6	0	3.118420	0.579150	1.808309
55	6	0	3.045352	-0.268393	2.915133
56	6	0	4.299010	0.599748	1.057569
57	6	0	4.129595	-1.069921	3.269358
58	1	0	2.126215	-0.303480	3.491885
59	6	0	5.383065	-0.199367	1.406386
60	1	0	4.363520	1.256452	0.190797
61	6	0	5.302583	-1.034950	2.519173
62	1	0	4.058307	-1.721221	4.135293
63	1	0	6.292266	-0.167947	0.812598
64	1	0	6.148900	-1.655668	2.797256
65	6	0	0.587102	2.002293	-0.780717
66	8	0	0.448594	1.394954	-2.070144
67	6	0	-0.848215	2.265318	-0.287828
68	8	0	-1.585454	2.961466	-1.015964
69	6	0	1.404765	3.276551	-0.902968
70	6	0	2.532809	3.280406	-1.727595
71	6	0	1.093796	4.421990	-0.168643
72	6	0	3.343528	4.409172	-1.808819
73	1	0	2.766198	2.392460	-2.309010
74	6	0	1.902327	5.553244	-0.252620
75	1	0	0.215880	4.430224	0.470986
76	6	0	3.029758	5.549185	-1.070470
77	1	0	4.219415	4.400683	-2.449971
78	1	0	1.648869	6.439114	0.320864
79	1	0	3.659904	6.430539	-1.133488
80	7	0	-1.093192	1.597975	0.827982
81	1	0	-0.227568	1.929645	-2.517646
82	6	0	-2.294911	1.643318	1.540591

83	6	0	-2.272837	1.041476	2.810860
84	6	0	-3.500569	2.212231	1.088447
85	6	0	-3.419504	0.975530	3.590220
86	1	0	-1.334227	0.613719	3.151738
87	6	0	-4.645399	2.138365	1.879621
88	1	0	-3.523045	2.709044	0.126454
89	6	0	-4.618478	1.517808	3.125812
90	1	0	-3.380309	0.496823	4.564517
91	1	0	-5.570400	2.575209	1.513106
92	1	0	-5.517250	1.465405	3.731915

TS7SR

Total energy= -2219.82485601

Sum of electronic and zero-point Energies= -2219.067569

Sum of electronic and thermal Energies= -2219.024974

Sum of electronic and thermal Enthalpies= -2219.024030

Sum of electronic and thermal Free Energies= -2219.141947

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.525805	-0.552517	-0.622091
2	6	0	4.899556	-0.700302	-0.426014
3	6	0	5.792760	-0.064028	-1.275607
4	6	0	5.286491	0.689538	-2.337792
5	6	0	3.912753	0.783319	-2.557036
6	6	0	3.012460	0.157652	-1.693290
7	6	0	2.806773	-1.288672	0.487309
8	6	0	3.826919	-2.388482	0.838226
9	6	0	5.159935	-1.639426	0.733110
10	1	0	6.864509	-0.167556	-1.133926
11	1	0	5.972690	1.187929	-3.015395
12	1	0	3.537881	1.355783	-3.399449
13	1	0	1.940620	0.230321	-1.849374
14	1	0	2.609491	-0.640991	1.346812
15	1	0	3.637596	-2.860939	1.809642
16	1	0	5.350936	-1.089750	1.662132
17	6	0	1.448825	-3.156026	-0.413205
18	6	0	2.630842	-4.081209	-0.340851
19	6	0	0.310338	-1.347791	0.061658
20	1	0	2.700306	-4.677311	-1.251542
21	1	0	5.986285	-2.332784	0.562130
22	7	0	1.538753	-1.888242	0.088603

23	7	0	0.227512	-3.426416	-0.772015
24	7	0	-0.470041	-2.291801	-0.471274
25	8	0	3.832654	-3.362339	-0.202561
26	1	0	2.470827	-4.758104	0.510602
27	6	0	-1.874685	-2.224106	-0.783830
28	6	0	-2.230765	-2.057067	-2.125569
29	6	0	-2.806757	-2.335501	0.252313
30	6	0	-3.589252	-1.919919	-2.407717
31	6	0	-4.151214	-2.190574	-0.088411
32	6	0	-4.557703	-1.959319	-1.402906
33	1	0	-3.895375	-1.773244	-3.440756
34	1	0	-4.895802	-2.258252	0.700623
35	6	0	-1.214874	-2.069815	-3.235491
36	1	0	-0.249485	-1.681988	-2.908743
37	1	0	-1.066058	-3.092451	-3.596598
38	1	0	-1.565231	-1.462512	-4.072605
39	6	0	-6.012263	-1.739663	-1.725375
40	1	0	-6.228860	-1.978834	-2.768492
41	1	0	-6.655165	-2.349426	-1.086484
42	1	0	-6.281918	-0.690889	-1.560387
43	6	0	-2.400199	-2.576046	1.681780
44	1	0	-1.502750	-3.197177	1.746472
45	1	0	-2.196985	-1.633292	2.201098
46	1	0	-3.209721	-3.077527	2.215433
47	6	0	-0.162727	-0.166893	0.948062
48	8	0	0.028071	-0.418897	2.127039
49	1	0	-0.852355	2.026478	2.097349
50	6	0	-1.226810	0.765080	0.395098
51	6	0	-1.717996	1.682941	1.524496
52	1	0	-2.065598	0.137139	0.063159
53	1	0	-2.195295	2.561286	1.080334
54	6	0	-2.712926	0.983374	2.422289
55	6	0	-3.968180	0.623640	1.921409
56	6	0	-2.401531	0.656441	3.743840
57	6	0	-4.886191	-0.056509	2.717236
58	1	0	-4.222441	0.874711	0.892213
59	6	0	-3.317323	-0.022912	4.544348
60	1	0	-1.422507	0.917765	4.134293
61	6	0	-4.560859	-0.385724	4.032312
62	1	0	-5.856910	-0.327307	2.311832
63	1	0	-3.056986	-0.273869	5.568064
64	1	0	-5.273504	-0.918476	4.653935
65	6	0	-0.718215	1.489263	-0.864779
66	8	0	-0.504103	0.454967	-1.837556

67	6	0	0.670876	2.109905	-0.583038
68	8	0	1.125264	2.945590	-1.385074
69	6	0	-1.771610	2.451367	-1.387774
70	6	0	-1.695441	3.833627	-1.207638
71	6	0	-2.900294	1.907193	-2.009951
72	6	0	-2.734117	4.655765	-1.641422
73	1	0	-0.815089	4.263937	-0.743590
74	6	0	-3.937238	2.728792	-2.442137
75	1	0	-2.956732	0.830378	-2.154961
76	6	0	-3.856253	4.107960	-2.257850
77	1	0	-2.662894	5.729478	-1.498536
78	1	0	-4.808100	2.292035	-2.921524
79	1	0	-4.662774	4.751954	-2.593807
80	7	0	1.207757	1.547158	0.492725
81	1	0	-0.169831	0.892696	-2.634247
82	6	0	2.441587	1.917548	1.028912
83	6	0	3.461619	2.608986	0.345706
84	6	0	2.682225	1.533079	2.362564
85	6	0	4.676570	2.864719	0.974136
86	1	0	3.287958	2.917271	-0.675705
87	6	0	3.904006	1.786396	2.977333
88	1	0	1.882363	1.025683	2.896280
89	6	0	4.914665	2.451942	2.284645
90	1	0	5.454425	3.388046	0.424475
91	1	0	4.063108	1.471392	4.004904
92	1	0	5.868930	2.652765	2.761227

TS7SS

Total energy= -2219.82633682
Sum of electronic and zero-point Energies= -2219.067884
Sum of electronic and thermal Energies= -2219.026184
Sum of electronic and thermal Enthalpies= -2219.025240
Sum of electronic and thermal Free Energies= -2219.138892

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.926070	0.489727	-0.467497
2	6	0	5.193915	1.070450	-0.365553
3	6	0	6.315290	0.403722	-0.840080
4	6	0	6.154438	-0.859078	-1.412307
5	6	0	4.887141	-1.429917	-1.521159
6	6	0	3.757531	-0.751724	-1.062374

7	6	0	2.903571	1.465208	0.081863
8	6	0	3.766690	2.362413	1.004868
9	6	0	5.107844	2.433472	0.279475
10	1	0	7.300512	0.852623	-0.755754
11	1	0	7.023207	-1.399943	-1.774372
12	1	0	4.768280	-2.412525	-1.966634
13	1	0	2.773725	-1.184842	-1.173190
14	1	0	2.460581	2.056998	-0.722765
15	1	0	3.299944	3.336482	1.201270
16	1	0	5.089410	3.228798	-0.473871
17	6	0	1.714851	1.065997	2.239528
18	6	0	2.878221	1.573489	3.035132
19	6	0	0.522908	0.548278	0.485445
20	1	0	3.103158	0.879675	3.847377
21	1	0	5.914413	2.645701	0.984618
22	7	0	1.760104	0.938433	0.875805
23	7	0	0.529422	0.796496	2.702998
24	7	0	-0.206236	0.483750	1.602687
25	8	0	4.016719	1.676338	2.223401
26	1	0	2.601759	2.545061	3.468389
27	6	0	-1.644620	0.450162	1.750366
28	6	0	-2.289391	1.687891	1.614778
29	6	0	-2.303524	-0.727937	2.094410
30	6	0	-3.676535	1.695309	1.710117
31	6	0	-3.693816	-0.656674	2.203961
32	6	0	-4.394292	0.526821	1.986833
33	1	0	-4.206054	2.636465	1.581924
34	1	0	-4.240709	-1.561787	2.450838
35	6	0	-1.500830	2.954791	1.414703
36	1	0	-0.794189	3.097049	2.239224
37	1	0	-0.930951	2.946510	0.478482
38	1	0	-2.168094	3.815913	1.380361
39	6	0	-5.896442	0.564846	2.079853
40	1	0	-6.327094	1.028776	1.187833
41	1	0	-6.310530	-0.440875	2.176147
42	1	0	-6.217507	1.154595	2.944128
43	6	0	-1.563639	-2.003300	2.380279
44	1	0	-0.995770	-2.320638	1.502641
45	1	0	-0.860515	-1.862961	3.208385
46	1	0	-2.266712	-2.792755	2.652289
47	6	0	0.177928	0.228424	-0.967789
48	8	0	1.087853	0.422279	-1.761344
49	1	0	-0.696859	0.920542	-3.350140
50	6	0	-1.283222	0.136005	-1.434116

51	6	0	-1.471222	1.121798	-2.607543
52	1	0	-1.931781	0.448258	-0.614597
53	1	0	-2.430756	0.907113	-3.083207
54	6	0	-1.435871	2.566102	-2.171267
55	6	0	-2.612758	3.202864	-1.762998
56	6	0	-0.241784	3.295228	-2.157662
57	6	0	-2.600886	4.533599	-1.354722
58	1	0	-3.548501	2.648066	-1.774237
59	6	0	-0.224456	4.624958	-1.738001
60	1	0	0.672773	2.813448	-2.493048
61	6	0	-1.404000	5.247831	-1.336216
62	1	0	-3.525709	5.013492	-1.048583
63	1	0	0.709560	5.178587	-1.738260
64	1	0	-1.392515	6.285306	-1.017691
65	6	0	-1.680603	-1.320514	-1.831896
66	8	0	-1.874537	-1.405808	-3.230961
67	6	0	-0.554706	-2.311367	-1.475109
68	8	0	-0.504306	-3.350011	-2.160120
69	6	0	-2.982676	-1.741215	-1.134510
70	6	0	-3.102931	-2.943001	-0.434463
71	6	0	-4.118697	-0.937874	-1.280818
72	6	0	-4.325492	-3.324634	0.118395
73	1	0	-2.242672	-3.596594	-0.325831
74	6	0	-5.340478	-1.318576	-0.737824
75	1	0	-4.050281	-0.006550	-1.837428
76	6	0	-5.447875	-2.516973	-0.032522
77	1	0	-4.397408	-4.261768	0.662331
78	1	0	-6.210689	-0.681649	-0.865898
79	1	0	-6.400504	-2.817471	0.393307
80	7	0	0.174018	-1.916828	-0.438547
81	1	0	-1.591522	-2.316146	-3.434420
82	6	0	1.266508	-2.657260	0.036524
83	6	0	1.758475	-2.335166	1.314565
84	6	0	1.949863	-3.648745	-0.696486
85	6	0	2.896568	-2.943616	1.829490
86	1	0	1.227456	-1.602303	1.913518
87	6	0	3.085463	-4.256714	-0.169051
88	1	0	1.583569	-3.922871	-1.675982
89	6	0	3.574971	-3.907648	1.087948
90	1	0	3.251916	-2.662263	2.816505
91	1	0	3.599169	-5.012780	-0.756616
92	1	0	4.465909	-4.382793	1.485104

M6RR

Total energy= -2219.83843426
Sum of electronic and zero-point Energies= -2219.079989
Sum of electronic and thermal Energies= -2219.037471
Sum of electronic and thermal Enthalpies= -2219.036527
Sum of electronic and thermal Free Energies= -2219.152827

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.408961	-0.384322	-1.184564
2	6	0	-4.742763	-0.062258	-1.442586
3	6	0	-5.617928	-1.038408	-1.897241
4	6	0	-5.131575	-2.332794	-2.093512
5	6	0	-3.794837	-2.640945	-1.840427
6	6	0	-2.910198	-1.663254	-1.379306
7	6	0	-2.708751	0.853024	-0.663239
8	6	0	-3.579151	1.990916	-1.245430
9	6	0	-4.990579	1.404386	-1.166970
10	1	0	-6.655899	-0.799700	-2.109020
11	1	0	-5.801193	-3.106959	-2.454909
12	1	0	-3.436952	-3.653193	-1.999699
13	1	0	-1.870496	-1.896267	-1.150248
14	1	0	-2.737152	0.893578	0.426156
15	1	0	-3.445879	2.940119	-0.708922
16	1	0	-5.402773	1.555453	-0.162234
17	6	0	-0.985789	1.724776	-2.198106
18	6	0	-1.986762	2.621767	-2.860255
19	6	0	-0.174667	0.425402	-0.616276
20	1	0	-1.817682	2.638680	-3.937280
21	1	0	-5.652655	1.888566	-1.888147
22	7	0	-1.311641	0.993954	-1.085258
23	7	0	0.272807	1.608134	-2.479433
24	7	0	0.764565	0.787125	-1.503730
25	8	0	-3.293501	2.160390	-2.625776
26	1	0	-1.849811	3.638850	-2.463595
27	6	0	2.163219	0.441258	-1.618406
28	6	0	2.515050	-0.793009	-2.173361
29	6	0	3.098770	1.436559	-1.315809
30	6	0	3.877452	-1.049610	-2.322870
31	6	0	4.445718	1.120556	-1.472331
32	6	0	4.851723	-0.120993	-1.962948
33	1	0	4.182890	-2.009736	-2.729722
34	1	0	5.192488	1.869454	-1.218657

35	6	0	1.485766	-1.780437	-2.645038
36	1	0	0.914863	-2.154592	-1.791128
37	1	0	0.784231	-1.301767	-3.338084
38	1	0	1.971325	-2.608533	-3.164915
39	6	0	6.313791	-0.432802	-2.144542
40	1	0	6.486962	-1.511407	-2.133303
41	1	0	6.678468	-0.040854	-3.099815
42	1	0	6.912583	0.021533	-1.350954
43	6	0	2.673647	2.817924	-0.898820
44	1	0	2.481142	3.431517	-1.785646
45	1	0	1.757392	2.809376	-0.305653
46	1	0	3.456995	3.302599	-0.313205
47	6	0	0.054582	-0.595417	0.574910
48	8	0	0.100441	-1.773550	0.051110
49	1	0	2.372440	-1.070455	3.037273
50	6	0	1.288832	-0.115990	1.456309
51	6	0	1.931664	-1.366271	2.083896
52	1	0	2.035860	0.405517	0.853609
53	1	0	1.145497	-2.097868	2.299114
54	6	0	3.014188	-2.010683	1.245024
55	6	0	2.765758	-3.125550	0.439092
56	6	0	4.324244	-1.527938	1.324609
57	6	0	3.803014	-3.756220	-0.243537
58	1	0	1.745021	-3.481465	0.352813
59	6	0	5.364252	-2.152807	0.640221
60	1	0	4.533191	-0.660304	1.947550
61	6	0	5.108090	-3.277726	-0.139896
62	1	0	3.590648	-4.627608	-0.856738
63	1	0	6.375991	-1.765946	0.723766
64	1	0	5.918133	-3.774892	-0.665964
65	6	0	0.696817	0.841089	2.522005
66	8	0	1.368742	0.745588	3.758614
67	6	0	-0.711769	0.285768	2.722360
68	8	0	-1.328072	0.449495	3.766392
69	6	0	0.662261	2.302696	2.077443
70	6	0	1.758559	3.116317	2.377003
71	6	0	-0.421400	2.858756	1.395476
72	6	0	1.781200	4.447917	1.975570
73	1	0	2.587340	2.692460	2.934122
74	6	0	-0.394773	4.188743	0.977403
75	1	0	-1.308643	2.261239	1.209522
76	6	0	0.710321	4.986088	1.262856
77	1	0	2.640023	5.066963	2.215510
78	1	0	-1.247618	4.603526	0.448206

79	1	0	0.731182	6.023513	0.945427
80	7	0	-1.091518	-0.423768	1.629943
81	1	0	0.695148	0.944438	4.429321
82	6	0	-2.211436	-1.306930	1.742756
83	6	0	-2.056258	-2.688244	1.598965
84	6	0	-3.466334	-0.781519	2.061107
85	6	0	-3.169307	-3.518568	1.698150
86	1	0	-1.073657	-3.083327	1.380175
87	6	0	-4.571634	-1.619102	2.162275
88	1	0	-3.571549	0.284145	2.242274
89	6	0	-4.429930	-2.990445	1.963304
90	1	0	-3.045619	-4.589410	1.568803
91	1	0	-5.543596	-1.197069	2.397460
92	1	0	-5.293714	-3.643876	2.031777

M6RS

Total energy= -2219.83902912

Sum of electronic and zero-point Energies= -2219.080202

Sum of electronic and thermal Energies= -2219.037628

Sum of electronic and thermal Enthalpies= -2219.036683

Sum of electronic and thermal Free Energies= -2219.154011

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.753973	-0.775898	-0.087333
2	6	0	-5.097624	-0.728190	-0.460080
3	6	0	-6.081673	-1.131401	0.432198
4	6	0	-5.693304	-1.590175	1.692624
5	6	0	-4.345436	-1.648656	2.048637
6	6	0	-3.352224	-1.240534	1.156386
7	6	0	-2.914158	-0.241915	-1.228667
8	6	0	-3.831676	-0.487143	-2.449677
9	6	0	-5.228000	-0.223881	-1.880340
10	1	0	-7.130675	-1.105022	0.152454
11	1	0	-6.449177	-1.915214	2.400804
12	1	0	-4.064324	-2.010737	3.032443
13	1	0	-2.298498	-1.257943	1.436119
14	1	0	-2.713186	0.826408	-1.127251
15	1	0	-3.564104	0.139078	-3.310074
16	1	0	-5.443666	0.850802	-1.902978
17	6	0	-1.473350	-1.949366	-2.290205
18	6	0	-2.540355	-2.266048	-3.293523

19	6	0	-0.472179	-0.793644	-0.709789
20	1	0	-2.574817	-3.341179	-3.472535
21	1	0	-5.989740	-0.740540	-2.468396
22	7	0	-1.628364	-0.922871	-1.394997
23	7	0	-0.300061	-2.487745	-2.181966
24	7	0	0.309707	-1.771942	-1.188735
25	8	0	-3.797965	-1.860571	-2.811118
26	1	0	-2.296685	-1.757495	-4.237590
27	6	0	1.646334	-2.180472	-0.823387
28	6	0	2.687208	-1.858008	-1.702594
29	6	0	1.826771	-2.971800	0.313680
30	6	0	3.969641	-2.275900	-1.357689
31	6	0	3.133005	-3.359801	0.612707
32	6	0	4.211641	-3.016422	-0.199827
33	1	0	4.798495	-2.019892	-2.013279
34	1	0	3.307757	-3.953967	1.506137
35	6	0	2.431668	-1.117457	-2.988011
36	1	0	1.964762	-1.783503	-3.721168
37	1	0	1.756562	-0.269479	-2.841129
38	1	0	3.371394	-0.754165	-3.409115
39	6	0	5.604321	-3.476383	0.141367
40	1	0	5.729333	-3.568133	1.222807
41	1	0	5.808559	-4.454892	-0.306065
42	1	0	6.353667	-2.775781	-0.235114
43	6	0	0.667402	-3.429732	1.152786
44	1	0	0.205026	-2.567254	1.639643
45	1	0	-0.090072	-3.914926	0.526967
46	1	0	1.004528	-4.148673	1.901922
47	6	0	-0.058070	0.164914	0.482433
48	8	0	-0.077672	-0.514294	1.578319
49	1	0	2.560865	2.270795	1.098080
50	6	0	1.273952	0.889920	0.051510
51	6	0	1.985497	1.368924	1.326183
52	1	0	1.944684	0.233508	-0.506807
53	1	0	1.233577	1.640378	2.075432
54	6	0	2.941803	0.345813	1.902812
55	6	0	2.583994	-0.486350	2.966734
56	6	0	4.240275	0.257763	1.392989
57	6	0	3.508700	-1.369863	3.517880
58	1	0	1.566634	-0.440951	3.339326
59	6	0	5.167477	-0.625930	1.940159
60	1	0	4.527886	0.899921	0.562129
61	6	0	4.804875	-1.439855	3.010546
62	1	0	3.217006	-2.004141	4.350091

63	1	0	6.173757	-0.675996	1.533879
64	1	0	5.527449	-2.124115	3.445993
65	6	0	0.799390	2.014346	-0.883955
66	8	0	0.429417	1.378535	-2.114040
67	6	0	-0.521080	2.460643	-0.238295
68	8	0	-1.056810	3.545674	-0.410410
69	6	0	1.806444	3.114663	-1.132095
70	6	0	2.799358	2.903023	-2.093603
71	6	0	1.824641	4.295570	-0.384755
72	6	0	3.793561	3.854596	-2.305051
73	1	0	2.787670	1.985863	-2.675526
74	6	0	2.819628	5.246354	-0.597707
75	1	0	1.056345	4.474352	0.359145
76	6	0	3.805441	5.030177	-1.557622
77	1	0	4.558995	3.677673	-3.054003
78	1	0	2.821476	6.159968	-0.012004
79	1	0	4.578614	5.773774	-1.721911
80	7	0	-1.000517	1.413191	0.488829
81	1	0	0.116433	2.068639	-2.715874
82	6	0	-2.070387	1.611268	1.409909
83	6	0	-1.920344	1.263845	2.756490
84	6	0	-3.261984	2.203548	0.979780
85	6	0	-2.980968	1.446983	3.638477
86	1	0	-0.984978	0.827852	3.080020
87	6	0	-4.312183	2.391792	1.872104
88	1	0	-3.359803	2.529162	-0.050083
89	6	0	-4.182580	1.999510	3.201848
90	1	0	-2.861451	1.161159	4.679076
91	1	0	-5.235005	2.844079	1.522385
92	1	0	-5.005286	2.138437	3.895901

M6SR

Total energy= -2219.83737541
Sum of electronic and zero-point Energies= -2219.079233
Sum of electronic and thermal Energies= -2219.036409
Sum of electronic and thermal Enthalpies= -2219.035465
Sum of electronic and thermal Free Energies= -2219.154015

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.635995	0.455793	-0.744730
2	6	0	-5.023712	0.558740	-0.643658

3	6	0	-5.833618	0.002847	-1.624258
4	6	0	-5.229947	-0.626452	-2.716151
5	6	0	-3.840751	-0.674399	-2.836110
6	6	0	-3.025007	-0.125986	-1.844323
7	6	0	-3.013698	1.079960	0.483850
8	6	0	-4.092872	2.099806	0.902772
9	6	0	-5.394802	1.352875	0.590362
10	1	0	-6.915207	0.072950	-1.557771
11	1	0	-5.850151	-1.060720	-3.493810
12	1	0	-3.390595	-1.141666	-3.705828
13	1	0	-1.941754	-0.154395	-1.929717
14	1	0	-2.856834	0.352882	1.286152
15	1	0	-3.992995	2.419420	1.947450
16	1	0	-5.654143	0.694571	1.427659
17	6	0	-1.654927	3.079648	-0.023315
18	6	0	-2.851426	3.967597	0.155072
19	6	0	-0.506617	1.200670	0.118533
20	1	0	-2.859700	4.744996	-0.609876
21	1	0	-6.218293	2.052859	0.432936
22	7	0	-1.742053	1.739085	0.227091
23	7	0	-0.436187	3.418158	-0.307813
24	7	0	0.266648	2.242835	-0.224666
25	8	0	-4.042211	3.224419	0.032657
26	1	0	-2.783522	4.445319	1.142940
27	6	0	1.660064	2.295781	-0.586575
28	6	0	1.979438	2.300690	-1.946590
29	6	0	2.618293	2.383068	0.427720
30	6	0	3.334041	2.307289	-2.281588
31	6	0	3.956191	2.391646	0.037193
32	6	0	4.331623	2.330987	-1.306064
33	1	0	3.613375	2.294754	-3.332740
34	1	0	4.721594	2.431523	0.808227
35	6	0	0.923444	2.356600	-3.017383
36	1	0	-0.008731	1.891098	-2.694879
37	1	0	0.710834	3.398528	-3.278121
38	1	0	1.270142	1.846497	-3.918799
39	6	0	5.786481	2.270177	-1.692356
40	1	0	5.954374	2.709736	-2.678122
41	1	0	6.410960	2.795146	-0.965974
42	1	0	6.127273	1.229886	-1.730867
43	6	0	2.219441	2.452758	1.875956
44	1	0	1.766420	3.426739	2.094530
45	1	0	1.488188	1.676511	2.127876
46	1	0	3.095581	2.321368	2.515183

47	6	0	-0.071303	-0.165127	0.833436
48	8	0	-0.123363	0.152219	2.082363
49	1	0	1.091188	-2.170453	1.839301
50	6	0	1.252360	-0.731875	0.227229
51	6	0	1.882460	-1.671681	1.268989
52	1	0	1.971037	0.043959	-0.036730
53	1	0	2.450671	-2.450424	0.750626
54	6	0	2.823877	-0.953474	2.209045
55	6	0	4.071653	-0.529646	1.743219
56	6	0	2.492723	-0.713033	3.543810
57	6	0	4.973287	0.110214	2.590532
58	1	0	4.337313	-0.706025	0.701663
59	6	0	3.390555	-0.075114	4.395974
60	1	0	1.512966	-1.013863	3.901305
61	6	0	4.635664	0.337030	3.923524
62	1	0	5.940211	0.427835	2.210721
63	1	0	3.117878	0.102868	5.431896
64	1	0	5.336934	0.831099	4.588837
65	6	0	0.798764	-1.428861	-1.060601
66	8	0	0.485062	-0.379529	-1.983761
67	6	0	-0.541076	-2.057723	-0.640584
68	8	0	-1.078006	-3.006952	-1.189994
69	6	0	1.827581	-2.358724	-1.663210
70	6	0	1.798648	-3.745758	-1.505232
71	6	0	2.899227	-1.769788	-2.345004
72	6	0	2.825932	-4.530061	-2.027219
73	1	0	0.970921	-4.212068	-0.983500
74	6	0	3.923842	-2.555310	-2.862827
75	1	0	2.921588	-0.688453	-2.461603
76	6	0	3.888478	-3.940080	-2.706223
77	1	0	2.792493	-5.607656	-1.902044
78	1	0	4.750934	-2.086082	-3.386407
79	1	0	4.685962	-4.555435	-3.110252
80	7	0	-1.026509	-1.330633	0.409848
81	1	0	0.258554	-0.788744	-2.831126
82	6	0	-2.082464	-1.847427	1.216886
83	6	0	-3.251525	-2.335758	0.618456
84	6	0	-1.946383	-1.909548	2.610478
85	6	0	-4.279267	-2.843631	1.407551
86	1	0	-3.345787	-2.320650	-0.459094
87	6	0	-2.989379	-2.406734	3.387579
88	1	0	-1.033442	-1.544831	3.060930
89	6	0	-4.160815	-2.870896	2.795039
90	1	0	-5.179322	-3.217125	0.928875

91	1	0	-2.875112	-2.440875	4.466656
92	1	0	-4.967843	-3.260980	3.406920

M6SS

Total energy= -2219.83320881
Sum of electronic and zero-point Energies= -2219.073968
Sum of electronic and thermal Energies= -2219.031819
Sum of electronic and thermal Enthalpies= -2219.030875
Sum of electronic and thermal Free Energies= -2219.146265

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.924667	0.090818	-0.518795
2	6	0	-5.234280	0.559486	-0.377988
3	6	0	-6.294090	-0.168537	-0.897343
4	6	0	-6.022511	-1.356360	-1.583084
5	6	0	-4.711104	-1.793270	-1.756462
6	6	0	-3.644348	-1.066542	-1.223063
7	6	0	-2.994723	1.065339	0.176196
8	6	0	-3.793086	2.377926	0.046844
9	6	0	-5.229346	1.911505	0.305254
10	1	0	-7.314403	0.189752	-0.797592
11	1	0	-6.840997	-1.932215	-2.003383
12	1	0	-4.512662	-2.708753	-2.304576
13	1	0	-2.622766	-1.413230	-1.348526
14	1	0	-2.806824	0.796210	1.218559
15	1	0	-3.431157	3.170623	0.714364
16	1	0	-5.408349	1.826197	1.382900
17	6	0	-1.498641	2.058335	-1.500607
18	6	0	-2.502301	3.131441	-1.808913
19	6	0	-0.519119	0.526293	-0.251217
20	1	0	-2.588978	3.270457	-2.887404
21	1	0	-5.951476	2.616250	-0.112410
22	7	0	-1.678799	1.202406	-0.454641
23	7	0	-0.317991	1.917353	-2.019698
24	7	0	0.277243	0.957905	-1.246835
25	8	0	-3.776263	2.813084	-1.310121
26	1	0	-2.123431	4.064430	-1.365769
27	6	0	1.592068	0.546267	-1.677422
28	6	0	2.604727	1.515398	-1.706922
29	6	0	1.768424	-0.746738	-2.174163
30	6	0	3.842553	1.129525	-2.210966

31	6	0	3.028065	-1.076486	-2.675426
32	6	0	4.073439	-0.157867	-2.700035
33	1	0	4.648420	1.859848	-2.229032
34	1	0	3.188749	-2.080299	-3.059177
35	6	0	2.375830	2.928686	-1.245891
36	1	0	1.963044	3.531398	-2.060875
37	1	0	1.672660	2.979758	-0.412114
38	1	0	3.317890	3.379222	-0.927941
39	6	0	5.419021	-0.524922	-3.266349
40	1	0	6.221513	-0.218650	-2.589242
41	1	0	5.499726	-1.602108	-3.426773
42	1	0	5.584984	-0.022541	-4.224724
43	6	0	0.645931	-1.745677	-2.206129
44	1	0	0.388502	-2.065912	-1.194433
45	1	0	-0.255729	-1.318303	-2.658671
46	1	0	0.936037	-2.625936	-2.782245
47	6	0	-0.194231	-0.167909	1.190254
48	8	0	-1.019613	0.314559	2.054446
49	1	0	0.751950	0.849166	3.410055
50	6	0	1.354537	0.063401	1.510271
51	6	0	1.518048	1.067164	2.662945
52	1	0	1.871805	0.463223	0.638648
53	1	0	2.493534	0.900971	3.127179
54	6	0	1.430219	2.511059	2.218740
55	6	0	2.585770	3.297470	2.176565
56	6	0	0.215451	3.097098	1.833771
57	6	0	2.540764	4.623987	1.750725
58	1	0	3.534555	2.863391	2.483931
59	6	0	0.169433	4.420120	1.400024
60	1	0	-0.685721	2.493443	1.890609
61	6	0	1.332363	5.188998	1.352518
62	1	0	3.451832	5.214344	1.727643
63	1	0	-0.781820	4.858470	1.109296
64	1	0	1.294429	6.220641	1.017148
65	6	0	1.946497	-1.332814	1.811074
66	8	0	2.338771	-1.429618	3.173007
67	6	0	0.788611	-2.307513	1.625031
68	8	0	0.843815	-3.472615	1.996177
69	6	0	3.138590	-1.692702	0.923391
70	6	0	3.235523	-2.897830	0.225699
71	6	0	4.226766	-0.812328	0.902763
72	6	0	4.403139	-3.221789	-0.466578
73	1	0	2.409883	-3.601326	0.236247
74	6	0	5.390887	-1.136210	0.217372

75	1	0	4.160898	0.131133	1.440775
76	6	0	5.484820	-2.349407	-0.465693
77	1	0	4.464164	-4.164888	-1.001175
78	1	0	6.227247	-0.443427	0.214745
79	1	0	6.396117	-2.606794	-0.996693
80	7	0	-0.271196	-1.683151	1.054418
81	1	0	2.397928	-2.380029	3.355431
82	6	0	-1.508693	-2.395034	0.964740
83	6	0	-1.590219	-3.478427	0.085337
84	6	0	-2.595269	-2.083865	1.786752
85	6	0	-2.764224	-4.217930	-0.004774
86	1	0	-0.726328	-3.748414	-0.513564
87	6	0	-3.771638	-2.822360	1.678685
88	1	0	-2.495084	-1.271840	2.493768
89	6	0	-3.863601	-3.884396	0.784612
90	1	0	-2.818380	-5.056963	-0.691173
91	1	0	-4.618984	-2.567545	2.307575
92	1	0	-4.783566	-4.455065	0.707386

TS8RR

Total energy= -2219.83054215

Sum of electronic and zero-point Energies= -2219.073206

Sum of electronic and thermal Energies= -2219.030818

Sum of electronic and thermal Enthalpies= -2219.029873

Sum of electronic and thermal Free Energies= -2219.147257

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.385708	-0.238326	-1.231334
2	6	0	-4.726448	0.071932	-1.464532
3	6	0	-5.581432	-0.885860	-1.992526
4	6	0	-5.069438	-2.151535	-2.284458
5	6	0	-3.727436	-2.451688	-2.048791
6	6	0	-2.864582	-1.491672	-1.515384
7	6	0	-2.703341	0.967342	-0.621758
8	6	0	-3.613109	2.131064	-1.079139
9	6	0	-5.009749	1.503857	-1.068224
10	1	0	-6.624496	-0.653787	-2.186261
11	1	0	-5.723239	-2.910126	-2.703312
12	1	0	-3.349724	-3.443178	-2.277800
13	1	0	-1.822895	-1.728917	-1.303064
14	1	0	-2.708178	0.902340	0.469427

15	1	0	-3.507180	3.020997	-0.443921
16	1	0	-5.436456	1.556689	-0.059544
17	6	0	-1.013969	2.049745	-2.064922
18	6	0	-2.041939	2.985929	-2.621845
19	6	0	-0.199240	0.540179	-0.643440
20	1	0	-1.887140	3.123225	-3.692626
21	1	0	-5.677570	2.032987	-1.751792
22	7	0	-1.327239	1.180693	-1.053274
23	7	0	0.246138	1.978295	-2.357366
24	7	0	0.727780	1.035178	-1.480138
25	8	0	-3.333899	2.457486	-2.433255
26	1	0	-1.938917	3.961141	-2.123497
27	6	0	2.114671	0.680120	-1.628995
28	6	0	2.437625	-0.524486	-2.262116
29	6	0	3.079144	1.616319	-1.244274
30	6	0	3.790558	-0.802487	-2.451367
31	6	0	4.417477	1.285530	-1.448129
32	6	0	4.789499	0.083626	-2.050595
33	1	0	4.068798	-1.738805	-2.927988
34	1	0	5.184952	1.992650	-1.141157
35	6	0	1.375053	-1.467700	-2.753497
36	1	0	0.886231	-1.953293	-1.904685
37	1	0	0.609448	-0.930429	-3.323844
38	1	0	1.816975	-2.228307	-3.400216
39	6	0	6.241078	-0.229219	-2.302934
40	1	0	6.396792	-1.304983	-2.411143
41	1	0	6.586189	0.256083	-3.222012
42	1	0	6.870003	0.131134	-1.484651
43	6	0	2.687950	2.954064	-0.679446
44	1	0	2.525931	3.673409	-1.489140
45	1	0	1.761653	2.897629	-0.104017
46	1	0	3.474597	3.344385	-0.030705
47	6	0	0.088747	-0.912482	0.715581
48	8	0	0.138123	-1.957523	0.054530
49	1	0	2.628134	-1.200546	2.961340
50	6	0	1.312085	-0.346580	1.498898
51	6	0	2.104400	-1.545020	2.068384
52	1	0	1.965600	0.232809	0.844202
53	1	0	1.400435	-2.319599	2.393057
54	6	0	3.127402	-2.132534	1.119908
55	6	0	2.842557	-3.222993	0.292417
56	6	0	4.426921	-1.616595	1.115111
57	6	0	3.831979	-3.783364	-0.511661
58	1	0	1.833916	-3.620546	0.281762

59	6	0	5.421389	-2.179981	0.319920
60	1	0	4.665003	-0.771780	1.758261
61	6	0	5.127032	-3.268819	-0.496530
62	1	0	3.592179	-4.633212	-1.144170
63	1	0	6.427765	-1.772016	0.343072
64	1	0	5.901148	-3.714632	-1.114508
65	6	0	0.699880	0.547993	2.609164
66	8	0	1.333413	0.333184	3.853317
67	6	0	-0.730331	0.020690	2.746002
68	8	0	-1.414602	0.244163	3.731199
69	6	0	0.704605	2.040551	2.288891
70	6	0	1.824890	2.796894	2.643570
71	6	0	-0.380152	2.682053	1.688908
72	6	0	1.865066	4.163382	2.383898
73	1	0	2.656668	2.304256	3.136613
74	6	0	-0.334755	4.046730	1.409316
75	1	0	-1.280225	2.120709	1.454727
76	6	0	0.789861	4.791221	1.756421
77	1	0	2.740757	4.739404	2.666035
78	1	0	-1.186691	4.527759	0.938212
79	1	0	0.824157	5.855750	1.548975
80	7	0	-1.051290	-0.745876	1.667771
81	1	0	0.693783	0.621745	4.523230
82	6	0	-2.225619	-1.559481	1.668224
83	6	0	-2.140545	-2.929880	1.410842
84	6	0	-3.460894	-0.983474	1.973873
85	6	0	-3.300980	-3.697333	1.390963
86	1	0	-1.174827	-3.373107	1.210853
87	6	0	-4.613954	-1.760853	1.954014
88	1	0	-3.514531	0.066696	2.241117
89	6	0	-4.540560	-3.116828	1.645797
90	1	0	-3.231639	-4.759066	1.176410
91	1	0	-5.571241	-1.302168	2.180347
92	1	0	-5.442280	-3.719998	1.621926

TS8RS

Total energy= -2219.83119876
Sum of electronic and zero-point Energies= -2219.073332
Sum of electronic and thermal Energies= -2219.031069
Sum of electronic and thermal Enthalpies= -2219.030125
Sum of electronic and thermal Free Energies= -2219.147307

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-3.668720	-0.842998	-0.111341
2	6	0	-5.020917	-0.812020	-0.447374
3	6	0	-5.977493	-1.206450	0.480062
4	6	0	-5.552043	-1.639954	1.736479
5	6	0	-4.193867	-1.683477	2.057735
6	6	0	-3.232011	-1.282942	1.130885
7	6	0	-2.856874	-0.312572	-1.272258
8	6	0	-3.806296	-0.527336	-2.475129
9	6	0	-5.197688	-0.320992	-1.867665
10	1	0	-7.034226	-1.191352	0.229856
11	1	0	-6.286049	-1.957391	2.470710
12	1	0	-3.883317	-2.024960	3.039916
13	1	0	-2.173250	-1.287289	1.387308
14	1	0	-2.638496	0.755454	-1.161018
15	1	0	-3.578200	0.145198	-3.312096
16	1	0	-5.460392	0.743013	-1.889124
17	6	0	-1.412304	-1.957824	-2.438484
18	6	0	-2.483490	-2.215679	-3.453038
19	6	0	-0.476206	-0.915654	-0.709964
20	1	0	-2.504210	-3.272451	-3.720984
21	1	0	-5.952140	-0.869405	-2.436633
22	7	0	-1.594145	-1.006564	-1.470465
23	7	0	-0.238317	-2.498920	-2.335717
24	7	0	0.318525	-1.845227	-1.258538
25	8	0	-3.740679	-1.879402	-2.907835
26	1	0	-2.277839	-1.625530	-4.357829
27	6	0	1.621169	-2.272747	-0.828970
28	6	0	2.720400	-1.965993	-1.636930
29	6	0	1.724677	-3.046452	0.331998
30	6	0	3.968562	-2.439248	-1.233949
31	6	0	2.995137	-3.494196	0.690865
32	6	0	4.122824	-3.205436	-0.079348
33	1	0	4.840239	-2.202039	-1.839449
34	1	0	3.104143	-4.092429	1.592608
35	6	0	2.559519	-1.171775	-2.906447
36	1	0	2.175121	-1.808404	-3.710022
37	1	0	1.848448	-0.349604	-2.778092
38	1	0	3.521803	-0.765216	-3.225518
39	6	0	5.472785	-3.741108	0.319404
40	1	0	5.614652	-3.672243	1.400875
41	1	0	5.568331	-4.795250	0.038722
42	1	0	6.278821	-3.190367	-0.171017

43	6	0	0.508254	-3.408520	1.140993
44	1	0	0.753276	-4.187015	1.865898
45	1	0	0.140091	-2.526461	1.672796
46	1	0	-0.295264	-3.778086	0.495481
47	6	0	0.103728	0.333637	0.785051
48	8	0	0.204997	-0.357449	1.801429
49	1	0	2.793658	2.410118	0.696474
50	6	0	1.305524	0.980564	0.057496
51	6	0	2.211068	1.600785	1.144237
52	1	0	1.882183	0.250670	-0.514565
53	1	0	1.589183	2.050607	1.927512
54	6	0	3.178552	0.607374	1.747062
55	6	0	2.960887	0.015347	2.993278
56	6	0	4.349111	0.293182	1.051121
57	6	0	3.897629	-0.861502	3.535106
58	1	0	2.044473	0.240111	3.529278
59	6	0	5.288481	-0.581578	1.589214
60	1	0	4.524660	0.746461	0.076895
61	6	0	5.066681	-1.159160	2.837301
62	1	0	3.716609	-1.310597	4.507008
63	1	0	6.193454	-0.812396	1.034507
64	1	0	5.800550	-1.836436	3.263987
65	6	0	0.665874	2.000825	-0.902502
66	8	0	0.324807	1.305060	-2.102859
67	6	0	-0.667417	2.348386	-0.218713
68	8	0	-1.386134	3.276206	-0.551849
69	6	0	1.527804	3.204719	-1.223765
70	6	0	2.516988	3.059399	-2.200846
71	6	0	1.420463	4.415199	-0.536166
72	6	0	3.386260	4.107843	-2.486533
73	1	0	2.600777	2.116208	-2.733252
74	6	0	2.290397	5.464361	-0.824401
75	1	0	0.654643	4.544114	0.221464
76	6	0	3.274152	5.314406	-1.798717
77	1	0	4.151515	3.982160	-3.245774
78	1	0	2.196165	6.402382	-0.286794
79	1	0	3.949949	6.133872	-2.021045
80	7	0	-0.929162	1.409291	0.739429
81	1	0	-0.100718	1.945916	-2.690711
82	6	0	-2.009362	1.532479	1.662696
83	6	0	-1.804654	1.232628	3.013154
84	6	0	-3.264438	1.977269	1.234813
85	6	0	-2.863691	1.329701	3.910163
86	1	0	-0.826163	0.911184	3.341804

87	6	0	-4.312355	2.077480	2.143484
88	1	0	-3.418280	2.252220	0.199004
89	6	0	-4.122249	1.743905	3.481637
90	1	0	-2.696856	1.086297	4.954808
91	1	0	-5.284335	2.413463	1.796547
92	1	0	-4.944343	1.816835	4.186261

TS8SR

Total energy= -2219.83325934
Sum of electronic and zero-point Energies= -2219.076252
Sum of electronic and thermal Energies= -2219.033594
Sum of electronic and thermal Enthalpies= -2219.032650
Sum of electronic and thermal Free Energies= -2219.151714

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.704057	-0.155833	-0.833499
2	6	0	5.087956	-0.003914	-0.916260
3	6	0	5.656140	0.565179	-2.048290
4	6	0	4.818378	0.952806	-3.097247
5	6	0	3.438935	0.754571	-3.022942
6	6	0	2.865178	0.190416	-1.881855
7	6	0	3.353292	-0.722490	0.521972
8	6	0	4.652776	-1.452886	0.921326
9	6	0	5.744906	-0.551176	0.332567
10	1	0	6.731805	0.691907	-2.127500
11	1	0	5.248361	1.394282	-3.990680
12	1	0	2.807812	1.042756	-3.857378
13	1	0	1.790695	0.033017	-1.812802
14	1	0	3.137611	0.067474	1.249289
15	1	0	4.733331	-1.604839	2.005123
16	1	0	5.980593	0.252773	1.040005
17	6	0	2.368009	-2.989810	0.456066
18	6	0	3.721165	-3.606062	0.653082
19	6	0	0.912241	-1.305334	0.344563
20	1	0	3.816059	-4.508797	0.048716
21	1	0	6.658301	-1.118388	0.139252
22	7	0	2.221215	-1.630422	0.490972
23	7	0	1.218860	-3.569797	0.296609
24	7	0	0.336091	-2.513105	0.229162
25	8	0	4.726956	-2.702331	0.245987
26	1	0	3.842766	-3.875256	1.712186

27	6	0	-1.045334	-2.820761	-0.011069
28	6	0	-1.470628	-2.984810	-1.331205
29	6	0	-1.892564	-2.979762	1.087772
30	6	0	-2.825884	-3.244565	-1.538661
31	6	0	-3.233919	-3.258687	0.829576
32	6	0	-3.721377	-3.365168	-0.474492
33	1	0	-3.189642	-3.357426	-2.557178
34	1	0	-3.918244	-3.377692	1.667228
35	6	0	-0.494415	-2.928323	-2.473816
36	1	0	-1.020437	-2.820327	-3.424218
37	1	0	0.196589	-2.090590	-2.357541
38	1	0	0.096192	-3.849531	-2.512265
39	6	0	-5.192050	-3.573390	-0.725018
40	1	0	-5.654588	-4.147359	0.081451
41	1	0	-5.705054	-2.606840	-0.778982
42	1	0	-5.366231	-4.094603	-1.668915
43	6	0	-1.367215	-2.815329	2.488763
44	1	0	-0.567730	-3.536554	2.687358
45	1	0	-0.939549	-1.815616	2.635403
46	1	0	-2.163404	-2.971718	3.218976
47	6	0	0.230022	0.344312	1.180637
48	8	0	0.477076	0.086448	2.371494
49	1	0	-1.689120	1.047353	2.597928
50	6	0	-1.200555	0.462843	0.611634
51	6	0	-1.995657	1.352570	1.591337
52	1	0	-1.678888	-0.513482	0.523050
53	1	0	-1.693855	2.401134	1.473902
54	6	0	-3.497861	1.230508	1.472252
55	6	0	-4.309785	2.338270	1.229202
56	6	0	-4.107122	-0.017975	1.632055
57	6	0	-5.690958	2.198336	1.112345
58	1	0	-3.855089	3.316856	1.105727
59	6	0	-5.485162	-0.165516	1.513635
60	1	0	-3.490996	-0.885752	1.850189
61	6	0	-6.284321	0.945650	1.246042
62	1	0	-6.302479	3.071467	0.905085
63	1	0	-5.934197	-1.147473	1.636119
64	1	0	-7.359768	0.835648	1.147990
65	6	0	-1.001651	1.076746	-0.781745
66	8	0	-0.680336	0.015246	-1.680861
67	6	0	0.285529	1.909588	-0.607285
68	8	0	0.668636	2.767298	-1.381982
69	6	0	-2.191228	1.851833	-1.310886
70	6	0	-2.273308	3.243850	-1.285786

71	6	0	-3.271924	1.109988	-1.801784
72	6	0	-3.425185	3.885169	-1.741537
73	1	0	-1.437250	3.831009	-0.922565
74	6	0	-4.422415	1.750615	-2.244340
75	1	0	-3.206477	0.024733	-1.814381
76	6	0	-4.501073	3.142916	-2.216582
77	1	0	-3.477674	4.969256	-1.722083
78	1	0	-5.261552	1.164434	-2.605752
79	1	0	-5.398664	3.644864	-2.564221
80	7	0	0.937313	1.475652	0.520433
81	1	0	-0.625950	0.400984	-2.567301
82	6	0	2.030517	2.192147	1.092797
83	6	0	3.049709	2.701982	0.279952
84	6	0	2.067964	2.419607	2.474151
85	6	0	4.110658	3.397688	0.853484
86	1	0	3.008494	2.555711	-0.790643
87	6	0	3.140088	3.108395	3.033192
88	1	0	1.266178	2.044040	3.094469
89	6	0	4.168804	3.595226	2.230401
90	1	0	4.896788	3.782500	0.211413
91	1	0	3.162237	3.272149	4.105898
92	1	0	5.001625	4.131802	2.673258

TS8SS

Total energy= -2219.83092939

Sum of electronic and zero-point Energies= -2219.071978

Sum of electronic and thermal Energies= -2219.030069

Sum of electronic and thermal Enthalpies= -2219.029125

Sum of electronic and thermal Free Energies= -2219.144133

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.998383	0.124457	0.336008
2	6	0	5.299335	0.626378	0.246705
3	6	0	6.377612	-0.152700	0.641899
4	6	0	6.133802	-1.434262	1.142566
5	6	0	4.832079	-1.921346	1.246940
6	6	0	3.747262	-1.141724	0.838660
7	6	0	3.032852	1.171582	-0.183943
8	6	0	3.835449	2.474319	0.027844
9	6	0	5.275229	2.047381	-0.273236
10	1	0	7.391207	0.232608	0.581797

11	1	0	6.966586	-2.051736	1.464120
12	1	0	4.655305	-2.915762	1.643971
13	1	0	2.733528	-1.526119	0.911610
14	1	0	2.799578	1.006499	-1.239801
15	1	0	3.467443	3.306121	-0.587701
16	1	0	5.460121	2.082862	-1.352701
17	6	0	1.556257	2.085241	1.584655
18	6	0	2.541037	3.172614	1.889869
19	6	0	0.667842	0.436436	0.387879
20	1	0	2.619852	3.320312	2.967774
21	1	0	5.988702	2.711044	0.220362
22	7	0	1.759475	1.232103	0.532119
23	7	0	0.410068	1.860193	2.150431
24	7	0	-0.116974	0.835457	1.401521
25	8	0	3.817995	2.831520	1.405902
26	1	0	2.182627	4.107898	1.435172
27	6	0	-1.340836	0.229583	1.844671
28	6	0	-2.516010	0.982924	1.842180
29	6	0	-1.284219	-1.082783	2.336200
30	6	0	-3.671868	0.371255	2.333556
31	6	0	-2.466845	-1.649966	2.797338
32	6	0	-3.669243	-0.936130	2.808850
33	1	0	-4.601838	0.934489	2.325928
34	1	0	-2.446860	-2.667761	3.179937
35	6	0	-2.563140	2.402695	1.342741
36	1	0	-2.469638	3.105500	2.177037
37	1	0	-1.759669	2.626583	0.636308
38	1	0	-3.519098	2.591676	0.846339
39	6	0	-4.918960	-1.563621	3.367414
40	1	0	-5.807244	-1.000184	3.074098
41	1	0	-5.032505	-2.590718	3.011110
42	1	0	-4.878089	-1.593388	4.461240
43	6	0	0.022047	-1.825224	2.425926
44	1	0	0.462876	-1.979075	1.439011
45	1	0	0.749102	-1.260375	3.020136
46	1	0	-0.122872	-2.800513	2.894033
47	6	0	0.203525	-0.253004	-1.391350
48	8	0	1.075012	0.231730	-2.137632
49	1	0	-0.689271	1.079732	-3.386987
50	6	0	-1.290713	0.194719	-1.521390
51	6	0	-1.456055	1.253780	-2.628759
52	1	0	-1.632017	0.617249	-0.578173
53	1	0	-2.426222	1.120097	-3.112126
54	6	0	-1.351656	2.654803	-2.074101

55	6	0	-2.478729	3.476376	-2.001768
56	6	0	-0.139356	3.137373	-1.562226
57	6	0	-2.412421	4.736289	-1.407596
58	1	0	-3.422152	3.125101	-2.413830
59	6	0	-0.070365	4.395058	-0.969739
60	1	0	0.744835	2.510668	-1.646368
61	6	0	-1.209278	5.196287	-0.880728
62	1	0	-3.301932	5.356757	-1.358387
63	1	0	0.878904	4.762904	-0.590150
64	1	0	-1.153321	6.175430	-0.415970
65	6	0	-2.089136	-1.101658	-1.738915
66	8	0	-2.309313	-1.268070	-3.139265
67	6	0	-1.108769	-2.228909	-1.373386
68	8	0	-1.390641	-3.416900	-1.397417
69	6	0	-3.427896	-1.123288	-1.006251
70	6	0	-3.966543	-2.287007	-0.451013
71	6	0	-4.203337	0.043590	-0.992109
72	6	0	-5.250896	-2.282349	0.092521
73	1	0	-3.384206	-3.199927	-0.450827
74	6	0	-5.483561	0.047723	-0.450900
75	1	0	-3.801053	0.967926	-1.397528
76	6	0	-6.015173	-1.120369	0.092058
77	1	0	-5.653549	-3.197305	0.516775
78	1	0	-6.063763	0.965543	-0.449067
79	1	0	-7.015762	-1.122667	0.513627
80	7	0	0.142692	-1.711254	-1.205103
81	1	0	-2.705419	-2.143676	-3.254888
82	6	0	1.297604	-2.545965	-1.160342
83	6	0	1.313616	-3.649685	-0.300541
84	6	0	2.397163	-2.294936	-1.987577
85	6	0	2.435241	-4.470751	-0.243721
86	1	0	0.442238	-3.870630	0.303955
87	6	0	3.514705	-3.121605	-1.916551
88	1	0	2.366226	-1.456790	-2.668468
89	6	0	3.543869	-4.205748	-1.044961
90	1	0	2.437436	-5.323662	0.427389
91	1	0	4.369176	-2.911338	-2.551987
92	1	0	4.420049	-4.844113	-0.994526

M7RR

Total energy= -2219.85102851
Sum of electronic and zero-point Energies= -2219.093030
Sum of electronic and thermal Energies= -2219.049816

Sum of electronic and thermal Enthalpies= -2219.048872
Sum of electronic and thermal Free Energies= -2219.168681

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.641403	0.325872	-1.149276
2	6	0	-5.019442	0.531528	-1.085584
3	6	0	-5.864687	-0.146996	-1.953114
4	6	0	-5.304746	-1.008052	-2.901010
5	6	0	-3.922308	-1.177972	-2.983667
6	6	0	-3.074411	-0.507748	-2.099818
7	6	0	-2.967401	1.143120	-0.068090
8	6	0	-3.991570	2.276318	0.152943
9	6	0	-5.338285	1.564660	-0.025850
10	1	0	-6.939478	0.005128	-1.915274
11	1	0	-5.952235	-1.535913	-3.594355
12	1	0	-3.504744	-1.835713	-3.739420
13	1	0	-1.995264	-0.635578	-2.143806
14	1	0	-2.843540	0.562088	0.853102
15	1	0	-3.868643	2.775825	1.122557
16	1	0	-5.636142	1.089287	0.916194
17	6	0	-1.516622	2.920438	-0.980729
18	6	0	-2.650029	3.900668	-0.940069
19	6	0	-0.494063	0.972477	-0.483854
20	1	0	-2.643252	4.533807	-1.828073
21	1	0	-6.119555	2.270214	-0.318248
22	7	0	-1.669772	1.669420	-0.444883
23	7	0	-0.297442	3.096481	-1.385808
24	7	0	0.304311	1.893508	-1.068531
25	8	0	-3.889258	3.223055	-0.905850
26	1	0	-2.533757	4.540498	-0.052750
27	6	0	1.688119	1.696305	-1.363494
28	6	0	2.073967	0.544126	-2.064133
29	6	0	2.621664	2.644034	-0.921313
30	6	0	3.439455	0.330254	-2.262373
31	6	0	3.968497	2.403176	-1.188328
32	6	0	4.400105	1.244039	-1.833426
33	1	0	3.754730	-0.572063	-2.780072
34	1	0	4.703946	3.131786	-0.852384
35	6	0	1.080796	-0.438267	-2.636227
36	1	0	0.667688	-1.105427	-1.872786
37	1	0	0.236874	0.083124	-3.097669
38	1	0	1.570290	-1.055447	-3.392822

39	6	0	5.869396	0.983546	-2.041286
40	1	0	6.029606	0.207833	-2.793447
41	1	0	6.391023	1.891248	-2.356394
42	1	0	6.335155	0.641317	-1.110391
43	6	0	2.215671	3.859231	-0.128419
44	1	0	1.746365	4.614793	-0.762436
45	1	0	1.493103	3.590448	0.648760
46	1	0	3.091406	4.296574	0.355938
47	6	0	0.014139	-2.296467	0.745841
48	8	0	-0.124404	-3.269785	0.039481
49	1	0	3.177549	-2.068370	1.939664
50	6	0	1.311909	-1.553968	1.024004
51	6	0	2.547429	-2.460693	1.135528
52	1	0	1.409191	-0.831697	0.202247
53	1	0	2.228655	-3.459344	1.455462
54	6	0	3.372471	-2.584685	-0.126025
55	6	0	2.839078	-3.150981	-1.289442
56	6	0	4.709769	-2.179710	-0.131706
57	6	0	3.631830	-3.325459	-2.420661
58	1	0	1.800396	-3.470044	-1.292002
59	6	0	5.507653	-2.360870	-1.260316
60	1	0	5.134915	-1.733328	0.764344
61	6	0	4.972299	-2.939675	-2.407717
62	1	0	3.204471	-3.773528	-3.312807
63	1	0	6.548700	-2.053046	-1.239888
64	1	0	5.592461	-3.087081	-3.286549
65	6	0	0.985986	-0.767609	2.297636
66	8	0	1.169077	-1.570035	3.466832
67	6	0	-0.537505	-0.566421	2.174844
68	8	0	-1.221078	0.284593	2.686691
69	6	0	1.782659	0.488574	2.548053
70	6	0	2.880828	0.849872	1.767477
71	6	0	1.471861	1.243584	3.686139
72	6	0	3.668535	1.941601	2.136445
73	1	0	3.143700	0.295024	0.867803
74	6	0	2.241725	2.346054	4.033664
75	1	0	0.624386	0.953165	4.296705
76	6	0	3.351843	2.691871	3.262844
77	1	0	4.526378	2.205710	1.526190
78	1	0	1.985073	2.927896	4.913029
79	1	0	3.965171	3.543252	3.540621
80	7	0	-1.019112	-1.675428	1.458337
81	1	0	0.656989	-2.387511	3.383157
82	6	0	-2.402715	-2.021422	1.377336

83	6	0	-2.933941	-2.568006	0.209671
84	6	0	-3.225703	-1.788688	2.483935
85	6	0	-4.295622	-2.850192	0.141995
86	1	0	-2.294377	-2.757240	-0.641061
87	6	0	-4.584590	-2.068416	2.399318
88	1	0	-2.808437	-1.376089	3.393527
89	6	0	-5.126696	-2.593765	1.227145
90	1	0	-4.705418	-3.245695	-0.781696
91	1	0	-5.220283	-1.874715	3.257099
92	1	0	-6.189352	-2.803403	1.163534

M7RS

Total energy= -2219.84833906

Sum of electronic and zero-point Energies= -2219.092029

Sum of electronic and thermal Energies= -2219.047772

Sum of electronic and thermal Enthalpies= -2219.046828

Sum of electronic and thermal Free Energies= -2219.171973

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.494002	-1.011550	0.400469
2	6	0	-4.882018	-1.101688	0.310229
3	6	0	-5.666345	-0.945440	1.447120
4	6	0	-5.036476	-0.703143	2.668526
5	6	0	-3.645038	-0.620757	2.751741
6	6	0	-2.857281	-0.775011	1.611572
7	6	0	-2.890971	-1.130406	-0.981412
8	6	0	-4.010937	-1.828506	-1.790121
9	6	0	-5.302907	-1.345548	-1.121996
10	1	0	-6.748700	-1.017169	1.389352
11	1	0	-5.634974	-0.580724	3.566134
12	1	0	-3.172848	-0.427910	3.709834
13	1	0	-1.773879	-0.690287	1.656804
14	1	0	-2.693187	-0.139053	-1.405418
15	1	0	-3.954094	-1.596305	-2.861853
16	1	0	-5.643503	-0.415970	-1.593142
17	6	0	-1.570666	-3.153138	-1.552697
18	6	0	-2.775334	-3.797753	-2.165699
19	6	0	-0.443111	-1.481821	-0.538307
20	1	0	-2.782915	-4.867726	-1.954574
21	1	0	-6.094191	-2.090958	-1.233338
22	7	0	-1.651349	-1.885442	-1.040948

23	7	0	-0.367771	-3.620126	-1.426014
24	7	0	0.297717	-2.575655	-0.808817
25	8	0	-3.942982	-3.235927	-1.602248
26	1	0	-2.762202	-3.652958	-3.255894
27	6	0	1.659860	-2.800394	-0.430073
28	6	0	2.635183	-2.857589	-1.433104
29	6	0	1.955532	-3.029498	0.916128
30	6	0	3.939616	-3.168961	-1.054470
31	6	0	3.270492	-3.365582	1.242724
32	6	0	4.272742	-3.436639	0.276393
33	1	0	4.712750	-3.216356	-1.818190
34	1	0	3.514404	-3.568626	2.282915
35	6	0	2.269852	-2.586837	-2.867622
36	1	0	1.575735	-3.345175	-3.241042
37	1	0	1.773848	-1.614892	-2.952336
38	1	0	3.160966	-2.587005	-3.497940
39	6	0	5.695954	-3.755215	0.656788
40	1	0	5.751043	-4.187362	1.658695
41	1	0	6.145878	-4.459001	-0.048250
42	1	0	6.309254	-2.847448	0.648678
43	6	0	0.903310	-2.886073	1.982732
44	1	0	1.249806	-3.317153	2.923759
45	1	0	0.682147	-1.825630	2.147325
46	1	0	-0.032890	-3.372484	1.693993
47	6	0	0.356619	1.340276	0.821835
48	8	0	0.432998	1.111526	2.002964
49	1	0	3.450034	1.751613	-0.656998
50	6	0	1.457175	1.146373	-0.207143
51	6	0	2.771252	1.830590	0.200686
52	1	0	1.598695	0.063362	-0.292570
53	1	0	2.598361	2.899513	0.358672
54	6	0	3.433814	1.241590	1.423132
55	6	0	3.609591	2.013547	2.572620
56	6	0	3.919072	-0.068694	1.411570
57	6	0	4.263696	1.496328	3.687925
58	1	0	3.229481	3.031674	2.592389
59	6	0	4.577382	-0.586845	2.523554
60	1	0	3.788043	-0.688811	0.525221
61	6	0	4.753987	0.193558	3.664548
62	1	0	4.391289	2.111784	4.573167
63	1	0	4.957200	-1.603481	2.496394
64	1	0	5.269064	-0.212803	4.529205
65	6	0	0.830175	1.624968	-1.530880
66	8	0	0.976770	0.633215	-2.517311

67	6	0	-0.654404	1.787094	-1.191166
68	8	0	-1.522107	1.879388	-2.033420
69	6	0	1.347765	2.979706	-2.021188
70	6	0	2.266384	3.020025	-3.069390
71	6	0	0.942257	4.175640	-1.420731
72	6	0	2.774096	4.239535	-3.512719
73	1	0	2.577470	2.090815	-3.534251
74	6	0	1.449221	5.392812	-1.865837
75	1	0	0.226756	4.166593	-0.601513
76	6	0	2.367156	5.428048	-2.913571
77	1	0	3.487701	4.258512	-4.330280
78	1	0	1.122620	6.314453	-1.395212
79	1	0	2.759876	6.377604	-3.262136
80	7	0	-0.805525	1.845600	0.184351
81	1	0	0.336350	0.836736	-3.216125
82	6	0	-1.988924	2.258763	0.877426
83	6	0	-1.869129	2.777147	2.170692
84	6	0	-3.246997	2.175240	0.274397
85	6	0	-3.008934	3.165337	2.865991
86	1	0	-0.896124	2.864700	2.633577
87	6	0	-4.376377	2.574263	0.982088
88	1	0	-3.346296	1.807582	-0.736256
89	6	0	-4.267816	3.058103	2.281852
90	1	0	-2.904754	3.558950	3.871790
91	1	0	-5.349780	2.489124	0.509587
92	1	0	-5.154467	3.354887	2.832248

M7SR

Total energy= -2219.85884258
Sum of electronic and zero-point Energies= -2219.102172
Sum of electronic and thermal Energies= -2219.058097
Sum of electronic and thermal Enthalpies= -2219.057153
Sum of electronic and thermal Free Energies= -2219.181158

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.005710	-0.876659	-1.076817
2	6	0	4.379216	-0.867265	-1.322090
3	6	0	4.882756	-0.224787	-2.446918
4	6	0	3.991586	0.408162	-3.316152
5	6	0	2.617787	0.392420	-3.065719
6	6	0	2.110086	-0.255728	-1.938701

7	6	0	2.736941	-1.539227	0.255059
8	6	0	4.030651	-2.347500	0.522273
9	6	0	5.122983	-1.551030	-0.198821
10	1	0	5.950333	-0.210596	-2.646689
11	1	0	4.370537	0.915918	-4.197463
12	1	0	1.938087	0.892149	-3.748694
13	1	0	1.041047	-0.268269	-1.739322
14	1	0	2.607778	-0.777900	1.035846
15	1	0	4.218473	-2.476448	1.596124
16	1	0	5.547801	-0.802933	0.482217
17	6	0	1.634679	-3.768708	0.404526
18	6	0	2.967378	-4.445809	0.499034
19	6	0	0.271516	-1.987693	0.204128
20	1	0	2.952389	-5.394423	-0.039006
21	1	0	5.929029	-2.210374	-0.529686
22	7	0	1.570158	-2.405435	0.284496
23	7	0	0.442115	-4.283810	0.422123
24	7	0	-0.363736	-3.168978	0.300000
25	8	0	3.946394	-3.621747	-0.101895
26	1	0	3.217185	-4.640913	1.551915
27	6	0	-1.788523	-3.293632	0.319242
28	6	0	-2.452253	-3.627011	-0.862675
29	6	0	-2.463389	-3.008428	1.510213
30	6	0	-3.846958	-3.660147	-0.835738
31	6	0	-3.856456	-3.046032	1.488389
32	6	0	-4.562329	-3.359214	0.324537
33	1	0	-4.386129	-3.910394	-1.746632
34	1	0	-4.404549	-2.814079	2.398528
35	6	0	-1.671812	-3.899605	-2.120195
36	1	0	-2.340390	-4.136788	-2.949210
37	1	0	-1.072220	-3.025030	-2.393525
38	1	0	-0.977808	-4.733017	-1.978493
39	6	0	-6.067772	-3.318803	0.312145
40	1	0	-6.412694	-2.287079	0.177931
41	1	0	-6.475660	-3.916666	-0.506047
42	1	0	-6.483626	-3.686889	1.253223
43	6	0	-1.696726	-2.663175	2.759764
44	1	0	-1.053202	-3.496470	3.060161
45	1	0	-1.044291	-1.799382	2.593906
46	1	0	-2.379067	-2.439215	3.581619
47	6	0	0.452992	1.123798	1.222253
48	8	0	0.632461	0.532543	2.260184
49	1	0	-1.989940	0.244420	1.895325
50	6	0	-0.800481	1.119060	0.373691

51	6	0	-2.069016	1.112194	1.230180
52	1	0	-0.730312	0.157430	-0.155501
53	1	0	-2.100356	2.002002	1.866465
54	6	0	-3.340508	1.020694	0.419506
55	6	0	-4.289328	2.043295	0.472195
56	6	0	-3.596184	-0.095291	-0.382648
57	6	0	-5.472727	1.956905	-0.257503
58	1	0	-4.086835	2.923473	1.079063
59	6	0	-4.778489	-0.185681	-1.112758
60	1	0	-2.869891	-0.905456	-0.428228
61	6	0	-5.721156	0.840180	-1.051792
62	1	0	-6.197914	2.763320	-0.206597
63	1	0	-4.963089	-1.064525	-1.724682
64	1	0	-6.642526	0.769514	-1.621562
65	6	0	-0.578769	2.232947	-0.662001
66	8	0	-0.836607	1.733431	-1.954341
67	6	0	0.930642	2.517495	-0.560829
68	8	0	1.554619	3.168279	-1.365582
69	6	0	-1.334680	3.525277	-0.373662
70	6	0	-1.064971	4.251668	0.790358
71	6	0	-2.317900	3.978976	-1.249649
72	6	0	-1.778763	5.410132	1.078523
73	1	0	-0.294759	3.915226	1.482270
74	6	0	-3.028900	5.143178	-0.963476
75	1	0	-2.544351	3.403116	-2.140370
76	6	0	-2.764764	5.858760	0.200479
77	1	0	-1.562070	5.963994	1.986044
78	1	0	-3.797305	5.484534	-1.649822
79	1	0	-3.321289	6.763003	0.424195
80	7	0	1.432771	1.909680	0.581482
81	1	0	-0.425287	2.350249	-2.579655
82	6	0	2.783022	2.034237	1.030661
83	6	0	3.827202	1.977651	0.106744
84	6	0	3.039273	2.207488	2.391815
85	6	0	5.138941	2.088184	0.560559
86	1	0	3.616608	1.844388	-0.948222
87	6	0	4.355764	2.309741	2.829531
88	1	0	2.215516	2.253155	3.093662
89	6	0	5.407941	2.248974	1.917840
90	1	0	5.951754	2.038949	-0.157648
91	1	0	4.556801	2.441454	3.887426
92	1	0	6.432862	2.330346	2.264482

M7SS

Total energy= -2219.85346026
Sum of electronic and zero-point Energies= -2219.096359
Sum of electronic and thermal Energies= -2219.052459
Sum of electronic and thermal Enthalpies= -2219.051515
Sum of electronic and thermal Free Energies= -2219.173688

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.002744	0.164321	0.116563
2	6	0	5.301425	0.596834	-0.159138
3	6	0	6.391113	-0.167348	0.237641
4	6	0	6.159354	-1.363617	0.920232
5	6	0	4.859165	-1.789716	1.190236
6	6	0	3.761567	-1.029562	0.780249
7	6	0	3.009693	1.168526	-0.430623
8	6	0	3.868056	2.449836	-0.568115
9	6	0	5.269767	1.921758	-0.887895
10	1	0	7.405338	0.164453	0.035030
11	1	0	7.001306	-1.966062	1.246911
12	1	0	4.694283	-2.724487	1.716517
13	1	0	2.742953	-1.358819	0.971385
14	1	0	2.637699	0.845717	-1.408975
15	1	0	3.468509	3.141968	-1.322282
16	1	0	5.382299	1.780920	-1.968803
17	6	0	1.716964	2.533105	1.196322
18	6	0	2.729701	3.633742	1.125013
19	6	0	0.822818	0.535840	0.649763
20	1	0	2.882292	4.071905	2.112275
21	1	0	6.032646	2.629692	-0.555232
22	7	0	1.855939	1.407602	0.425839
23	7	0	0.644716	2.463045	1.922234
24	7	0	0.120265	1.236141	1.564704
25	8	0	3.964060	3.108571	0.688720
26	1	0	2.381953	4.425311	0.444813
27	6	0	-1.051023	0.774655	2.243165
28	6	0	-2.244329	1.485339	2.092885
29	6	0	-0.948921	-0.352193	3.071780
30	6	0	-3.358228	1.045985	2.811375
31	6	0	-2.093695	-0.762587	3.751771
32	6	0	-3.302004	-0.068660	3.645319
33	1	0	-4.296630	1.585104	2.702488
34	1	0	-2.036066	-1.634586	4.399373

35	6	0	-2.329043	2.683474	1.186540
36	1	0	-1.901654	3.569328	1.666319
37	1	0	-1.766253	2.523437	0.262128
38	1	0	-3.368971	2.895934	0.929564
39	6	0	-4.510100	-0.523719	4.424491
40	1	0	-4.723737	-1.580559	4.237145
41	1	0	-4.343885	-0.412335	5.500364
42	1	0	-5.395860	0.058346	4.158927
43	6	0	0.355882	-1.084954	3.242361
44	1	0	0.652730	-1.578645	2.313190
45	1	0	1.162628	-0.391552	3.501190
46	1	0	0.272090	-1.833977	4.031963
47	6	0	0.010996	-0.880982	-1.864335
48	8	0	0.998066	-0.405300	-2.372737
49	1	0	-1.057554	0.520953	-3.782100
50	6	0	-1.383270	-0.283849	-1.813727
51	6	0	-1.694972	0.731339	-2.917301
52	1	0	-1.455348	0.183374	-0.821148
53	1	0	-2.730296	0.583971	-3.240707
54	6	0	-1.508946	2.158394	-2.457380
55	6	0	-2.594591	3.032995	-2.401510
56	6	0	-0.253399	2.615314	-2.037875
57	6	0	-2.437688	4.338162	-1.936199
58	1	0	-3.574839	2.685290	-2.717212
59	6	0	-0.096099	3.916987	-1.571364
60	1	0	0.596529	1.938618	-2.084238
61	6	0	-1.187539	4.783633	-1.516785
62	1	0	-3.294747	5.003327	-1.897933
63	1	0	0.884855	4.261959	-1.257931
64	1	0	-1.062344	5.797235	-1.149881
65	6	0	-2.264047	-1.537785	-1.800766
66	8	0	-2.327498	-1.988744	-3.143632
67	6	0	-1.366088	-2.551293	-1.059120
68	8	0	-1.724308	-3.571217	-0.521008
69	6	0	-3.630535	-1.348694	-1.184764
70	6	0	-3.779207	-1.216217	0.198735
71	6	0	-4.754442	-1.265745	-2.007715
72	6	0	-5.044357	-1.027951	0.745819
73	1	0	-2.911589	-1.263542	0.856401
74	6	0	-6.018911	-1.068268	-1.456356
75	1	0	-4.636693	-1.355080	-3.082533
76	6	0	-6.166693	-0.955991	-0.078100
77	1	0	-5.153813	-0.937677	1.821204
78	1	0	-6.885678	-1.006791	-2.106426

79	1	0	-7.150620	-0.811500	0.356312
80	7	0	-0.049339	-2.136900	-1.240756
81	1	0	-2.814516	-2.825203	-3.158656
82	6	0	1.088196	-2.917319	-0.886715
83	6	0	1.099101	-3.596075	0.332849
84	6	0	2.171101	-3.009411	-1.761583
85	6	0	2.203948	-4.371061	0.673616
86	1	0	0.244641	-3.527268	0.995214
87	6	0	3.272343	-3.780978	-1.403395
88	1	0	2.147786	-2.480446	-2.705268
89	6	0	3.291727	-4.465889	-0.191717
90	1	0	2.210949	-4.901864	1.620080
91	1	0	4.117859	-3.846872	-2.080090
92	1	0	4.152907	-5.067503	0.080287

PRR

Total energy= -1167.91245120
Sum of electronic and zero-point Energies= -1167.540591
Sum of electronic and thermal Energies= -1167.519026
Sum of electronic and thermal Enthalpies= -1167.518082
Sum of electronic and thermal Free Energies= -1167.591751

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.115043	0.171078	1.407371
2	8	0	0.277624	0.620349	2.455373
3	1	0	0.096602	-2.422566	2.455361
4	6	0	-0.971291	-1.066131	1.192070
5	6	0	-0.069139	-2.314408	1.379565
6	1	0	-1.780455	-1.092278	1.924306
7	1	0	-0.634876	-3.183854	1.037546
8	6	0	1.271137	-2.241111	0.676917
9	6	0	1.441459	-2.710803	-0.629005
10	6	0	2.372343	-1.681776	1.336179
11	6	0	2.682276	-2.624965	-1.258659
12	1	0	0.593561	-3.145305	-1.147875
13	6	0	3.611379	-1.592033	0.708074
14	1	0	2.252315	-1.311240	2.351019
15	6	0	3.770761	-2.066269	-0.592557
16	1	0	2.798220	-3.001790	-2.270065
17	1	0	4.452620	-1.153680	1.235633
18	1	0	4.736880	-2.000736	-1.082952

19	6	0	-1.498579	-0.871799	-0.243438
20	8	0	-1.602640	-2.091201	-0.927634
21	6	0	-0.408581	-0.002137	-0.878974
22	8	0	-0.195656	0.094638	-2.063843
23	6	0	-2.832504	-0.118720	-0.236185
24	6	0	-2.912026	1.272882	-0.144641
25	6	0	-4.009820	-0.869413	-0.273342
26	6	0	-4.154043	1.902056	-0.090812
27	1	0	-2.012503	1.881903	-0.125855
28	6	0	-5.248469	-0.238610	-0.216224
29	1	0	-3.943552	-1.949136	-0.352741
30	6	0	-5.324443	1.149554	-0.123877
31	1	0	-4.203004	2.984164	-0.026782
32	1	0	-6.155954	-0.833115	-0.244736
33	1	0	-6.290384	1.642060	-0.080863
34	7	0	0.250169	0.664739	0.143898
35	1	0	-1.634848	-1.879686	-1.873330
36	6	0	1.292061	1.616780	-0.059884
37	6	0	1.235850	2.846630	0.589764
38	6	0	2.356240	1.284462	-0.895118
39	6	0	2.267237	3.760765	0.395760
40	1	0	0.398919	3.074417	1.240780
41	6	0	3.375044	2.211787	-1.089619
42	1	0	2.379389	0.308075	-1.369052
43	6	0	3.332676	3.447204	-0.445617
44	1	0	2.234207	4.720547	0.900259
45	1	0	4.208293	1.963199	-1.738451
46	1	0	4.131620	4.165425	-0.597152

PRS

Total energy= -1167.90742300
Sum of electronic and zero-point Energies= -1167.536205
Sum of electronic and thermal Energies= -1167.514244
Sum of electronic and thermal Enthalpies= -1167.513300
Sum of electronic and thermal Free Energies= -1167.589832

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.165827	-0.844577	0.030513
2	8	0	0.057189	-1.720887	0.826611
3	1	0	2.627450	1.147202	-0.419737
4	6	0	0.838502	0.027078	-0.706031

5	6	0	2.125555	0.306631	0.073164
6	1	0	1.081243	-0.511345	-1.632395
7	1	0	1.875984	0.634296	1.087126
8	6	0	3.057757	-0.882929	0.117560
9	6	0	3.215788	-1.633988	1.282544
10	6	0	3.780441	-1.248649	-1.021898
11	6	0	4.078462	-2.727134	1.311982
12	1	0	2.650095	-1.362876	2.169057
13	6	0	4.640854	-2.342777	-0.998284
14	1	0	3.671942	-0.665751	-1.934284
15	6	0	4.792589	-3.085352	0.170994
16	1	0	4.190513	-3.300339	2.226998
17	1	0	5.196787	-2.612364	-1.890766
18	1	0	5.463832	-3.937854	0.192301
19	6	0	0.001271	1.244843	-1.139303
20	8	0	0.387077	1.640831	-2.429253
21	6	0	-1.423591	0.677642	-1.178144
22	8	0	-2.349403	1.170936	-1.776714
23	6	0	0.064932	2.396228	-0.136136
24	6	0	0.877387	3.494653	-0.418968
25	6	0	-0.629001	2.352673	1.077045
26	6	0	0.996420	4.535991	0.498333
27	1	0	1.414098	3.526809	-1.361010
28	6	0	-0.508831	3.395095	1.991571
29	1	0	-1.276209	1.513137	1.318325
30	6	0	0.305099	4.488894	1.705596
31	1	0	1.630942	5.385213	0.266212
32	1	0	-1.056680	3.352563	2.927157
33	1	0	0.396984	5.300422	2.419843
34	7	0	-1.455715	-0.468716	-0.395933
35	1	0	-0.299365	2.239367	-2.760740
36	6	0	-2.650596	-1.174975	-0.061379
37	6	0	-2.890321	-1.535192	1.263701
38	6	0	-3.564223	-1.484672	-1.067128
39	6	0	-4.059930	-2.220353	1.578599
40	1	0	-2.165942	-1.288772	2.031173
41	6	0	-4.735167	-2.159180	-0.736108
42	1	0	-3.357583	-1.194113	-2.090408
43	6	0	-4.983575	-2.530767	0.583295
44	1	0	-4.250072	-2.506513	2.607611
45	1	0	-5.451547	-2.398503	-1.514810
46	1	0	-5.895337	-3.061701	0.835625

PSR

Total energy= -1167.90028615
Sum of electronic and zero-point Energies= -1167.528866
Sum of electronic and thermal Energies= -1167.507011
Sum of electronic and thermal Enthalpies= -1167.506067
Sum of electronic and thermal Free Energies= -1167.581849

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.774622	-0.488056	0.863790
2	8	0	-1.377591	-1.480189	1.189016
3	1	0	0.909697	-0.608265	-1.270890
4	6	0	0.729997	-0.273051	0.866662
5	6	0	1.343599	-1.009096	-0.347263
6	1	0	1.163677	-0.669312	1.789472
7	1	0	2.410771	-0.768085	-0.368085
8	6	0	1.149936	-2.504518	-0.288417
9	6	0	1.923291	-3.275901	0.583401
10	6	0	0.197578	-3.140354	-1.085814
11	6	0	1.745278	-4.653679	0.660086
12	1	0	2.675251	-2.791714	1.202404
13	6	0	0.017676	-4.519931	-1.013922
14	1	0	-0.405842	-2.549430	-1.771009
15	6	0	0.790166	-5.279505	-0.138950
16	1	0	2.355280	-5.240634	1.339426
17	1	0	-0.725942	-5.000379	-1.641832
18	1	0	0.651480	-6.354318	-0.081928
19	6	0	0.871774	1.266745	0.822354
20	8	0	0.899601	1.809432	2.133461
21	6	0	-0.465294	1.719464	0.191080
22	8	0	-0.721341	2.804417	-0.268541
23	6	0	2.092652	1.778887	0.094817
24	6	0	3.291639	1.899417	0.800515
25	6	0	2.070149	2.060395	-1.272442
26	6	0	4.453876	2.296999	0.146286
27	1	0	3.303597	1.685281	1.863725
28	6	0	3.234566	2.457294	-1.925002
29	1	0	1.143167	1.985179	-1.832113
30	6	0	4.428120	2.576628	-1.218444
31	1	0	5.380539	2.388880	0.703641
32	1	0	3.205177	2.678951	-2.986762
33	1	0	5.333801	2.888670	-1.728392
34	7	0	-1.375213	0.673192	0.347239

35	1	0	0.239865	1.364615	2.682631
36	6	0	-2.765873	0.773401	0.042981
37	6	0	-3.390771	-0.267486	-0.642465
38	6	0	-3.478335	1.907631	0.427995
39	6	0	-4.746133	-0.169266	-0.938870
40	1	0	-2.819595	-1.143272	-0.928931
41	6	0	-4.831064	1.998688	0.115088
42	1	0	-2.975177	2.708263	0.957235
43	6	0	-5.467411	0.962669	-0.564884
44	1	0	-5.237447	-0.978918	-1.467834
45	1	0	-5.388653	2.881753	0.408370
46	1	0	-6.523276	1.036865	-0.802792

PSS

Total energy= -1167.91029185
Sum of electronic and zero-point Energies= -1167.539119
Sum of electronic and thermal Energies= -1167.517340
Sum of electronic and thermal Enthalpies= -1167.516396
Sum of electronic and thermal Free Energies= -1167.591935

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.344120	-1.254970	-0.609276
2	8	0	1.842192	-2.224308	-1.126664
3	1	0	-0.794132	-2.892868	-1.023215
4	6	0	-0.135984	-0.931595	-0.511540
5	6	0	-0.986632	-2.170521	-0.223231
6	1	0	-0.413635	-0.520238	-1.490642
7	1	0	-0.654886	-2.622171	0.714700
8	6	0	-2.457992	-1.835412	-0.140186
9	6	0	-3.153484	-1.987802	1.059799
10	6	0	-3.137725	-1.328337	-1.251130
11	6	0	-4.496504	-1.628975	1.155172
12	1	0	-2.628828	-2.370971	1.930486
13	6	0	-4.477162	-0.962730	-1.159257
14	1	0	-2.612625	-1.210192	-2.196501
15	6	0	-5.159926	-1.107845	0.047315
16	1	0	-5.021655	-1.751810	2.097382
17	1	0	-4.988230	-0.562336	-2.029268
18	1	0	-6.204145	-0.820934	0.120701
19	6	0	-0.218760	0.206756	0.522438
20	8	0	-0.504751	-0.366298	1.782482

21	6	0	1.237334	0.712126	0.613502
22	8	0	1.600390	1.696801	1.211026
23	6	0	-1.177450	1.317404	0.139801
24	6	0	-2.425895	1.423245	0.749307
25	6	0	-0.827392	2.213223	-0.873316
26	6	0	-3.317988	2.414222	0.343875
27	1	0	-2.710365	0.711701	1.517783
28	6	0	-1.717551	3.202534	-1.276032
29	1	0	0.147850	2.141145	-1.350773
30	6	0	-2.967619	3.304298	-0.667012
31	1	0	-4.292813	2.482865	0.816490
32	1	0	-1.434441	3.895281	-2.061828
33	1	0	-3.663998	4.074973	-0.981436
34	7	0	2.066402	-0.209397	-0.015202
35	1	0	-0.481936	0.345205	2.438722
36	6	0	3.491743	-0.130754	-0.014231
37	6	0	4.188580	-0.356844	-1.199966
38	6	0	4.166001	0.177169	1.165831
39	6	0	5.577240	-0.277006	-1.198855
40	1	0	3.645870	-0.596713	-2.106992
41	6	0	5.554631	0.265260	1.151079
42	1	0	3.607145	0.352518	2.077444
43	6	0	6.262077	0.037106	-0.026861
44	1	0	6.122930	-0.455781	-2.119193
45	1	0	6.083623	0.509014	2.066220
46	1	0	7.344848	0.104212	-0.031784

Cartesian coordinates of the structures at M06-2X/6-31G(d, p)//SMD$_{DCM}$ level

Cat

Total energy= -1051.94747524
Sum of electronic and zero-point Energies= -1051.564091
Sum of electronic and thermal Energies= -1051.544071
Sum of electronic and thermal Enthalpies= -1051.543127
Sum of electronic and thermal Free Energies= -1051.613112

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.922319	0.578538	-0.621335
2	6	0	-4.258039	0.331769	-0.297120
3	6	0	-5.131855	1.390130	-0.079077
4	6	0	-4.647018	2.695675	-0.181965

5	6	0	-3.309182	2.935495	-0.498027
6	6	0	-2.431800	1.873230	-0.723513
7	6	0	-2.207843	-0.737773	-0.848484
8	6	0	-3.114140	-1.748481	-0.102558
9	6	0	-4.519790	-1.156381	-0.240824
10	1	0	-6.171023	1.206152	0.178941
11	1	0	-5.316103	3.532458	-0.005697
12	1	0	-2.946422	3.956363	-0.566595
13	1	0	-1.388559	2.051168	-0.967519
14	1	0	-2.182765	-0.980409	-1.915977
15	1	0	-3.017100	-2.765423	-0.503941
16	1	0	-4.985685	-1.509136	-1.167805
17	6	0	-0.495242	-1.454897	0.801675
18	6	0	-1.513811	-2.256601	1.550985
19	6	0	0.245912	-0.159393	-0.891239
20	1	0	-1.339611	-2.186245	2.626022
21	1	0	-5.151470	-1.462490	0.596822
22	7	0	-0.841720	-0.789953	-0.344713
23	7	0	0.768833	-1.304118	1.051035
24	7	0	1.191228	-0.511330	0.001856
25	8	0	-2.802520	-1.743912	1.284761
26	1	0	-1.446375	-3.313207	1.253204
27	6	0	2.562711	-0.097915	-0.023560
28	6	0	3.456443	-0.756576	-0.871326
29	6	0	2.957722	0.946297	0.818874
30	6	0	4.785167	-0.329594	-0.872343
31	6	0	4.295798	1.337041	0.787363
32	6	0	5.221558	0.710471	-0.049846
33	1	0	5.495878	-0.825839	-1.529299
34	1	0	4.621288	2.151877	1.430016
35	6	0	2.993401	-1.883796	-1.754098
36	1	0	2.442505	-2.632815	-1.176253
37	1	0	2.320123	-1.519074	-2.535705
38	1	0	3.844554	-2.371681	-2.233341
39	6	0	6.668826	1.128568	-0.039697
40	1	0	7.224665	0.578735	0.727731
41	1	0	7.147341	0.928563	-1.001584
42	1	0	6.770898	2.194024	0.182221
43	6	0	1.959911	1.619227	1.721479
44	1	0	1.092211	1.970011	1.153190
45	1	0	1.586286	0.922801	2.478843
46	1	0	2.412683	2.473060	2.229208

R1

Total energy= -422.80878260
Sum of electronic and zero-point Energies= -422.663817
Sum of electronic and thermal Energies= -422.655234
Sum of electronic and thermal Enthalpies= -422.654289
Sum of electronic and thermal Free Energies= -422.698277

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.408865	0.384566	0.000030
2	8	0	-3.849405	-0.749469	-0.000209
3	1	0	-4.099281	1.248915	0.000120
4	6	0	-1.973238	0.719828	0.000039
5	6	0	-1.053051	-0.258959	0.000183
6	1	0	-1.713014	1.774370	-0.000163
7	1	0	-1.424569	-1.283831	0.000211
8	6	0	0.404486	-0.110770	0.000090
9	6	0	1.193490	-1.269678	0.000090
10	6	0	1.041806	1.139936	0.000041
11	6	0	2.582182	-1.186134	-0.000041
12	1	0	0.705795	-2.240940	0.000159
13	6	0	2.427728	1.222678	-0.000064
14	1	0	0.451722	2.051216	0.000142
15	6	0	3.202317	0.060680	-0.000118
16	1	0	3.178701	-2.092861	-0.000060
17	1	0	2.909109	2.195665	-0.000063
18	1	0	4.285641	0.130328	-0.000181

R2

Total energy= -745.05766364
Sum of electronic and zero-point Energies= -422.663817
Sum of electronic and thermal Energies= -422.655234
Sum of electronic and thermal Enthalpies= -422.654289
Sum of electronic and thermal Free Energies= -422.698277

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.153789	0.861406	-0.023685
2	8	0	0.989757	2.066407	0.011775
3	6	0	-0.099763	-0.040276	-0.149510
4	8	0	-0.028244	-1.215054	-0.474926

5	6	0	2.504399	0.247080	0.009245
6	6	0	2.733381	-1.078887	0.398190
7	6	0	3.586915	1.076005	-0.315688
8	6	0	4.036470	-1.564184	0.452491
9	1	0	1.901471	-1.719631	0.660315
10	6	0	4.882873	0.580940	-0.274252
11	1	0	3.392403	2.104583	-0.602501
12	6	0	5.107515	-0.741344	0.110758
13	1	0	4.215296	-2.589539	0.759539
14	1	0	5.718057	1.221795	-0.537312
15	1	0	6.120872	-1.129364	0.146982
16	7	0	-1.229785	0.654342	0.112584
17	1	0	-1.087296	1.640543	0.306908
18	6	0	-2.563220	0.208457	0.058482
19	6	0	-3.559823	1.169120	0.271648
20	6	0	-2.919588	-1.122014	-0.188585
21	6	0	-4.899201	0.805442	0.236339
22	1	0	-3.274569	2.199685	0.465124
23	6	0	-4.268605	-1.468983	-0.220187
24	1	0	-2.154143	-1.866280	-0.354311
25	6	0	-5.262932	-0.517641	-0.011018
26	1	0	-5.660813	1.560977	0.401532
27	1	0	-4.538485	-2.502600	-0.414611
28	1	0	-6.309666	-0.802108	-0.039916

Si-M3

Total energy= -1474.79416537
Sum of electronic and zero-point Energies= -1474.261453
Sum of electronic and thermal Energies= -1474.231712
Sum of electronic and thermal Enthalpies= -1474.230768
Sum of electronic and thermal Free Energies= -1474.323170

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.800502	-0.949556	0.020325
2	6	0	-4.036841	-1.597836	0.072125
3	6	0	-5.095602	-1.026276	0.766466
4	6	0	-4.895413	0.196310	1.411735
5	6	0	-3.656422	0.834770	1.360685
6	6	0	-2.592667	0.267201	0.655660
7	6	0	-1.856942	-1.758919	-0.842120
8	6	0	-2.481621	-3.172266	-0.802509

9	6	0	-3.983826	-2.897123	-0.699273
10	1	0	-6.059157	-1.525399	0.817383
11	1	0	-5.711651	0.652180	1.963910
12	1	0	-3.515117	1.784427	1.867854
13	1	0	-1.628262	0.767743	0.616495
14	1	0	-1.808296	-1.349946	-1.854440
15	1	0	-2.193421	-3.780912	-1.668189
16	1	0	-4.412034	-2.777554	-1.700544
17	6	0	0.076325	-2.901809	0.266166
18	6	0	-0.734288	-4.149017	0.446632
19	6	0	0.479677	-0.862356	-0.426129
20	1	0	-0.520053	-4.598624	1.417596
21	1	0	-4.494689	-3.726726	-0.204746
22	7	0	-0.471795	-1.815519	-0.356976
23	7	0	1.319042	-2.682823	0.582415
24	7	0	1.556520	-1.409732	0.141876
25	8	0	-2.104972	-3.828623	0.403433
26	1	0	-0.469459	-4.867404	-0.342036
27	6	0	2.882233	-0.862235	0.239140
28	6	0	3.654989	-0.797603	-0.922071
29	6	0	3.334831	-0.439030	1.491179
30	6	0	4.939370	-0.266426	-0.801986
31	6	0	4.624539	0.083762	1.557308
32	6	0	5.435791	0.181709	0.423516
33	1	0	5.564589	-0.203694	-1.689134
34	1	0	5.002763	0.428094	2.516824
35	6	0	3.116417	-1.271763	-2.244595
36	1	0	2.701859	-2.282001	-2.162640
37	1	0	2.316545	-0.614780	-2.605463
38	1	0	3.908921	-1.284139	-2.995099
39	6	0	6.810486	0.787889	0.524707
40	1	0	6.746109	1.880828	0.559230
41	1	0	7.319782	0.461596	1.435379
42	1	0	7.427963	0.517274	-0.334796
43	6	0	2.452156	-0.532936	2.705967
44	1	0	1.491696	-0.035197	2.533957
45	1	0	2.237062	-1.575802	2.959030
46	1	0	2.934005	-0.061947	3.564548
47	6	0	0.306419	0.461319	-1.128539
48	8	0	-0.414637	0.395522	-2.179311
49	1	0	1.724319	3.477907	-0.968677
50	6	0	0.921576	1.529579	-0.539184
51	6	0	0.808006	2.903706	-1.145524
52	1	0	1.472014	1.399744	0.386863

53	1	0	0.694755	2.786592	-2.230229
54	6	0	-0.380486	3.688658	-0.623212
55	6	0	-1.675904	3.215578	-0.873190
56	6	0	-0.225903	4.859094	0.120653
57	6	0	-2.786447	3.899837	-0.388874
58	1	0	-1.785646	2.295918	-1.446190
59	6	0	-1.338196	5.546073	0.609665
60	1	0	0.774268	5.236157	0.321198
61	6	0	-2.621195	5.069396	0.356232
62	1	0	-3.784431	3.519693	-0.590079
63	1	0	-1.199472	6.455431	1.187681
64	1	0	-3.487828	5.603486	0.734404

TS5RR

Total energy= -2219.86445776

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.449109	-1.970795	-0.791764
2	6	0	4.836731	-2.084034	-0.914113
3	6	0	5.404875	-3.256526	-1.395491
4	6	0	4.566929	-4.319797	-1.735682
5	6	0	3.183706	-4.207406	-1.595566
6	6	0	2.609704	-3.024390	-1.126453
7	6	0	3.123972	-0.578158	-0.281556
8	6	0	4.437071	-0.174274	0.429494
9	6	0	5.512574	-0.815472	-0.446363
10	1	0	6.482930	-3.350222	-1.490008
11	1	0	4.995578	-5.246432	-2.104862
12	1	0	2.546343	-5.046280	-1.856638
13	1	0	1.532321	-2.931025	-1.035626
14	1	0	2.890614	0.102409	-1.103565
15	1	0	4.536522	0.908547	0.552300
16	1	0	5.748052	-0.154539	-1.288699
17	6	0	2.180953	-0.547269	2.026100
18	6	0	3.549027	-0.366905	2.608011
19	6	0	0.671889	-0.574074	0.450076
20	1	0	3.643683	-0.941413	3.530625
21	1	0	6.428432	-0.987135	0.124216
22	7	0	2.000614	-0.522048	0.671712
23	7	0	1.041955	-0.661909	2.648554
24	7	0	0.112108	-0.684567	1.657360

25	8	0	4.515416	-0.825161	1.695170
26	1	0	3.689806	0.700295	2.835374
27	6	0	-1.269012	-0.937291	1.976117
28	6	0	-1.869356	-2.082995	1.440603
29	6	0	-1.947524	-0.027567	2.797532
30	6	0	-3.231174	-2.261580	1.684557
31	6	0	-3.306627	-0.256679	3.003051
32	6	0	-3.967285	-1.352589	2.443335
33	1	0	-3.727568	-3.129830	1.258461
34	1	0	-3.864914	0.446483	3.617091
35	6	0	-1.110083	-3.091813	0.619064
36	1	0	-1.030617	-2.778382	-0.428442
37	1	0	-0.099457	-3.253450	1.007410
38	1	0	-1.637214	-4.048029	0.630336
39	6	0	-5.440480	-1.550893	2.680367
40	1	0	-5.636114	-1.782043	3.732662
41	1	0	-5.998969	-0.641686	2.438119
42	1	0	-5.832435	-2.369608	2.073095
43	6	0	-1.261895	1.140683	3.453805
44	1	0	-0.726726	0.812645	4.350811
45	1	0	-0.542309	1.612286	2.783479
46	1	0	-2.002965	1.884719	3.754923
47	6	0	0.037491	-0.471835	-0.927662
48	8	0	0.776671	-0.768379	-1.870137
49	1	0	-2.331804	0.476457	-2.868875
50	6	0	-1.277813	0.071721	-1.030947
51	6	0	-2.074283	-0.387806	-2.243725
52	1	0	-1.835853	0.137995	-0.103403
53	1	0	-1.432950	-1.027142	-2.857983
54	6	0	-3.325947	-1.136052	-1.846498
55	6	0	-3.421688	-2.521826	-2.000367
56	6	0	-4.415472	-0.449488	-1.296149
57	6	0	-4.572038	-3.209366	-1.613057
58	1	0	-2.588719	-3.065853	-2.439804
59	6	0	-5.565349	-1.131480	-0.907885
60	1	0	-4.357841	0.630764	-1.177408
61	6	0	-5.647713	-2.515971	-1.063151
62	1	0	-4.628057	-4.285949	-1.746568
63	1	0	-6.401986	-0.581062	-0.486479
64	1	0	-6.546665	-3.047706	-0.765335
65	6	0	-0.895878	1.965051	-1.475555
66	8	0	-0.505965	2.015892	-2.678786
67	6	0	0.191566	2.259525	-0.416407
68	8	0	-0.002715	2.324643	0.795047

69	6	0	-2.281003	2.512756	-1.146836
70	6	0	-2.847017	2.534147	0.135432
71	6	0	-3.036765	2.982615	-2.223609
72	6	0	-4.140144	3.011252	0.325573
73	1	0	-2.274856	2.168376	0.980462
74	6	0	-4.335509	3.452854	-2.033498
75	1	0	-2.582298	2.968559	-3.209109
76	6	0	-4.892943	3.467312	-0.757737
77	1	0	-4.566339	3.015732	1.324996
78	1	0	-4.910984	3.806710	-2.883953
79	1	0	-5.904812	3.831130	-0.606417
80	7	0	1.404284	2.394228	-1.012220
81	1	0	1.335467	2.307533	-2.027094
82	6	0	2.631011	2.752174	-0.436368
83	6	0	3.735839	2.853931	-1.295175
84	6	0	2.797007	3.009179	0.932057
85	6	0	4.980157	3.224309	-0.800648
86	1	0	3.603892	2.647679	-2.354270
87	6	0	4.052004	3.388179	1.410111
88	1	0	1.950646	2.931283	1.599962
89	6	0	5.146994	3.499274	0.557480
90	1	0	5.821336	3.301915	-1.482621
91	1	0	4.166202	3.600599	2.469236
92	1	0	6.116975	3.795998	0.942381

TS5RS

Total energy= -2219.85961845
Sum of electronic and zero-point Energies= -2219.103458
Sum of electronic and thermal Energies= -2219.060546
Sum of electronic and thermal Enthalpies= -2219.059602
Sum of electronic and thermal Free Energies= -2219.178267

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.531449	-1.664445	-0.730843
2	6	0	4.924365	-1.667715	-0.618701
3	6	0	5.690812	-2.463106	-1.460859
4	6	0	5.042568	-3.263741	-2.403224
5	6	0	3.651307	-3.263008	-2.502463
6	6	0	2.879366	-2.452704	-1.667146
7	6	0	2.972655	-0.684930	0.282591
8	6	0	4.095265	-0.633026	1.341805

9	6	0	5.363916	-0.744581	0.495838
10	1	0	6.773689	-2.474480	-1.377471
11	1	0	5.627983	-3.899127	-3.060753
12	1	0	3.163464	-3.895497	-3.237429
13	1	0	1.798252	-2.429911	-1.754723
14	1	0	2.810522	0.292761	-0.173875
15	1	0	4.043179	0.264176	1.971195
16	1	0	5.636488	0.245007	0.107996
17	6	0	1.664610	-1.749335	2.117308
18	6	0	2.899417	-1.899072	2.951390
19	6	0	0.443072	-0.963523	0.491197
20	1	0	2.904113	-2.872656	3.444250
21	1	0	6.197857	-1.127868	1.088425
22	7	0	1.712372	-1.091951	0.921287
23	7	0	0.442055	-2.085627	2.417853
24	7	0	-0.306379	-1.595217	1.394343
25	8	0	4.046362	-1.810759	2.142251
26	1	0	2.889834	-1.113581	3.721169
27	6	0	-1.717368	-1.872835	1.334252
28	6	0	-2.535952	-1.384143	2.360922
29	6	0	-2.205327	-2.593853	0.239410
30	6	0	-3.907458	-1.584420	2.221663
31	6	0	-3.587652	-2.767075	0.155794
32	6	0	-4.451277	-2.256416	1.123401
33	1	0	-4.571337	-1.196489	2.991072
34	1	0	-3.994752	-3.309456	-0.693481
35	6	0	-1.972673	-0.664373	3.556711
36	1	0	-2.777588	-0.173264	4.108383
37	1	0	-1.475420	-1.366304	4.232906
38	1	0	-1.244582	0.089447	3.242069
39	6	0	-5.941124	-2.436643	1.005946
40	1	0	-6.458091	-1.479316	1.120875
41	1	0	-6.213435	-2.861054	0.036977
42	1	0	-6.314662	-3.105045	1.788748
43	6	0	-1.305398	-3.152764	-0.831574
44	1	0	-1.040920	-2.387913	-1.570592
45	1	0	-0.378185	-3.558128	-0.414254
46	1	0	-1.818917	-3.955016	-1.365303
47	6	0	0.042612	-0.199032	-0.753859
48	8	0	0.903797	-0.151165	-1.642635
49	1	0	-1.055951	0.717993	-2.831859
50	6	0	-1.198585	0.490045	-0.711013
51	6	0	-1.785432	0.919804	-2.041928
52	1	0	-1.922717	0.123039	0.007274

53	1	0	-1.982255	1.996543	-2.052486
54	6	0	-3.072868	0.166390	-2.291355
55	6	0	-4.250120	0.573648	-1.653082
56	6	0	-3.108119	-0.976049	-3.095476
57	6	0	-5.432196	-0.143650	-1.813533
58	1	0	-4.231194	1.463299	-1.025603
59	6	0	-4.291068	-1.695888	-3.261508
60	1	0	-2.200516	-1.298388	-3.601231
61	6	0	-5.456775	-1.282524	-2.619738
62	1	0	-6.338138	0.188889	-1.314417
63	1	0	-4.301710	-2.578268	-3.895014
64	1	0	-6.380323	-1.838724	-2.750976
65	6	0	-0.711527	1.989107	0.606417
66	8	0	-0.383161	1.446393	1.705203
67	6	0	0.444923	2.570146	-0.235027
68	8	0	0.333698	3.063608	-1.349019
69	6	0	-2.045775	2.705568	0.548447
70	6	0	-2.353620	3.769365	-0.306348
71	6	0	-3.024688	2.254728	1.443001
72	6	0	-3.619319	4.357196	-0.267555
73	1	0	-1.606173	4.137477	-0.998923
74	6	0	-4.286332	2.834841	1.474799
75	1	0	-2.772226	1.434582	2.107407
76	6	0	-4.589916	3.892220	0.615388
77	1	0	-3.843888	5.184443	-0.934301
78	1	0	-5.034081	2.464317	2.170110
79	1	0	-5.574097	4.350418	0.637408
80	7	0	1.620933	2.424471	0.439540
81	1	0	1.487973	2.072399	1.385022
82	6	0	2.912564	2.772779	0.018483
83	6	0	3.892405	2.959848	1.002120
84	6	0	3.260205	2.863086	-1.334806
85	6	0	5.206037	3.234012	0.637578
86	1	0	3.612016	2.893897	2.050495
87	6	0	4.578596	3.144850	-1.683739
88	1	0	2.502632	2.703841	-2.090673
89	6	0	5.557072	3.330534	-0.708614
90	1	0	5.955669	3.376817	1.409866
91	1	0	4.841887	3.210474	-2.735071
92	1	0	6.581277	3.548422	-0.993201

TS5SR

Total energy= -2219.84911724

Sum of electronic and zero-point Energies= -2219.093429
Sum of electronic and thermal Energies= -2219.049918
Sum of electronic and thermal Enthalpies= -2219.048974
Sum of electronic and thermal Free Energies= -2219.171224

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.232705	-1.918850	-0.023880
2	6	0	4.419535	-2.641345	0.113109
3	6	0	5.608941	-2.126374	-0.384546
4	6	0	5.583378	-0.891739	-1.036681
5	6	0	4.386697	-0.192604	-1.192894
6	6	0	3.190472	-0.699598	-0.679482
7	6	0	2.112869	-2.695134	0.628448
8	6	0	2.646737	-4.144841	0.589384
9	6	0	4.152113	-3.960538	0.802627
10	1	0	6.538048	-2.680407	-0.287043
11	1	0	6.502358	-0.478729	-1.440920
12	1	0	4.386742	0.755490	-1.721303
13	1	0	2.254968	-0.161259	-0.814741
14	1	0	1.942496	-2.364824	1.653090
15	1	0	2.161144	-4.793206	1.329218
16	1	0	4.374713	-3.904130	1.873963
17	6	0	0.374663	-3.598449	-0.893093
18	6	0	1.137955	-4.877415	-1.058811
19	6	0	-0.120685	-1.625811	-0.072397
20	1	0	1.091475	-5.201429	-2.099614
21	1	0	4.706751	-4.800946	0.378834
22	7	0	0.821190	-2.601532	-0.076322
23	7	0	-0.788429	-3.304464	-1.397123
24	7	0	-1.085641	-2.083475	-0.880223
25	8	0	2.486723	-4.683481	-0.716764
26	1	0	0.671127	-5.647283	-0.427467
27	6	0	-2.387814	-1.546174	-1.191255
28	6	0	-2.580368	-0.973573	-2.448377
29	6	0	-3.406825	-1.715870	-0.249703
30	6	0	-3.851547	-0.467178	-2.719239
31	6	0	-4.653083	-1.179408	-0.566034
32	6	0	-4.885286	-0.533898	-1.783554
33	1	0	-4.032442	-0.000451	-3.684819
34	1	0	-5.459788	-1.271444	0.157235
35	6	0	-1.465843	-0.910926	-3.456394
36	1	0	-0.607338	-0.371885	-3.041584

37	1	0	-1.138871	-1.917025	-3.737300
38	1	0	-1.801331	-0.396168	-4.359271
39	6	0	-6.218584	0.101448	-2.073585
40	1	0	-6.449884	0.070042	-3.141058
41	1	0	-7.023685	-0.394278	-1.526289
42	1	0	-6.207039	1.153921	-1.768896
43	6	0	-3.160503	-2.443870	1.042077
44	1	0	-2.702428	-3.421339	0.857586
45	1	0	-2.493314	-1.873498	1.698106
46	1	0	-4.099213	-2.595438	1.576979
47	6	0	-0.077061	-0.416420	0.868389
48	8	0	0.853698	-0.455455	1.688994
49	1	0	-0.502853	1.488409	2.609068
50	6	0	-1.047989	0.603837	0.740467
51	6	0	-1.405137	1.347211	2.012981
52	1	0	-1.879433	0.408353	0.072617
53	1	0	-1.799186	2.337656	1.768980
54	6	0	-2.444257	0.578817	2.799241
55	6	0	-3.796892	0.653919	2.449188
56	6	0	-2.070461	-0.266432	3.848524
57	6	0	-4.752944	-0.094598	3.131419
58	1	0	-4.095728	1.304384	1.628969
59	6	0	-3.023934	-1.020654	4.531159
60	1	0	-1.020371	-0.333836	4.122359
61	6	0	-4.368561	-0.936463	4.175196
62	1	0	-5.800003	-0.020343	2.850889
63	1	0	-2.717130	-1.669665	5.346204
64	1	0	-5.113149	-1.518740	4.709343
65	6	0	-0.071993	1.869887	-0.734232
66	8	0	0.340681	1.140037	-1.671920
67	6	0	1.012419	2.475444	0.191441
68	8	0	0.809500	3.007769	1.273275
69	6	0	-1.290280	2.739128	-0.970408
70	6	0	-1.645373	3.847092	-0.189623
71	6	0	-2.079039	2.418816	-2.081136
72	6	0	-2.784504	4.588915	-0.500985
73	1	0	-1.029045	4.130563	0.654932
74	6	0	-3.218559	3.154050	-2.384819
75	1	0	-1.773036	1.586263	-2.703922
76	6	0	-3.579981	4.241715	-1.589905
77	1	0	-3.047438	5.445494	0.112177
78	1	0	-3.822195	2.884558	-3.246969
79	1	0	-4.467908	4.820349	-1.825333
80	7	0	2.234055	2.407777	-0.408273

81	1	0	2.214577	2.016996	-1.344856
82	6	0	3.435956	2.961123	0.066024
83	6	0	4.387369	3.374026	-0.873764
84	6	0	3.712884	3.077673	1.431904
85	6	0	5.606516	3.892611	-0.453530
86	1	0	4.160193	3.288369	-1.933401
87	6	0	4.933530	3.609702	1.838628
88	1	0	2.979189	2.747069	2.154907
89	6	0	5.884664	4.017639	0.906450
90	1	0	6.336619	4.207864	-1.192518
91	1	0	5.143754	3.695981	2.900338
92	1	0	6.834214	4.426121	1.236455

TS5SS

Total energy= -2219.85052651
Sum of electronic and zero-point Energies= -2219.094573
Sum of electronic and thermal Energies= -2219.051572
Sum of electronic and thermal Enthalpies= -2219.050628
Sum of electronic and thermal Free Energies= -2219.169246

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.488272	-1.719114	0.060087
2	6	0	4.609114	-2.554968	0.040979
3	6	0	5.878923	-2.034442	0.253236
4	6	0	6.010857	-0.664136	0.479479
5	6	0	4.890715	0.167301	0.486553
6	6	0	3.611918	-0.353754	0.276567
7	6	0	2.252012	-2.576529	-0.107831
8	6	0	2.806161	-3.834666	-0.814011
9	6	0	4.202850	-3.987562	-0.214394
10	1	0	6.751962	-2.680555	0.236215
11	1	0	6.995553	-0.237267	0.644558
12	1	0	5.014323	1.230813	0.662261
13	1	0	2.736228	0.287958	0.277548
14	1	0	1.837352	-2.836040	0.867456
15	1	0	2.157413	-4.709623	-0.680365
16	1	0	4.149165	-4.556653	0.720320
17	6	0	0.865183	-2.468204	-2.168213
18	6	0	1.761480	-3.437885	-2.877833
19	6	0	0.085852	-1.242254	-0.530208
20	1	0	1.968991	-3.078957	-3.887959

21	1	0	4.862959	-4.519974	-0.903428
22	7	0	1.131125	-2.023761	-0.902769
23	7	0	-0.278954	-2.019800	-2.594652
24	7	0	-0.755319	-1.269332	-1.566868
25	8	0	2.983335	-3.560330	-2.197322
26	1	0	1.241824	-4.403837	-2.948901
27	6	0	-2.101571	-0.767109	-1.682659
28	6	0	-2.326036	0.361542	-2.471694
29	6	0	-3.118793	-1.497100	-1.061994
30	6	0	-3.641300	0.812787	-2.562037
31	6	0	-4.413273	-0.988954	-1.165199
32	6	0	-4.687598	0.169083	-1.896109
33	1	0	-3.852790	1.693818	-3.162072
34	1	0	-5.224539	-1.519483	-0.672892
35	6	0	-1.199160	1.024218	-3.214336
36	1	0	-0.370057	1.249703	-2.537388
37	1	0	-0.822949	0.365927	-4.005040
38	1	0	-1.543188	1.952270	-3.675208
39	6	0	-6.084095	0.724825	-1.974424
40	1	0	-6.816432	0.022421	-1.570439
41	1	0	-6.152546	1.656285	-1.401669
42	1	0	-6.357856	0.957800	-3.007328
43	6	0	-2.825613	-2.766263	-0.309413
44	1	0	-2.196187	-3.436245	-0.904561
45	1	0	-2.305853	-2.560557	0.634029
46	1	0	-3.753696	-3.289144	-0.071833
47	6	0	-0.045258	-0.632639	0.861449
48	8	0	0.917429	-0.888125	1.601567
49	1	0	-0.650182	-0.084479	3.266904
50	6	0	-1.185049	0.137988	1.216874
51	6	0	-1.565800	0.035763	2.681927
52	1	0	-2.016427	0.123062	0.522885
53	1	0	-2.029704	0.968603	3.014057
54	6	0	-2.496673	-1.131626	2.907646
55	6	0	-3.847067	-1.032932	2.550631
56	6	0	-2.025696	-2.351497	3.402356
57	6	0	-4.703214	-2.122472	2.682962
58	1	0	-4.222722	-0.091695	2.153107
59	6	0	-2.879405	-3.446691	3.533872
60	1	0	-0.978157	-2.440499	3.680245
61	6	0	-4.220644	-3.336371	3.174214
62	1	0	-5.748731	-2.026311	2.403443
63	1	0	-2.496143	-4.386304	3.921259
64	1	0	-4.887369	-4.186911	3.278135

65	6	0	-0.685819	2.203566	1.153695
66	8	0	-0.676966	2.600697	2.343950
67	6	0	0.682464	2.108029	0.440833
68	8	0	0.861302	1.602067	-0.665561
69	6	0	-1.820625	2.697367	0.269477
70	6	0	-1.596861	3.335904	-0.951999
71	6	0	-3.119097	2.681746	0.792707
72	6	0	-2.651880	3.941032	-1.637149
73	1	0	-0.596926	3.374255	-1.371364
74	6	0	-4.173819	3.264744	0.101041
75	1	0	-3.290610	2.225779	1.763348
76	6	0	-3.941951	3.904038	-1.118523
77	1	0	-2.458148	4.445792	-2.579595
78	1	0	-5.174812	3.240681	0.522312
79	1	0	-4.761777	4.374665	-1.653368
80	7	0	1.639602	2.718010	1.176045
81	1	0	1.306192	3.002284	2.095029
82	6	0	2.944559	3.076286	0.799074
83	6	0	3.376738	3.071540	-0.533163
84	6	0	3.814532	3.504098	1.809484
85	6	0	4.667065	3.500043	-0.834220
86	1	0	2.708859	2.733755	-1.313658
87	6	0	5.100623	3.925263	1.492889
88	1	0	3.471550	3.505317	2.840431
89	6	0	5.535657	3.926454	0.167790
90	1	0	4.993888	3.495409	-1.869622
91	1	0	5.763658	4.254354	2.287044
92	1	0	6.539843	4.254611	-0.079749

Cartesian coordinates of the structures at WB97XD/6-31G(d, p)//IEFPCM$_{DCM}$ level

Cat

Total energy= -1052.03089747
Sum of electronic and zero-point Energies= -1051.646417
Sum of electronic and thermal Energies= -1051.625574
Sum of electronic and thermal Enthalpies= -1051.624630
Sum of electronic and thermal Free Energies= -1051.698004

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.929241	-0.589395	-0.593099

2	6	0	4.260382	-0.317495	-0.280303
3	6	0	5.143073	-1.358203	-0.022267
4	6	0	4.669950	-2.670081	-0.076126
5	6	0	3.335406	-2.934548	-0.384891
6	6	0	2.450334	-1.889787	-0.651030
7	6	0	2.196892	0.706700	-0.863886
8	6	0	3.098599	1.763419	-0.175045
9	6	0	4.508574	1.172791	-0.281737
10	1	0	6.180819	-1.157739	0.226762
11	1	0	5.346920	-3.492855	0.131517
12	1	0	2.982725	-3.960519	-0.417255
13	1	0	1.407857	-2.076817	-0.890137
14	1	0	2.157393	0.903322	-1.940193
15	1	0	2.999787	2.752584	-0.640952
16	1	0	4.979930	1.492627	-1.217761
17	6	0	0.482810	1.494179	0.749717
18	6	0	1.491020	2.352481	1.445369
19	6	0	-0.241323	0.082749	-0.856305
20	1	0	1.323640	2.343305	2.522891
21	1	0	5.135315	1.518473	0.543660
22	7	0	0.837303	0.765944	-0.354244
23	7	0	-0.777924	1.342470	1.015972
24	7	0	-1.189790	0.474823	0.015756
25	8	0	2.787823	1.849928	1.208699
26	1	0	1.401192	3.389364	1.088252
27	6	0	-2.559785	0.065803	-0.010622
28	6	0	-3.491097	0.876929	-0.663913
29	6	0	-2.919428	-1.124927	0.623928
30	6	0	-4.821530	0.462854	-0.673725
31	6	0	-4.261785	-1.501290	0.588367
32	6	0	-5.224494	-0.719786	-0.050947
33	1	0	-5.560966	1.077281	-1.181554
34	1	0	-4.561881	-2.427082	1.072882
35	6	0	-3.055070	2.149492	-1.339448
36	1	0	-2.617238	2.844673	-0.616471
37	1	0	-2.289317	1.945618	-2.094278
38	1	0	-3.899176	2.642697	-1.825490
39	6	0	-6.676193	-1.126561	-0.048070
40	1	0	-7.213119	-0.634573	0.770333
41	1	0	-7.170027	-0.842526	-0.981086
42	1	0	-6.788572	-2.205253	0.085868
43	6	0	-1.880383	-1.969426	1.311981
44	1	0	-1.115936	-2.298756	0.601673
45	1	0	-1.367039	-1.399762	2.092772

46	1	0	-2.333178	-2.851525	1.768908

R1

Total energy= -422.84309747

Sum of electronic and zero-point Energies= -422.698001

Sum of electronic and thermal Energies= -422.689392

Sum of electronic and thermal Enthalpies= -422.688447

Sum of electronic and thermal Free Energies= -422.732777

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.409927	0.384867	0.000012
2	8	0	-3.862483	-0.747105	-0.000018
3	1	0	-4.093582	1.255837	-0.000017
4	6	0	-1.976642	0.715646	0.000006
5	6	0	-1.050426	-0.258080	0.000010
6	1	0	-1.719277	1.770655	-0.000002
7	1	0	-1.424035	-1.281487	0.000017
8	6	0	0.406329	-0.110451	0.000005
9	6	0	1.195947	-1.268565	0.000004
10	6	0	1.045826	1.138709	0.000000
11	6	0	2.583967	-1.185577	-0.000001
12	1	0	0.712505	-2.241254	0.000008
13	6	0	2.431234	1.221536	-0.000005
14	1	0	0.460123	2.052196	0.000001
15	6	0	3.204514	0.060227	-0.000006
16	1	0	3.179234	-2.092684	-0.000001
17	1	0	2.912517	2.193879	-0.000008
18	1	0	4.287446	0.129825	-0.000009

R2

Total energy= -745.10564476

Sum of electronic and zero-point Energies= -744.884058

Sum of electronic and thermal Energies= -744.870418

Sum of electronic and thermal Enthalpies= -744.869474

Sum of electronic and thermal Free Energies= -744.927136

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.149166	0.819820	-0.028104

2	8	0	0.965030	2.025877	-0.001818
3	6	0	-0.104702	-0.093320	-0.126352
4	8	0	-0.039968	-1.288882	-0.374924
5	6	0	2.510746	0.235529	0.004040
6	6	0	2.774767	-1.102049	0.328504
7	6	0	3.578338	1.105420	-0.262512
8	6	0	4.088912	-1.554235	0.379020
9	1	0	1.958614	-1.779165	0.539881
10	6	0	4.885769	0.644916	-0.222905
11	1	0	3.363716	2.141131	-0.501583
12	6	0	5.141959	-0.687607	0.099004
13	1	0	4.289591	-2.589103	0.634679
14	1	0	5.705020	1.321910	-0.440010
15	1	0	6.164510	-1.049762	0.134073
16	7	0	-1.229920	0.628221	0.073196
17	1	0	-1.056527	1.618178	0.207568
18	6	0	-2.572226	0.206935	0.039823
19	6	0	-3.551964	1.186462	0.238092
20	6	0	-2.950830	-1.121866	-0.174845
21	6	0	-4.896826	0.842654	0.219270
22	1	0	-3.257266	2.218271	0.406877
23	6	0	-4.304058	-1.449786	-0.189812
24	1	0	-2.195156	-1.878611	-0.328627
25	6	0	-5.281495	-0.479288	0.004393
26	1	0	-5.645905	1.612580	0.372567
27	1	0	-4.590495	-2.483058	-0.357914
28	1	0	-6.332497	-0.747381	-0.011645

Si-M3

Total energy= -1474.92405135
Sum of electronic and zero-point Energies= -1474.389475
Sum of electronic and thermal Energies= -1474.360007
Sum of electronic and thermal Enthalpies= -1474.359063
Sum of electronic and thermal Free Energies= -1474.450594

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.734016	-1.010577	0.053618
2	6	0	-3.950504	-1.691763	0.107250
3	6	0	-5.022543	-1.151453	0.804015
4	6	0	-4.857154	0.077215	1.445553
5	6	0	-3.638677	0.751746	1.388154

6	6	0	-2.561239	0.212223	0.685307
7	6	0	-1.771609	-1.786162	-0.817223
8	6	0	-2.363194	-3.215470	-0.805212
9	6	0	-3.870525	-2.981783	-0.674875
10	1	0	-5.971987	-1.675677	0.855206
11	1	0	-5.686635	0.511075	1.995011
12	1	0	-3.526092	1.711912	1.880753
13	1	0	-1.616766	0.745511	0.629792
14	1	0	-1.725663	-1.357779	-1.822741
15	1	0	-2.076737	-3.791231	-1.693905
16	1	0	-4.320046	-2.867946	-1.667405
17	6	0	0.194482	-2.898228	0.260127
18	6	0	-0.576178	-4.171931	0.413503
19	6	0	0.539383	-0.843846	-0.414458
20	1	0	-0.353464	-4.635684	1.374799
21	1	0	-4.349946	-3.831360	-0.183468
22	7	0	-0.387615	-1.819765	-0.341835
23	7	0	1.434250	-2.655364	0.570484
24	7	0	1.633137	-1.367427	0.141108
25	8	0	-1.955558	-3.902358	0.373245
26	1	0	-0.278919	-4.865616	-0.386394
27	6	0	2.931121	-0.766578	0.246493
28	6	0	3.721152	-0.697736	-0.902569
29	6	0	3.341210	-0.286612	1.490835
30	6	0	4.976689	-0.107986	-0.774936
31	6	0	4.606374	0.290744	1.566325
32	6	0	5.432421	0.392723	0.445592
33	1	0	5.615536	-0.039881	-1.651373
34	1	0	4.953228	0.675294	2.521769
35	6	0	3.228809	-1.235827	-2.220009
36	1	0	2.926837	-2.283831	-2.125938
37	1	0	2.359905	-0.675952	-2.581466
38	1	0	4.011825	-1.173965	-2.977536
39	6	0	6.779511	1.059701	0.547929
40	1	0	6.683011	2.139662	0.393272
41	1	0	7.225564	0.907109	1.533837
42	1	0	7.471740	0.679078	-0.206999
43	6	0	2.440676	-0.383301	2.693472
44	1	0	1.474892	0.097215	2.503648
45	1	0	2.237422	-1.427436	2.948773
46	1	0	2.896909	0.100276	3.558687
47	6	0	0.346996	0.461828	-1.135276
48	8	0	-0.274917	0.337952	-2.246070
49	1	0	1.546644	3.562286	-0.876930

50	6	0	0.838801	1.568135	-0.507527
51	6	0	0.675088	2.939110	-1.106914
52	1	0	1.334418	1.470515	0.452654
53	1	0	0.628862	2.832297	-2.196935
54	6	0	-0.583996	3.642338	-0.634389
55	6	0	-1.835666	3.100393	-0.951394
56	6	0	-0.536424	4.803566	0.137498
57	6	0	-3.005153	3.702376	-0.501737
58	1	0	-1.870891	2.188007	-1.541729
59	6	0	-1.708200	5.411316	0.588674
60	1	0	0.427582	5.237621	0.391456
61	6	0	-2.946785	4.861791	0.272217
62	1	0	-3.966177	3.260061	-0.746985
63	1	0	-1.650825	6.314488	1.189236
64	1	0	-3.859923	5.331358	0.624935

TS5RR

Total energy= -2220.05429485

Sum of electronic and zero-point Energies= -2219.295008

Sum of electronic and thermal Energies= -2219.252166

Sum of electronic and thermal Enthalpies= -2219.251222

Sum of electronic and thermal Free Energies= -2219.370225

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.443109	1.968659	-0.811796
2	6	0	-4.829847	2.081961	-0.923953
3	6	0	-5.400730	3.245995	-1.418707
4	6	0	-4.565875	4.302526	-1.783612
5	6	0	-3.182247	4.189718	-1.656209
6	6	0	-2.607351	3.014098	-1.174206
7	6	0	-3.113763	0.587091	-0.277315
8	6	0	-4.421408	0.199871	0.453509
9	6	0	-5.502100	0.825280	-0.425690
10	1	0	-6.478671	3.340411	-1.506302
11	1	0	-4.998130	5.222726	-2.163481
12	1	0	-2.544411	5.021075	-1.938184
13	1	0	-1.531125	2.917346	-1.098777
14	1	0	-2.894802	-0.109791	-1.087655
15	1	0	-4.526584	-0.878442	0.590771
16	1	0	-5.745346	0.145016	-1.249824
17	6	0	-2.148626	0.602517	2.014148

18	6	0	-3.507547	0.432391	2.615574
19	6	0	-0.654268	0.571298	0.425840
20	1	0	-3.593423	1.025087	3.526332
21	1	0	-6.414826	1.005821	0.145925
22	7	0	-1.981725	0.540157	0.660691
23	7	0	-1.007316	0.735233	2.626456
24	7	0	-0.084219	0.722170	1.624184
25	8	0	-4.490656	0.865057	1.711688
26	1	0	-3.637868	-0.630189	2.869422
27	6	0	1.294245	1.006532	1.919136
28	6	0	1.855966	2.166441	1.374968
29	6	0	2.010161	0.123237	2.736878
30	6	0	3.210935	2.390113	1.607091
31	6	0	3.361126	0.396484	2.929372
32	6	0	3.982222	1.508952	2.358845
33	1	0	3.677233	3.264465	1.164181
34	1	0	3.946865	-0.283541	3.542425
35	6	0	1.063061	3.145273	0.549565
36	1	0	1.010066	2.827755	-0.497093
37	1	0	0.042487	3.268024	0.923432
38	1	0	1.546606	4.123406	0.563715
39	6	0	5.452004	1.750912	2.575283
40	1	0	5.798355	2.619456	2.011807
41	1	0	5.667374	1.917562	3.635470
42	1	0	6.036229	0.883694	2.253444
43	6	0	1.363316	-1.058618	3.406925
44	1	0	0.774746	-0.731069	4.269234
45	1	0	0.696296	-1.589763	2.726199
46	1	0	2.126658	-1.755179	3.760544
47	6	0	-0.027784	0.429446	-0.948997
48	8	0	-0.761237	0.739042	-1.897903
49	1	0	2.383160	-0.629239	-2.821472
50	6	0	1.271269	-0.135433	-1.037709
51	6	0	2.086408	0.262021	-2.257514
52	1	0	1.823891	-0.188067	-0.107928
53	1	0	1.447235	0.846641	-2.924455
54	6	0	3.311409	1.060047	-1.874186
55	6	0	3.364809	2.441402	-2.069596
56	6	0	4.414473	0.426989	-1.291042
57	6	0	4.484858	3.177408	-1.687451
58	1	0	2.519520	2.946377	-2.530587
59	6	0	5.534542	1.157111	-0.909522
60	1	0	4.390020	-0.647886	-1.134528
61	6	0	5.574136	2.536838	-1.104046

62	1	0	4.506424	4.251028	-1.849296
63	1	0	6.381263	0.648533	-0.458269
64	1	0	6.449449	3.105994	-0.806237
65	6	0	0.889638	-2.105827	-1.412119
66	8	0	0.501800	-2.199998	-2.610531
67	6	0	-0.205482	-2.350420	-0.346804
68	8	0	-0.023287	-2.389464	0.867709
69	6	0	2.282594	-2.611672	-1.066541
70	6	0	2.849139	-2.576320	0.213375
71	6	0	3.046509	-3.105248	-2.125664
72	6	0	4.150868	-3.018369	0.419411
73	1	0	2.270591	-2.194108	1.043638
74	6	0	4.352767	-3.542132	-1.920937
75	1	0	2.592166	-3.133787	-3.109902
76	6	0	4.910949	-3.498083	-0.646931
77	1	0	4.578686	-2.975725	1.416495
78	1	0	4.934009	-3.915302	-2.758509
79	1	0	5.930390	-3.833601	-0.483959
80	7	0	-1.409373	-2.496574	-0.953945
81	1	0	-1.310116	-2.433586	-1.967504
82	6	0	-2.654074	-2.800620	-0.389123
83	6	0	-3.753705	-2.879492	-1.254457
84	6	0	-2.839700	-3.024971	0.981064
85	6	0	-5.014744	-3.188923	-0.761012
86	1	0	-3.612501	-2.700433	-2.316344
87	6	0	-4.109923	-3.341737	1.458851
88	1	0	-1.993462	-2.959907	1.650045
89	6	0	-5.202071	-3.426034	0.600043
90	1	0	-5.853634	-3.245194	-1.446988
91	1	0	-4.241125	-3.521564	2.521315
92	1	0	-6.186526	-3.668330	0.985055

TS5RS

Total energy= -2220.04968493
Sum of electronic and zero-point Energies= -2219.291218
Sum of electronic and thermal Energies= -2219.248242
Sum of electronic and thermal Enthalpies= -2219.247298
Sum of electronic and thermal Free Energies= -2219.366841

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.542666	-1.639170	-0.723134

2	6	0	4.932252	-1.574798	-0.606780
3	6	0	5.740045	-2.330378	-1.444272
4	6	0	5.137231	-3.161368	-2.389194
5	6	0	3.748515	-3.227298	-2.494612
6	6	0	2.935276	-2.455849	-1.663955
7	6	0	2.937664	-0.678693	0.279490
8	6	0	4.050501	-0.568537	1.344086
9	6	0	5.326004	-0.631182	0.505456
10	1	0	6.821267	-2.287170	-1.355699
11	1	0	5.755412	-3.767793	-3.043538
12	1	0	3.294897	-3.881540	-3.232014
13	1	0	1.856392	-2.481352	-1.762725
14	1	0	2.747069	0.286464	-0.188094
15	1	0	3.959531	0.335444	1.958062
16	1	0	5.559092	0.367353	0.116777
17	6	0	1.657226	-1.760324	2.116682
18	6	0	2.895231	-1.879188	2.950953
19	6	0	0.417366	-0.977552	0.504761
20	1	0	2.937420	-2.857532	3.430535
21	1	0	6.172897	-0.975089	1.102892
22	7	0	1.691243	-1.108753	0.918798
23	7	0	0.440222	-2.100823	2.434114
24	7	0	-0.321206	-1.609251	1.416373
25	8	0	4.046620	-1.735223	2.161015
26	1	0	2.845959	-1.108793	3.734478
27	6	0	-1.733173	-1.872923	1.369279
28	6	0	-2.549610	-1.323524	2.366026
29	6	0	-2.228961	-2.634119	0.307439
30	6	0	-3.921586	-1.507235	2.227667
31	6	0	-3.611799	-2.785855	0.222461
32	6	0	-4.471383	-2.215613	1.156467
33	1	0	-4.582760	-1.074829	2.974233
34	1	0	-4.024038	-3.343943	-0.612196
35	6	0	-1.979244	-0.552779	3.525167
36	1	0	-2.783176	-0.090590	4.102284
37	1	0	-1.414037	-1.211239	4.190486
38	1	0	-1.304822	0.231200	3.165676
39	6	0	-5.964081	-2.364055	1.030727
40	1	0	-6.450429	-1.384220	1.036814
41	1	0	-6.234816	-2.869038	0.101374
42	1	0	-6.371907	-2.938425	1.868589
43	6	0	-1.334487	-3.250758	-0.736038
44	1	0	-1.077969	-2.525679	-1.514950
45	1	0	-0.403973	-3.633421	-0.306685

46	1	0	-1.846549	-4.081684	-1.224571
47	6	0	-0.000179	-0.237503	-0.746450
48	8	0	0.828753	-0.255028	-1.669219
49	1	0	-1.108099	0.684374	-2.813881
50	6	0	-1.218018	0.485826	-0.690342
51	6	0	-1.832964	0.880295	-2.019801
52	1	0	-1.928762	0.148493	0.054104
53	1	0	-2.049651	1.951322	-2.044236
54	6	0	-3.108985	0.103118	-2.251016
55	6	0	-4.298434	0.514412	-1.641140
56	6	0	-3.120992	-1.062540	-3.019372
57	6	0	-5.467653	-0.223726	-1.791162
58	1	0	-4.300853	1.421290	-1.041100
59	6	0	-4.290363	-1.804477	-3.172765
60	1	0	-2.204464	-1.390506	-3.503481
61	6	0	-5.467685	-1.388042	-2.557208
62	1	0	-6.382346	0.111062	-1.311072
63	1	0	-4.281198	-2.708266	-3.774956
64	1	0	-6.380990	-1.962859	-2.676336
65	6	0	-0.707659	2.052801	0.577159
66	8	0	-0.378462	1.557770	1.697839
67	6	0	0.465764	2.589742	-0.278778
68	8	0	0.380755	3.047343	-1.411268
69	6	0	-2.038275	2.769002	0.487350
70	6	0	-2.329159	3.790563	-0.421260
71	6	0	-3.030574	2.369158	1.389309
72	6	0	-3.590691	4.384364	-0.432941
73	1	0	-1.570051	4.112887	-1.122940
74	6	0	-4.288543	2.956029	1.372990
75	1	0	-2.799505	1.583765	2.098802
76	6	0	-4.575296	3.968052	0.456849
77	1	0	-3.802023	5.173923	-1.147292
78	1	0	-5.047178	2.624710	2.075399
79	1	0	-5.557809	4.428996	0.439754
80	7	0	1.623824	2.455770	0.425199
81	1	0	1.445641	2.117770	1.368889
82	6	0	2.937485	2.726086	0.014958
83	6	0	3.897027	2.977717	1.001466
84	6	0	3.322493	2.670126	-1.328974
85	6	0	5.228423	3.168030	0.650069
86	1	0	3.592672	3.025539	2.043128
87	6	0	4.657694	2.867773	-1.666981
88	1	0	2.579054	2.462178	-2.086700
89	6	0	5.616315	3.115658	-0.687421

90	1	0	5.963307	3.360078	1.425057
91	1	0	4.949516	2.816325	-2.711042
92	1	0	6.655075	3.265705	-0.961440

TS5SR

Total energy= -2220.04266939
Sum of electronic and zero-point Energies= -2219.283803
Sum of electronic and thermal Energies= -2219.240948
Sum of electronic and thermal Enthalpies= -2219.240004
Sum of electronic and thermal Free Energies= -2219.358884

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.403986	-0.878454	-0.812526
2	6	0	4.764975	-1.115166	-0.615601
3	6	0	5.684717	-0.713231	-1.570516
4	6	0	5.219133	-0.095091	-2.734380
5	6	0	3.854684	0.098755	-2.940972
6	6	0	2.925924	-0.299445	-1.975197
7	6	0	2.652960	-1.373503	0.406933
8	6	0	3.597241	-2.485669	0.906733
9	6	0	4.976111	-1.856031	0.684824
10	1	0	6.746167	-0.889572	-1.427213
11	1	0	5.927664	0.220108	-3.493463
12	1	0	3.506364	0.560799	-3.858665
13	1	0	1.862483	-0.130428	-2.126352
14	1	0	2.517039	-0.593776	1.161048
15	1	0	3.389682	-2.796750	1.936594
16	1	0	5.208375	-1.162188	1.501512
17	6	0	1.180757	-3.210708	-0.320447
18	6	0	2.280697	-4.211077	-0.119833
19	6	0	0.132848	-1.322344	0.031948
20	1	0	2.335043	-4.894031	-0.968030
21	1	0	5.757748	-2.616695	0.641491
22	7	0	1.336167	-1.927408	0.106119
23	7	0	-0.044509	-3.430964	-0.707912
24	7	0	-0.679436	-2.241335	-0.492530
25	8	0	3.535681	-3.594488	0.012439
26	1	0	2.022844	-4.793130	0.777330
27	6	0	-2.064663	-2.108520	-0.853346
28	6	0	-2.356724	-1.646126	-2.139871
29	6	0	-3.033148	-2.456731	0.085463

30	6	0	-3.702502	-1.491671	-2.460308
31	6	0	-4.364291	-2.297860	-0.293854
32	6	0	-4.714816	-1.801913	-1.548695
33	1	0	-3.966549	-1.121720	-3.447407
34	1	0	-5.142329	-2.550561	0.420250
35	6	0	-1.261980	-1.302239	-3.112103
36	1	0	-0.715187	-0.409477	-2.779365
37	1	0	-0.542882	-2.121976	-3.206673
38	1	0	-1.680269	-1.101389	-4.100390
39	6	0	-6.159915	-1.574668	-1.907672
40	1	0	-6.343866	-1.776255	-2.965943
41	1	0	-6.822622	-2.207565	-1.312942
42	1	0	-6.437126	-0.531953	-1.718713
43	6	0	-2.652061	-2.939623	1.456535
44	1	0	-1.914150	-3.745463	1.407648
45	1	0	-2.224681	-2.120575	2.045102
46	1	0	-3.529316	-3.301801	1.993451
47	6	0	-0.252821	-0.075474	0.831810
48	8	0	0.418020	0.050787	1.863258
49	1	0	-1.339870	2.091126	2.055115
50	6	0	-1.299686	0.767380	0.373996
51	6	0	-2.054536	1.538330	1.443531
52	1	0	-1.922742	0.346185	-0.408418
53	1	0	-2.690467	2.278051	0.949855
54	6	0	-2.911352	0.650923	2.318355
55	6	0	-4.191645	0.268986	1.909766
56	6	0	-2.439943	0.186181	3.550478
57	6	0	-4.983586	-0.549862	2.709489
58	1	0	-4.569397	0.617016	0.951380
59	6	0	-3.227956	-0.636039	4.352478
60	1	0	-1.443878	0.471703	3.874717
61	6	0	-4.504166	-1.006295	3.935222
62	1	0	-5.977912	-0.830925	2.374767
63	1	0	-2.844465	-0.985905	5.306321
64	1	0	-5.121675	-1.642951	4.561103
65	6	0	-0.323304	2.029012	-0.924078
66	8	0	0.200727	1.337055	-1.850566
67	6	0	0.653478	2.593795	0.140331
68	8	0	0.343511	3.331959	1.070160
69	6	0	-1.530848	2.870993	-1.295502
70	6	0	-1.821667	4.123801	-0.749096
71	6	0	-2.386472	2.351283	-2.273893
72	6	0	-2.945676	4.833082	-1.169847
73	1	0	-1.175756	4.533566	0.016105

74	6	0	-3.515270	3.050299	-2.680243
75	1	0	-2.155336	1.385098	-2.709303
76	6	0	-3.799412	4.299557	-2.129051
77	1	0	-3.154238	5.806304	-0.736181
78	1	0	-4.173352	2.624011	-3.431453
79	1	0	-4.679570	4.849873	-2.446750
80	7	0	1.909887	2.126951	-0.076376
81	1	0	2.002328	1.635705	-0.958929
82	6	0	3.025116	2.215229	0.773190
83	6	0	4.297612	2.091200	0.208394
84	6	0	2.894296	2.347212	2.159988
85	6	0	5.426036	2.084255	1.020009
86	1	0	4.399116	1.976812	-0.866397
87	6	0	4.032613	2.354408	2.959411
88	1	0	1.908265	2.429825	2.595031
89	6	0	5.301537	2.219328	2.400398
90	1	0	6.404912	1.970912	0.564900
91	1	0	3.920875	2.457754	4.034259
92	1	0	6.182765	2.219419	3.033680

TS5SS

Total energy= -2220.03854105
Sum of electronic and zero-point Energies= -2219.279723
Sum of electronic and thermal Energies= -2219.236728
Sum of electronic and thermal Enthalpies= -2219.235784
Sum of electronic and thermal Free Energies= -2219.355968

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.551054	-1.729027	0.113255
2	6	0	4.665079	-2.568988	0.177073
3	6	0	5.938964	-2.036701	0.311501
4	6	0	6.081297	-0.650738	0.372729
5	6	0	4.966965	0.182927	0.293536
6	6	0	3.683938	-0.350656	0.164603
7	6	0	2.308933	-2.588806	0.059132
8	6	0	2.845029	-3.917999	-0.519509
9	6	0	4.247338	-4.016879	0.079888
10	1	0	6.808110	-2.686051	0.357201
11	1	0	7.070010	-0.214265	0.474703
12	1	0	5.098424	1.257623	0.333397
13	1	0	2.817910	0.297976	0.090235

14	1	0	1.912696	-2.737838	1.063644
15	1	0	2.194962	-4.770039	-0.283211
16	1	0	4.199130	-4.486703	1.068482
17	6	0	0.909510	-2.654426	-1.984713
18	6	0	1.784690	-3.700674	-2.603868
19	6	0	0.140389	-1.295379	-0.448665
20	1	0	1.993798	-3.443174	-3.643203
21	1	0	4.896754	-4.625610	-0.553052
22	7	0	1.179048	-2.112122	-0.761071
23	7	0	-0.228214	-2.230828	-2.450500
24	7	0	-0.699193	-1.395352	-1.483883
25	8	0	3.007381	-3.796145	-1.925922
26	1	0	1.239179	-4.655435	-2.587207
27	6	0	-2.038687	-0.895606	-1.647570
28	6	0	-2.246343	0.189614	-2.498325
29	6	0	-3.070249	-1.587576	-1.008130
30	6	0	-3.556487	0.636898	-2.637336
31	6	0	-4.359446	-1.085653	-1.167468
32	6	0	-4.616336	0.032755	-1.960368
33	1	0	-3.751581	1.491554	-3.277449
34	1	0	-5.179568	-1.583144	-0.657549
35	6	0	-1.104448	0.818387	-3.246121
36	1	0	-0.299875	1.091862	-2.558541
37	1	0	-0.700403	0.119526	-3.985924
38	1	0	-1.438487	1.717364	-3.767118
39	6	0	-6.006999	0.595920	-2.082383
40	1	0	-6.757343	-0.096789	-1.694384
41	1	0	-6.082114	1.531647	-1.518203
42	1	0	-6.251124	0.822504	-3.124041
43	6	0	-2.796944	-2.808909	-0.174517
44	1	0	-2.188417	-3.533991	-0.724117
45	1	0	-2.270438	-2.548561	0.749335
46	1	0	-3.731443	-3.290411	0.115946
47	6	0	-0.003981	-0.606369	0.903451
48	8	0	0.935863	-0.834495	1.682674
49	1	0	-0.726864	-0.101625	3.261627
50	6	0	-1.146565	0.183670	1.192599
51	6	0	-1.595082	0.132488	2.640895
52	1	0	-1.945583	0.151026	0.464178
53	1	0	-1.938266	1.121721	2.960199
54	6	0	-2.675048	-0.904845	2.845108
55	6	0	-3.961957	-0.702297	2.334445
56	6	0	-2.404813	-2.109667	3.498359
57	6	0	-4.946781	-1.674689	2.468504

58	1	0	-4.186317	0.220930	1.806486
59	6	0	-3.388044	-3.088282	3.634481
60	1	0	-1.409772	-2.283345	3.899570
61	6	0	-4.663032	-2.874933	3.118509
62	1	0	-5.937605	-1.497907	2.060354
63	1	0	-3.156576	-4.018627	4.144416
64	1	0	-5.430262	-3.635751	3.222068
65	6	0	-0.657384	2.266088	1.050178
66	8	0	-0.645936	2.702042	2.229242
67	6	0	0.717606	2.157546	0.347877
68	8	0	0.917071	1.637053	-0.749443
69	6	0	-1.808930	2.712175	0.165342
70	6	0	-1.621228	3.255157	-1.105814
71	6	0	-3.093005	2.739811	0.720468
72	6	0	-2.694987	3.796873	-1.810722
73	1	0	-0.634576	3.261448	-1.553165
74	6	0	-4.168850	3.251911	0.008151
75	1	0	-3.239010	2.371666	1.730050
76	6	0	-3.972673	3.788721	-1.263969
77	1	0	-2.526837	4.224174	-2.794712
78	1	0	-5.158718	3.252753	0.454455
79	1	0	-4.809633	4.202793	-1.817480
80	7	0	1.661094	2.775025	1.092139
81	1	0	1.297707	3.057794	1.999587
82	6	0	2.975656	3.122601	0.739384
83	6	0	3.395968	3.204337	-0.592542
84	6	0	3.863845	3.453969	1.767411
85	6	0	4.692459	3.621196	-0.877869
86	1	0	2.713010	2.935318	-1.386277
87	6	0	5.156423	3.866899	1.468088
88	1	0	3.536589	3.383696	2.800338
89	6	0	5.578846	3.954456	0.142982
90	1	0	5.009779	3.683553	-1.913948
91	1	0	5.835872	4.120263	2.275339
92	1	0	6.588565	4.275600	-0.089581

Cartesian coordinates of the structures at WB97XD/6-31G(d, p)//SMD$_{DCM}$ level

Cat

Total energy= -1052.05770365
Sum of electronic and zero-point Energies= -1051.673685
Sum of electronic and thermal Energies= -1051.652723
Sum of electronic and thermal Enthalpies= -1051.651779

Sum of electronic and thermal Free Energies= -1051.724838

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.956109	0.585252	-0.582474
2	6	0	-4.285711	0.281959	-0.286913
3	6	0	-5.202238	1.300769	-0.059824
4	6	0	-4.765738	2.625097	-0.122945
5	6	0	-3.433343	2.922136	-0.410392
6	6	0	-2.514257	1.899094	-0.647194
7	6	0	-2.194129	-0.697077	-0.842643
8	6	0	-3.075017	-1.768809	-0.151804
9	6	0	-4.496641	-1.213696	-0.275364
10	1	0	-6.238673	1.073786	0.172701
11	1	0	-5.469891	3.431411	0.059004
12	1	0	-3.108538	3.957323	-0.450766
13	1	0	-1.475829	2.120757	-0.873467
14	1	0	-2.151572	-0.898251	-1.917580
15	1	0	-2.947770	-2.758750	-0.608224
16	1	0	-4.950108	-1.553330	-1.213311
17	6	0	-0.468875	-1.456815	0.771716
18	6	0	-1.468324	-2.313107	1.483213
19	6	0	0.245017	-0.063400	-0.851018
20	1	0	-1.301302	-2.280295	2.560937
21	1	0	-5.123916	-1.565317	0.547442
22	7	0	-0.832160	-0.732893	-0.331740
23	7	0	0.795530	-1.307675	1.021755
24	7	0	1.201912	-0.449979	0.012421
25	8	0	-2.770858	-1.832646	1.235294
26	1	0	-1.363003	-3.355968	1.148581
27	6	0	2.576416	-0.051746	-0.020704
28	6	0	3.491374	-0.848527	-0.715911
29	6	0	2.959225	1.106089	0.661482
30	6	0	4.825715	-0.445974	-0.730124
31	6	0	4.305483	1.470021	0.620983
32	6	0	5.249892	0.708010	-0.067787
33	1	0	5.551292	-1.049900	-1.269649
34	1	0	4.622796	2.369807	1.142373
35	6	0	3.040788	-2.098542	-1.422599
36	1	0	2.572303	-2.797388	-0.721897
37	1	0	2.299228	-1.869300	-2.194251
38	1	0	3.885721	-2.602399	-1.897439
39	6	0	6.704766	1.099971	-0.069625

40	1	0	7.252851	0.556648	0.708671
41	1	0	7.179568	0.866680	-1.026882
42	1	0	6.830382	2.168666	0.123780
43	6	0	1.946487	1.932755	1.406562
44	1	0	1.241862	2.405622	0.714717
45	1	0	1.359086	1.314423	2.092431
46	1	0	2.436712	2.720001	1.983623

R1

Total energy= -422.85251530

Sum of electronic and zero-point Energies=	-422.707372
Sum of electronic and thermal Energies=	-422.698763
Sum of electronic and thermal Enthalpies=	-422.697819
Sum of electronic and thermal Free Energies=	-422.742313

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.410048	0.384720	0.000199
2	8	0	-3.862963	-0.747355	-0.000550
3	1	0	-4.093675	1.255724	0.001058
4	6	0	-1.977063	0.715899	-0.000051
5	6	0	-1.050661	-0.257730	0.000393
6	1	0	-1.720124	1.771465	-0.000711
7	1	0	-1.418437	-1.283377	0.000896
8	6	0	0.406357	-0.108728	0.000172
9	6	0	1.194591	-1.268254	0.000162
10	6	0	1.046821	1.140311	0.000062
11	6	0	2.582944	-1.186653	-0.000067
12	1	0	0.708617	-2.239965	0.000292
13	6	0	2.432797	1.221005	-0.000125
14	1	0	0.461063	2.054213	0.000203
15	6	0	3.205104	0.058673	-0.000202
16	1	0	3.177244	-2.094958	-0.000105
17	1	0	2.915400	2.193203	-0.000159
18	1	0	4.288554	0.127078	-0.000330

R2

Total energy= -745.12024270

Sum of electronic and zero-point Energies=	-744.898500
Sum of electronic and thermal Energies=	-744.884950
Sum of electronic and thermal Enthalpies=	-744.884006

Sum of electronic and thermal Free Energies= -744.940997

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.147922	0.806224	-0.047518
2	8	0	0.963350	2.012375	-0.031258
3	6	0	-0.107696	-0.104899	-0.130064
4	8	0	-0.049633	-1.305807	-0.353730
5	6	0	2.513474	0.228123	-0.007170
6	6	0	2.785656	-1.121382	0.256720
7	6	0	3.578658	1.120439	-0.203866
8	6	0	4.103663	-1.562169	0.317897
9	1	0	1.972823	-1.817696	0.411926
10	6	0	4.890042	0.672711	-0.150286
11	1	0	3.360886	2.164614	-0.400163
12	6	0	5.153798	-0.671359	0.112479
13	1	0	4.309042	-2.607020	0.526454
14	1	0	5.706380	1.369690	-0.309345
15	1	0	6.179691	-1.023689	0.158998
16	7	0	-1.231341	0.622863	0.054394
17	1	0	-1.063237	1.616459	0.173625
18	6	0	-2.574070	0.205011	0.034961
19	6	0	-3.548251	1.196286	0.205595
20	6	0	-2.961340	-1.127439	-0.139712
21	6	0	-4.895096	0.859822	0.199904
22	1	0	-3.243236	2.230173	0.342744
23	6	0	-4.316831	-1.447894	-0.142024
24	1	0	-2.212004	-1.894848	-0.272411
25	6	0	-5.288262	-0.466141	0.025587
26	1	0	-5.639876	1.638557	0.331116
27	1	0	-4.609559	-2.484415	-0.279068
28	1	0	-6.341261	-0.728415	0.020257

Si-M3

Total energy= -1474.95388385
Sum of electronic and zero-point Energies= -1474.419287
Sum of electronic and thermal Energies= -1474.390034
Sum of electronic and thermal Enthalpies= -1474.389090
Sum of electronic and thermal Free Energies= -1474.479573

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

1	6	0	-2.668635	-1.096266	0.083287
2	6	0	-3.850060	-1.840224	0.101673
3	6	0	-4.955810	-1.377568	0.802405
4	6	0	-4.861290	-0.162699	1.483568
5	6	0	-3.678779	0.575665	1.461135
6	6	0	-2.568141	0.115087	0.752761
7	6	0	-1.658271	-1.800845	-0.796076
8	6	0	-2.177182	-3.258058	-0.828019
9	6	0	-3.695056	-3.102645	-0.713114
10	1	0	-5.877537	-1.951761	0.826001
11	1	0	-5.717179	0.209986	2.038059
12	1	0	-3.620129	1.522488	1.988477
13	1	0	-1.652049	0.697831	0.725842
14	1	0	-1.629510	-1.350794	-1.792489
15	1	0	-1.849848	-3.793747	-1.726868
16	1	0	-4.135033	-2.981753	-1.709202
17	6	0	0.353228	-2.847278	0.262224
18	6	0	-0.358299	-4.157162	0.389143
19	6	0	0.609748	-0.768511	-0.373805
20	1	0	-0.122306	-4.625409	1.345753
21	1	0	-4.141156	-3.986642	-0.251578
22	7	0	-0.277399	-1.781027	-0.311438
23	7	0	1.584949	-2.558391	0.565878
24	7	0	1.727840	-1.254956	0.161913
25	8	0	-1.748885	-3.952304	0.339101
26	1	0	-0.020186	-4.824385	-0.416987
27	6	0	3.008978	-0.614665	0.245032
28	6	0	3.782874	-0.544724	-0.915834
29	6	0	3.425936	-0.110781	1.478232
30	6	0	5.026842	0.075159	-0.814029
31	6	0	4.678722	0.497118	1.527756
32	6	0	5.488255	0.600581	0.394393
33	1	0	5.651120	0.145034	-1.701010
34	1	0	5.030092	0.901766	2.473424
35	6	0	3.287764	-1.115340	-2.217877
36	1	0	3.036048	-2.175840	-2.109043
37	1	0	2.387453	-0.598798	-2.568190
38	1	0	4.053476	-1.025989	-2.991142
39	6	0	6.821284	1.296947	0.470223
40	1	0	6.700256	2.373471	0.304858
41	1	0	7.284462	1.165566	1.451959
42	1	0	7.512046	0.922498	-0.289952
43	6	0	2.546137	-0.210701	2.694743

44	1	0	1.584929	0.287868	2.528898
45	1	0	2.331502	-1.255043	2.942744
46	1	0	3.025906	0.255161	3.557788
47	6	0	0.364719	0.540486	-1.075317
48	8	0	-0.189123	0.400813	-2.218217
49	1	0	1.284116	3.729458	-0.631650
50	6	0	0.749029	1.661107	-0.398642
51	6	0	0.507364	3.034364	-0.968882
52	1	0	1.199353	1.568993	0.584627
53	1	0	0.574356	2.975051	-2.061716
54	6	0	-0.855348	3.586613	-0.592647
55	6	0	-2.011725	3.006602	-1.130928
56	6	0	-0.997112	4.637553	0.315146
57	6	0	-3.272684	3.471301	-0.772725
58	1	0	-1.899926	2.171590	-1.818582
59	6	0	-2.260764	5.103255	0.679221
60	1	0	-0.109305	5.095464	0.744862
61	6	0	-3.403089	4.523435	0.134719
62	1	0	-4.158445	3.007615	-1.197568
63	1	0	-2.350194	5.919915	1.390042
64	1	0	-4.387779	4.886117	0.414514

TS5RR

Total energy= -2220.09077883
Sum of electronic and zero-point Energies= -2219.332325
Sum of electronic and thermal Energies= -2219.289530
Sum of electronic and thermal Enthalpies= -2219.288585
Sum of electronic and thermal Free Energies= -2219.406862

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.475632	1.923781	-0.839451
2	6	0	-4.866988	1.988814	-0.941573
3	6	0	-5.474538	3.092721	-1.524226
4	6	0	-4.671995	4.137878	-1.984695
5	6	0	-3.284363	4.074675	-1.863667
6	6	0	-2.671865	2.958381	-1.293085
7	6	0	-3.103599	0.601042	-0.197945
8	6	0	-4.385941	0.249457	0.590472
9	6	0	-5.496437	0.761148	-0.325567
10	1	0	-6.555934	3.152010	-1.605238
11	1	0	-5.133310	5.012707	-2.432702

12	1	0	-2.673189	4.898916	-2.217996
13	1	0	-1.592445	2.897807	-1.215288
14	1	0	-2.890667	-0.155925	-0.953522
15	1	0	-4.452405	-0.815201	0.832472
16	1	0	-5.724291	0.005202	-1.085451
17	6	0	-2.095047	0.835999	2.059476
18	6	0	-3.441769	0.745825	2.704653
19	6	0	-0.631731	0.630132	0.453012
20	1	0	-3.512938	1.467317	3.519984
21	1	0	-6.409609	0.965534	0.237722
22	7	0	-1.954193	0.649978	0.715170
23	7	0	-0.938291	0.986788	2.637551
24	7	0	-0.035198	0.862834	1.624412
25	8	0	-4.453328	1.036788	1.775984
26	1	0	-3.554536	-0.265755	3.121612
27	6	0	1.354732	1.122326	1.886429
28	6	0	1.934280	2.254433	1.305474
29	6	0	2.057287	0.242650	2.717976
30	6	0	3.294596	2.458690	1.528422
31	6	0	3.413905	0.494536	2.902062
32	6	0	4.050996	1.585638	2.307004
33	1	0	3.773733	3.318304	1.069534
34	1	0	3.990313	-0.183097	3.526716
35	6	0	1.147164	3.213953	0.454100
36	1	0	1.010910	2.824484	-0.560359
37	1	0	0.158165	3.413396	0.877939
38	1	0	1.677695	4.164237	0.367230
39	6	0	5.523315	1.811689	2.523308
40	1	0	5.734598	2.008274	3.579879
41	1	0	6.098886	0.926056	2.236210
42	1	0	5.887620	2.660044	1.939563
43	6	0	1.386615	-0.918763	3.398358
44	1	0	0.799630	-0.574698	4.256251
45	1	0	0.712262	-1.446382	2.720053
46	1	0	2.134020	-1.626848	3.764079
47	6	0	-0.030985	0.404330	-0.921644
48	8	0	-0.776652	0.672595	-1.873905
49	1	0	2.338021	-0.710715	-2.798498
50	6	0	1.265772	-0.164622	-1.005089
51	6	0	2.066895	0.195750	-2.245072
52	1	0	1.826723	-0.201988	-0.079435
53	1	0	1.425835	0.777778	-2.913041
54	6	0	3.314267	0.981409	-1.909648
55	6	0	3.400398	2.350328	-2.173239

56	6	0	4.412677	0.347819	-1.317694
57	6	0	4.550752	3.071101	-1.855677
58	1	0	2.558071	2.855625	-2.639042
59	6	0	5.563118	1.062000	-1.000073
60	1	0	4.361208	-0.717004	-1.107451
61	6	0	5.637226	2.428620	-1.267763
62	1	0	4.598619	4.134624	-2.071485
63	1	0	6.406556	0.551120	-0.544908
64	1	0	6.536891	2.985586	-1.023376
65	6	0	0.860450	-2.153700	-1.348970
66	8	0	0.479944	-2.254542	-2.546845
67	6	0	-0.241296	-2.380122	-0.284907
68	8	0	-0.062199	-2.417733	0.930220
69	6	0	2.246910	-2.669673	-0.992380
70	6	0	2.815653	-2.612417	0.285766
71	6	0	3.000357	-3.206015	-2.038710
72	6	0	4.108070	-3.076867	0.503484
73	1	0	2.245597	-2.196518	1.105926
74	6	0	4.297089	-3.666062	-1.822790
75	1	0	2.546129	-3.252421	-3.022634
76	6	0	4.856825	-3.601597	-0.550013
77	1	0	4.537321	-3.017903	1.499436
78	1	0	4.868805	-4.074765	-2.650704
79	1	0	5.868527	-3.956758	-0.378270
80	7	0	-1.441557	-2.529245	-0.897897
81	1	0	-1.346145	-2.455262	-1.910989
82	6	0	-2.692539	-2.832832	-0.346819
83	6	0	-3.792214	-2.839789	-1.216115
84	6	0	-2.885826	-3.125440	1.008707
85	6	0	-5.062517	-3.136092	-0.738993
86	1	0	-3.640635	-2.611103	-2.267533
87	6	0	-4.166117	-3.423812	1.471278
88	1	0	-2.040791	-3.118157	1.682850
89	6	0	-5.259480	-3.430312	0.609813
90	1	0	-5.901416	-3.137132	-1.428114
91	1	0	-4.303966	-3.651975	2.523924
92	1	0	-6.252115	-3.660811	0.982429

TS5RS

Total energy= -2220.08668604
Sum of electronic and zero-point Energies= -2219.328941
Sum of electronic and thermal Energies= -2219.285869
Sum of electronic and thermal Enthalpies= -2219.284925

Sum of electronic and thermal Free Energies= -2219.404483

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.531582	-1.671634	0.714271
2	6	0	-4.923638	-1.650620	0.605856
3	6	0	-5.702431	-2.433956	1.446494
4	6	0	-5.067855	-3.248822	2.385372
5	6	0	-3.676895	-3.273267	2.480891
6	6	0	-2.893157	-2.474718	1.646706
7	6	0	-2.959848	-0.694515	-0.293070
8	6	0	-4.082604	-0.617788	-1.350566
9	6	0	-5.351379	-0.719833	-0.504867
10	1	0	-6.785333	-2.425454	1.364592
11	1	0	-5.663389	-3.875544	3.042173
12	1	0	-3.197922	-3.916419	3.212543
13	1	0	-1.812665	-2.470631	1.734651
14	1	0	-2.791806	0.278381	0.169093
15	1	0	-4.019776	0.287743	-1.965329
16	1	0	-5.614454	0.269942	-0.113424
17	6	0	-1.665265	-1.757235	-2.130871
18	6	0	-2.900420	-1.891909	-2.964984
19	6	0	-0.432898	-0.964148	-0.516377
20	1	0	-2.919548	-2.865437	-3.456740
21	1	0	-6.190943	-1.090345	-1.097194
22	7	0	-1.705436	-1.101267	-0.935409
23	7	0	-0.445357	-2.091032	-2.442400
24	7	0	0.311552	-1.592696	-1.425434
25	8	0	-4.051296	-1.784370	-2.167665
26	1	0	-2.871673	-1.110709	-3.738887
27	6	0	1.723951	-1.854967	-1.383274
28	6	0	2.531654	-1.321238	-2.395778
29	6	0	2.228410	-2.604485	-0.316387
30	6	0	3.905582	-1.504342	-2.268916
31	6	0	3.612639	-2.754256	-0.241310
32	6	0	4.464360	-2.198553	-1.192948
33	1	0	4.560257	-1.082011	-3.027256
34	1	0	4.032034	-3.307010	0.594209
35	6	0	1.951979	-0.565754	-3.560005
36	1	0	2.749538	-0.086389	-4.132501
37	1	0	1.408523	-1.238405	-4.230373
38	1	0	1.257493	0.204463	-3.208801
39	6	0	5.957312	-2.353906	-1.082437

40	1	0	6.460485	-1.392066	-1.219666
41	1	0	6.244042	-2.755442	-0.107744
42	1	0	6.335585	-3.033553	-1.853928
43	6	0	1.343211	-3.208129	0.741378
44	1	0	1.099437	-2.476975	1.518908
45	1	0	0.405570	-3.588062	0.324722
46	1	0	1.857044	-4.038341	1.230444
47	6	0	-0.020816	-0.215806	0.732903
48	8	0	-0.857908	-0.213363	1.647026
49	1	0	1.058560	0.735008	2.801919
50	6	0	1.205815	0.496208	0.684764
51	6	0	1.804086	0.896801	2.019187
52	1	0	1.923771	0.148469	-0.047795
53	1	0	2.048632	1.962459	2.028503
54	6	0	3.052825	0.091125	2.299081
55	6	0	4.258269	0.427080	1.673532
56	6	0	3.025414	-1.026060	3.137086
57	6	0	5.405674	-0.331134	1.883091
58	1	0	4.290508	1.291678	1.014172
59	6	0	4.172484	-1.789266	3.349601
60	1	0	2.095712	-1.295696	3.632309
61	6	0	5.367336	-1.443878	2.722793
62	1	0	6.333382	-0.053678	1.391145
63	1	0	4.133075	-2.650552	4.010366
64	1	0	6.264458	-2.032401	2.890485
65	6	0	0.719196	2.058205	-0.593408
66	8	0	0.376861	1.559648	-1.708240
67	6	0	-0.435757	2.621049	0.268532
68	8	0	-0.323860	3.110568	1.385522
69	6	0	2.063784	2.753627	-0.519597
70	6	0	2.385870	3.782193	0.371171
71	6	0	3.039294	2.321671	-1.425562
72	6	0	3.658855	4.352557	0.358118
73	1	0	1.641987	4.132216	1.076171
74	6	0	4.308807	2.883848	-1.433261
75	1	0	2.783548	1.531268	-2.121018
76	6	0	4.625406	3.904705	-0.536584
77	1	0	3.893126	5.149771	1.057226
78	1	0	5.052542	2.527315	-2.139844
79	1	0	5.616093	4.348984	-0.539091
80	7	0	-1.609248	2.471609	-0.405073
81	1	0	-1.459446	2.108264	-1.343993
82	6	0	-2.910422	2.784129	0.009840
83	6	0	-3.889885	2.939044	-0.978622

84	6	0	-3.267613	2.874268	1.359862
85	6	0	-5.212348	3.176114	-0.622583
86	1	0	-3.606096	2.870737	-2.025478
87	6	0	-4.594882	3.118136	1.701304
88	1	0	-2.509733	2.746997	2.121232
89	6	0	-5.572895	3.268469	0.720967
90	1	0	-5.962410	3.290790	-1.399108
91	1	0	-4.863869	3.184759	2.751096
92	1	0	-6.605012	3.455644	0.998932

TS5SR

Total energy= -2220.07603384
Sum of electronic and zero-point Energies= -2219.318346
Sum of electronic and thermal Energies= -2219.275862
Sum of electronic and thermal Enthalpies= -2219.274917
Sum of electronic and thermal Free Energies= -2219.394379

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.265980	-1.899348	-0.023511
2	6	0	4.459956	-2.604617	0.136867
3	6	0	5.645004	-2.095404	-0.375124
4	6	0	5.610746	-0.881934	-1.064682
5	6	0	4.409259	-0.197380	-1.238419
6	6	0	3.218294	-0.698120	-0.709775
7	6	0	2.154602	-2.660948	0.660187
8	6	0	2.703488	-4.106224	0.680918
9	6	0	4.207380	-3.898714	0.874500
10	1	0	6.579191	-2.636410	-0.256321
11	1	0	6.526313	-0.472289	-1.480122
12	1	0	4.401870	0.738808	-1.786466
13	1	0	2.285718	-0.158362	-0.850277
14	1	0	1.987927	-2.290367	1.670951
15	1	0	2.231546	-4.722170	1.455906
16	1	0	4.434420	-3.798078	1.941725
17	6	0	0.415601	-3.641001	-0.806148
18	6	0	1.189031	-4.916843	-0.926043
19	6	0	-0.103820	-1.653994	-0.038797
20	1	0	1.141875	-5.284836	-1.952014
21	1	0	4.770001	-4.749656	0.484175
22	7	0	0.856375	-2.611136	-0.030019
23	7	0	-0.758607	-3.384531	-1.303580

24	7	0	-1.069646	-2.150051	-0.821410
25	8	0	2.536559	-4.708018	-0.596449
26	1	0	0.724169	-5.664704	-0.266736
27	6	0	-2.373189	-1.632873	-1.147471
28	6	0	-2.556319	-1.051705	-2.403206
29	6	0	-3.401568	-1.811565	-0.219990
30	6	0	-3.826447	-0.553839	-2.686611
31	6	0	-4.649325	-1.287846	-0.550766
32	6	0	-4.871879	-0.637123	-1.765267
33	1	0	-3.998229	-0.078064	-3.648650
34	1	0	-5.461855	-1.385924	0.163848
35	6	0	-1.428568	-0.959204	-3.392554
36	1	0	-0.606091	-0.364853	-2.978464
37	1	0	-1.041717	-1.952618	-3.641306
38	1	0	-1.769741	-0.485627	-4.315789
39	6	0	-6.205511	-0.009232	-2.068816
40	1	0	-6.455264	-0.098107	-3.129669
41	1	0	-7.007378	-0.466504	-1.483617
42	1	0	-6.182351	1.059351	-1.825882
43	6	0	-3.165798	-2.521880	1.082413
44	1	0	-2.689454	-3.494557	0.921794
45	1	0	-2.518248	-1.932729	1.739783
46	1	0	-4.109423	-2.683229	1.605841
47	6	0	-0.092130	-0.426210	0.876672
48	8	0	0.789062	-0.461486	1.750148
49	1	0	-0.587884	1.518652	2.561053
50	6	0	-1.042986	0.604607	0.681861
51	6	0	-1.460290	1.368696	1.924930
52	1	0	-1.847192	0.389299	-0.011665
53	1	0	-1.827841	2.357675	1.642572
54	6	0	-2.551721	0.648137	2.684852
55	6	0	-3.885002	0.751339	2.275275
56	6	0	-2.253872	-0.154400	3.790293
57	6	0	-4.894474	0.070034	2.949629
58	1	0	-4.128473	1.370753	1.414810
59	6	0	-3.261263	-0.838606	4.468286
60	1	0	-1.220771	-0.243617	4.115671
61	6	0	-4.585541	-0.728380	4.050360
62	1	0	-5.924705	0.165579	2.618495
63	1	0	-3.011229	-1.454448	5.327522
64	1	0	-5.372680	-1.256798	4.579790
65	6	0	-0.046647	1.885547	-0.758070
66	8	0	0.393714	1.167768	-1.695556
67	6	0	1.022013	2.502128	0.183595

68	8	0	0.804069	3.040976	1.260787
69	6	0	-1.265791	2.748566	-1.022304
70	6	0	-1.624273	3.867722	-0.261348
71	6	0	-2.055709	2.409180	-2.125176
72	6	0	-2.765880	4.600917	-0.580441
73	1	0	-1.007562	4.165264	0.578072
74	6	0	-3.198349	3.134406	-2.437893
75	1	0	-1.751094	1.567761	-2.734434
76	6	0	-3.562890	4.232990	-1.660372
77	1	0	-3.030192	5.465380	0.021374
78	1	0	-3.803114	2.846970	-3.293237
79	1	0	-4.455546	4.802446	-1.901282
80	7	0	2.250004	2.429949	-0.397896
81	1	0	2.236675	2.027836	-1.328719
82	6	0	3.455817	2.963584	0.085764
83	6	0	4.425742	3.346307	-0.847219
84	6	0	3.722032	3.088810	1.452520
85	6	0	5.650713	3.843599	-0.419007
86	1	0	4.211172	3.251833	-1.908297
87	6	0	4.948596	3.599107	1.867947
88	1	0	2.974984	2.786136	2.173639
89	6	0	5.917363	3.977545	0.942061
90	1	0	6.394948	4.135500	-1.153424
91	1	0	5.147602	3.694461	2.931108
92	1	0	6.871275	4.371709	1.277645

TS5SS

Total energy= -2220.07606396
Sum of electronic and zero-point Energies= -2219.318007
Sum of electronic and thermal Energies= -2219.275251
Sum of electronic and thermal Enthalpies= -2219.274307
Sum of electronic and thermal Free Energies= -2219.392636

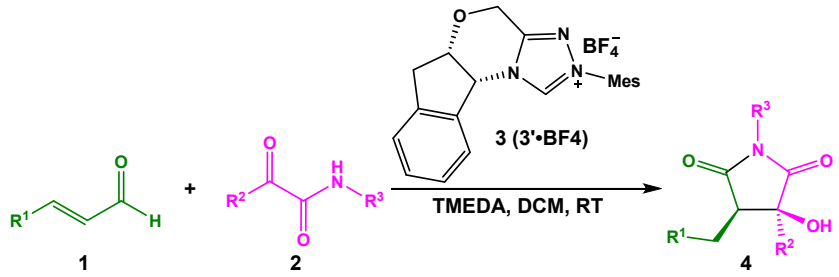
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.541997	-1.736737	0.112158
2	6	0	4.661997	-2.572058	0.132251
3	6	0	5.932713	-2.041172	0.305419
4	6	0	6.067517	-0.661135	0.455255
5	6	0	4.947131	0.168200	0.430691
6	6	0	3.668518	-0.363956	0.259679
7	6	0	2.303615	-2.599155	0.004955

8	6	0	2.850969	-3.900961	-0.626076
9	6	0	4.253742	-4.015841	-0.032957
10	1	0	6.805192	-2.688168	0.317520
11	1	0	7.053238	-0.225897	0.589145
12	1	0	5.070614	1.238262	0.551090
13	1	0	2.795126	0.277932	0.245148
14	1	0	1.899962	-2.796503	0.998298
15	1	0	2.205771	-4.764708	-0.423072
16	1	0	4.208849	-4.526497	0.935437
17	6	0	0.903900	-2.608775	-2.041285
18	6	0	1.789020	-3.619405	-2.700768
19	6	0	0.130998	-1.295276	-0.468959
20	1	0	1.993320	-3.316495	-3.729471
21	1	0	4.908416	-4.592224	-0.690656
22	7	0	1.174951	-2.095976	-0.805199
23	7	0	-0.241725	-2.186192	-2.487613
24	7	0	-0.715392	-1.378673	-1.499446
25	8	0	3.013216	-3.722964	-2.026517
26	1	0	1.256454	-4.581096	-2.723541
27	6	0	-2.054551	-0.874136	-1.657686
28	6	0	-2.257002	0.219482	-2.500225
29	6	0	-3.092184	-1.570090	-1.031228
30	6	0	-3.566857	0.668708	-2.645700
31	6	0	-4.380487	-1.065416	-1.193756
32	6	0	-4.632444	0.058181	-1.982160
33	1	0	-3.757641	1.525724	-3.284524
34	1	0	-5.205567	-1.569322	-0.697701
35	6	0	-1.111375	0.854193	-3.236695
36	1	0	-0.307767	1.118324	-2.543997
37	1	0	-0.704339	0.162805	-3.982748
38	1	0	-1.441598	1.757612	-3.753060
39	6	0	-6.024336	0.614040	-2.118141
40	1	0	-6.774398	-0.085374	-1.740569
41	1	0	-6.115729	1.547585	-1.552047
42	1	0	-6.258264	0.842534	-3.162141
43	6	0	-2.830065	-2.804763	-0.215131
44	1	0	-2.279970	-3.550842	-0.798319
45	1	0	-2.242414	-2.574991	0.679350
46	1	0	-3.768900	-3.252588	0.114475
47	6	0	-0.009308	-0.626897	0.893167
48	8	0	0.934589	-0.864227	1.664521
49	1	0	-0.688170	-0.095439	3.263194
50	6	0	-1.150303	0.160371	1.199724
51	6	0	-1.573219	0.107904	2.655462

52	1	0	-1.961631	0.123737	0.484908
53	1	0	-1.941981	1.089072	2.969953
54	6	0	-2.620011	-0.956905	2.889317
55	6	0	-3.940748	-0.760025	2.469626
56	6	0	-2.288812	-2.178762	3.481852
57	6	0	-4.901342	-1.752593	2.636962
58	1	0	-4.213427	0.178966	1.994786
59	6	0	-3.247216	-3.177314	3.650009
60	1	0	-1.266598	-2.348858	3.810469
61	6	0	-4.557572	-2.968036	3.228126
62	1	0	-5.921380	-1.577628	2.306831
63	1	0	-2.969493	-4.118857	4.114980
64	1	0	-5.306490	-3.743106	3.360075
65	6	0	-0.671376	2.247765	1.055605
66	8	0	-0.665116	2.682242	2.234489
67	6	0	0.703236	2.150679	0.352044
68	8	0	0.903206	1.632687	-0.745673
69	6	0	-1.820858	2.698866	0.168131
70	6	0	-1.620771	3.294613	-1.078072
71	6	0	-3.113715	2.688043	0.703603
72	6	0	-2.689804	3.857486	-1.775032
73	1	0	-0.628040	3.330091	-1.511627
74	6	0	-4.183896	3.223922	-0.000636
75	1	0	-3.273350	2.268556	1.690853
76	6	0	-3.974528	3.818371	-1.245203
77	1	0	-2.512080	4.327588	-2.737877
78	1	0	-5.180041	3.196507	0.431121
79	1	0	-4.807125	4.252231	-1.790692
80	7	0	1.644238	2.777112	1.092877
81	1	0	1.286096	3.064564	2.001258
82	6	0	2.955533	3.134101	0.741926
83	6	0	3.410105	3.133843	-0.581675
84	6	0	3.810281	3.552869	1.767881
85	6	0	4.707155	3.554919	-0.860480
86	1	0	2.753574	2.798885	-1.372844
87	6	0	5.103352	3.968129	1.474561
88	1	0	3.452420	3.550508	2.793564
89	6	0	5.560495	3.972415	0.157467
90	1	0	5.051741	3.550956	-1.890078
91	1	0	5.755851	4.289320	2.280491
92	1	0	6.571140	4.294889	-0.070913

Cartesian coordinates for different substiuent of TS5s at M06-2X/6-31G(d,

p)//IEFPCM$_{DCM}$ level



4-OMeC$_6$H$_4$/Ph/Ph

TS5RR

Total energy= -2334.30585370

Sum of electronic and zero-point Energies= -2333.516795

Sum of electronic and thermal Energies= -2333.471211

Sum of electronic and thermal Enthalpies= -2333.470267

Sum of electronic and thermal Free Energies= -2333.596007

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.504873	2.273254	-0.775667
2	6	0	-4.866675	2.550211	-0.917942
3	6	0	-5.286416	3.799537	-1.355159
4	6	0	-4.325534	4.772905	-1.631871
5	6	0	-2.967968	4.495951	-1.473955
6	6	0	-2.543806	3.235793	-1.049740
7	6	0	-3.351107	0.835344	-0.314533
8	6	0	-4.719152	0.558355	0.353815
9	6	0	-5.693464	1.349886	-0.517128
10	1	0	-6.344047	4.020382	-1.463599
11	1	0	-4.638265	5.757731	-1.963739
12	1	0	-2.232587	5.265704	-1.683845
13	1	0	-1.487237	3.013616	-0.947812
14	1	0	-3.174436	0.160843	-1.156091
15	1	0	-4.946566	-0.508593	0.432341
16	1	0	-5.981307	0.751021	-1.389044
17	6	0	-2.481444	0.592443	2.010612
18	6	0	-3.876334	0.552908	2.554518
19	6	0	-0.933838	0.534172	0.474318
20	1	0	-3.924623	1.096266	3.498730
21	1	0	-6.597375	1.600750	0.041705
22	7	0	-2.266575	0.616925	0.661249
23	7	0	-1.355888	0.554426	2.666044
24	7	0	-0.401232	0.526705	1.699246
25	8	0	-4.752827	1.165737	1.642636

26	1	0	-4.152089	-0.497775	2.728192
27	6	0	0.992104	0.602617	2.056532
28	6	0	1.735353	1.687923	1.577015
29	6	0	1.545053	-0.413753	2.846151
30	6	0	3.104410	1.689465	1.838535
31	6	0	2.919043	-0.358220	3.071854
32	6	0	3.717384	0.665079	2.557425
33	1	0	3.707784	2.507322	1.455141
34	1	0	3.378849	-1.147612	3.662614
35	6	0	1.115652	2.816335	0.794241
36	1	0	1.007468	2.554296	-0.265129
37	1	0	0.129957	3.090886	1.182392
38	1	0	1.759231	3.696573	0.842438
39	6	0	5.206237	0.655128	2.779985
40	1	0	5.442418	0.577757	3.848810
41	1	0	5.656740	-0.211789	2.278756
42	1	0	5.674825	1.557403	2.372709
43	6	0	0.715843	-1.514999	3.452350
44	1	0	0.190427	-1.150529	4.339872
45	1	0	-0.027583	-1.890561	2.748066
46	1	0	1.362333	-2.341748	3.754843
47	6	0	-0.275145	0.416560	-0.890242
48	8	0	-0.948801	0.831026	-1.839478
49	1	0	2.028596	-0.716805	-2.809923
50	6	0	0.971696	-0.262907	-0.981681
51	6	0	1.854914	0.143692	-2.152900
52	1	0	1.488865	-0.441809	-0.045809
53	1	0	1.314945	0.884650	-2.750097
54	6	0	3.168982	0.713341	-1.670925
55	6	0	3.424120	2.086382	-1.703528
56	6	0	4.147804	-0.133401	-1.135922
57	6	0	4.610930	2.611923	-1.195344
58	1	0	2.681456	2.757690	-2.127941
59	6	0	5.335343	0.378963	-0.624740
60	1	0	3.970333	-1.206717	-1.116224
61	6	0	5.557354	1.754496	-0.641590
62	1	0	4.806535	3.680173	-1.208115
63	1	0	6.094592	-0.274082	-0.203932
64	6	0	0.370526	-2.089890	-1.519952
65	8	0	-0.000244	-2.038531	-2.727712
66	6	0	-0.763550	-2.287716	-0.487930
67	8	0	-0.604625	-2.402640	0.724781
68	6	0	1.676867	-2.801704	-1.193354
69	6	0	2.206286	-2.945178	0.096780

70	6	0	2.397407	-3.307374	-2.277474
71	6	0	3.429989	-3.578425	0.287574
72	1	0	1.662317	-2.548438	0.946329
73	6	0	3.627939	-3.933924	-2.085878
74	1	0	1.969734	-3.193657	-3.268098
75	6	0	4.148994	-4.070880	-0.802094
76	1	0	3.829423	-3.676931	1.292546
77	1	0	4.178643	-4.313661	-2.940906
78	1	0	5.108238	-4.555648	-0.649734
79	7	0	-1.971502	-2.269476	-1.108913
80	1	0	-1.866897	-2.162707	-2.118467
81	6	0	-3.241396	-2.499995	-0.562257
82	6	0	-4.336748	-2.448799	-1.437326
83	6	0	-3.457761	-2.777337	0.795296
84	6	0	-5.623363	-2.687119	-0.970223
85	1	0	-4.167964	-2.228411	-2.487944
86	6	0	-4.755407	-3.022851	1.244970
87	1	0	-2.619075	-2.817181	1.475731
88	6	0	-5.842250	-2.981023	0.376167
89	1	0	-6.457006	-2.646220	-1.663855
90	1	0	-4.910798	-3.250598	2.295340
91	1	0	-6.845617	-3.171824	0.740756
92	8	0	6.704066	2.271261	-0.077109
93	6	0	7.783846	2.370219	-0.998832
94	1	0	7.526666	3.037276	-1.831823
95	1	0	8.633620	2.780173	-0.452361
96	1	0	8.048200	1.383558	-1.400832

TS5RS

Total energy= -2334.30011744
Sum of electronic and zero-point Energies= -2333.510927
Sum of electronic and thermal Energies= -2333.465314
Sum of electronic and thermal Enthalpies= -2333.464370
Sum of electronic and thermal Free Energies= -2333.589278

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.664997	-1.895002	-0.765680
2	6	0	5.062374	-1.900708	-0.765712
3	6	0	5.756995	-2.771717	-1.594168
4	6	0	5.033380	-3.645023	-2.408395
5	6	0	3.638895	-3.640860	-2.395081

6	6	0	2.937843	-2.755013	-1.574360
7	6	0	3.197071	-0.814758	0.187598
8	6	0	4.395319	-0.685240	1.149659
9	6	0	5.592909	-0.884346	0.222252
10	1	0	6.842737	-2.784470	-1.598149
11	1	0	5.562143	-4.339360	-3.053683
12	1	0	3.092134	-4.329748	-3.030674
13	1	0	1.853627	-2.726937	-1.577164
14	1	0	3.016265	0.114684	-0.352618
15	1	0	4.399932	0.263744	1.701258
16	1	0	5.833038	0.066057	-0.272476
17	6	0	2.015250	-1.627741	2.226396
18	6	0	3.316569	-1.777278	2.957426
19	6	0	0.692036	-0.927403	0.643046
20	1	0	3.332029	-2.716591	3.511813
21	1	0	6.470744	-1.219366	0.779008
22	7	0	1.985851	-1.111377	0.962865
23	7	0	0.809206	-1.831195	2.678181
24	7	0	-0.003396	-1.395224	1.679214
25	8	0	4.391704	-1.788411	2.051287
26	1	0	3.403715	-0.945511	3.671256
27	6	0	-1.433081	-1.528747	1.785414
28	6	0	-2.093992	-0.832441	2.806128
29	6	0	-2.097823	-2.306737	0.832216
30	6	0	-3.486099	-0.879414	2.799567
31	6	0	-3.491608	-2.321813	0.881845
32	6	0	-4.200874	-1.598450	1.838218
33	1	0	-4.027075	-0.327936	3.564559
34	1	0	-4.034470	-2.896829	0.136683
35	6	0	-1.348275	-0.051676	3.855205
36	1	0	-2.051521	0.534523	4.450479
37	1	0	-0.805600	-0.723233	4.526032
38	1	0	-0.628949	0.623985	3.383775
39	6	0	-5.706537	-1.612339	1.856628
40	1	0	-6.100195	-0.609428	2.046924
41	1	0	-6.111354	-1.965670	0.906162
42	1	0	-6.076312	-2.266218	2.653467
43	6	0	-1.371095	-3.085523	-0.233319
44	1	0	-1.123672	-2.450098	-1.090935
45	1	0	-0.442202	-3.525545	0.142452
46	1	0	-2.007807	-3.892315	-0.600775
47	6	0	0.231974	-0.280339	-0.646644
48	8	0	1.004418	-0.418928	-1.605099
49	1	0	-0.992429	0.475174	-2.717426

50	6	0	-0.936819	0.522918	-0.580785
51	6	0	-1.613370	0.851377	-1.899350
52	1	0	-1.612487	0.303870	0.238786
53	1	0	-1.701410	1.933630	-2.034230
54	6	0	-2.985634	0.217469	-1.925358
55	6	0	-4.045258	0.823937	-1.240823
56	6	0	-3.206581	-1.018878	-2.537212
57	6	0	-5.286726	0.203948	-1.150729
58	1	0	-3.885304	1.790317	-0.765300
59	6	0	-4.445380	-1.650884	-2.452724
60	1	0	-2.395320	-1.498411	-3.079374
61	6	0	-5.478054	-1.042173	-1.744430
62	1	0	-6.110779	0.662692	-0.611730
63	1	0	-4.614620	-2.620022	-2.912273
64	6	0	-0.195958	2.097592	0.497198
65	8	0	0.163927	1.659146	1.633775
66	6	0	0.951292	2.457695	-0.474476
67	8	0	0.819514	2.767994	-1.650011
68	6	0	-1.446929	2.948091	0.433900
69	6	0	-1.703232	3.910500	-0.548144
70	6	0	-2.390183	2.749340	1.449763
71	6	0	-2.889070	4.644897	-0.518714
72	1	0	-0.976915	4.081420	-1.333877
73	6	0	-3.572683	3.478829	1.475455
74	1	0	-2.176117	2.006853	2.212763
75	6	0	-3.827834	4.431098	0.486832
76	1	0	-3.074842	5.389166	-1.286818
77	1	0	-4.297072	3.307461	2.265493
78	1	0	-4.750245	5.002925	0.503415
79	7	0	2.145589	2.345052	0.175521
80	1	0	2.023295	2.144282	1.165731
81	6	0	3.437855	2.536640	-0.337009
82	6	0	4.464168	2.837522	0.566529
83	6	0	3.734432	2.364406	-1.694566
84	6	0	5.774144	2.967672	0.119666
85	1	0	4.225351	2.973955	1.617924
86	6	0	5.050320	2.504259	-2.127974
87	1	0	2.937115	2.119267	-2.384214
88	6	0	6.074566	2.804949	-1.232144
89	1	0	6.560126	3.200817	0.830860
90	1	0	5.274678	2.367592	-3.181077
91	1	0	7.095620	2.909347	-1.582946
92	8	0	-6.688893	-1.684865	-1.594143
93	6	0	-7.548431	-1.530744	-2.720578

94	1	0	-7.092015	-1.952902	-3.627359
95	1	0	-8.468835	-2.069504	-2.491919
96	1	0	-7.776285	-0.469336	-2.896142

TS5SR

Total energy= -2334.28613826
Sum of electronic and zero-point Energies= -2333.497758
Sum of electronic and thermal Energies= -2333.451402
Sum of electronic and thermal Enthalpies= -2333.450458
Sum of electronic and thermal Free Energies= -2333.580416

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.461487	-1.929916	0.198790
2	6	0	4.616451	-2.661401	0.479428
3	6	0	5.860697	-2.156803	0.127861
4	6	0	5.921923	-0.925715	-0.528737
5	6	0	4.757948	-0.220244	-0.832011
6	6	0	3.505059	-0.714500	-0.463224
7	6	0	2.262960	-2.695798	0.705562
8	6	0	2.785081	-4.150632	0.727871
9	6	0	4.254249	-3.979126	1.128080
10	1	0	6.767002	-2.716354	0.338797
11	1	0	6.885179	-0.521177	-0.822860
12	1	0	4.832293	0.721569	-1.366012
13	1	0	2.595444	-0.172527	-0.713721
14	1	0	1.966987	-2.366944	1.701288
15	1	0	2.206217	-4.797276	1.399087
16	1	0	4.342220	-3.927729	2.218856
17	6	0	0.732803	-3.565663	-1.041758
18	6	0	1.487330	-4.859772	-1.099088
19	6	0	0.168539	-1.583875	-0.291548
20	1	0	1.568463	-5.193489	-2.134209
21	1	0	4.849146	-4.824626	0.775535
22	7	0	1.075309	-2.582987	-0.159995
23	7	0	-0.333551	-3.241421	-1.713767
24	7	0	-0.674789	-2.014793	-1.238940
25	8	0	2.784441	-4.685366	-0.588944
26	1	0	0.930545	-5.615655	-0.526672
27	6	0	-1.893668	-1.434003	-1.747805
28	6	0	-1.861263	-0.831822	-3.005738
29	6	0	-3.055380	-1.582853	-0.986854

30	6	0	-3.055471	-0.279947	-3.467869
31	6	0	-4.217630	-1.003828	-1.491717
32	6	0	-4.230100	-0.331175	-2.715315
33	1	0	-3.062055	0.212852	-4.437618
34	1	0	-5.132923	-1.081246	-0.910593
35	6	0	-0.590188	-0.771469	-3.807910
36	1	0	0.172666	-0.208061	-3.259418
37	1	0	-0.204965	-1.776822	-4.003177
38	1	0	-0.770318	-0.279480	-4.765648
39	6	0	-5.480674	0.347752	-3.207531
40	1	0	-5.554329	0.302053	-4.296541
41	1	0	-6.375927	-0.106214	-2.777494
42	1	0	-5.471452	1.404933	-2.920702
43	6	0	-3.041396	-2.325068	0.320475
44	1	0	-2.581404	-3.311956	0.206041
45	1	0	-2.479337	-1.770847	1.080587
46	1	0	-4.057395	-2.454585	0.696227
47	6	0	0.094769	-0.384663	0.660799
48	8	0	0.896132	-0.446479	1.605336
49	1	0	-0.637635	1.407623	2.390711
50	6	0	-0.829217	0.655304	0.398361
51	6	0	-1.394511	1.379064	1.605905
52	1	0	-1.537331	0.480127	-0.404150
53	1	0	-1.629155	2.414721	1.345843
54	6	0	-2.650928	0.698724	2.101660
55	6	0	-3.852061	0.837493	1.398896
56	6	0	-2.634175	-0.118999	3.235327
57	6	0	-5.007523	0.184748	1.816911
58	1	0	-3.876400	1.462285	0.507342
59	6	0	-3.781209	-0.786270	3.658509
60	1	0	-1.704054	-0.242608	3.784175
61	6	0	-4.967467	-0.633439	2.944359
62	1	0	-5.945225	0.291847	1.279712
63	1	0	-3.764464	-1.430405	4.532680
64	6	0	0.379176	1.932317	-0.826237
65	8	0	0.907934	1.239306	-1.737218
66	6	0	1.332639	2.445598	0.282341
67	8	0	0.986800	2.922826	1.354047
68	6	0	-0.762255	2.858632	-1.189504
69	6	0	-1.132296	3.989513	-0.451504
70	6	0	-1.460985	2.564174	-2.365459
71	6	0	-2.200912	4.781790	-0.869931
72	1	0	-0.586368	4.249616	0.447487
73	6	0	-2.535477	3.344996	-2.772844

74	1	0	-1.140854	1.710217	-2.950979
75	6	0	-2.912948	4.458780	-2.021450
76	1	0	-2.476288	5.656132	-0.288534
77	1	0	-3.074220	3.090624	-3.681348
78	1	0	-3.749675	5.073949	-2.337138
79	7	0	2.626250	2.360252	-0.133260
80	1	0	2.728746	2.016907	-1.082470
81	6	0	3.765055	2.791881	0.569198
82	6	0	4.875301	3.222724	-0.164658
83	6	0	3.821994	2.769700	1.966103
84	6	0	6.035228	3.619848	0.490114
85	1	0	4.819374	3.250255	-1.249618
86	6	0	4.985267	3.181884	2.609527
87	1	0	2.961102	2.432369	2.527677
88	6	0	6.095190	3.605466	1.882137
89	1	0	6.891181	3.947369	-0.091201
90	1	0	5.023951	3.161897	3.694140
91	1	0	6.998229	3.919852	2.394621
92	8	0	-6.106701	-1.309208	3.322353
93	6	0	-6.745571	-0.744297	4.460039
94	1	0	-7.624591	-1.355249	4.667798
95	1	0	-6.083456	-0.752389	5.333175
96	1	0	-7.055343	0.287787	4.258091

TS5SS

Total energy= -2334.28963490
Sum of electronic and zero-point Energies= -2333.500290
Sum of electronic and thermal Energies= -2333.454628
Sum of electronic and thermal Enthalpies= -2333.453684
Sum of electronic and thermal Free Energies= -2333.578283

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.407901	-2.219447	-0.009175
2	6	0	-4.351184	-3.249495	0.033752
3	6	0	-5.660501	-3.021632	-0.366238
4	6	0	-6.012180	-1.744878	-0.804393
5	6	0	-5.070376	-0.716651	-0.832969
6	6	0	-3.750957	-0.944591	-0.435554
7	6	0	-2.065729	-2.785267	0.400640
8	6	0	-2.464853	-4.019815	1.242530
9	6	0	-3.725554	-4.526628	0.544152

10	1	0	-6.397111	-3.818829	-0.328669
11	1	0	-7.032374	-1.545545	-1.117568
12	1	0	-5.365807	0.271230	-1.169259
13	1	0	-3.015398	-0.146011	-0.447027
14	1	0	-1.496237	-3.083919	-0.480599
15	1	0	-1.657905	-4.760521	1.313089
16	1	0	-3.455011	-5.195117	-0.280656
17	6	0	-0.990437	-2.116526	2.539071
18	6	0	-1.776785	-3.136805	3.306237
19	6	0	-0.243000	-1.007190	0.806208
20	1	0	-2.171985	-2.690141	4.220111
21	1	0	-4.356080	-5.081975	1.242311
22	7	0	-1.168887	-1.918946	1.198075
23	7	0	-0.011009	-1.393531	2.997716
24	7	0	0.450187	-0.719838	1.911297
25	8	0	-2.859489	-3.597614	2.541169
26	1	0	-1.100953	-3.959227	3.580786
27	6	0	1.661270	0.045738	2.069270
28	6	0	1.586752	1.289096	2.694232
29	6	0	2.859169	-0.548198	1.658416
30	6	0	2.780891	1.994587	2.833411
31	6	0	4.018406	0.210578	1.799801
32	6	0	3.993530	1.487210	2.367027
33	1	0	2.756777	2.972663	3.305735
34	1	0	4.962838	-0.211447	1.465179
35	6	0	0.281008	1.818948	3.219165
36	1	0	-0.497265	1.746882	2.454631
37	1	0	-0.040625	1.242841	4.092908
38	1	0	0.389323	2.864762	3.513486
39	6	0	5.248994	2.311987	2.462333
40	1	0	6.141464	1.682618	2.469710
41	1	0	5.318445	2.985766	1.601650
42	1	0	5.248802	2.930047	3.363279
43	6	0	2.889051	-1.939685	1.086207
44	1	0	2.407118	-2.650926	1.765374
45	1	0	2.373676	-1.987066	0.120425
46	1	0	3.918889	-2.259251	0.919617
47	6	0	-0.047886	-0.593768	-0.647876
48	8	0	-0.847050	-1.138041	-1.426004
49	1	0	0.816184	-0.385671	-3.010373
50	6	0	0.971540	0.326262	-1.008080
51	6	0	1.574382	0.084588	-2.378628
52	1	0	1.683324	0.587192	-0.234855
53	1	0	1.823440	1.037982	-2.854200

54	6	0	2.795380	-0.800150	-2.276975
55	6	0	3.981362	-0.306264	-1.721143
56	6	0	2.753779	-2.142241	-2.664074
57	6	0	5.095938	-1.123007	-1.562735
58	1	0	4.024954	0.730522	-1.392047
59	6	0	3.860032	-2.973872	-2.502098
60	1	0	1.835979	-2.543522	-3.086386
61	6	0	5.029899	-2.460742	-1.948488
62	1	0	6.019111	-0.744215	-1.134017
63	1	0	3.824456	-4.019647	-2.793064
64	6	0	0.095247	2.231805	-1.344352
65	8	0	0.137286	2.430663	-2.583674
66	6	0	-1.301820	1.978898	-0.729765
67	8	0	-1.506607	1.607509	0.425023
68	6	0	1.030049	3.057247	-0.476571
69	6	0	0.595067	3.771236	0.640871
70	6	0	2.344851	3.239262	-0.921606
71	6	0	1.464563	4.633733	1.309267
72	1	0	-0.424801	3.660638	0.992893
73	6	0	3.219736	4.075084	-0.239399
74	1	0	2.666653	2.733146	-1.826639
75	6	0	2.779976	4.779781	0.882394
76	1	0	1.108057	5.190224	2.171603
77	1	0	4.238626	4.196511	-0.595406
78	1	0	3.457349	5.443258	1.411665
79	7	0	-2.265404	2.282462	-1.628339
80	1	0	-1.880755	2.487018	-2.548194
81	6	0	-3.648015	2.425705	-1.424008
82	6	0	-4.214468	2.539813	-0.148524
83	6	0	-4.465499	2.510100	-2.557020
84	6	0	-5.586730	2.740334	-0.026930
85	1	0	-3.582981	2.468919	0.726168
86	6	0	-5.833957	2.708860	-2.418893
87	1	0	-4.020554	2.417866	-3.543504
88	6	0	-6.403870	2.825222	-1.151775
89	1	0	-6.019315	2.830037	0.964526
90	1	0	-6.455323	2.770583	-3.306421
91	1	0	-7.472058	2.979586	-1.043320
92	8	0	6.123912	-3.275183	-1.751968
93	6	0	6.894447	-3.467009	-2.931319
94	1	0	7.726931	-4.119407	-2.665680
95	1	0	6.298007	-3.939628	-3.720202
96	1	0	7.281805	-2.511225	-3.303052

4-FC_6H_4/Ph/Ph

TS5RR

Total energy= -2319.03503752

Sum of electronic and zero-point Energies= -2318.286402

Sum of electronic and thermal Energies= -2318.242814

Sum of electronic and thermal Enthalpies= -2318.241870

Sum of electronic and thermal Free Energies= -2318.361561

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.466563	-2.112862	-0.796527
2	6	0	4.845423	-2.311167	-0.899642
3	6	0	5.347691	-3.521058	-1.359853
4	6	0	4.451518	-4.535095	-1.699981
5	6	0	3.076125	-4.336421	-1.583405
6	6	0	2.569374	-3.115481	-1.135692
7	6	0	3.218400	-0.701836	-0.293952
8	6	0	4.547364	-0.373206	0.427610
9	6	0	5.591075	-1.081816	-0.434357
10	1	0	6.418855	-3.681145	-1.437701
11	1	0	4.828324	-5.490252	-2.051457
12	1	0	2.392082	-5.136684	-1.845971
13	1	0	1.499395	-2.952209	-1.067607
14	1	0	3.027863	-0.009952	-1.117842
15	1	0	4.713876	0.700789	0.546563
16	1	0	5.873229	-0.440427	-1.277482
17	6	0	2.261767	-0.597726	2.008105
18	6	0	3.633906	-0.495686	2.599832
19	6	0	0.766204	-0.566261	0.421931
20	1	0	3.685133	-1.070273	3.525128
21	1	0	6.489218	-1.301627	0.146993
22	7	0	2.093871	-0.578598	0.651905
23	7	0	1.114999	-0.654792	2.624092
24	7	0	0.192556	-0.643679	1.625682
25	8	0	4.575329	-1.020658	1.697143
26	1	0	3.840025	0.562157	2.819897
27	6	0	-1.201581	-0.840298	1.931155
28	6	0	-1.842198	-1.961107	1.388776
29	6	0	-1.853076	0.091397	2.749366
30	6	0	-3.207903	-2.095812	1.632350
31	6	0	-3.221890	-0.087820	2.942470
32	6	0	-3.918055	-1.160322	2.381984

33	1	0	-3.730233	-2.947799	1.206248
34	1	0	-3.758649	0.637297	3.549726
35	6	0	-1.122922	-2.993422	0.559096
36	1	0	-1.036033	-2.673409	-0.486127
37	1	0	-0.118168	-3.198749	0.941225
38	1	0	-1.685893	-3.928377	0.563703
39	6	0	-5.398792	-1.313761	2.610374
40	1	0	-5.598177	-1.670334	3.626083
41	1	0	-5.908780	-0.353556	2.493910
42	1	0	-5.838429	-2.022952	1.905825
43	6	0	-1.129668	1.229399	3.420020
44	1	0	-0.606291	0.870330	4.311276
45	1	0	-0.393597	1.685279	2.756785
46	1	0	-1.846655	1.992512	3.730571
47	6	0	0.145287	-0.416549	-0.957202
48	8	0	0.858910	-0.769753	-1.900772
49	1	0	-2.176626	0.751298	-2.857300
50	6	0	-1.121461	0.229287	-1.048304
51	6	0	-1.966119	-0.143263	-2.258495
52	1	0	-1.665349	0.324575	-0.115113
53	1	0	-1.382092	-0.811992	-2.898184
54	6	0	-3.253440	-0.810154	-1.833631
55	6	0	-3.442986	-2.186192	-1.978115
56	6	0	-4.271406	-0.053414	-1.239497
57	6	0	-4.604391	-2.809151	-1.522471
58	1	0	-2.669969	-2.784530	-2.453694
59	6	0	-5.434494	-0.655641	-0.772837
60	1	0	-4.146581	1.022171	-1.136453
61	6	0	-5.574841	-2.028382	-0.917269
62	1	0	-4.758545	-3.877807	-1.625370
63	1	0	-6.226092	-0.081877	-0.302497
64	6	0	-0.612081	2.105985	-1.454081
65	8	0	-0.229120	2.160368	-2.659313
66	6	0	0.500851	2.300022	-0.398342
67	8	0	0.324205	2.333546	0.816972
68	6	0	-1.955050	2.732082	-1.096309
69	6	0	-2.505308	2.756380	0.192595
70	6	0	-2.688173	3.277395	-2.152229
71	6	0	-3.761376	3.313173	0.410159
72	1	0	-1.953760	2.326549	1.020467
73	6	0	-3.950856	3.826870	-1.934654
74	1	0	-2.244820	3.256028	-3.142357
75	6	0	-4.492334	3.846253	-0.652339
76	1	0	-4.176451	3.319466	1.413854

77	1	0	-4.510222	4.240407	-2.768329
78	1	0	-5.475942	4.272164	-0.480534
79	7	0	1.713074	2.385115	-1.004105
80	1	0	1.623381	2.333394	-2.019374
81	6	0	2.963737	2.645962	-0.426939
82	6	0	4.075155	2.670118	-1.282447
83	6	0	3.144312	2.884248	0.943197
84	6	0	5.342334	2.943820	-0.782713
85	1	0	3.934464	2.479330	-2.342923
86	6	0	4.422410	3.166010	1.426033
87	1	0	2.292370	2.863070	1.607790
88	6	0	5.525170	3.198556	0.576886
89	1	0	6.189341	2.960717	-1.460882
90	1	0	4.549716	3.362259	2.486466
91	1	0	6.513465	3.416289	0.966754
92	9	0	-6.687228	-2.622754	-0.434582

TS5RS

Total energy= -2319.02885516
Sum of electronic and zero-point Energies= -2318.281210
Sum of electronic and thermal Energies= -2318.237246
Sum of electronic and thermal Enthalpies= -2318.236302
Sum of electronic and thermal Free Energies= -2318.358356

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.579656	-1.775800	-0.710422
2	6	0	4.975154	-1.795833	-0.647020
3	6	0	5.698440	-2.652661	-1.465659
4	6	0	5.004506	-3.495887	-2.335313
5	6	0	3.611003	-3.476920	-2.385922
6	6	0	2.882168	-2.605680	-1.574496
7	6	0	3.074405	-0.725694	0.257459
8	6	0	4.231548	-0.632982	1.274272
9	6	0	5.467619	-0.813747	0.393565
10	1	0	6.782991	-2.678041	-1.419930
11	1	0	5.555914	-4.178869	-2.973686
12	1	0	3.087567	-4.142795	-3.064230
13	1	0	1.799413	-2.567378	-1.625827
14	1	0	2.916756	0.223596	-0.254977
15	1	0	4.216775	0.300026	1.852101
16	1	0	5.736343	0.148540	-0.061305

17	6	0	1.805262	-1.633184	2.201488
18	6	0	3.068868	-1.776546	2.995565
19	6	0	0.551077	-0.907261	0.574488
20	1	0	3.068290	-2.723402	3.536937
21	1	0	6.317485	-1.172052	0.978481
22	7	0	1.829940	-1.058011	0.963425
23	7	0	0.584099	-1.902664	2.569791
24	7	0	-0.185024	-1.451343	1.543686
25	8	0	4.186578	-1.761594	2.142310
26	1	0	3.110745	-0.953440	3.723384
27	6	0	-1.607753	-1.670856	1.545875
28	6	0	-2.375047	-1.076439	2.555221
29	6	0	-2.158910	-2.440032	0.515247
30	6	0	-3.758363	-1.214973	2.458207
31	6	0	-3.548100	-2.551835	0.476886
32	6	0	-4.362411	-1.930787	1.421649
33	1	0	-4.381258	-0.740927	3.213163
34	1	0	-4.003041	-3.127851	-0.324381
35	6	0	-1.747556	-0.309415	3.688278
36	1	0	-2.519445	0.222062	4.249015
37	1	0	-1.229998	-0.986885	4.373049
38	1	0	-1.022673	0.413582	3.302740
39	6	0	-5.861551	-2.051365	1.344466
40	1	0	-6.341610	-1.108880	1.620638
41	1	0	-6.185225	-2.320652	0.336645
42	1	0	-6.223701	-2.819813	2.035208
43	6	0	-1.318567	-3.112377	-0.539581
44	1	0	-1.059498	-2.416645	-1.345722
45	1	0	-0.389976	-3.517938	-0.126764
46	1	0	-1.878014	-3.934277	-0.989817
47	6	0	0.135623	-0.207439	-0.702758
48	8	0	0.960055	-0.258941	-1.624813
49	1	0	-1.003402	0.631837	-2.792135
50	6	0	-1.068560	0.545722	-0.655515
51	6	0	-1.690238	0.916757	-1.989790
52	1	0	-1.778672	0.247608	0.107841
53	1	0	-1.841610	1.997745	-2.063783
54	6	0	-3.013883	0.199892	-2.129879
55	6	0	-4.141562	0.684861	-1.456946
56	6	0	-3.122100	-0.994712	-2.844542
57	6	0	-5.343441	-0.015424	-1.473005
58	1	0	-4.069594	1.619195	-0.902998
59	6	0	-4.317370	-1.711964	-2.875505
60	1	0	-2.256953	-1.376010	-3.381298

61	6	0	-5.401856	-1.209076	-2.176443
62	1	0	-6.223358	0.342363	-0.948984
63	1	0	-4.413249	-2.645553	-3.419169
64	6	0	-0.472930	2.079535	0.541554
65	8	0	-0.139588	1.591508	1.667119
66	6	0	0.692785	2.549548	-0.356712
67	8	0	0.588071	2.959081	-1.504577
68	6	0	-1.767923	2.862327	0.470966
69	6	0	-2.043921	3.867398	-0.461957
70	6	0	-2.741063	2.539114	1.424206
71	6	0	-3.277328	4.519730	-0.446307
72	1	0	-1.296509	4.134245	-1.199747
73	6	0	-3.970572	3.186255	1.435126
74	1	0	-2.512026	1.764938	2.149785
75	6	0	-4.244958	4.180558	0.494463
76	1	0	-3.478227	5.297080	-1.176995
77	1	0	-4.716972	2.916912	2.176579
78	1	0	-5.204577	4.687892	0.498754
79	7	0	1.871197	2.403661	0.314505
80	1	0	1.728847	2.129114	1.284254
81	6	0	3.171458	2.641903	-0.158228
82	6	0	4.174277	2.915874	0.778976
83	6	0	3.498614	2.528928	-1.515022
84	6	0	5.492331	3.077418	0.365932
85	1	0	3.911642	3.004427	1.829788
86	6	0	4.821280	2.699710	-1.914053
87	1	0	2.719974	2.298275	-2.230860
88	6	0	5.822958	2.973607	-0.984393
89	1	0	6.260703	3.287927	1.102961
90	1	0	5.069807	2.607894	-2.966617
91	1	0	6.850187	3.102182	-1.308244
92	9	0	-6.553853	-1.914385	-2.162280

TS5SR

Total energy= -2319.01504863
Sum of electronic and zero-point Energies= -2318.266338
Sum of electronic and thermal Energies= -2318.222191
Sum of electronic and thermal Enthalpies= -2318.221247
Sum of electronic and thermal Free Energies= -2318.344810

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

1	6	0	3.351628	-1.952758	0.137891
2	6	0	4.515166	-2.695042	0.345480
3	6	0	5.746330	-2.180471	-0.036421
4	6	0	5.785917	-0.925470	-0.646783
5	6	0	4.613602	-0.205465	-0.874544
6	6	0	3.374353	-0.711752	-0.476748
7	6	0	2.174647	-2.733982	0.670698
8	6	0	2.692891	-4.189380	0.625877
9	6	0	4.178994	-4.034051	0.963595
10	1	0	6.658323	-2.749582	0.116913
11	1	0	6.738148	-0.511643	-0.963120
12	1	0	4.670749	0.759636	-1.367121
13	1	0	2.457239	-0.160507	-0.672187
14	1	0	1.926312	-2.434071	1.688692
15	1	0	2.142134	-4.854547	1.303012
16	1	0	4.317777	-4.021568	2.050177
17	6	0	0.547871	-3.568420	-1.006405
18	6	0	1.309210	-4.851670	-1.153425
19	6	0	0.019279	-1.609002	-0.176396
20	1	0	1.338516	-5.142756	-2.204157
21	1	0	4.754199	-4.867260	0.553610
22	7	0	0.943650	-2.600155	-0.130937
23	7	0	-0.568932	-3.244455	-1.590539
24	7	0	-0.888405	-2.032093	-1.066402
25	8	0	2.629416	-4.683373	-0.705553
26	1	0	0.789747	-5.635756	-0.584263
27	6	0	-2.154230	-1.466579	-1.467371
28	6	0	-2.245825	-0.896444	-2.737244
29	6	0	-3.240881	-1.609807	-0.600664
30	6	0	-3.484281	-0.368534	-3.100927
31	6	0	-4.449747	-1.049809	-1.007629
32	6	0	-4.582536	-0.408148	-2.241473
33	1	0	-3.586364	0.098440	-4.077936
34	1	0	-5.306773	-1.120572	-0.342444
35	6	0	-1.057071	-0.845594	-3.657252
36	1	0	-0.229187	-0.321794	-3.168421
37	1	0	-0.725263	-1.854371	-3.920016
38	1	0	-1.313786	-0.316924	-4.577287
39	6	0	-5.880235	0.249796	-2.628935
40	1	0	-6.037149	0.211735	-3.709289
41	1	0	-6.730526	-0.225407	-2.135065
42	1	0	-5.868863	1.304406	-2.332696
43	6	0	-3.102751	-2.331716	0.711166
44	1	0	-2.648785	-3.317825	0.569168

45	1	0	-2.476939	-1.764775	1.409082
46	1	0	-4.080196	-2.462226	1.177850
47	6	0	0.017415	-0.422195	0.793475
48	8	0	0.895895	-0.489977	1.666713
49	1	0	-0.545963	1.371511	2.583137
50	6	0	-0.929248	0.614352	0.619024
51	6	0	-1.372107	1.345981	1.871514
52	1	0	-1.715469	0.435216	-0.105672
53	1	0	-1.625342	2.382215	1.633144
54	6	0	-2.582235	0.671318	2.477393
55	6	0	-3.839313	0.823823	1.881318
56	6	0	-2.471088	-0.154954	3.598523
57	6	0	-4.961180	0.174158	2.386430
58	1	0	-3.936226	1.458678	1.002151
59	6	0	-3.580981	-0.818037	4.119604
60	1	0	-1.499371	-0.286269	4.066969
61	6	0	-4.807209	-0.638677	3.500117
62	1	0	-5.942034	0.289332	1.937602
63	1	0	-3.509584	-1.459933	4.990680
64	6	0	0.138681	1.873275	-0.755737
65	8	0	0.587218	1.157129	-1.690529
66	6	0	1.188367	2.439947	0.232500
67	8	0	0.950587	2.918744	1.332006
68	6	0	-1.049018	2.771244	-1.032185
69	6	0	-1.393074	3.895750	-0.272094
70	6	0	-1.825153	2.450857	-2.150963
71	6	0	-2.514519	4.653360	-0.610068
72	1	0	-0.784632	4.178202	0.579088
73	6	0	-2.950269	3.196984	-2.477789
74	1	0	-1.523265	1.604513	-2.755983
75	6	0	-3.302972	4.302261	-1.702602
76	1	0	-2.770824	5.523066	-0.013234
77	1	0	-3.547904	2.922250	-3.342494
78	1	0	-4.178915	4.891052	-1.956027
79	7	0	2.426851	2.402168	-0.333876
80	1	0	2.431456	2.043999	-1.283274
81	6	0	3.617543	2.909944	0.215228
82	6	0	4.598679	3.392881	-0.657515
83	6	0	3.852809	2.907164	1.593291
84	6	0	5.807678	3.863153	-0.157973
85	1	0	4.404729	3.399374	-1.726877
86	6	0	5.062443	3.393488	2.080855
87	1	0	3.093559	2.523482	2.261622
88	6	0	6.044121	3.870643	1.215270

89	1	0	6.561983	4.232228	-0.845416
90	1	0	5.240578	3.388446	3.151570
91	1	0	6.984826	4.243506	1.606247
92	9	0	-5.888245	-1.271831	3.996980

TS5SS

Total energy= -2319.01808731
Sum of electronic and zero-point Energies= -2318.270344
Sum of electronic and thermal Energies= -2318.226369
Sum of electronic and thermal Enthalpies= -2318.225425
Sum of electronic and thermal Free Energies= -2318.347059

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.396814	-1.924876	0.083775
2	6	0	-4.431188	-2.860226	0.177779
3	6	0	-5.728545	-2.511391	-0.170841
4	6	0	-5.975931	-1.210296	-0.608898
5	6	0	-4.942800	-0.276666	-0.688585
6	6	0	-3.635346	-0.626928	-0.343691
7	6	0	-2.097840	-2.615365	0.438341
8	6	0	-2.574328	-3.800793	1.309434
9	6	0	-3.908880	-4.188111	0.674979
10	1	0	-6.535120	-3.234649	-0.094627
11	1	0	-6.984829	-0.917592	-0.882596
12	1	0	-5.156290	0.732667	-1.024233
13	1	0	-2.827050	0.095491	-0.398923
14	1	0	-1.602997	-2.973254	-0.465746
15	1	0	-1.839387	-4.615074	1.351872
16	1	0	-3.743459	-4.887168	-0.152201
17	6	0	-0.849891	-2.063447	2.515504
18	6	0	-1.707258	-2.983744	3.331547
19	6	0	-0.080191	-1.039019	0.741285
20	1	0	-2.013394	-2.484370	4.252431
21	1	0	-4.557218	-4.673066	1.408356
22	7	0	-1.079859	-1.842376	1.185552
23	7	0	0.231737	-1.461295	2.915729
24	7	0	0.703412	-0.839536	1.803507
25	8	0	-2.865248	-3.333644	2.619854
26	1	0	-1.112904	-3.870455	3.593086
27	6	0	2.005395	-0.227399	1.878367
28	6	0	2.129906	1.001081	2.527790

29	6	0	3.083418	-0.943388	1.351836
30	6	0	3.403955	1.561621	2.567061
31	6	0	4.330722	-0.322375	1.391030
32	6	0	4.503685	0.932089	1.979787
33	1	0	3.536975	2.524375	3.052850
34	1	0	5.185209	-0.837840	0.959338
35	6	0	0.944025	1.654279	3.182497
36	1	0	0.100209	1.703846	2.488553
37	1	0	0.632002	1.080406	4.061016
38	1	0	1.198505	2.666989	3.499786
39	6	0	5.852239	1.600752	2.007900
40	1	0	6.587819	1.041052	1.426925
41	1	0	5.780412	2.611998	1.595890
42	1	0	6.222791	1.689943	3.033530
43	6	0	2.901176	-2.315687	0.760354
44	1	0	2.318077	-2.955476	1.430741
45	1	0	2.382807	-2.271716	-0.204498
46	1	0	3.870623	-2.786490	0.590076
47	6	0	0.070299	-0.625640	-0.716822
48	8	0	-0.811208	-1.096969	-1.454714
49	1	0	0.676002	-0.178715	-3.172738
50	6	0	1.131751	0.220012	-1.129086
51	6	0	1.566476	-0.000691	-2.564972
52	1	0	1.936884	0.373800	-0.422445
53	1	0	2.038348	0.902843	-2.958018
54	6	0	2.509468	-1.176493	-2.643667
55	6	0	3.861947	-1.019059	-2.321255
56	6	0	2.040026	-2.458410	-2.945397
57	6	0	4.730556	-2.106003	-2.296377
58	1	0	4.238038	-0.029430	-2.070977
59	6	0	2.891954	-3.561213	-2.924000
60	1	0	0.988982	-2.592249	-3.186069
61	6	0	4.223885	-3.361440	-2.597954
62	1	0	5.780936	-1.995922	-2.049507
63	1	0	2.541911	-4.560437	-3.158588
64	6	0	0.442100	2.226045	-1.304075
65	8	0	0.438633	2.486064	-2.531456
66	6	0	-0.937545	2.070380	-0.620874
67	8	0	-1.111054	1.669856	0.529034
68	6	0	1.495776	2.914801	-0.453108
69	6	0	1.166504	3.671414	0.672702
70	6	0	2.810914	2.955008	-0.929965
71	6	0	2.135057	4.446021	1.312035
72	1	0	0.150589	3.665472	1.053268

73	6	0	3.780898	3.709153	-0.282316
74	1	0	3.062995	2.402886	-1.830116
75	6	0	3.443839	4.464889	0.842021
76	1	0	1.859405	5.037591	2.180308
77	1	0	4.797735	3.723840	-0.663461
78	1	0	4.197406	5.065900	1.342203
79	7	0	-1.916115	2.496836	-1.450939
80	1	0	-1.562343	2.714107	-2.380248
81	6	0	-3.268354	2.751118	-1.167622
82	6	0	-3.770159	2.818378	0.137918
83	6	0	-4.119104	2.995024	-2.252140
84	6	0	-5.112234	3.131061	0.336858
85	1	0	-3.114256	2.620664	0.974387
86	6	0	-5.456569	3.304371	-2.036797
87	1	0	-3.723995	2.939782	-3.262380
88	6	0	-5.962157	3.374253	-0.739288
89	1	0	-5.495215	3.181723	1.351226
90	1	0	-6.104076	3.491813	-2.887266
91	1	0	-7.006278	3.614365	-0.569825
92	9	0	5.056213	-4.421559	-2.576497

Furan/Ph/Ph

TS5RR

Total energy= -2217.61552264

Sum of electronic and zero-point Energies= -2216.888733

Sum of electronic and thermal Energies= -2216.846949

Sum of electronic and thermal Enthalpies= -2216.846004

Sum of electronic and thermal Free Energies= -2216.961074

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.510503	-1.798256	-0.895255
2	6	0	4.900981	-1.800810	-1.030570
3	6	0	5.552309	-2.909847	-1.553379
4	6	0	4.794460	-4.022251	-1.922645
5	6	0	3.408185	-4.019959	-1.770996
6	6	0	2.750314	-2.900025	-1.260390
7	6	0	3.084917	-0.454196	-0.332912
8	6	0	4.370074	0.019968	0.386577
9	6	0	5.481937	-0.500691	-0.522763
10	1	0	6.633023	-2.918132	-1.658120
11	1	0	5.289278	-4.900991	-2.323769

12	1	0	2.833570	-4.895274	-2.055312
13	1	0	1.670106	-2.887745	-1.165300
14	1	0	2.791372	0.235688	-1.127998
15	1	0	4.391194	1.100531	0.555213
16	1	0	5.652166	0.210018	-1.339901
17	6	0	2.162111	-0.553669	1.982420
18	6	0	3.523286	-0.321106	2.562975
19	6	0	0.645577	-0.640609	0.417151
20	1	0	3.659656	-0.937336	3.452447
21	1	0	6.415223	-0.617805	0.032226
22	7	0	1.970252	-0.513015	0.629985
23	7	0	1.038123	-0.750327	2.612290
24	7	0	0.104350	-0.809924	1.627158
25	8	0	4.506055	-0.676383	1.622937
26	1	0	3.604166	0.739026	2.844389
27	6	0	-1.262548	-1.138609	1.935053
28	6	0	-1.809619	-2.288175	1.354622
29	6	0	-1.994594	-0.277672	2.764881
30	6	0	-3.171158	-2.515613	1.551186
31	6	0	-3.353894	-0.546853	2.907420
32	6	0	-3.965367	-1.638012	2.284369
33	1	0	-3.621627	-3.395126	1.100667
34	1	0	-3.953627	0.122077	3.520173
35	6	0	-1.010761	-3.249115	0.512706
36	1	0	-1.055851	-2.970004	-0.546467
37	1	0	0.038647	-3.296381	0.816871
38	1	0	-1.433574	-4.251703	0.600029
39	6	0	-5.449664	-1.852938	2.407462
40	1	0	-5.768207	-1.821525	3.452996
41	1	0	-5.988122	-1.064708	1.871752
42	1	0	-5.746693	-2.811436	1.977445
43	6	0	-1.362659	0.879370	3.491771
44	1	0	-0.807707	0.519500	4.363257
45	1	0	-0.671451	1.424693	2.848757
46	1	0	-2.136788	1.567040	3.838123
47	6	0	-0.009783	-0.551169	-0.950397
48	8	0	0.729373	-0.790422	-1.911783
49	1	0	-2.279813	0.279563	-2.933300
50	6	0	-1.353100	-0.098155	-1.020707
51	6	0	-2.142834	-0.556551	-2.235692
52	1	0	-1.903074	-0.066998	-0.089305
53	1	0	-1.566261	-1.315071	-2.775906
54	6	0	-1.102352	1.856784	-1.439123
55	8	0	-0.691484	1.950440	-2.629321

56	6	0	-0.059511	2.177271	-0.347243
57	8	0	-0.283766	2.185806	0.859638
58	6	0	-2.529811	2.288680	-1.132531
59	6	0	-3.136436	2.208536	0.128660
60	6	0	-3.269767	2.788722	-2.206244
61	6	0	-4.450526	2.628903	0.302823
62	1	0	-2.578243	1.813894	0.970135
63	6	0	-4.588127	3.206366	-2.031092
64	1	0	-2.784901	2.849034	-3.174893
65	6	0	-5.182510	3.130256	-0.774273
66	1	0	-4.908308	2.556982	1.285178
67	1	0	-5.148647	3.592999	-2.876830
68	1	0	-6.208767	3.454987	-0.633453
69	7	0	1.156291	2.405402	-0.910723
70	1	0	1.109307	2.357405	-1.928497
71	6	0	2.344379	2.818504	-0.291792
72	6	0	3.447581	3.067797	-1.121713
73	6	0	2.472918	2.990510	1.093962
74	6	0	4.652254	3.499606	-0.581073
75	1	0	3.347980	2.928863	-2.194799
76	6	0	3.687878	3.432542	1.618562
77	1	0	1.627048	2.797515	1.739066
78	6	0	4.780396	3.690330	0.795139
79	1	0	5.492350	3.691927	-1.240696
80	1	0	3.772801	3.576264	2.691641
81	1	0	5.718762	4.033652	1.216634
82	6	0	-3.465122	-1.127152	-1.850010
83	6	0	-4.670674	-0.572554	-1.547964
84	8	0	-3.534295	-2.481848	-1.706414
85	6	0	-5.542390	-1.658039	-1.201249
86	1	0	-4.902805	0.483399	-1.572568
87	6	0	-4.799732	-2.787364	-1.317706
88	1	0	-6.581850	-1.603122	-0.913011
89	1	0	-5.013246	-3.835913	-1.178432

TS5RS

Total energy= -2217.60844850
Sum of electronic and zero-point Energies= -2216.883436
Sum of electronic and thermal Energies= -2216.840812
Sum of electronic and thermal Enthalpies= -2216.839868
Sum of electronic and thermal Free Energies= -2216.959350

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-3.564678	-1.496398	0.809803
2	6	0	-4.946947	-1.383528	0.640254
3	6	0	-5.812036	-2.036201	1.507562
4	6	0	-5.273081	-2.811694	2.535740
5	6	0	-3.892152	-2.925287	2.694187
6	6	0	-3.019916	-2.258161	1.832325
7	6	0	-2.886844	-0.646213	-0.243918
8	6	0	-3.958650	-0.579105	-1.352128
9	6	0	-5.261191	-0.511598	-0.556163
10	1	0	-6.887567	-1.957239	1.380404
11	1	0	-5.936031	-3.337272	3.215711
12	1	0	-3.491063	-3.535646	3.496684
13	1	0	-1.944837	-2.319941	1.965765
14	1	0	-2.660516	0.342644	0.155347
15	1	0	-3.803654	0.257023	-2.046454
16	1	0	-5.452084	0.526523	-0.254319
17	6	0	-1.598702	-1.914687	-1.961122
18	6	0	-2.821629	-2.055065	-2.817110
19	6	0	-0.378622	-1.082932	-0.359098
20	1	0	-2.884798	-3.064898	-3.224439
21	1	0	-6.105494	-0.861770	-1.153977
22	7	0	-1.642844	-1.187443	-0.806256
23	7	0	-0.385497	-2.318852	-2.215104
24	7	0	0.361625	-1.798114	-1.206194
25	8	0	-3.980169	-1.816920	-2.057023
26	1	0	-2.737265	-1.342559	-3.650341
27	6	0	1.766235	-2.092267	-1.103712
28	6	0	2.608238	-1.689616	-2.148934
29	6	0	2.232129	-2.707757	0.063574
30	6	0	3.978109	-1.858418	-1.954108
31	6	0	3.611522	-2.854824	0.196625
32	6	0	4.498665	-2.413947	-0.783635
33	1	0	4.657970	-1.526045	-2.735006
34	1	0	4.000357	-3.310849	1.103062
35	6	0	2.077699	-1.066889	-3.412506
36	1	0	2.906737	-0.693484	-4.017262
37	1	0	1.519738	-1.798173	-4.002949
38	1	0	1.410281	-0.235154	-3.169364
39	6	0	5.983891	-2.566977	-0.591527
40	1	0	6.534854	-1.816677	-1.169867
41	1	0	6.244513	-2.453583	0.466908
42	1	0	6.318067	-3.559941	-0.921356

43	6	0	1.324630	-3.163325	1.177260
44	1	0	1.185989	-2.367011	1.917967
45	1	0	0.341448	-3.473861	0.813422
46	1	0	1.777530	-4.011314	1.694173
47	6	0	0.025496	-0.252345	0.840736
48	8	0	-0.844620	-0.116865	1.710624
49	1	0	1.202597	0.643931	2.896242
50	6	0	1.286131	0.396095	0.767500
51	6	0	1.857353	0.933563	2.067378
52	1	0	2.014049	-0.049602	0.099943
53	1	0	1.895320	2.026183	2.059485
54	6	0	0.888094	1.801683	-0.646293
55	8	0	0.579388	1.198251	-1.720973
56	6	0	-0.281985	2.478581	0.102043
57	8	0	-0.205146	3.033776	1.189663
58	6	0	2.237708	2.491032	-0.587980
59	6	0	2.518279	3.640261	0.157547
60	6	0	3.250865	1.932967	-1.376902
61	6	0	3.790186	4.214028	0.109682
62	1	0	1.743295	4.088041	0.768175
63	6	0	4.518718	2.497083	-1.413763
64	1	0	3.019861	1.045871	-1.958724
65	6	0	4.793155	3.646718	-0.670648
66	1	0	3.993671	5.110866	0.686682
67	1	0	5.294307	2.044813	-2.024606
68	1	0	5.781344	4.094990	-0.701985
69	7	0	-1.431472	2.339157	-0.619375
70	1	0	-1.265823	1.936336	-1.538756
71	6	0	-2.726445	2.745738	-0.258230
72	6	0	-3.649545	3.007231	-1.277023
73	6	0	-3.129325	2.813921	1.081119
74	6	0	-4.963520	3.337167	-0.961186
75	1	0	-3.327664	2.956113	-2.313648
76	6	0	-4.445651	3.152153	1.381742
77	1	0	-2.413135	2.592873	1.862354
78	6	0	-5.368109	3.415317	0.370493
79	1	0	-5.670323	3.537426	-1.760069
80	1	0	-4.753139	3.200765	2.421508
81	1	0	-6.392015	3.675338	0.616897
82	6	0	3.234943	0.408865	2.287851
83	6	0	4.467684	0.885635	1.967688
84	8	0	3.348883	-0.831250	2.842262
85	6	0	5.408198	-0.125333	2.359271
86	1	0	4.667016	1.839531	1.498218

87	6	0	4.672384	-1.138176	2.882745
88	1	0	6.484201	-0.096296	2.270969
89	1	0	4.925213	-2.090911	3.322444

TS5SR

Total energy= -2217.59660150
Sum of electronic and zero-point Energies= -2216.870380
Sum of electronic and thermal Energies= -2216.827906
Sum of electronic and thermal Enthalpies= -2216.826962
Sum of electronic and thermal Free Energies= -2216.946672

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.212878	-1.889426	0.037510
2	6	0	4.410138	-2.594442	0.170809
3	6	0	5.587473	-2.067358	-0.341241
4	6	0	5.538160	-0.839158	-1.003620
5	6	0	4.330811	-0.157654	-1.155869
6	6	0	3.146306	-0.676843	-0.627957
7	6	0	2.110571	-2.673678	0.708467
8	6	0	2.661504	-4.116912	0.672562
9	6	0	4.166591	-3.912698	0.871382
10	1	0	6.525047	-2.607145	-0.247901
11	1	0	6.447547	-0.417208	-1.419490
12	1	0	4.316210	0.785632	-1.692017
13	1	0	2.198843	-0.159455	-0.760723
14	1	0	1.948448	-2.335200	1.731896
15	1	0	2.190796	-4.768641	1.419308
16	1	0	4.399042	-3.849262	1.940077
17	6	0	0.363390	-3.613024	-0.781125
18	6	0	1.148935	-4.877590	-0.959883
19	6	0	-0.153624	-1.647983	0.041875
20	1	0	1.099302	-5.197879	-2.001320
21	1	0	4.726512	-4.748922	0.446653
22	7	0	0.807769	-2.603769	0.022064
23	7	0	-0.817721	-3.347178	-1.258502
24	7	0	-1.127883	-2.130269	-0.739315
25	8	0	2.496949	-4.662502	-0.629879
26	1	0	0.701795	-5.658660	-0.328338
27	6	0	-2.455254	-1.629500	-0.999236
28	6	0	-2.728995	-1.116223	-2.266954
29	6	0	-3.414871	-1.772204	0.006274

30	6	0	-4.022828	-0.647120	-2.487289
31	6	0	-4.687396	-1.272944	-0.262788
32	6	0	-5.001321	-0.690780	-1.492480
33	1	0	-4.266852	-0.224433	-3.459423
34	1	0	-5.451545	-1.347475	0.506783
35	6	0	-1.669874	-1.071772	-3.334345
36	1	0	-0.797487	-0.514927	-2.976396
37	1	0	-1.348529	-2.082233	-3.603872
38	1	0	-2.056628	-0.583491	-4.231134
39	6	0	-6.363192	-0.099160	-1.742388
40	1	0	-6.702921	-0.304019	-2.760524
41	1	0	-7.102872	-0.491541	-1.041747
42	1	0	-6.327181	0.988459	-1.618961
43	6	0	-3.080582	-2.425990	1.318652
44	1	0	-2.554321	-3.373039	1.162341
45	1	0	-2.443227	-1.781475	1.936106
46	1	0	-3.990565	-2.627088	1.885094
47	6	0	-0.111640	-0.430956	0.969580
48	8	0	0.846546	-0.435704	1.758698
49	1	0	-0.502088	1.513550	2.678072
50	6	0	-1.109978	0.561420	0.856787
51	6	0	-1.422134	1.334865	2.122193
52	1	0	-1.964259	0.340063	0.229295
53	1	0	-1.855096	2.309013	1.874473
54	6	0	-0.211100	1.789033	-0.699325
55	8	0	0.174351	1.029476	-1.624599
56	6	0	0.901255	2.444967	0.157062
57	8	0	0.741558	2.980906	1.244419
58	6	0	-1.451110	2.630954	-0.910484
59	6	0	-1.783790	3.762560	-0.154950
60	6	0	-2.285177	2.258099	-1.969473
61	6	0	-2.945057	4.478828	-0.441829
62	1	0	-1.133229	4.083611	0.649942
63	6	0	-3.448196	2.965659	-2.245839
64	1	0	-1.996528	1.405981	-2.572752
65	6	0	-3.785246	4.080170	-1.478008
66	1	0	-3.191833	5.354615	0.150094
67	1	0	-4.088005	2.653351	-3.066328
68	1	0	-4.690803	4.638752	-1.692818
69	7	0	2.085444	2.416876	-0.515425
70	1	0	2.020771	2.002989	-1.439584
71	6	0	3.292977	3.020874	-0.122604
72	6	0	4.178113	3.438621	-1.122669
73	6	0	3.637496	3.184406	1.222561

74	6	0	5.399086	4.008437	-0.782447
75	1	0	3.899792	3.317735	-2.166329
76	6	0	4.858198	3.768735	1.548713
77	1	0	2.953303	2.853189	1.991930
78	6	0	5.744227	4.181056	0.556496
79	1	0	6.077671	4.325421	-1.567872
80	1	0	5.120128	3.893329	2.594730
81	1	0	6.694390	4.631632	0.823055
82	6	0	-2.375615	0.590027	2.997872
83	6	0	-2.245725	-0.063718	4.185301
84	8	0	-3.660468	0.482004	2.556751
85	6	0	-3.537944	-0.604920	4.498909
86	1	0	-1.337708	-0.140454	4.765109
87	6	0	-4.351933	-0.240588	3.477261
88	1	0	-3.818560	-1.180822	5.368156
89	1	0	-5.397257	-0.403403	3.264772

TS5SS

Total energy= -2217.60140989
Sum of electronic and zero-point Energies= -2216.874640
Sum of electronic and thermal Energies= -2216.832472
Sum of electronic and thermal Enthalpies= -2216.831528
Sum of electronic and thermal Free Energies= -2216.948659

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.590254	-1.586708	0.281816
2	6	0	4.754917	-2.357842	0.329857
3	6	0	5.997720	-1.749409	0.437191
4	6	0	6.057326	-0.356795	0.490709
5	6	0	4.893118	0.409151	0.429942
6	6	0	3.641073	-0.200876	0.326175
7	6	0	2.400926	-2.522486	0.254415
8	6	0	3.009942	-3.823448	-0.318286
9	6	0	4.425471	-3.830575	0.256719
10	1	0	6.904661	-2.345842	0.469823
11	1	0	7.020359	0.137548	0.572967
12	1	0	4.959564	1.491187	0.466922
13	1	0	2.732212	0.390022	0.272228
14	1	0	2.023499	-2.683577	1.265372
15	1	0	2.415921	-4.712059	-0.068926
16	1	0	4.425053	-4.289087	1.251871

17	6	0	0.970206	-2.722812	-1.769290
18	6	0	1.905244	-3.718975	-2.386798
19	6	0	0.152279	-1.370329	-0.255723
20	1	0	2.074713	-3.468648	-3.435300
21	1	0	5.097925	-4.405095	-0.384363
22	7	0	1.232729	-2.129902	-0.565707
23	7	0	-0.203201	-2.384157	-2.216459
24	7	0	-0.704518	-1.553454	-1.264382
25	8	0	3.144234	-3.700440	-1.727860
26	1	0	1.437381	-4.712260	-2.333405
27	6	0	-2.076109	-1.132361	-1.426301
28	6	0	-2.359293	-0.163621	-2.390848
29	6	0	-3.057854	-1.802896	-0.690478
30	6	0	-3.697678	0.178429	-2.564922
31	6	0	-4.378837	-1.405463	-0.891493
32	6	0	-4.713927	-0.413318	-1.813326
33	1	0	-3.949729	0.937891	-3.300286
34	1	0	-5.163028	-1.896773	-0.320831
35	6	0	-1.269664	0.448918	-3.226621
36	1	0	-0.448347	0.794600	-2.593011
37	1	0	-0.872812	-0.284491	-3.936032
38	1	0	-1.661960	1.298761	-3.788551
39	6	0	-6.141545	0.025096	-1.999285
40	1	0	-6.841826	-0.691731	-1.563998
41	1	0	-6.301643	0.993289	-1.517175
42	1	0	-6.380778	0.145703	-3.060084
43	6	0	-2.711932	-2.891111	0.289508
44	1	0	-2.004860	-3.606982	-0.141837
45	1	0	-2.262898	-2.477395	1.200671
46	1	0	-3.612285	-3.431364	0.586232
47	6	0	0.018231	-0.622236	1.064195
48	8	0	1.012089	-0.723885	1.798916
49	1	0	-0.672193	-0.139065	3.425051
50	6	0	-1.166844	0.099763	1.353787
51	6	0	-1.537219	0.150240	2.822836
52	1	0	-1.998422	-0.050536	0.679927
53	1	0	-1.791713	1.178915	3.111802
54	6	0	-0.822733	2.157448	0.971829
55	8	0	-0.829101	2.731119	2.089618
56	6	0	0.540323	2.056394	0.250849
57	8	0	0.734833	1.420769	-0.783832
58	6	0	-2.002591	2.426378	0.052560
59	6	0	-1.839625	2.974251	-1.220835
60	6	0	-3.293636	2.307928	0.578594

61	6	0	-2.948766	3.398326	-1.953836
62	1	0	-0.846265	3.077794	-1.645672
63	6	0	-4.398738	2.716363	-0.156853
64	1	0	-3.423961	1.893145	1.574095
65	6	0	-4.229520	3.270664	-1.426963
66	1	0	-2.805578	3.831634	-2.939561
67	1	0	-5.394232	2.614314	0.265440
68	1	0	-5.092604	3.597613	-1.999412
69	7	0	1.466483	2.811827	0.882829
70	1	0	1.118976	3.193483	1.759721
71	6	0	2.746212	3.188417	0.439361
72	6	0	3.151631	3.052290	-0.893834
73	6	0	3.611918	3.770999	1.372193
74	6	0	4.412244	3.504742	-1.273775
75	1	0	2.485635	2.594748	-1.612184
76	6	0	4.868293	4.216107	0.977543
77	1	0	3.292762	3.871167	2.405470
78	6	0	5.276481	4.086199	-0.349111
79	1	0	4.719523	3.396946	-2.309208
80	1	0	5.529550	4.664820	1.711737
81	1	0	6.256878	4.432933	-0.657460
82	6	0	-2.662194	-0.781708	3.123083
83	6	0	-2.817921	-1.848192	3.954436
84	8	0	-3.803914	-0.598332	2.401386
85	6	0	-4.144075	-2.352500	3.731467
86	1	0	-2.075834	-2.228374	4.640850
87	6	0	-4.690786	-1.556941	2.779315
88	1	0	-4.619851	-3.191951	4.216026
89	1	0	-5.653298	-1.530317	2.292512

Me/Ph/Ph

TS5RR

Total energy= -2028.15521100
Sum of electronic and zero-point Energies= -2027.452810
Sum of electronic and thermal Energies= -2027.412445
Sum of electronic and thermal Enthalpies= -2027.411501
Sum of electronic and thermal Free Energies= -2027.525780

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.402101	-1.338936	-1.149110
2	6	0	4.786562	-1.149711	-1.163103

3	6	0	5.609054	-2.031657	-1.850536
4	6	0	5.029386	-3.116881	-2.509233
5	6	0	3.648779	-3.310232	-2.479378
6	6	0	2.818864	-2.415169	-1.802606
7	6	0	2.772324	-0.211578	-0.350087
8	6	0	3.942455	0.230304	0.562232
9	6	0	5.162164	0.061946	-0.340909
10	1	0	6.685464	-1.889467	-1.860732
11	1	0	5.659407	-3.821564	-3.042576
12	1	0	3.212556	-4.162890	-2.989313
13	1	0	1.743229	-2.550835	-1.801122
14	1	0	2.441502	0.602197	-0.999988
15	1	0	3.812351	1.237716	0.967567
16	1	0	5.283858	0.952533	-0.968644
17	6	0	1.739056	-0.917906	1.806718
18	6	0	3.028955	-0.687343	2.532841
19	6	0	0.329809	-0.803048	0.143823
20	1	0	3.187606	-1.474638	3.270555
21	1	0	6.070121	-0.068836	0.251895
22	7	0	1.619800	-0.603294	0.481572
23	7	0	0.609648	-1.350318	2.290380
24	7	0	-0.256851	-1.280807	1.245095
25	8	0	4.097440	-0.711706	1.620562
26	1	0	2.967440	0.282026	3.048452
27	6	0	-1.587769	-1.811543	1.392927
28	6	0	-1.977059	-2.869651	0.563182
29	6	0	-2.425383	-1.262846	2.374365
30	6	0	-3.286624	-3.333705	0.691016
31	6	0	-3.723266	-1.763257	2.448433
32	6	0	-4.177975	-2.781931	1.608641
33	1	0	-3.612619	-4.150538	0.052182
34	1	0	-4.398373	-1.344208	3.190528
35	6	0	-1.060473	-3.504015	-0.450967
36	1	0	-1.105239	-2.975347	-1.410649
37	1	0	-0.019137	-3.515739	-0.116953
38	1	0	-1.367301	-4.535633	-0.631481
39	6	0	-5.600023	-3.267502	1.702735
40	1	0	-5.884812	-3.445922	2.742884
41	1	0	-6.286972	-2.517510	1.298769
42	1	0	-5.741785	-4.192373	1.140683
43	6	0	-1.963144	-0.205197	3.340818
44	1	0	-1.354520	-0.654927	4.130717
45	1	0	-1.365149	0.557252	2.841198
46	1	0	-2.827343	0.273513	3.805249

47	6	0	-0.247204	-0.497710	-1.228904
48	8	0	0.571582	-0.480905	-2.153370
49	1	0	-2.279641	0.462202	-3.275121
50	6	0	-1.623325	-0.154990	-1.326828
51	6	0	-2.284189	-0.446457	-2.660101
52	1	0	-2.223081	-0.346003	-0.442402
53	1	0	-1.675826	-1.178044	-3.205158
54	6	0	-1.509998	1.835483	-1.338647
55	8	0	-0.971360	2.208138	-2.421951
56	6	0	-0.640445	2.019753	-0.076657
57	8	0	-0.981680	1.731416	1.067366
58	6	0	-3.000118	2.086090	-1.152977
59	6	0	-3.729790	1.753865	-0.002945
60	6	0	-3.671787	2.649971	-2.239408
61	6	0	-5.101278	1.982836	0.046777
62	1	0	-3.223149	1.306871	0.845328
63	6	0	-5.046959	2.868733	-2.191370
64	1	0	-3.090067	2.908235	-3.117598
65	6	0	-5.767149	2.535219	-1.047718
66	1	0	-5.655567	1.719231	0.942650
67	1	0	-5.554762	3.302874	-3.047396
68	1	0	-6.838740	2.704000	-1.006807
69	7	0	0.583387	2.501865	-0.420021
70	1	0	0.638199	2.683114	-1.423166
71	6	0	1.645407	2.875701	0.413286
72	6	0	2.765438	3.460166	-0.196972
73	6	0	1.638843	2.687037	1.802876
74	6	0	3.853240	3.863873	0.567227
75	1	0	2.771015	3.601178	-1.274332
76	6	0	2.736324	3.106526	2.555165
77	1	0	0.779732	2.235399	2.279479
78	6	0	3.845613	3.692779	1.951927
79	1	0	4.708728	4.316944	0.076763
80	1	0	2.715787	2.968186	3.632150
81	1	0	4.692936	4.010651	2.549360
82	6	0	-3.708889	-0.969330	-2.484185
83	1	0	-3.711726	-1.908008	-1.920037
84	1	0	-4.319869	-0.246246	-1.935122
85	1	0	-4.183174	-1.151160	-3.451930

TS5RS

Total energy= -2028.14807034

Sum of electronic and zero-point Energies= -2027.445991

Sum of electronic and thermal Energies= -2027.405638
Sum of electronic and thermal Enthalpies= -2027.404694
Sum of electronic and thermal Free Energies= -2027.518726

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.234617	-1.530420	0.691950
2	6	0	-4.596282	-1.452238	0.390398
3	6	0	-5.523668	-2.137230	1.163809
4	6	0	-5.066269	-2.910623	2.231106
5	6	0	-3.704651	-2.989467	2.522548
6	6	0	-2.771622	-2.288834	1.756351
7	6	0	-2.479210	-0.652915	-0.284327
8	6	0	-3.440141	-0.599978	-1.490769
9	6	0	-4.815461	-0.575241	-0.823775
10	1	0	-6.583572	-2.083783	0.933616
11	1	0	-5.777477	-3.461286	2.838556
12	1	0	-3.367780	-3.597245	3.355946
13	1	0	-1.713832	-2.321278	1.994823
14	1	0	-2.317404	0.337245	0.142502
15	1	0	-3.242375	0.250148	-2.154855
16	1	0	-5.062790	0.454725	-0.535384
17	6	0	-1.001243	-1.880295	-1.872448
18	6	0	-2.127521	-2.026647	-2.852353
19	6	0	0.035082	-1.059187	-0.139792
20	1	0	-2.125126	-3.030045	-3.279937
21	1	0	-5.586853	-0.941601	-1.504685
22	7	0	-1.173010	-1.162108	-0.723959
23	7	0	0.232138	-2.282802	-1.996199
24	7	0	0.863337	-1.769546	-0.906233
25	8	0	-3.361543	-1.826906	-2.210629
26	1	0	-1.975423	-1.297133	-3.660805
27	6	0	2.233330	-2.112441	-0.633107
28	6	0	3.215371	-1.741604	-1.559734
29	6	0	2.517036	-2.796412	0.552717
30	6	0	4.537315	-2.021871	-1.221437
31	6	0	3.858581	-3.051042	0.836452
32	6	0	4.879600	-2.659496	-0.027554
33	1	0	5.324586	-1.727803	-1.913398
34	1	0	4.107311	-3.572853	1.757394
35	6	0	2.873626	-1.064325	-2.860231
36	1	0	3.780487	-0.668540	-3.322369
37	1	0	2.416341	-1.774868	-3.555472

38	1	0	2.170383	-0.243993	-2.689682
39	6	0	6.324568	-2.932791	0.298412
40	1	0	6.909317	-2.010444	0.269336
41	1	0	6.430618	-3.374922	1.290479
42	1	0	6.761883	-3.621703	-0.430224
43	6	0	1.441115	-3.249911	1.508257
44	1	0	1.122697	-2.439373	2.173834
45	1	0	0.556921	-3.615882	0.977466
46	1	0	1.819389	-4.058381	2.134850
47	6	0	0.298845	-0.229241	1.101778
48	8	0	-0.676960	-0.110946	1.859159
49	1	0	1.056234	1.075134	3.143805
50	6	0	1.547462	0.440414	1.173365
51	6	0	1.948192	1.014498	2.509915
52	1	0	2.353647	-0.002922	0.594843
53	1	0	2.321273	2.039026	2.391096
54	6	0	3.029950	0.149455	3.172628
55	6	0	1.275162	1.814618	-0.337262
56	8	0	1.100133	1.178980	-1.421917
57	6	0	0.019903	2.479627	0.268203
58	8	0	-0.033810	3.042794	1.351442
59	6	0	2.593131	2.537132	-0.151431
60	6	0	2.740361	3.754717	0.518100
61	6	0	3.717990	1.947483	-0.741673
62	6	0	3.993779	4.365074	0.595153
63	1	0	1.880629	4.221532	0.982576
64	6	0	4.966061	2.548983	-0.651153
65	1	0	3.591578	1.006264	-1.268064
66	6	0	5.108695	3.765150	0.018674
67	1	0	4.093759	5.313467	1.113065
68	1	0	5.829607	2.073560	-1.107527
69	1	0	6.081580	4.239983	0.087952
70	7	0	-1.035826	2.323616	-0.584388
71	1	0	-0.756041	1.908713	-1.470178
72	6	0	-2.366200	2.730600	-0.396638
73	6	0	-3.163651	2.924085	-1.530489
74	6	0	-2.926362	2.864786	0.879237
75	6	0	-4.508861	3.248857	-1.391221
76	1	0	-2.721164	2.823629	-2.517473
77	6	0	-4.272792	3.196202	1.002711
78	1	0	-2.307934	2.696258	1.751147
79	6	0	-5.071424	3.389629	-0.123499
80	1	0	-5.116888	3.396570	-2.278865
81	1	0	-4.702833	3.296336	1.994177

82	1	0	-6.119827	3.646026	-0.015312
83	1	0	3.353643	0.577389	4.126229
84	1	0	2.664305	-0.869201	3.364030
85	1	0	3.911017	0.067166	2.520283

TS5SR

Total energy= -2028.13590684
Sum of electronic and zero-point Energies= -2027.433226
Sum of electronic and thermal Energies= -2027.392833
Sum of electronic and thermal Enthalpies= -2027.391889
Sum of electronic and thermal Free Energies= -2027.507100

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.990832	-1.840189	-0.031610
2	6	0	4.216893	-2.505698	-0.062804
3	6	0	5.281253	-1.966234	-0.772029
4	6	0	5.086534	-0.766763	-1.460205
5	6	0	3.847614	-0.126485	-1.444426
6	6	0	2.778528	-0.657509	-0.719990
7	6	0	2.030482	-2.625794	0.828940
8	6	0	2.617918	-4.053728	0.763247
9	6	0	4.128172	-3.799924	0.715307
10	1	0	6.239976	-2.474795	-0.808776
11	1	0	5.904647	-0.334750	-2.027828
12	1	0	3.718487	0.794214	-2.003974
13	1	0	1.805339	-0.171658	-0.715543
14	1	0	2.013659	-2.249437	1.851813
15	1	0	2.291737	-4.683694	1.600267
16	1	0	4.522761	-3.686064	1.730796
17	6	0	0.115073	-3.662878	-0.355276
18	6	0	0.896916	-4.921127	-0.584654
19	6	0	-0.329074	-1.669559	0.447494
20	1	0	0.699878	-5.299678	-1.588406
21	1	0	4.642225	-4.637925	0.239325
22	7	0	0.639384	-2.613748	0.341152
23	7	0	-1.121464	-3.433207	-0.688337
24	7	0	-1.385753	-2.199015	-0.184352
25	8	0	2.273310	-4.663502	-0.473701
26	1	0	0.570254	-5.674118	0.146967
27	6	0	-2.734866	-1.711953	-0.338429
28	6	0	-3.122027	-1.228616	-1.587509

29	6	0	-3.606523	-1.844101	0.745448
30	6	0	-4.432599	-0.765363	-1.701802
31	6	0	-4.898007	-1.349122	0.583290
32	6	0	-5.317852	-0.784282	-0.624098
33	1	0	-4.762809	-0.363595	-2.657058
34	1	0	-5.592875	-1.411787	1.416638
35	6	0	-2.164218	-1.209451	-2.746822
36	1	0	-1.275341	-0.626039	-2.486574
37	1	0	-1.851502	-2.225151	-3.006945
38	1	0	-2.637965	-0.760462	-3.622103
39	6	0	-6.691932	-0.184407	-0.758745
40	1	0	-7.101096	-0.350735	-1.757989
41	1	0	-7.383696	-0.600686	-0.023622
42	1	0	-6.642408	0.898059	-0.597814
43	6	0	-3.158258	-2.498885	2.023289
44	1	0	-2.790216	-3.511834	1.830438
45	1	0	-2.348732	-1.934097	2.495477
46	1	0	-3.984187	-2.560406	2.733409
47	6	0	-0.182463	-0.418666	1.325403
48	8	0	0.898515	-0.363622	1.933239
49	1	0	-0.383344	1.588727	3.024309
50	6	0	-1.225816	0.533584	1.370682
51	6	0	-1.372924	1.319470	2.653162
52	1	0	-2.154778	0.262831	0.881479
53	1	0	-1.901134	2.255680	2.451452
54	6	0	-2.140371	0.536824	3.724925
55	6	0	-0.600468	1.741433	-0.318648
56	8	0	-0.298993	0.969931	-1.268709
57	6	0	0.581839	2.477644	0.361209
58	8	0	0.529946	3.095528	1.414686
59	6	0	-1.889201	2.532859	-0.410044
60	6	0	-2.208445	3.642660	0.384085
61	6	0	-2.790624	2.135345	-1.402547
62	6	0	-3.421409	4.305672	0.205844
63	1	0	-1.503225	3.989330	1.129457
64	6	0	-4.004233	2.790912	-1.571682
65	1	0	-2.511569	1.308282	-2.043715
66	6	0	-4.328211	3.877928	-0.761134
67	1	0	-3.656632	5.164452	0.826936
68	1	0	-4.694612	2.458439	-2.342022
69	1	0	-5.273932	4.394847	-0.890936
70	7	0	1.686490	2.419622	-0.435655
71	1	0	1.522579	1.947614	-1.318807
72	6	0	2.906973	3.086175	-0.235489

73	6	0	3.654523	3.448762	-1.362190
74	6	0	3.397069	3.373126	1.042443
75	6	0	4.881774	4.083664	-1.214314
76	1	0	3.261019	3.238877	-2.353494
77	6	0	4.622030	4.021099	1.175538
78	1	0	2.818947	3.088495	1.910683
79	6	0	5.371156	4.377808	0.056786
80	1	0	5.451470	4.356232	-2.096903
81	1	0	4.997113	4.240167	2.170412
82	1	0	6.326853	4.877553	0.173783
83	1	0	-1.590253	-0.364222	4.017099
84	1	0	-2.290546	1.142790	4.623995
85	1	0	-3.125255	0.226916	3.358121

TS5SS

Total energy= -2028.14069684
Sum of electronic and zero-point Energies= -2027.438464
Sum of electronic and thermal Energies= -2027.398363
Sum of electronic and thermal Enthalpies= -2027.397419
Sum of electronic and thermal Free Energies= -2027.509221

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.447722	-1.343359	0.267000
2	6	0	4.683022	-1.995996	0.254798
3	6	0	5.856023	-1.276744	0.070428
4	6	0	5.772247	0.104151	-0.109624
5	6	0	4.535194	0.748323	-0.112802
6	6	0	3.354300	0.027636	0.077183
7	6	0	2.371742	-2.363995	0.569974
8	6	0	3.029558	-3.687216	0.114909
9	6	0	4.503750	-3.482047	0.462232
10	1	0	6.817914	-1.780863	0.056685
11	1	0	6.678865	0.682505	-0.258674
12	1	0	4.488086	1.821849	-0.261563
13	1	0	2.388065	0.521598	0.066330
14	1	0	2.160486	-2.385976	1.640057
15	1	0	2.572947	-4.568896	0.583025
16	1	0	4.687532	-3.765057	1.504626
17	6	0	0.710826	-2.993513	-1.167380
18	6	0	1.646033	-4.008351	-1.754464
19	6	0	-0.030817	-1.484984	0.235668

20	1	0	1.644720	-3.927431	-2.842548
21	1	0	5.138722	-4.099349	-0.177228
22	7	0	1.066979	-2.205061	-0.109321
23	7	0	-0.534260	-2.810279	-1.494771
24	7	0	-0.984943	-1.878887	-0.612215
25	8	0	2.955953	-3.788478	-1.300818
26	1	0	1.288078	-5.009641	-1.475140
27	6	0	-2.397101	-1.586028	-0.648129
28	6	0	-2.888566	-0.802765	-1.694154
29	6	0	-3.213238	-2.225177	0.288565
30	6	0	-4.267011	-0.611210	-1.741185
31	6	0	-4.582726	-1.977231	0.210881
32	6	0	-5.122810	-1.169678	-0.790620
33	1	0	-4.681158	0.004455	-2.535305
34	1	0	-5.242303	-2.442340	0.938900
35	6	0	-1.975744	-0.240847	-2.748490
36	1	0	-1.105092	0.236470	-2.292405
37	1	0	-1.624710	-1.038698	-3.411300
38	1	0	-2.508566	0.499260	-3.348705
39	6	0	-6.603414	-0.908952	-0.867131
40	1	0	-7.136758	-1.390822	-0.045450
41	1	0	-6.801390	0.166756	-0.824920
42	1	0	-7.016500	-1.280474	-1.809542
43	6	0	-2.636978	-3.148473	1.329049
44	1	0	-2.019601	-3.923958	0.863704
45	1	0	-2.007884	-2.604994	2.042349
46	1	0	-3.435998	-3.637745	1.887907
47	6	0	-0.051258	-0.550271	1.439213
48	8	0	1.055576	-0.431899	1.987465
49	1	0	-0.357548	0.962871	3.573153
50	6	0	-1.243356	0.103659	1.846036
51	6	0	-1.281894	0.435397	3.321821
52	1	0	-2.167560	-0.260003	1.412682
53	1	0	-2.089154	1.147584	3.511106
54	6	0	-1.443038	-0.799329	4.209255
55	6	0	-1.212325	2.057023	1.082384
56	8	0	-1.145205	2.825526	2.076272
57	6	0	0.054079	1.975914	0.195701
58	8	0	0.192123	1.214711	-0.760788
59	6	0	-2.517968	2.070631	0.300357
60	6	0	-2.567573	2.500520	-1.026870
61	6	0	-3.719435	1.872894	0.988273
62	6	0	-3.793704	2.730672	-1.651846
63	1	0	-1.647422	2.664021	-1.579176

64	6	0	-4.941331	2.089386	0.364127
65	1	0	-3.687747	1.561430	2.028599
66	6	0	-4.983238	2.530058	-0.959236
67	1	0	-3.813811	3.073611	-2.682286
68	1	0	-5.864452	1.927701	0.913302
69	1	0	-5.937558	2.711775	-1.444913
70	7	0	0.961675	2.896291	0.589876
71	1	0	0.674622	3.369860	1.444733
72	6	0	2.125256	3.323056	-0.072222
73	6	0	2.351102	3.074174	-1.431532
74	6	0	3.050425	4.077003	0.658172
75	6	0	3.492089	3.589943	-2.040169
76	1	0	1.639755	2.484263	-1.993163
77	6	0	4.186124	4.583359	0.037207
78	1	0	2.870243	4.263903	1.712743
79	6	0	4.413749	4.344060	-1.317351
80	1	0	3.659537	3.395532	-3.094853
81	1	0	4.893999	5.167639	0.616177
82	1	0	5.299669	4.740138	-1.801998
83	1	0	-0.623102	-1.505693	4.042251
84	1	0	-1.441562	-0.528150	5.269571
85	1	0	-2.385418	-1.316609	3.999056

Ph/4-MeC$_6$H$_4$/Ph

TS5RR

Total energy= -2259.12747002

Sum of electronic and zero-point Energies= -2258.342699

Sum of electronic and thermal Energies= -2258.298340

Sum of electronic and thermal Enthalpies= -2258.297395

Sum of electronic and thermal Free Energies= -2258.418729

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.739502	-1.769268	-0.831337
2	6	0	5.129446	-1.759947	-0.971572
3	6	0	5.792213	-2.878662	-1.458082
4	6	0	5.046612	-4.012381	-1.785049
5	6	0	3.661034	-4.021863	-1.627084
6	6	0	2.991646	-2.892719	-1.152900
7	6	0	3.299336	-0.411410	-0.315499
8	6	0	4.580479	0.103333	0.382849
9	6	0	5.695994	-0.436243	-0.510902

10	1	0	6.872608	-2.877826	-1.566462
11	1	0	5.550806	-4.898646	-2.156960
12	1	0	3.096338	-4.913654	-1.878051
13	1	0	1.912008	-2.891099	-1.050297
14	1	0	2.997668	0.247127	-1.133356
15	1	0	4.589196	1.189320	0.511301
16	1	0	5.855942	0.247387	-1.352867
17	6	0	2.382829	-0.445352	2.002696
18	6	0	3.740628	-0.166705	2.570472
19	6	0	0.863700	-0.612721	0.446592
20	1	0	3.888326	-0.742035	3.485112
21	1	0	6.631894	-0.522901	0.045262
22	7	0	2.186604	-0.452006	0.650657
23	7	0	1.264933	-0.645706	2.641953
24	7	0	0.329839	-0.755898	1.662754
25	8	0	4.727709	-0.544966	1.643720
26	1	0	3.804752	0.905864	2.805636
27	6	0	-1.028600	-1.098688	1.992304
28	6	0	-1.560370	-2.273291	1.447413
29	6	0	-1.762045	-0.236767	2.818661
30	6	0	-2.911713	-2.529266	1.676334
31	6	0	-3.106499	-0.546075	3.012349
32	6	0	-3.702784	-1.669058	2.434347
33	1	0	-3.357617	-3.414053	1.230192
34	1	0	-3.706762	0.116615	3.631502
35	6	0	-0.741502	-3.236270	0.626428
36	1	0	-0.718889	-2.940575	-0.428689
37	1	0	0.289206	-3.308260	0.987061
38	1	0	-1.188485	-4.231078	0.671603
39	6	0	-5.166323	-1.947246	2.651477
40	1	0	-5.371769	-2.147935	3.707395
41	1	0	-5.769244	-1.083056	2.357558
42	1	0	-5.493296	-2.806814	2.063349
43	6	0	-1.148098	0.959663	3.495976
44	1	0	-0.570570	0.644378	4.370029
45	1	0	-0.480271	1.500008	2.824522
46	1	0	-1.934646	1.638369	3.832406
47	6	0	0.207095	-0.565066	-0.923391
48	8	0	0.954168	-0.818540	-1.873369
49	1	0	-2.255681	0.210276	-2.831736
50	6	0	-1.142021	-0.114534	-1.012865
51	6	0	-1.921759	-0.631424	-2.212512
52	1	0	-1.690760	-0.078379	-0.079077
53	1	0	-1.243951	-1.222096	-2.836378

54	6	0	-3.107618	-1.468550	-1.789829
55	6	0	-3.110160	-2.856420	-1.947418
56	6	0	-4.228049	-0.860156	-1.210816
57	6	0	-4.197149	-3.624274	-1.529779
58	1	0	-2.253393	-3.340993	-2.409915
59	6	0	-5.314058	-1.622568	-0.792404
60	1	0	-4.244023	0.221242	-1.090828
61	6	0	-5.302658	-3.009061	-0.948106
62	1	0	-4.180554	-4.701718	-1.664510
63	1	0	-6.175726	-1.133431	-0.346819
64	1	0	-6.152634	-3.602777	-0.625217
65	6	0	-0.900223	1.802145	-1.451387
66	8	0	-0.514811	1.889374	-2.655400
67	6	0	0.165812	2.165347	-0.392383
68	8	0	-0.019395	2.176593	0.822164
69	6	0	-2.319750	2.241132	-1.115600
70	6	0	-2.883063	2.227686	0.165790
71	6	0	-3.120517	2.640031	-2.189107
72	6	0	-4.211273	2.597468	0.354993
73	1	0	-2.284297	1.915024	1.013697
74	6	0	-4.450245	2.999272	-1.994006
75	1	0	-2.673488	2.657552	-3.177704
76	6	0	-5.020441	2.982355	-0.717827
77	1	0	-4.632270	2.572521	1.357528
78	1	0	-5.057538	3.296946	-2.845598
79	7	0	1.355793	2.423471	-0.993587
80	1	0	1.277508	2.352260	-2.008915
81	6	0	2.553633	2.861971	-0.413058
82	6	0	3.646071	3.066334	-1.268982
83	6	0	2.700547	3.104463	0.960443
84	6	0	4.859272	3.520241	-0.766418
85	1	0	3.531831	2.873664	-2.332226
86	6	0	3.923758	3.567722	1.446227
87	1	0	1.862762	2.947863	1.625384
88	6	0	5.006391	3.778390	0.596780
89	1	0	5.690991	3.675444	-1.446090
90	1	0	4.023221	3.765529	2.509374
91	1	0	5.951561	4.137804	0.988572
92	6	0	-6.464086	3.366639	-0.516474
93	1	0	-6.642899	4.400887	-0.837710
94	1	0	-7.126275	2.721930	-1.108129
95	1	0	-6.753073	3.281359	0.536602

TS5RS

Total energy= -2259.12174083
Sum of electronic and zero-point Energies= -2258.337111
Sum of electronic and thermal Energies= -2258.292553
Sum of electronic and thermal Enthalpies= -2258.291609
Sum of electronic and thermal Free Energies= -2258.413642

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.827175	-1.451430	-0.664237
2	6	0	5.198313	-1.230948	-0.509152
3	6	0	6.108335	-1.897464	-1.317936
4	6	0	5.626539	-2.795505	-2.272447
5	6	0	4.256868	-3.015888	-2.416114
6	6	0	3.338704	-2.335332	-1.614494
7	6	0	3.091120	-0.553170	0.307594
8	6	0	4.150473	-0.314559	1.402764
9	6	0	5.449517	-0.235301	0.602744
10	1	0	7.175632	-1.734560	-1.201658
11	1	0	6.325598	-3.332611	-2.905609
12	1	0	3.899871	-3.719877	-3.160701
13	1	0	2.270705	-2.479472	-1.738860
14	1	0	2.803549	0.377494	-0.181824
15	1	0	3.937217	0.571026	2.015659
16	1	0	5.572845	0.780979	0.206191
17	6	0	1.872717	-1.722144	2.142174
18	6	0	3.104169	-1.726036	2.998942
19	6	0	0.609538	-1.092547	0.482663
20	1	0	3.227839	-2.697337	3.479440
21	1	0	6.312316	-0.474290	1.228319
22	7	0	1.880185	-1.108859	0.922823
23	7	0	0.677782	-2.145841	2.446841
24	7	0	-0.096134	-1.751813	1.401121
25	8	0	4.248325	-1.478029	2.219758
26	1	0	2.976937	-0.960676	3.777820
27	6	0	-1.494273	-2.089441	1.352048
28	6	0	-2.332549	-1.598587	2.362523
29	6	0	-1.958561	-2.842109	0.269054
30	6	0	-3.698178	-1.825647	2.211435
31	6	0	-3.336278	-3.040301	0.173959
32	6	0	-4.219592	-2.521631	1.117661
33	1	0	-4.376375	-1.434429	2.966341
34	1	0	-3.724964	-3.594505	-0.675876

35	6	0	-1.799395	-0.842520	3.550189
36	1	0	-2.626378	-0.395033	4.105841
37	1	0	-1.253972	-1.510122	4.222521
38	1	0	-1.120868	-0.050173	3.221091
39	6	0	-5.706144	-2.715586	0.978087
40	1	0	-6.225277	-1.754084	1.029994
41	1	0	-5.953131	-3.183999	0.023279
42	1	0	-6.095158	-3.344364	1.784915
43	6	0	-1.040751	-3.407856	-0.783976
44	1	0	-0.810872	-2.663985	-1.554531
45	1	0	-0.096777	-3.759941	-0.357722
46	1	0	-1.525913	-4.249332	-1.281940
47	6	0	0.172956	-0.394642	-0.789207
48	8	0	1.034060	-0.339864	-1.678556
49	1	0	-0.955898	0.432662	-2.888761
50	6	0	-1.096182	0.241960	-0.765016
51	6	0	-1.696770	0.619806	-2.106131
52	1	0	-1.805978	-0.145264	-0.042955
53	1	0	-1.935405	1.687261	-2.136522
54	6	0	-2.951112	-0.191833	-2.338570
55	6	0	-4.150020	0.194762	-1.728911
56	6	0	-2.931090	-1.368846	-3.090682
57	6	0	-5.296892	-0.582616	-1.859392
58	1	0	-4.174591	1.114139	-1.145900
59	6	0	-4.078427	-2.149405	-3.224767
60	1	0	-2.007553	-1.672697	-3.578507
61	6	0	-5.264083	-1.761064	-2.605149
62	1	0	-6.219935	-0.267846	-1.380614
63	1	0	-4.046385	-3.060175	-3.815577
64	1	0	-6.159274	-2.367139	-2.708004
65	6	0	-0.688274	1.771332	0.521462
66	8	0	-0.331799	1.260828	1.630137
67	6	0	0.440764	2.416179	-0.313536
68	8	0	0.328229	2.848870	-1.451780
69	6	0	-2.054850	2.416770	0.450361
70	6	0	-2.414577	3.450041	-0.417053
71	6	0	-3.019865	1.927838	1.341066
72	6	0	-3.711493	3.967234	-0.395476
73	1	0	-1.684731	3.849479	-1.111539
74	6	0	-4.307913	2.439803	1.350729
75	1	0	-2.735949	1.128429	2.017905
76	6	0	-4.678643	3.472337	0.478331
77	1	0	-3.973132	4.772830	-1.076694
78	1	0	-5.042958	2.036934	2.043984

79	7	0	1.601794	2.406305	0.404904
80	1	0	1.461106	2.089135	1.361200
81	6	0	2.877930	2.816451	-0.015096
82	6	0	3.793010	3.248536	0.951402
83	6	0	3.274180	2.716711	-1.354112
84	6	0	5.091256	3.585414	0.581558
85	1	0	3.478093	3.322214	1.988788
86	6	0	4.574200	3.063917	-1.710647
87	1	0	2.566133	2.356306	-2.089894
88	6	0	5.487750	3.498888	-0.751847
89	1	0	5.792102	3.920689	1.339424
90	1	0	4.876612	2.982057	-2.749754
91	1	0	6.499289	3.764583	-1.039651
92	6	0	-6.079808	4.026345	0.499499
93	1	0	-6.311050	4.467914	1.477299
94	1	0	-6.211553	4.799417	-0.264318
95	1	0	-6.816447	3.233884	0.317329

TS5SR

Total energy= -2259.10877490
Sum of electronic and zero-point Energies= -2258.325556
Sum of electronic and thermal Energies= -2258.280967
Sum of electronic and thermal Enthalpies= -2258.280023
Sum of electronic and thermal Free Energies= -2258.404701

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.606104	-1.540822	-0.085180
2	6	0	4.892297	-2.075597	0.000813
3	6	0	5.971292	-1.378021	-0.524135
4	6	0	5.733845	-0.153857	-1.152829
5	6	0	4.440036	0.355802	-1.257610
6	6	0	3.353501	-0.333795	-0.715120
7	6	0	2.637296	-2.489937	0.578494
8	6	0	3.383977	-3.841092	0.490715
9	6	0	4.849964	-3.432251	0.668123
10	1	0	6.976530	-1.784578	-0.466901
11	1	0	6.563682	0.399832	-1.580518
12	1	0	4.281200	1.298501	-1.770688
13	1	0	2.341464	0.053391	-0.811656
14	1	0	2.447093	-2.210769	1.614483
15	1	0	3.025421	-4.570429	1.227737

16	1	0	5.093109	-3.363552	1.734158
17	6	0	1.015579	-3.608092	-0.928244
18	6	0	1.953590	-4.759173	-1.133146
19	6	0	0.260880	-1.740464	-0.061447
20	1	0	1.927502	-5.073741	-2.177077
21	1	0	5.512750	-4.170879	0.211963
22	7	0	1.328767	-2.575395	-0.094003
23	7	0	-0.183707	-3.470494	-1.414860
24	7	0	-0.641063	-2.313451	-0.868982
25	8	0	3.267800	-4.372433	-0.822541
26	1	0	1.623566	-5.597518	-0.503120
27	6	0	-2.003196	-1.941803	-1.166030
28	6	0	-2.273893	-1.374065	-2.411293
29	6	0	-2.985313	-2.245771	-0.220445
30	6	0	-3.598324	-1.019454	-2.664052
31	6	0	-4.289349	-1.856265	-0.519031
32	6	0	-4.608100	-1.222822	-1.722060
33	1	0	-3.841672	-0.556460	-3.617776
34	1	0	-5.071104	-2.051681	0.210462
35	6	0	-1.180678	-1.142568	-3.418087
36	1	0	-0.435734	-0.453215	-3.006591
37	1	0	-0.680935	-2.081297	-3.674712
38	1	0	-1.593858	-0.711110	-4.331919
39	6	0	-6.008717	-0.740905	-1.992047
40	1	0	-6.259786	-0.824935	-3.051995
41	1	0	-6.743504	-1.304176	-1.412928
42	1	0	-6.100917	0.314804	-1.713181
43	6	0	-2.642167	-2.952434	1.061590
44	1	0	-2.073641	-3.866919	0.863406
45	1	0	-2.043445	-2.311824	1.718408
46	1	0	-3.550105	-3.214334	1.606362
47	6	0	0.147059	-0.561327	0.911459
48	8	0	1.089099	-0.485027	1.715098
49	1	0	-0.542872	1.121832	2.753721
50	6	0	-0.961641	0.313203	0.820694
51	6	0	-1.413220	0.958149	2.116973
52	1	0	-1.762113	0.014486	0.153284
53	1	0	-1.858937	1.935716	1.915983
54	6	0	-2.431998	0.087485	2.817869
55	6	0	-3.748050	0.028362	2.346896
56	6	0	-2.076161	-0.708702	3.909754
57	6	0	-4.685729	-0.802439	2.953578
58	1	0	-4.030973	0.638009	1.489864
59	6	0	-3.010727	-1.546164	4.517278

60	1	0	-1.054218	-0.672144	4.278955
61	6	0	-4.318937	-1.595108	4.041441
62	1	0	-5.705166	-0.831993	2.579211
63	1	0	-2.718087	-2.156884	5.366069
64	1	0	-5.049359	-2.243498	4.515112
65	6	0	-0.211744	1.732581	-0.601553
66	8	0	0.275523	1.100742	-1.578362
67	6	0	0.805781	2.451670	0.320172
68	8	0	0.569372	2.898437	1.433592
69	6	0	-1.536484	2.440120	-0.779600
70	6	0	-2.004796	3.477347	0.035127
71	6	0	-2.329417	2.034770	-1.858435
72	6	0	-3.248388	4.057191	-0.208907
73	1	0	-1.397463	3.832076	0.859575
74	6	0	-3.572288	2.607977	-2.088062
75	1	0	-1.946572	1.260628	-2.513021
76	6	0	-4.057009	3.629684	-1.263144
77	1	0	-3.596436	4.858758	0.437617
78	1	0	-4.177094	2.264586	-2.924994
79	7	0	1.999209	2.592316	-0.321655
80	1	0	1.994067	2.230500	-1.269691
81	6	0	3.131729	3.283782	0.141117
82	6	0	3.997348	3.844385	-0.805099
83	6	0	3.424511	3.400741	1.503619
84	6	0	5.148344	4.506640	-0.395454
85	1	0	3.757305	3.763315	-1.862078
86	6	0	4.574312	4.077893	1.900156
87	1	0	2.754184	2.963872	2.231013
88	6	0	5.441501	4.631062	0.961103
89	1	0	5.812903	4.933009	-1.140039
90	1	0	4.795654	4.165227	2.959306
91	1	0	6.336395	5.153718	1.281864
92	6	0	-5.393573	4.270975	-1.532605
93	1	0	-5.302248	5.058228	-2.288399
94	1	0	-6.113460	3.539272	-1.908629
95	1	0	-5.804204	4.726266	-0.628579

TS5SS

Total energy= -2259.11325616
Sum of electronic and zero-point Energies= -2258.328920
Sum of electronic and thermal Energies= -2258.284293
Sum of electronic and thermal Enthalpies= -2258.283349
Sum of electronic and thermal Free Energies= -2258.405277

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.762612	-1.400644	-0.117112
2	6	0	4.959468	-2.112858	-0.231338
3	6	0	6.175447	-1.484132	-0.001706
4	6	0	6.174457	-0.130535	0.336158
5	6	0	4.977749	0.579187	0.434976
6	6	0	3.752548	-0.052541	0.209702
7	6	0	2.614319	-2.361477	-0.333376
8	6	0	3.270264	-3.486767	-1.165804
9	6	0	4.691380	-3.551739	-0.607684
10	1	0	7.108469	-2.032531	-0.091985
11	1	0	7.116039	0.378932	0.516067
12	1	0	4.997892	1.632802	0.692405
13	1	0	2.816728	0.493511	0.278385
14	1	0	2.257126	-2.745227	0.623443
15	1	0	2.716716	-4.432660	-1.105981
16	1	0	4.719916	-4.205715	0.270811
17	6	0	1.165082	-2.205889	-2.346938
18	6	0	2.136844	-3.003978	-3.163914
19	6	0	0.308833	-1.234960	-0.582160
20	1	0	2.281220	-2.529598	-4.135894
21	1	0	5.380989	-3.950999	-1.354748
22	7	0	1.419153	-1.859966	-1.048595
23	7	0	-0.031534	-1.844719	-2.707415
24	7	0	-0.554426	-1.253741	-1.600934
25	8	0	3.382003	-3.067533	-2.519208
26	1	0	1.714277	-4.006362	-3.321472
27	6	0	-1.953649	-0.908947	-1.629134
28	6	0	-2.347749	0.230738	-2.328651
29	6	0	-2.845894	-1.797053	-1.020190
30	6	0	-3.711363	0.519914	-2.338642
31	6	0	-4.193518	-1.443533	-1.034956
32	6	0	-4.638808	-0.284025	-1.674936
33	1	0	-4.052616	1.403728	-2.871925
34	1	0	-4.911145	-2.098580	-0.546774
35	6	0	-1.346395	1.066122	-3.077158
36	1	0	-0.493086	1.309931	-2.438539
37	1	0	-0.975961	0.520128	-3.951027
38	1	0	-1.807892	1.994906	-3.417234
39	6	0	-6.093252	0.102413	-1.645252
40	1	0	-6.731012	-0.757439	-1.429339

41	1	0	-6.266349	0.853770	-0.866441
42	1	0	-6.406401	0.538630	-2.597487
43	6	0	-2.368954	-3.072006	-0.378336
44	1	0	-1.719290	-3.633070	-1.058404
45	1	0	-1.810751	-2.873295	0.543867
46	1	0	-3.218297	-3.702175	-0.111144
47	6	0	0.161218	-0.771340	0.862231
48	8	0	1.167809	-0.990332	1.554515
49	1	0	-0.413323	-0.396327	3.330363
50	6	0	-1.036694	-0.151105	1.306338
51	6	0	-1.351364	-0.397138	2.769794
52	1	0	-1.886972	-0.213257	0.638756
53	1	0	-1.953146	0.424681	3.166361
54	6	0	-2.067608	-1.716243	2.929912
55	6	0	-3.433719	-1.817050	2.642851
56	6	0	-1.371920	-2.877243	3.278998
57	6	0	-4.087225	-3.044399	2.700336
58	1	0	-3.983207	-0.922666	2.355045
59	6	0	-2.022128	-4.109159	3.334825
60	1	0	-0.308928	-2.809295	3.496389
61	6	0	-3.381917	-4.197341	3.045212
62	1	0	-5.148129	-3.102988	2.474502
63	1	0	-1.466020	-5.000776	3.608545
64	1	0	-3.889779	-5.155535	3.091066
65	6	0	-0.772519	1.940163	1.361485
66	8	0	-0.756065	2.267228	2.575057
67	6	0	0.569413	2.040867	0.598838
68	8	0	0.758775	1.628656	-0.544670
69	6	0	-1.986279	2.353157	0.546168
70	6	0	-1.884108	3.102312	-0.626432
71	6	0	-3.258272	2.139940	1.087017
72	6	0	-3.025709	3.604076	-1.248737
73	1	0	-0.910302	3.300276	-1.062211
74	6	0	-4.394648	2.623531	0.452433
75	1	0	-3.349305	1.606081	2.028211
76	6	0	-4.298630	3.362403	-0.731717
77	1	0	-2.923002	4.192384	-2.158231
78	1	0	-5.373132	2.445549	0.892763
79	7	0	1.483053	2.698649	1.347386
80	1	0	1.142447	2.883000	2.288988
81	6	0	2.731893	3.214119	0.961820
82	6	0	3.115143	3.340230	-0.379059
83	6	0	3.588793	3.662644	1.973691
84	6	0	4.344902	3.915801	-0.686455

85	1	0	2.455701	2.986371	-1.159304
86	6	0	4.814040	4.233237	1.650479
87	1	0	3.287094	3.560777	3.012021
88	6	0	5.200298	4.363792	0.317228
89	1	0	4.634970	4.010981	-1.728096
90	1	0	5.468140	4.576284	2.445566
91	1	0	6.156905	4.808890	0.065271
92	6	0	-5.530790	3.855436	-1.444388
93	1	0	-6.380679	3.932381	-0.761716
94	1	0	-5.362441	4.834662	-1.899788
95	1	0	-5.816901	3.166234	-2.248233

Ph/Me/Ph
TS5RR

Total energy= -2028.15623447
Sum of electronic and zero-point Energies= -2027.453352
Sum of electronic and thermal Energies= -2027.413474
Sum of electronic and thermal Enthalpies= -2027.412530
Sum of electronic and thermal Free Energies= -2027.524162

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.713534	2.347772	-0.214978
2	6	0	-4.058377	2.724172	-0.171782
3	6	0	-4.418828	4.058144	-0.304922
4	6	0	-3.413994	5.013473	-0.464007
5	6	0	-2.072351	4.634621	-0.491389
6	6	0	-1.709127	3.292090	-0.373703
7	6	0	-2.632982	0.837154	-0.075755
8	6	0	-3.959176	0.508705	0.653041
9	6	0	-4.938168	1.516173	0.053425
10	1	0	-5.462786	4.354840	-0.268911
11	1	0	-3.678361	6.061848	-0.558778
12	1	0	-1.301898	5.389434	-0.609267
13	1	0	-0.667928	2.993211	-0.419942
14	1	0	-2.578510	0.350365	-1.052761
15	1	0	-4.262416	-0.536395	0.543853
16	1	0	-5.337948	1.126951	-0.890296
17	6	0	-1.598347	0.057986	2.055956
18	6	0	-2.939815	0.009170	2.719845
19	6	0	-0.195991	0.199942	0.391376
20	1	0	-2.859645	0.361794	3.748704

21	1	0	-5.773457	1.697077	0.733520
22	7	0	-1.494766	0.346010	0.723385
23	7	0	-0.431850	-0.202274	2.574118
24	7	0	0.433241	-0.101646	1.529372
25	8	0	-3.837251	0.844899	2.032838
26	1	0	-3.288830	-1.033870	2.722576
27	6	0	1.852814	-0.153635	1.773720
28	6	0	2.613788	0.986902	1.489995
29	6	0	2.400873	-1.330305	2.297955
30	6	0	3.989795	0.901577	1.694494
31	6	0	3.781897	-1.355497	2.481090
32	6	0	4.591384	-0.259596	2.175261
33	1	0	4.606014	1.763391	1.453005
34	1	0	4.236564	-2.262606	2.872084
35	6	0	2.006596	2.267736	0.978643
36	1	0	1.855447	2.231848	-0.106599
37	1	0	1.043634	2.481254	1.453491
38	1	0	2.678348	3.103026	1.183681
39	6	0	6.080383	-0.328829	2.388008
40	1	0	6.320567	-0.299535	3.455606
41	1	0	6.487687	-1.260494	1.985804
42	1	0	6.585484	0.506617	1.899061
43	6	0	1.550651	-2.516430	2.665904
44	1	0	1.028454	-2.333182	3.609614
45	1	0	0.802960	-2.718690	1.897121
46	1	0	2.179274	-3.400248	2.789153
47	6	0	0.349290	0.345239	-1.016180
48	8	0	-0.331556	1.048160	-1.772896
49	1	0	2.439708	-0.500443	-3.319042
50	6	0	1.497712	-0.410281	-1.371488
51	6	0	2.355928	0.191859	-2.472266
52	1	0	2.035511	-0.874219	-0.550770
53	1	0	1.846138	1.078425	-2.861401
54	6	0	3.727111	0.568553	-1.956187
55	6	0	4.122159	1.904829	-1.858590
56	6	0	4.626030	-0.421134	-1.541758
57	6	0	5.381143	2.247498	-1.366246
58	1	0	3.436519	2.685792	-2.178974
59	6	0	5.883606	-0.085719	-1.051687
60	1	0	4.331644	-1.466889	-1.600159
61	6	0	6.267820	1.252339	-0.964111
62	1	0	5.669341	3.292579	-1.303161
63	1	0	6.567494	-0.868861	-0.737294
64	1	0	7.251132	1.515286	-0.585761

65	6	0	0.656379	-1.980955	-2.279795
66	8	0	0.186120	-1.599336	-3.386428
67	6	0	-0.365998	-2.342263	-1.183902
68	8	0	-0.061604	-2.805113	-0.087701
69	7	0	-1.630582	-2.065634	-1.598497
70	1	0	-1.631180	-1.717482	-2.558105
71	6	0	-2.845431	-2.360254	-0.966326
72	6	0	-4.025414	-2.088400	-1.674244
73	6	0	-2.924912	-2.899582	0.325452
74	6	0	-5.264129	-2.364625	-1.108713
75	1	0	-3.960959	-1.665029	-2.673019
76	6	0	-4.176857	-3.177985	0.874071
77	1	0	-2.017528	-3.111246	0.874265
78	6	0	-5.349166	-2.915309	0.170379
79	1	0	-6.165923	-2.148545	-1.672468
80	1	0	-4.228903	-3.606824	1.870459
81	1	0	-6.315837	-3.133268	0.610989
82	6	0	1.857210	-2.923460	-2.253564
83	1	0	2.642497	-2.550024	-2.911924
84	1	0	2.245338	-3.070545	-1.245757
85	1	0	1.524543	-3.889462	-2.645899

TS5RS

Total energy= -2028.15188111

Sum of electronic and zero-point Energies= -2027.449745

Sum of electronic and thermal Energies= -2027.409458

Sum of electronic and thermal Enthalpies= -2027.408514

Sum of electronic and thermal Free Energies= -2027.522034

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.634926	-1.880254	0.806420
2	6	0	-3.990513	-2.215337	0.775480
3	6	0	-4.513550	-3.093613	1.715107
4	6	0	-3.658061	-3.638038	2.674762
5	6	0	-2.304341	-3.303006	2.695384
6	6	0	-1.779215	-2.408966	1.760492
7	6	0	-2.364306	-0.875198	-0.294889
8	6	0	-3.511117	-1.160307	-1.288700
9	6	0	-4.681944	-1.505210	-0.367826
10	1	0	-5.565387	-3.362713	1.696773
11	1	0	-4.049872	-4.334259	3.409382

12	1	0	-1.653040	-3.736942	3.446972
13	1	0	-0.734311	-2.118783	1.786695
14	1	0	-2.411217	0.141131	0.098297
15	1	0	-3.701925	-0.323621	-1.973485
16	1	0	-5.166066	-0.581242	-0.027364
17	6	0	-0.914676	-1.746099	-2.131895
18	6	0	-2.116166	-2.227190	-2.887429
19	6	0	0.143673	-0.583812	-0.626429
20	1	0	-1.921631	-3.207454	-3.323909
21	1	0	-5.422155	-2.115474	-0.889772
22	7	0	-1.074308	-1.026477	-0.980863
23	7	0	0.343149	-1.830397	-2.465084
24	7	0	0.989618	-1.108337	-1.510319
25	8	0	-3.218509	-2.346239	-2.021179
26	1	0	-2.320125	-1.513136	-3.698220
27	6	0	2.425560	-1.111078	-1.408670
28	6	0	3.176357	-0.473035	-2.398836
29	6	0	2.989754	-1.705244	-0.272747
30	6	0	4.554111	-0.397090	-2.192052
31	6	0	4.368021	-1.595592	-0.117552
32	6	0	5.161693	-0.935780	-1.057364
33	1	0	5.163872	0.112278	-2.934299
34	1	0	4.829921	-2.020872	0.769786
35	6	0	2.524362	0.140054	-3.607712
36	1	0	3.245400	0.751183	-4.153649
37	1	0	2.154646	-0.637981	-4.282683
38	1	0	1.671658	0.760707	-3.310780
39	6	0	6.650310	-0.837768	-0.851608
40	1	0	7.084774	-0.041279	-1.465802
41	1	0	6.877380	-0.635463	0.201814
42	1	0	7.140339	-1.782068	-1.124882
43	6	0	2.159139	-2.430983	0.755191
44	1	0	1.681900	-1.731854	1.450135
45	1	0	1.376335	-3.037880	0.288509
46	1	0	2.795532	-3.090376	1.347402
47	6	0	0.418959	0.378338	0.507204
48	8	0	-0.335945	0.278862	1.488303
49	1	0	1.110943	2.223893	2.183249
50	6	0	1.393633	1.372881	0.247199
51	6	0	1.918631	2.121920	1.454353
52	1	0	2.142820	1.123056	-0.497057
53	1	0	2.242511	3.128417	1.179055
54	6	0	3.087582	1.361800	2.044527
55	6	0	4.400456	1.683364	1.693345

56	6	0	2.870265	0.275310	2.898706
57	6	0	5.473987	0.945519	2.187924
58	1	0	4.581596	2.522598	1.025444
59	6	0	3.938689	-0.473975	3.384338
60	1	0	1.848214	0.021845	3.173269
61	6	0	5.246445	-0.138695	3.033313
62	1	0	6.489119	1.219094	1.915326
63	1	0	3.751610	-1.314229	4.046755
64	1	0	6.081353	-0.716084	3.418594
65	6	0	0.383640	2.494580	-1.181396
66	8	0	0.095774	1.744789	-2.159157
67	6	0	-0.775784	2.902396	-0.253386
68	8	0	-0.653314	3.614586	0.732552
69	6	0	1.426641	3.582827	-1.367898
70	7	0	-1.946788	2.364458	-0.701977
71	1	0	-1.842451	1.922955	-1.612382
72	6	0	-3.216595	2.448593	-0.109604
73	6	0	-4.345137	2.321206	-0.926847
74	6	0	-3.369945	2.577014	1.275510
75	6	0	-5.617745	2.322436	-0.364293
76	1	0	-4.218189	2.235147	-2.002745
77	6	0	-4.649276	2.586492	1.822742
78	1	0	-2.490230	2.656170	1.901096
79	6	0	-5.776626	2.457189	1.013488
80	1	0	-6.485995	2.224897	-1.008344
81	1	0	-4.762974	2.684776	2.897702
82	1	0	-6.768914	2.461800	1.451635
83	1	0	2.372844	3.147520	-1.698616
84	1	0	1.059226	4.241629	-2.162359
85	1	0	1.574844	4.177992	-0.468125

TS5SR

Total energy= -2028.14242663
Sum of electronic and zero-point Energies= -2027.440493
Sum of electronic and thermal Energies= -2027.400019
Sum of electronic and thermal Enthalpies= -2027.399074
Sum of electronic and thermal Free Energies= -2027.515315

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.490422	2.357596	0.526775
2	6	0	-3.405921	3.350419	0.877075

3	6	0	-4.758499	3.174303	0.616298
4	6	0	-5.171993	1.994646	-0.004137
5	6	0	-4.246549	1.014002	-0.362187
6	6	0	-2.887231	1.186003	-0.097133
7	6	0	-1.114186	2.779202	0.981694
8	6	0	-1.246126	4.317902	1.079231
9	6	0	-2.697353	4.519355	1.522176
10	1	0	-5.479193	3.942456	0.880435
11	1	0	-6.224932	1.840655	-0.217709
12	1	0	-4.593039	0.104707	-0.842685
13	1	0	-2.154408	0.438063	-0.383750
14	1	0	-0.875023	2.341433	1.951918
15	1	0	-0.503961	4.761135	1.755030
16	1	0	-2.767600	4.473639	2.614381
17	6	0	0.622759	3.358831	-0.701821
18	6	0	0.168986	4.787084	-0.734752
19	6	0	0.678585	1.264178	-0.069510
20	1	0	0.155097	5.145593	-1.764934
21	1	0	-3.064083	5.495118	1.195746
22	7	0	-0.000661	2.426466	0.077888
23	7	0	1.655854	2.850276	-1.308378
24	7	0	1.682316	1.553617	-0.904035
25	8	0	-1.132485	4.890030	-0.216464
26	1	0	0.879862	5.395806	-0.158166
27	6	0	2.839867	0.771386	-1.266182
28	6	0	2.960261	0.330330	-2.583919
29	6	0	3.813356	0.558704	-0.282832
30	6	0	4.094680	-0.423108	-2.893630
31	6	0	4.918322	-0.206655	-0.645645
32	6	0	5.068415	-0.715114	-1.938803
33	1	0	4.212729	-0.793206	-3.908757
34	1	0	5.681155	-0.406386	0.103037
35	6	0	1.907106	0.639932	-3.611850
36	1	0	0.926293	0.300810	-3.259453
37	1	0	1.852738	1.717000	-3.797034
38	1	0	2.141208	0.139879	-4.553460
39	6	0	6.261450	-1.567199	-2.284578
40	1	0	6.379488	-1.665696	-3.365350
41	1	0	7.179971	-1.142571	-1.871833
42	1	0	6.148026	-2.571890	-1.865242
43	6	0	3.669265	1.108940	1.110475
44	1	0	3.341712	2.153252	1.093924
45	1	0	2.945517	0.527338	1.694354
46	1	0	4.624023	1.054100	1.635755

47	6	0	0.364918	-0.013336	0.706093
48	8	0	-0.454837	0.141331	1.623604
49	1	0	0.110586	-2.380643	1.884238
50	6	0	0.965584	-1.223821	0.289138
51	6	0	1.059171	-2.309071	1.346179
52	1	0	1.858518	-1.120677	-0.315978
53	1	0	1.232144	-3.278355	0.872384
54	6	0	2.184956	-1.977633	2.300150
55	6	0	3.509895	-2.273509	1.961162
56	6	0	1.937540	-1.284908	3.489504
57	6	0	4.561985	-1.884360	2.785938
58	1	0	3.714221	-2.805235	1.033908
59	6	0	2.988849	-0.892186	4.316639
60	1	0	0.911530	-1.041970	3.751804
61	6	0	4.304435	-1.189046	3.966938
62	1	0	5.584440	-2.124512	2.508370
63	1	0	2.779427	-0.355422	5.237092
64	1	0	5.123590	-0.885219	4.611026
65	6	0	-0.194818	-1.725540	-1.425616
66	8	0	-0.602319	-0.682932	-2.004776
67	6	0	-1.255462	-2.587619	-0.705215
68	8	0	-1.004079	-3.637861	-0.131483
69	6	0	0.872148	-2.592246	-2.076689
70	7	0	-2.509811	-2.083720	-0.890784
71	1	0	-2.525976	-1.307191	-1.545927
72	6	0	-3.717892	-2.711709	-0.541787
73	6	0	-4.841800	-2.494878	-1.346915
74	6	0	-3.824958	-3.524805	0.591304
75	6	0	-6.062338	-3.072488	-1.016433
76	1	0	-4.750029	-1.880633	-2.239045
77	6	0	-5.049699	-4.107671	0.902936
78	1	0	-2.953575	-3.695376	1.209176
79	6	0	-6.172789	-3.885367	0.109593
80	1	0	-6.926015	-2.891469	-1.648290
81	1	0	-5.123916	-4.737811	1.783729
82	1	0	-7.123455	-4.341205	0.364991
83	1	0	0.408239	-3.096958	-2.932619
84	1	0	1.689969	-1.970021	-2.443932
85	1	0	1.253618	-3.352834	-1.395007

TS5SS

Total energy= -2028.14502335

Sum of electronic and zero-point Energies= -2027.443220

Sum of electronic and thermal Energies= -2027.402778
Sum of electronic and thermal Enthalpies= -2027.401834
Sum of electronic and thermal Free Energies= -2027.517573

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.800757	1.957299	0.342295
2	6	0	-3.725022	3.000864	0.443239
3	6	0	-5.063087	2.733337	0.696096
4	6	0	-5.463250	1.404566	0.838992
5	6	0	-4.540080	0.365652	0.724229
6	6	0	-3.191327	0.633509	0.477422
7	6	0	-1.423784	2.555755	0.152791
8	6	0	-1.742626	3.946047	-0.444616
9	6	0	-3.046747	4.336630	0.248880
10	1	0	-5.784683	3.541383	0.772238
11	1	0	-6.506376	1.174780	1.032779
12	1	0	-4.873840	-0.661440	0.827272
13	1	0	-2.465957	-0.168436	0.384169
14	1	0	-0.917894	2.651917	1.114617
15	1	0	-0.924689	4.664404	-0.304881
16	1	0	-2.833098	4.819298	1.208861
17	6	0	-0.190135	2.316699	-1.993398
18	6	0	-0.909597	3.489150	-2.590316
19	6	0	0.406974	0.853064	-0.478420
20	1	0	-1.238252	3.246366	-3.602148
21	1	0	-3.615007	5.036757	-0.367725
22	7	0	-0.477994	1.847438	-0.740895
23	7	0	0.821962	1.687237	-2.513648
24	7	0	1.189757	0.790001	-1.561050
25	8	0	-2.043222	3.805404	-1.826466
26	1	0	-0.209749	4.335362	-2.640853
27	6	0	2.434294	0.089937	-1.763180
28	6	0	2.476655	-0.964967	-2.671883
29	6	0	3.559494	0.574913	-1.083705
30	6	0	3.703859	-1.614609	-2.826214
31	6	0	4.752849	-0.115906	-1.265621
32	6	0	4.839784	-1.218697	-2.122337
33	1	0	3.765833	-2.453462	-3.514456
34	1	0	5.638435	0.220726	-0.731515
35	6	0	1.258256	-1.376686	-3.452896
36	1	0	0.400669	-1.520073	-2.789318
37	1	0	0.995714	-0.604218	-4.182651

38	1	0	1.450997	-2.306265	-3.991501
39	6	0	6.150695	-1.940984	-2.292042
40	1	0	6.911239	-1.270326	-2.706912
41	1	0	6.523044	-2.299967	-1.330297
42	1	0	6.048714	-2.796494	-2.961368
43	6	0	3.475850	1.781640	-0.188221
44	1	0	2.960120	2.606690	-0.690415
45	1	0	2.939685	1.553630	0.740314
46	1	0	4.475999	2.116257	0.090267
47	6	0	0.471416	0.121247	0.860383
48	8	0	-0.345150	0.539926	1.696602
49	1	0	1.018411	-1.051564	3.140206
50	6	0	1.391859	-0.940252	1.042249
51	6	0	1.872525	-1.146621	2.464576
52	1	0	2.167124	-1.028103	0.291034
53	1	0	2.251470	-2.167535	2.570353
54	6	0	2.946551	-0.141299	2.801556
55	6	0	4.270536	-0.367225	2.409844
56	6	0	2.631137	1.070283	3.424128
57	6	0	5.255191	0.591986	2.630550
58	1	0	4.524253	-1.303219	1.915894
59	6	0	3.614012	2.034101	3.645035
60	1	0	1.602485	1.256474	3.721697
61	6	0	4.928713	1.798962	3.247970
62	1	0	6.278247	0.398569	2.320727
63	1	0	3.353054	2.969364	4.131360
64	1	0	5.694357	2.548630	3.420923
65	6	0	0.441138	-2.787558	0.773535
66	8	0	0.304886	-3.325258	1.898814
67	6	0	-0.859465	-2.337217	0.066404
68	8	0	-0.896598	-1.715754	-0.994419
69	6	0	1.469018	-3.355770	-0.196122
70	7	0	-1.939924	-2.785688	0.747480
71	1	0	-1.671977	-3.226855	1.625640
72	6	0	-3.287047	-2.816264	0.357955
73	6	0	-3.716526	-2.456900	-0.925516
74	6	0	-4.221007	-3.260480	1.302491
75	6	0	-5.069645	-2.544360	-1.241573
76	1	0	-2.995773	-2.106007	-1.650491
77	6	0	-5.567991	-3.340664	0.971346
78	1	0	-3.882974	-3.539420	2.296355
79	6	0	-6.002133	-2.980570	-0.303965
80	1	0	-5.395233	-2.260316	-2.237345
81	1	0	-6.279459	-3.686143	1.714520

82	1	0	-7.054048	-3.040188	-0.561879
83	1	0	1.521643	-2.783774	-1.121771
84	1	0	2.453089	-3.379492	0.279985
85	1	0	1.175012	-4.386464	-0.424795

Ph/Ph/4-OMeC$_6$H$_4$
TS5RR

Total energy= -2334.30857974
Sum of electronic and zero-point Energies= -2333.518479
Sum of electronic and thermal Energies= -2333.473180
Sum of electronic and thermal Enthalpies= -2333.472235
Sum of electronic and thermal Free Energies= -2333.596200

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.835235	2.575844	-0.760264
2	6	0	-4.194734	2.866607	-0.898248
3	6	0	-4.603696	4.124713	-1.319989
4	6	0	-3.634251	5.092941	-1.585014
5	6	0	-2.279187	4.802205	-1.430637
6	6	0	-1.865815	3.533258	-1.022210
7	6	0	-2.694806	1.130184	-0.320105
8	6	0	-4.063281	0.858302	0.348098
9	6	0	-5.032037	1.668651	-0.511449
10	1	0	-5.659388	4.356137	-1.425308
11	1	0	-3.938237	6.084515	-1.904706
12	1	0	-1.537256	5.568158	-1.631119
13	1	0	-0.811306	3.300126	-0.923358
14	1	0	-2.528565	0.466888	-1.172498
15	1	0	-4.299144	-0.207561	0.414388
16	1	0	-5.325847	1.082619	-1.390190
17	6	0	-1.822407	0.840478	1.998327
18	6	0	-3.216107	0.816583	2.546482
19	6	0	-0.280979	0.773154	0.456397
20	1	0	-3.253808	1.351368	3.496073
21	1	0	-5.932879	1.920641	0.052443
22	7	0	-1.611034	0.882293	0.648873
23	7	0	-0.696242	0.766949	2.649682
24	7	0	0.254639	0.733789	1.679550
25	8	0	-4.088271	1.450163	1.644000
26	1	0	-3.506258	-0.231761	2.711081
27	6	0	1.650820	0.751853	2.030995

28	6	0	2.434062	1.812684	1.560713
29	6	0	2.167653	-0.301871	2.796123
30	6	0	3.805732	1.748363	1.800261
31	6	0	3.545324	-0.310047	3.004806
32	6	0	4.380216	0.686944	2.496397
33	1	0	4.441296	2.538287	1.409367
34	1	0	3.978386	-1.128488	3.575558
35	6	0	1.854238	2.980967	0.805991
36	1	0	1.736456	2.749589	-0.258828
37	1	0	0.879605	3.280464	1.203455
38	1	0	2.529184	3.835940	0.875611
39	6	0	5.868315	0.613594	2.712156
40	1	0	6.110097	0.631101	3.779072
41	1	0	6.268045	-0.317513	2.299199
42	1	0	6.378122	1.446676	2.224427
43	6	0	1.299231	-1.376461	3.394832
44	1	0	0.809879	-1.006586	4.300792
45	1	0	0.526403	-1.701413	2.697636
46	1	0	1.912061	-2.238551	3.666485
47	6	0	0.370384	0.671574	-0.913079
48	8	0	-0.300742	1.121600	-1.848247
49	1	0	2.635771	-0.467649	-2.872144
50	6	0	1.604082	-0.026855	-1.028168
51	6	0	2.481019	0.385888	-2.200221
52	1	0	2.125830	-0.233753	-0.101403
53	1	0	1.944400	1.141984	-2.781577
54	6	0	3.811250	0.930799	-1.732530
55	6	0	4.091304	2.298549	-1.776735
56	6	0	4.787081	0.065784	-1.222377
57	6	0	5.310850	2.796812	-1.318772
58	1	0	3.348118	2.981339	-2.182118
59	6	0	6.005170	0.558759	-0.764456
60	1	0	4.585708	-1.003202	-1.191358
61	6	0	6.271768	1.927486	-0.808249
62	1	0	5.510006	3.863372	-1.365247
63	1	0	6.751926	-0.127877	-0.376089
64	1	0	7.223380	2.310857	-0.452551
65	6	0	0.969792	-1.838022	-1.593123
66	8	0	0.597807	-1.762222	-2.799056
67	6	0	-0.164416	-2.033126	-0.560912
68	8	0	-0.001017	-2.165658	0.650943
69	6	0	2.267218	-2.572579	-1.281410
70	6	0	2.798660	-2.741118	0.004901
71	6	0	2.978534	-3.070596	-2.375082

72	6	0	4.015006	-3.392037	0.182360
73	1	0	2.261936	-2.351058	0.861822
74	6	0	4.201623	-3.715295	-2.196659
75	1	0	2.549502	-2.937493	-3.362652
76	6	0	4.724549	-3.878014	-0.916686
77	1	0	4.416814	-3.510683	1.184503
78	1	0	4.745096	-4.089637	-3.058907
79	1	0	5.678394	-4.376333	-0.774385
80	7	0	-1.371304	-1.991852	-1.175896
81	1	0	-1.270612	-1.874239	-2.184318
82	6	0	-2.644408	-2.208964	-0.623064
83	6	0	-3.747510	-2.126292	-1.476839
84	6	0	-2.859496	-2.510021	0.731673
85	6	0	-5.042254	-2.347462	-1.013316
86	1	0	-3.592911	-1.891044	-2.526376
87	6	0	-4.150020	-2.738071	1.191772
88	1	0	-2.018723	-2.577306	1.407794
89	6	0	-5.250381	-2.661167	0.332359
90	1	0	-5.868674	-2.276992	-1.710082
91	1	0	-4.326477	-2.982137	2.234528
92	8	0	-6.466192	-2.901319	0.889674
93	6	0	-7.600640	-2.770734	0.052472
94	1	0	-7.572096	-3.492406	-0.771250
95	1	0	-8.467090	-2.973815	0.680021
96	1	0	-7.675546	-1.756792	-0.356889

TS5RS

Total energy= -2334.30272032
Sum of electronic and zero-point Energies= -2333.513233
Sum of electronic and thermal Energies= -2333.467541
Sum of electronic and thermal Enthalpies= -2333.466597
Sum of electronic and thermal Free Energies= -2333.592701

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.041145	-2.092499	0.652997
2	6	0	-4.421775	-2.215130	0.478249
3	6	0	-5.168093	-3.000420	1.346174
4	6	0	-4.510515	-3.670138	2.380040
5	6	0	-3.130858	-3.548339	2.544016
6	6	0	-2.380279	-2.746755	1.681866
7	6	0	-2.510659	-1.147624	-0.405728

8	6	0	-3.574201	-1.267177	-1.516662
9	6	0	-4.872448	-1.413519	-0.723141
10	1	0	-6.241035	-3.104573	1.215095
11	1	0	-5.079123	-4.296571	3.059940
12	1	0	-2.635657	-4.077533	3.351539
13	1	0	-1.310937	-2.624657	1.820387
14	1	0	-2.452034	-0.130899	-0.016259
15	1	0	-3.560470	-0.419186	-2.213821
16	1	0	-5.231572	-0.419323	-0.426599
17	6	0	-1.021220	-2.209799	-2.098794
18	6	0	-2.198563	-2.553620	-2.962081
19	6	0	0.035285	-1.178502	-0.496531
20	1	0	-2.095585	-3.565976	-3.354602
21	1	0	-5.646587	-1.900265	-1.320136
22	7	0	-1.191677	-1.481922	-0.956756
23	7	0	0.243263	-2.427815	-2.331610
24	7	0	0.887374	-1.785220	-1.321979
25	8	0	-3.389602	-2.494209	-2.216269
26	1	0	-2.220025	-1.849294	-3.806165
27	6	0	2.317194	-1.869885	-1.186123
28	6	0	3.118835	-1.344811	-2.208106
29	6	0	2.835528	-2.420850	-0.009852
30	6	0	4.492086	-1.318571	-1.977793
31	6	0	4.218748	-2.370824	0.162101
32	6	0	5.056715	-1.804302	-0.795329
33	1	0	5.139198	-0.893404	-2.741573
34	1	0	4.643987	-2.762269	1.082079
35	6	0	2.534594	-0.810945	-3.488571
36	1	0	3.310069	-0.303050	-4.066001
37	1	0	2.128112	-1.622683	-4.097725
38	1	0	1.729781	-0.102641	-3.270191
39	6	0	6.544697	-1.733213	-0.576157
40	1	0	6.919553	-0.728923	-0.793042
41	1	0	6.799641	-1.977400	0.457028
42	1	0	7.069484	-2.430467	-1.236891
43	6	0	1.963646	-3.024106	1.061412
44	1	0	1.597695	-2.258520	1.755068
45	1	0	1.099624	-3.545633	0.639042
46	1	0	2.542128	-3.740313	1.647921
47	6	0	0.284380	-0.284448	0.700702
48	8	0	-0.619302	-0.282186	1.546920
49	1	0	1.132186	0.952214	2.728644
50	6	0	1.431020	0.556596	0.649349
51	6	0	1.886210	1.161609	1.964752

52	1	0	2.233622	0.215992	0.004554
53	1	0	1.966801	2.249475	1.881802
54	6	0	3.225339	0.577258	2.353122
55	6	0	4.397356	1.066146	1.765017
56	6	0	3.319056	-0.496484	3.241377
57	6	0	5.630602	0.488716	2.053398
58	1	0	4.332570	1.905918	1.074476
59	6	0	4.552384	-1.077065	3.533561
60	1	0	2.414924	-0.876402	3.712154
61	6	0	5.712287	-0.587480	2.937251
62	1	0	6.532204	0.880009	1.590877
63	1	0	4.606837	-1.909513	4.228949
64	1	0	6.674960	-1.036356	3.163213
65	6	0	0.843504	1.850957	-0.787445
66	8	0	0.644464	1.188834	-1.856582
67	6	0	-0.426162	2.350885	-0.062638
68	8	0	-0.450712	2.922239	1.020183
69	6	0	2.069406	2.740924	-0.733010
70	6	0	2.183287	3.896997	0.045515
71	6	0	3.151095	2.358376	-1.535678
72	6	0	3.363512	4.641745	0.028883
73	1	0	1.351560	4.209482	0.665563
74	6	0	4.328210	3.096865	-1.545773
75	1	0	3.048949	1.465084	-2.143859
76	6	0	4.439567	4.244504	-0.759205
77	1	0	3.437084	5.537385	0.638059
78	1	0	5.160481	2.779828	-2.167227
79	1	0	5.356974	4.824611	-0.764141
80	7	0	-1.529137	2.019279	-0.789656
81	1	0	-1.291742	1.619771	-1.694838
82	6	0	-2.876528	2.219671	-0.435452
83	6	0	-3.831132	2.355158	-1.451709
84	6	0	-3.296738	2.200784	0.894995
85	6	0	-5.176406	2.473874	-1.141505
86	1	0	-3.510044	2.370517	-2.489659
87	6	0	-4.648699	2.332556	1.210727
88	1	0	-2.560706	2.072972	1.678860
89	6	0	-5.595683	2.470422	0.194010
90	1	0	-5.922811	2.581596	-1.921146
91	1	0	-4.945083	2.315567	2.252439
92	8	0	-6.933759	2.604189	0.396865
93	6	0	-7.390795	2.602580	1.737016
94	1	0	-8.471214	2.730688	1.690076
95	1	0	-7.156989	1.654879	2.234860

96	1	0	-6.950150	3.427963	2.306849

TS5SR

Total energy= -2334.29004740
Sum of electronic and zero-point Energies= -2333.500248
Sum of electronic and thermal Energies= -2333.454359
Sum of electronic and thermal Enthalpies= -2333.453415
Sum of electronic and thermal Free Energies= -2333.580781

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.314494	2.781879	-0.030901
2	6	0	-3.294396	3.766173	0.109726
3	6	0	-4.558387	3.570511	-0.429072
4	6	0	-4.812439	2.386748	-1.124646
5	6	0	-3.817280	1.421728	-1.280737
6	6	0	-2.548637	1.607360	-0.726364
7	6	0	-1.058912	3.242760	0.670067
8	6	0	-1.224327	4.779136	0.675929
9	6	0	-2.735106	4.959656	0.851515
10	1	0	-5.328249	4.329720	-0.329312
11	1	0	-5.791621	2.221277	-1.562687
12	1	0	-4.037103	0.518256	-1.839953
13	1	0	-1.764158	0.866057	-0.861348
14	1	0	-1.001640	2.847408	1.684056
15	1	0	-0.618403	5.265671	1.450750
16	1	0	-2.995094	4.929119	1.915330
17	6	0	0.895395	3.748290	-0.772587
18	6	0	0.465709	5.178221	-0.908732
19	6	0	0.868863	1.687581	-0.023379
20	1	0	0.618670	5.512823	-1.935556
21	1	0	-3.056815	5.922197	0.447658
22	7	0	0.191616	2.861999	-0.010722
23	7	0	1.972635	3.200144	-1.255082
24	7	0	1.946795	1.926623	-0.781731
25	8	0	-0.899552	5.304790	-0.603906
26	1	0	1.084285	5.794886	-0.241071
27	6	0	3.093112	1.097717	-1.062442
28	6	0	3.216701	0.551397	-2.339729
29	6	0	4.056898	0.957325	-0.060158
30	6	0	4.329210	-0.256889	-2.570538
31	6	0	5.138692	0.125162	-0.338794

32	6	0	5.276752	-0.506875	-1.577004
33	1	0	4.448429	-0.713249	-3.550602
34	1	0	5.890024	-0.029199	0.431525
35	6	0	2.189224	0.818448	-3.405208
36	1	0	1.202281	0.488900	-3.064639
37	1	0	2.138819	1.886458	-3.637092
38	1	0	2.444007	0.279127	-4.319702
39	6	0	6.415483	-1.458213	-1.832207
40	1	0	6.718922	-1.440970	-2.881495
41	1	0	7.282686	-1.217041	-1.213690
42	1	0	6.108963	-2.482372	-1.593302
43	6	0	3.921907	1.673887	1.254944
44	1	0	3.712885	2.737265	1.098935
45	1	0	3.109979	1.250217	1.856017
46	1	0	4.839833	1.578970	1.836170
47	6	0	0.496373	0.492712	0.861460
48	8	0	-0.415158	0.736374	1.668363
49	1	0	0.358007	-1.537387	2.504427
50	6	0	1.179265	-0.734652	0.700103
51	6	0	1.287860	-1.602753	1.938820
52	1	0	2.060104	-0.723578	0.068789
53	1	0	1.425764	-2.648615	1.650937
54	6	0	2.459832	-1.161663	2.786503
55	6	0	3.762677	-1.537742	2.442247
56	6	0	2.275117	-0.323692	3.889832
57	6	0	4.853312	-1.091012	3.183435
58	1	0	3.916738	-2.182076	1.578077
59	6	0	3.364829	0.129260	4.632073
60	1	0	1.266054	-0.021536	4.158632
61	6	0	4.657611	-0.254169	4.281888
62	1	0	5.858086	-1.397108	2.905986
63	1	0	3.203142	0.778483	5.487499
64	1	0	5.507051	0.092677	4.861967
65	6	0	0.017779	-1.642387	-0.876219
66	8	0	-0.128229	-0.796717	-1.797432
67	6	0	-1.251865	-1.993907	-0.061784
68	8	0	-1.272444	-2.561167	1.022337
69	6	0	0.989402	-2.785832	-1.081352
70	6	0	0.970510	-3.981009	-0.351886
71	6	0	1.943614	-2.628643	-2.092033
72	6	0	1.915073	-4.973979	-0.607181
73	1	0	0.218688	-4.131269	0.413696
74	6	0	2.893868	-3.612824	-2.335470
75	1	0	1.920925	-1.719056	-2.680442

76	6	0	2.886593	-4.790507	-1.587683
77	1	0	1.890184	-5.894717	-0.032762
78	1	0	3.637680	-3.464117	-3.113331
79	1	0	3.626328	-5.562557	-1.774844
80	7	0	-2.364972	-1.655784	-0.766996
81	1	0	-2.167146	-1.246516	-1.674051
82	6	0	-3.699747	-1.936350	-0.416883
83	6	0	-4.635537	-2.116510	-1.444216
84	6	0	-4.123594	-2.013128	0.908472
85	6	0	-5.965772	-2.360325	-1.150873
86	1	0	-4.310158	-2.067007	-2.480005
87	6	0	-5.460853	-2.274914	1.207498
88	1	0	-3.406094	-1.870853	1.705294
89	6	0	-6.388415	-2.447541	0.180329
90	1	0	-6.697281	-2.498241	-1.939693
91	1	0	-5.761650	-2.331352	2.246580
92	8	0	-7.711986	-2.701629	0.367838
93	6	0	-8.171111	-2.796038	1.703123
94	1	0	-8.012653	-1.856867	2.245092
95	1	0	-9.238653	-3.004166	1.644266
96	1	0	-7.670128	-3.610110	2.238707

TS5SS

Total energy= -2334.29322855
Sum of electronic and zero-point Energies= -2333.503614
Sum of electronic and thermal Energies= -2333.458049
Sum of electronic and thermal Enthalpies= -2333.457104
Sum of electronic and thermal Free Energies= -2333.581749

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.748948	2.525889	0.119090
2	6	0	-3.675798	3.571427	0.132162
3	6	0	-5.025774	3.311996	0.324000
4	6	0	-5.433543	1.989118	0.496218
5	6	0	-4.505832	0.948122	0.468525
6	6	0	-3.146260	1.206614	0.280150
7	6	0	-1.363543	3.118373	-0.020335
8	6	0	-1.648756	4.484273	-0.687670
9	6	0	-2.986227	4.899454	-0.076835
10	1	0	-5.749600	4.121664	0.330428
11	1	0	-6.485494	1.765461	0.644362

12	1	0	-4.843801	-0.074424	0.596322
13	1	0	-2.419979	0.400159	0.247694
14	1	0	-0.909790	3.254127	0.962372
15	1	0	-0.837656	5.207251	-0.532467
16	1	0	-2.820048	5.416738	0.874525
17	6	0	-0.035001	2.778193	-2.092483
18	6	0	-0.709127	3.934806	-2.767830
19	6	0	0.483468	1.380807	-0.488756
20	1	0	-0.987268	3.658362	-3.786114
21	1	0	-3.521509	5.576697	-0.746316
22	7	0	-0.377547	2.372002	-0.832904
23	7	0	0.984760	2.108815	-2.544428
24	7	0	1.302161	1.254302	-1.536548
25	8	0	-1.877301	4.292472	-2.077297
26	1	0	0.002890	4.771247	-2.812916
27	6	0	2.517093	0.490551	-1.669857
28	6	0	2.511034	-0.636637	-2.490106
29	6	0	3.657586	0.978508	-1.024622
30	6	0	3.707394	-1.344388	-2.591257
31	6	0	4.819574	0.219616	-1.141005
32	6	0	4.855595	-0.950795	-1.903231
33	1	0	3.735816	-2.234699	-3.213093
34	1	0	5.716421	0.555424	-0.626066
35	6	0	1.278874	-1.035400	-3.254088
36	1	0	0.408271	-1.063009	-2.593489
37	1	0	1.079450	-0.316052	-4.055062
38	1	0	1.413832	-2.023234	-3.698914
39	6	0	6.105806	-1.786405	-1.972932
40	1	0	6.993943	-1.197941	-1.733047
41	1	0	6.043398	-2.611363	-1.254953
42	1	0	6.233997	-2.225214	-2.965394
43	6	0	3.623113	2.258547	-0.234668
44	1	0	3.209416	3.076537	-0.833981
45	1	0	3.012131	2.152448	0.668814
46	1	0	4.628659	2.534059	0.086462
47	6	0	0.496014	0.732750	0.891382
48	8	0	-0.391203	1.162266	1.645355
49	1	0	1.062819	0.129352	3.275793
50	6	0	1.460632	-0.257165	1.218244
51	6	0	1.890457	-0.253887	2.672876
52	1	0	2.262346	-0.406496	0.506330
53	1	0	2.071834	-1.278398	3.012677
54	6	0	3.121707	0.601581	2.861887
55	6	0	4.361041	0.168759	2.374804

56	6	0	3.047499	1.861278	3.461442
57	6	0	5.492768	0.970099	2.485139
58	1	0	4.431636	-0.801642	1.886166
59	6	0	4.178322	2.670327	3.570233
60	1	0	2.090369	2.212331	3.839344
61	6	0	5.405478	2.227487	3.083431
62	1	0	6.445498	0.614510	2.103056
63	1	0	4.099072	3.646797	4.038691
64	1	0	6.287245	2.854693	3.168569
65	6	0	0.539831	-2.164943	1.123863
66	8	0	0.436034	-2.569796	2.308488
67	6	0	-0.771639	-1.778176	0.402846
68	8	0	-0.831086	-1.215639	-0.691090
69	6	0	1.559715	-2.863714	0.239769
70	6	0	1.238931	-3.391039	-1.012046
71	6	0	2.818851	-3.141964	0.784232
72	6	0	2.164792	-4.167923	-1.709451
73	1	0	0.262807	-3.202344	-1.446234
74	6	0	3.751879	-3.890486	0.078302
75	1	0	3.049859	-2.782981	1.782501
76	6	0	3.425974	-4.410406	-1.175370
77	1	0	1.894949	-4.581063	-2.677366
78	1	0	4.726450	-4.088877	0.515030
79	1	0	4.148898	-5.005857	-1.724853
80	7	0	-1.837920	-2.204947	1.111500
81	1	0	-1.573618	-2.578080	2.020402
82	6	0	-3.186000	-2.277229	0.711700
83	6	0	-3.583349	-2.176139	-0.629680
84	6	0	-4.151110	-2.520137	1.688109
85	6	0	-4.920042	-2.319479	-0.965399
86	1	0	-2.844471	-1.981730	-1.394783
87	6	0	-5.495565	-2.665347	1.351972
88	1	0	-3.850743	-2.598618	2.728912
89	6	0	-5.886883	-2.564527	0.015858
90	1	0	-5.241463	-2.242814	-1.998696
91	1	0	-6.216581	-2.853770	2.137679
92	8	0	-7.167367	-2.690236	-0.424302
93	6	0	-8.165389	-2.948498	0.545616
94	1	0	-9.107146	-3.016601	0.002787
95	1	0	-7.977030	-3.893288	1.067792
96	1	0	-8.226443	-2.136457	1.279086