Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

Computational exploration for possible reaction pathways, regioselectivity, and influence of substrate in gold-catalyzed cycloaddition of cyanamides with enynamides

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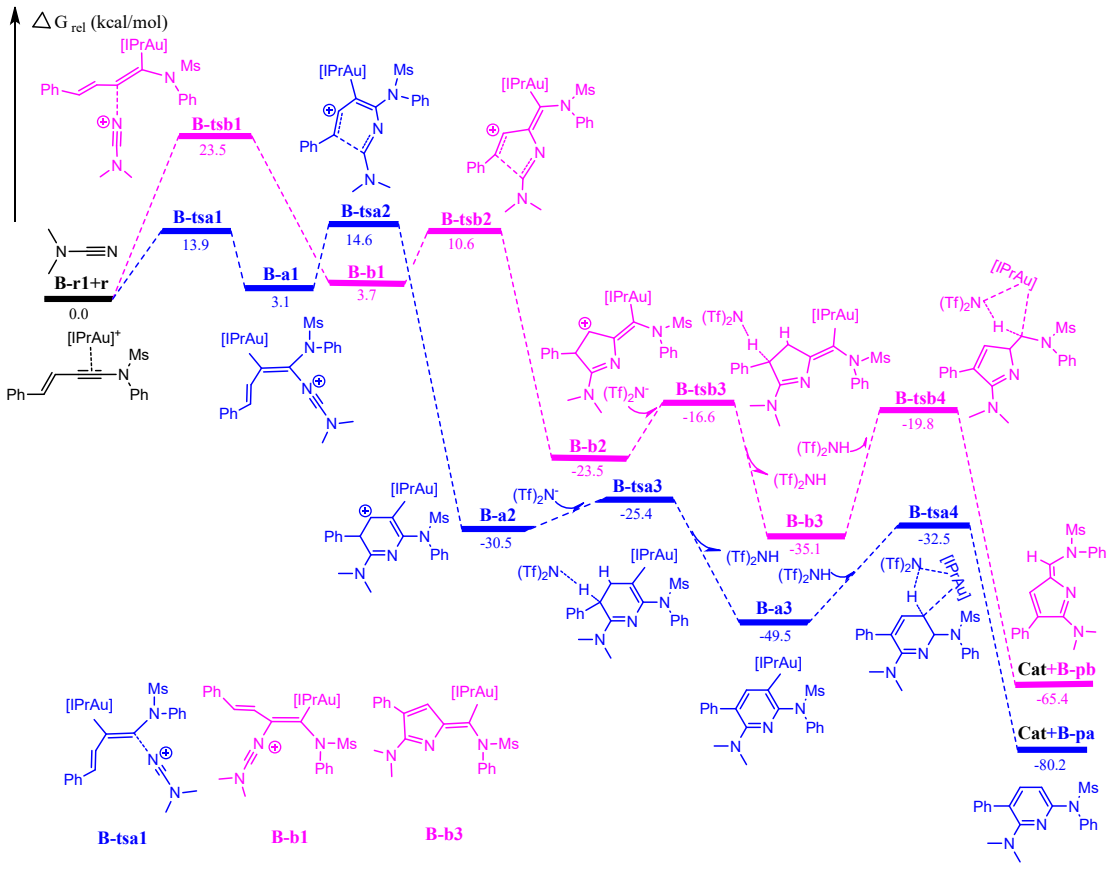

Fig.S1 Full energy profile for Au-catalyzed cycloaddition of dimethylcyanamide and enynamide B-r1 (R1=R2=Ph, R3=Me). Relative energies are in kcal/mol.

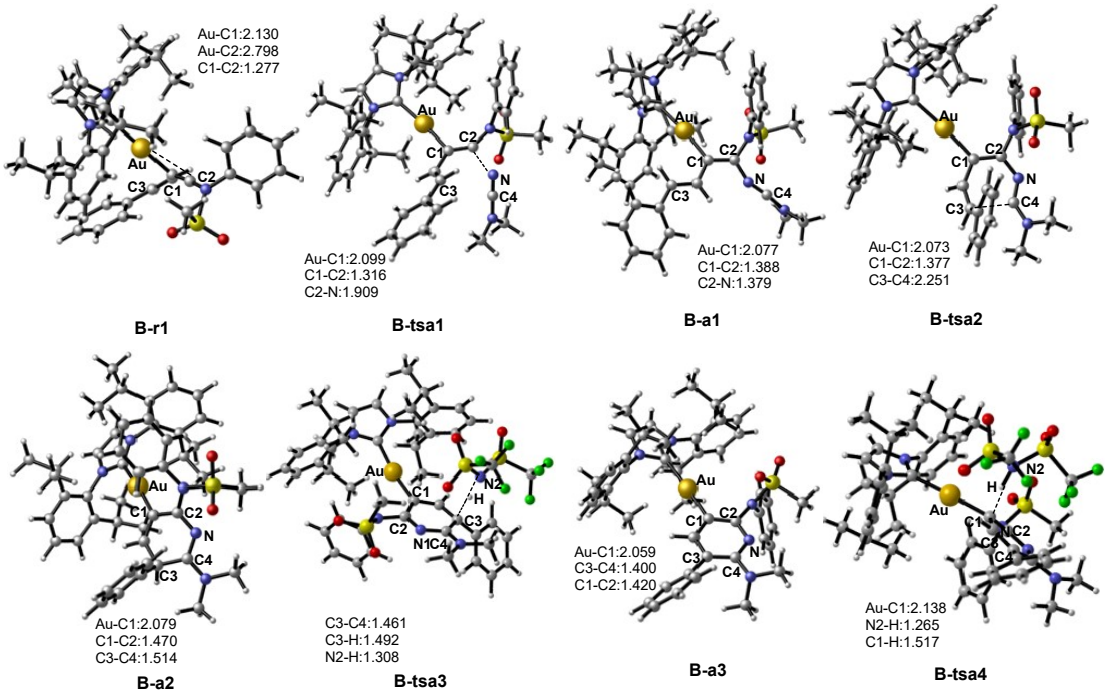

Fig.S2 Representative structures in Au-catalyzed pathway a of Fig.S1.

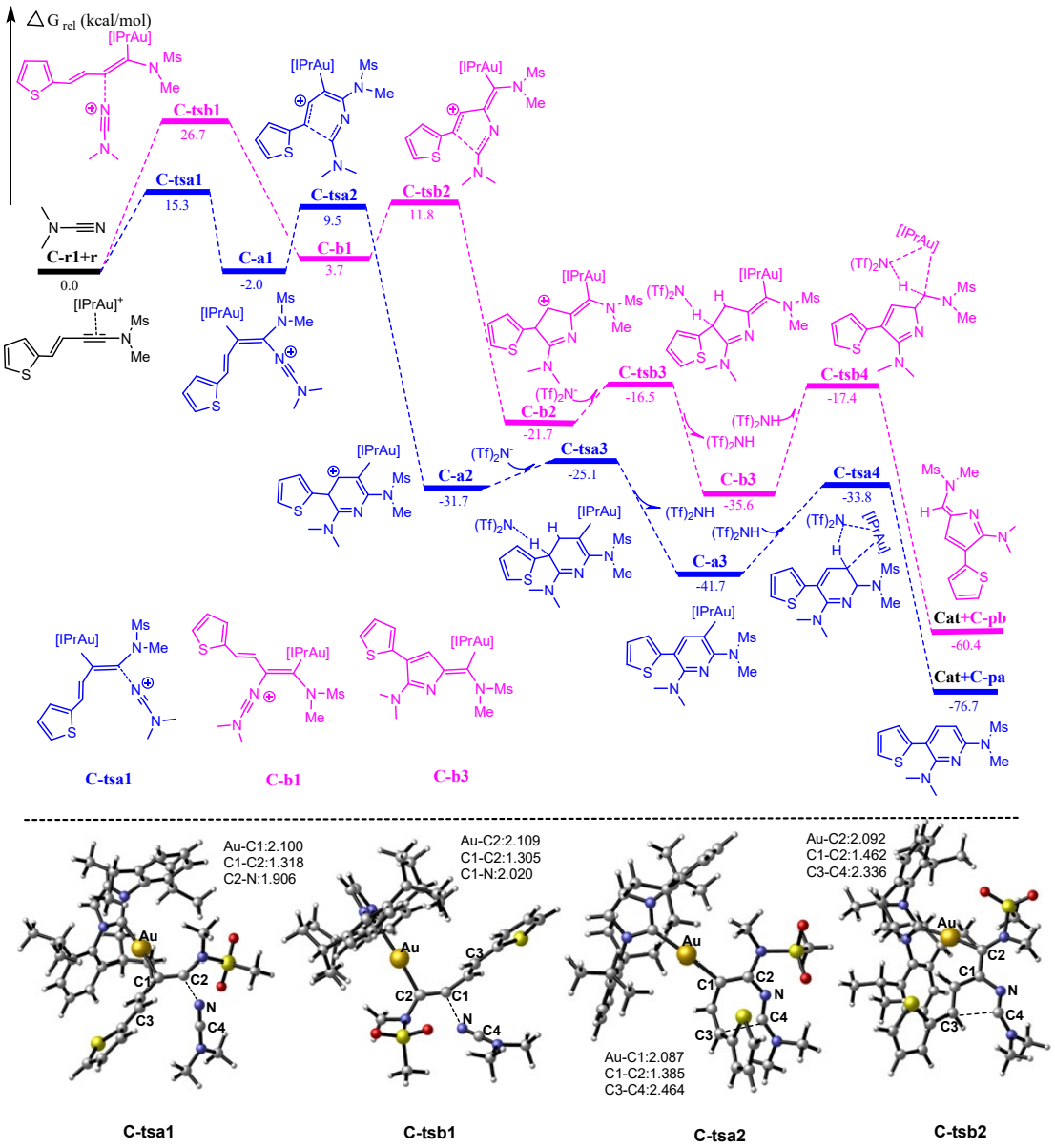

Fig.S3 Full energy profile for series C (C-r1:R1is thienyl, R2=Ms, R3=Me) with selected structures (selected bond lengths are in Å). Relative energies are in kcal/mol.

Cartesian Coordinates

A-r1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.496913	-1.453254	-1.641393
2	6	0	-1.592464	-2.600643	-1.084869
3	6	0	-1.931888	-0.995003	-2.967639
4	7	0	-1.749278	-3.689201	-0.423255
5	6	0	-2.647301	0.107354	-3.269482
6	79	0	-0.091069	-0.335751	-0.495678
7	7	0	2.721780	0.328008	0.485608
8	6	0	3.481807	1.282892	1.149848
9	6	0	2.628877	2.259988	1.544531
10	7	0	1.363914	1.904263	1.090824
11	6	0	3.298408	-0.822846	-0.190851
12	6	0	0.169655	2.663870	1.427616
13	6	0	-0.499371	2.311911	2.619724
14	6	0	-1.622781	3.063705	2.986261
15	6	0	-2.056427	4.128627	2.207548
16	6	0	-1.367224	4.461520	1.045659
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18	6	0	3.677249	-0.653334	-1.540393
19	6	0	4.241219	-1.751268	-2.203922
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A- tsa1

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5	6	0	3.743975	0.587829	-1.267132
6	79	0	-0.251715	0.055611	-0.089447

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8	7	0	-3.301508	0.348718	-0.529060
9	6	0	-4.389025	1.137137	-0.168732
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24	7	0	3.867775	-1.877612	-1.829674
25	6	0	4.953454	-1.692361	-1.406854
26	7	0	6.145853	-1.492325	-0.915337
27	6	0	6.523775	-2.095729	0.374782
28	6	0	7.181679	-0.810200	-1.703910
29	6	0	-2.167289	3.049579	-2.500980
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36	6	0	-4.294885	-1.545430	3.143885
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79	1	0	-2.777414	-3.009469	-1.793679
80	1	0	-4.253352	-3.690814	-1.086484
81	1	0	-4.184308	-3.343014	-2.813919
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85	1	0	-4.575819	-1.060875	2.205525
86	1	0	-2.893199	-3.624225	2.004135
87	1	0	-2.430112	-2.181242	1.092323
88	1	0	-1.252373	-2.973304	2.152576
89	1	0	-1.577267	2.871800	1.431312
90	1	0	0.896278	2.619800	1.342097
91	1	0	0.397494	4.319472	1.349938
92	1	0	1.056982	3.589719	2.815141
93	1	0	-2.716494	3.852427	3.427160
94	1	0	-1.705111	5.044966	2.594499
95	1	0	-1.149353	4.307527	4.103532
96	1	0	0.361853	-4.724405	-1.063191
97	1	0	-0.146073	-3.339028	-2.034239
98	1	0	-0.632621	-3.452304	-0.315923
99	1	0	4.008133	2.716838	1.834786
100	1	0	5.025187	4.973539	1.903336
101	1	0	5.344836	6.255058	-0.203098
102	1	0	4.638277	5.270123	-2.371701
103	1	0	3.623282	3.030084	-2.448561
104	1	0	3.741348	-4.611966	-0.856426
105	1	0	3.664009	-5.438605	0.745554
106	1	0	2.362946	-5.689448	-0.449446

Sum of electronic and zero-point Energies= -2590.591663
Sum of electronic and thermal Energies= -2590.534464
Sum of electronic and thermal Enthalpies= -2590.533520
Sum of electronic and thermal Free Energies= -2590.692132

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.013240	0.132180	-0.471973
2	6	0	2.855995	-0.967223	-0.431033
3	6	0	2.642005	1.428194	-0.627837
4	7	0	2.488603	-2.345801	-0.516862
5	6	0	1.969532	2.585602	-0.862181
6	79	0	-0.043955	0.018776	-0.183394
7	6	0	-2.098071	0.001414	0.145448
8	7	0	-3.059172	-0.575571	-0.636828

9	6	0	-4.326300	-0.345892	-0.112237
10	6	0	-4.158465	0.398069	1.007096
11	7	0	-2.790965	0.596783	1.160802
12	6	0	-2.814979	-1.456445	-1.765505
13	6	0	-2.234970	1.454072	2.195519
14	6	0	-1.828766	0.909249	3.435139
15	6	0	-1.310021	1.809617	4.377622
16	6	0	-1.218077	3.174161	4.124774
17	6	0	-1.665191	3.683294	2.911572
18	6	0	-2.186222	2.839815	1.922872
19	6	0	-2.746119	-2.842628	-1.493873
20	6	0	-2.488225	-3.705018	-2.567373
21	6	0	-2.317769	-3.215604	-3.857105
22	6	0	-2.437955	-1.850976	-4.100448
23	6	0	-2.703439	-0.932013	-3.074054
24	7	0	4.222219	-0.784418	-0.329149
25	6	0	5.325203	-1.194488	-0.186046
26	7	0	6.493391	-1.540734	0.236119
27	6	0	6.742944	-1.700991	1.690639
28	6	0	7.628930	-1.735104	-0.685906
29	6	0	-1.913454	-0.558125	3.872227
30	6	0	-3.328546	-1.166424	3.828508
31	6	0	-0.881426	-1.471319	3.188396
32	6	0	-2.734075	3.452117	0.635118
33	6	0	-4.122157	4.081963	0.878765
34	6	0	-1.779739	4.487897	0.014572
35	6	0	1.450405	-2.740395	-1.486510
36	6	0	3.162090	-4.816127	0.467441
37	16	0	2.490978	-3.217535	0.963042
38	8	0	1.128753	-3.448197	1.453156
39	8	0	3.486753	-2.553545	1.816151
40	6	0	2.559226	3.906784	-1.060795
41	6	0	1.780282	4.916314	-1.660340
42	6	0	2.303432	6.186430	-1.889754
43	6	0	3.614785	6.479691	-1.511002
44	6	0	4.398112	5.494129	-0.900633
45	6	0	3.879243	4.223430	-0.678227
46	6	0	-2.889074	0.529315	-3.504654
47	6	0	-4.241994	1.150167	-3.106628
48	6	0	-1.715564	1.455432	-3.136161
49	6	0	-3.030955	-3.434959	-0.113555
50	6	0	-4.461939	-4.014874	-0.073294
51	6	0	-2.009961	-4.501566	0.319876
52	1	0	3.730349	1.469567	-0.613499
53	1	0	0.886302	2.528263	-0.951314
54	1	0	-5.216273	-0.727388	-0.584567
55	1	0	-4.872650	0.794397	1.709688
56	1	0	-0.982190	1.422592	5.337989
57	1	0	-0.815341	3.841120	4.881246
58	1	0	-1.617413	4.751726	2.729628
59	1	0	-2.435900	-4.773947	-2.389126
60	1	0	-2.120130	-3.898108	-4.678550
61	1	0	-2.341969	-1.480853	-5.117116
62	1	0	5.786686	-1.745061	2.210425
63	1	0	7.284721	-2.637304	1.846663
64	1	0	7.345910	-0.864190	2.054409
65	1	0	7.295304	-1.585303	-1.712440
66	1	0	8.417091	-1.014211	-0.450496
67	1	0	8.020785	-2.749424	-0.571624

68	1	0	-1.639388	-0.534940	4.933729
69	1	0	-4.064767	-0.505835	4.298404
70	1	0	-3.333586	-2.112642	4.379333
71	1	0	-3.662185	-1.382539	2.810709
72	1	0	0.130534	-1.066929	3.278847
73	1	0	-0.888312	-2.461230	3.655888
74	1	0	-1.085317	-1.607723	2.124576
75	1	0	-2.859076	2.652995	-0.100707
76	1	0	-4.839599	3.350422	1.262570
77	1	0	-4.525666	4.493417	-0.052412
78	1	0	-4.058560	4.897049	1.607245
79	1	0	-0.772117	4.082065	-0.107361
80	1	0	-2.151058	4.795127	-0.968724
81	1	0	-1.701123	5.392134	0.626247
82	1	0	1.661688	-2.222017	-2.422883
83	1	0	0.438514	-2.488906	-1.158524
84	1	0	1.513866	-3.816113	-1.669674
85	1	0	3.219358	-5.412075	1.380199
86	1	0	2.491434	-5.297755	-0.243834
87	1	0	4.152680	-4.669470	0.037942
88	1	0	0.760617	4.690247	-1.959218
89	1	0	1.688945	6.947585	-2.360844
90	1	0	4.023466	7.470925	-1.682139
91	1	0	5.413542	5.723717	-0.591597
92	1	0	4.490945	3.476780	-0.181472
93	1	0	-2.899130	0.482819	-4.600043
94	1	0	-5.075507	0.485402	-3.355380
95	1	0	-4.389390	2.085341	-3.656687
96	1	0	-4.298145	1.386680	-2.041415
97	1	0	-1.848966	2.428729	-3.621629
98	1	0	-1.647852	1.621067	-2.058366
99	1	0	-0.760489	1.038055	-3.469078
100	1	0	-2.979269	-2.631013	0.625383
101	1	0	-5.215799	-3.264863	-0.331843
102	1	0	-4.691582	-4.393592	0.927910
103	1	0	-4.567353	-4.845389	-0.779345
104	1	0	-0.992705	-4.105007	0.348306
105	1	0	-2.253707	-4.852648	1.327640
106	1	0	-2.027816	-5.377327	-0.337418

Sum of electronic and zero-point Energies= -2590.624339
Sum of electronic and thermal Energies= -2590.567608
Sum of electronic and thermal Enthalpies= -2590.566664
Sum of electronic and thermal Free Energies= -2590.722311

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.655873	-0.577555	0.766901
2	6	0	-1.478962	-1.301756	0.710832
3	6	0	-2.745372	0.870474	0.601531
4	7	0	-1.563565	-2.717565	0.847338
5	6	0	-3.877759	1.592418	0.472662
6	79	0	0.356692	-0.431120	0.293976
7	6	0	2.186862	0.375612	-0.259808
8	7	0	2.636292	0.555091	-1.535525
9	6	0	3.904655	1.123304	-1.533667

10	6	0	4.264886	1.279221	-0.236226
11	7	0	3.199025	0.829292	0.535913
12	6	0	1.864936	0.329870	-2.748043
13	6	0	3.260491	0.713257	1.983249
14	6	0	2.844055	1.784628	2.806787
15	6	0	2.943243	1.591399	4.192248
16	6	0	3.442945	0.414056	4.740078
17	6	0	3.875114	-0.607050	3.903098
18	6	0	3.798607	-0.481925	2.510033
19	6	0	1.067876	1.400148	-3.210046
20	6	0	0.328692	1.206497	-4.383727
21	6	0	0.380694	0.001713	-5.072939
22	6	0	1.191891	-1.027390	-4.605656
23	6	0	1.963325	-0.899198	-3.441581
24	7	0	-3.842048	-1.252766	0.997917
25	6	0	-5.012960	-1.354168	1.084402
26	7	0	-6.263799	-1.671626	1.019922
27	6	0	-6.812418	-2.236745	-0.236761
28	6	0	-7.197019	-1.398744	2.130233
29	6	0	2.307513	3.145700	2.347774
30	6	0	3.261929	3.955573	1.449214
31	6	0	0.889395	3.081810	1.751516
32	6	0	4.350419	-1.605216	1.634750
33	6	0	5.892652	-1.625238	1.683773
34	6	0	3.776032	-2.983485	2.010674
35	6	0	2.828627	-2.109416	-3.067339
36	6	0	4.339334	-1.826680	-2.957788
37	6	0	2.307735	-2.889197	-1.845680
38	6	0	1.011991	2.760486	-2.518821
39	6	0	-0.432622	3.207175	-2.227779
40	6	0	1.760414	3.826385	-3.345908
41	6	0	-0.342545	-3.377557	1.362800
42	6	0	-3.985365	3.050050	0.362766
43	6	0	-5.192180	3.611465	-0.093894
44	6	0	-5.341894	4.990361	-0.226490
45	6	0	-4.287588	5.842574	0.105331
46	6	0	-3.086568	5.302173	0.575159
47	6	0	-2.936356	3.924720	0.706467
48	6	0	-3.141850	-4.951796	0.498064
49	16	0	-2.291771	-3.658164	-0.428275
50	8	0	-1.228005	-4.290977	-1.210847
51	8	0	-3.310815	-2.838925	-1.092889
52	1	0	-1.777504	1.362381	0.587296
53	1	0	-4.832897	1.070678	0.414118
54	1	0	4.426535	1.352697	-2.448062
55	1	0	5.166290	1.666886	0.209055
56	1	0	2.627969	2.393924	4.852718
57	1	0	3.510293	0.302236	5.818114
58	1	0	4.288885	-1.513219	4.333454
59	1	0	-0.289499	2.014212	-4.761796
60	1	0	-0.199228	-0.133861	-5.980921
61	1	0	1.238487	-1.960921	-5.158504
62	1	0	-5.988331	-2.466831	-0.912639
63	1	0	-7.361664	-3.151395	0.001757
64	1	0	-7.489752	-1.513769	-0.700091
65	1	0	-6.647397	-0.988191	2.976969
66	1	0	-7.954817	-0.680624	1.804555
67	1	0	-7.684212	-2.330998	2.428545
68	1	0	2.216798	3.723827	3.274785

69	1	0	2.911105	4.990795	1.384939
70	1	0	3.312186	3.565606	0.429969
71	1	0	4.276198	3.975544	1.860692
72	1	0	0.870108	2.552479	0.795899
73	1	0	0.200633	2.572088	2.432727
74	1	0	0.514500	4.097529	1.582806
75	1	0	4.059665	-1.412260	0.599209
76	1	0	6.318767	-0.668145	1.366949
77	1	0	6.286009	-2.405402	1.023947
78	1	0	6.253512	-1.829379	2.697242
79	1	0	2.682446	-2.978685	1.984333
80	1	0	4.130922	-3.741833	1.305553
81	1	0	4.087561	-3.298272	3.011641
82	1	0	2.720344	-2.787566	-3.921693
83	1	0	4.701396	-1.245776	-3.812418
84	1	0	4.886372	-2.775101	-2.947920
85	1	0	4.603049	-1.291113	-2.042615
86	1	0	2.889276	-3.809614	-1.720810
87	1	0	2.398955	-2.307756	-0.924365
88	1	0	1.257075	-3.167915	-1.968202
89	1	0	1.521985	2.680763	-1.555171
90	1	0	-0.979479	2.449279	-1.659388
91	1	0	-0.432360	4.135387	-1.647728
92	1	0	-0.992765	3.400751	-3.147979
93	1	0	2.805142	3.546144	-3.514337
94	1	0	1.747994	4.791048	-2.827899
95	1	0	1.292944	3.966746	-4.326050
96	1	0	-0.565784	-4.415117	1.620373
97	1	0	-0.049784	-2.859004	2.275536
98	1	0	0.478791	-3.357859	0.641746
99	1	0	-6.017061	2.953793	-0.358025
100	1	0	-6.281177	5.399495	-0.586549
101	1	0	-4.402140	6.917857	0.008794
102	1	0	-2.268403	5.960810	0.852320
103	1	0	-2.007281	3.524912	1.099961
104	1	0	-3.874754	-4.489894	1.158740
105	1	0	-3.628176	-5.584613	-0.247028
106	1	0	-2.420718	-5.539101	1.065513

Sum of electronic and zero-point Energies= -2590.622605
Sum of electronic and thermal Energies= -2590.565812
Sum of electronic and thermal Enthalpies= -2590.564867
Sum of electronic and thermal Free Energies= -2590.721302

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.605064	-0.098132	-1.002820
2	6	0	-2.426111	-1.203731	-0.926180
3	6	0	-2.141253	1.079476	-1.589243
4	7	0	-2.028803	-2.504235	-0.541566
5	6	0	-3.346940	1.724990	-1.311505
6	79	0	0.397640	0.062134	-0.471874
7	6	0	2.344638	0.339400	0.155092
8	7	0	3.233352	-0.600738	0.587271
9	6	0	4.439382	-0.007158	0.942482
10	6	0	4.293447	1.327010	0.751455

11	7	0	3.010437	1.525938	0.254414
12	6	0	3.036623	-2.039671	0.542785
13	6	0	2.432498	2.841155	0.035427
14	6	0	1.764020	3.438863	1.126122
15	6	0	1.214589	4.713633	0.937180
16	6	0	1.330980	5.371710	-0.280513
17	6	0	2.011228	4.764810	-1.332252
18	6	0	2.584864	3.490862	-1.211892
19	6	0	3.379638	-2.695808	-0.660310
20	6	0	3.210918	-4.085278	-0.718916
21	6	0	2.730620	-4.795928	0.374431
22	6	0	2.419995	-4.124975	1.553235
23	6	0	2.566103	-2.735458	1.681553
24	7	0	-3.712434	-1.193792	-1.431893
25	6	0	-4.436845	-0.231292	-1.744032
26	7	0	-5.721541	0.020149	-1.754570
27	6	0	-6.618520	-0.609065	-0.765319
28	6	0	-6.317512	1.010910	-2.652082
29	1	0	-3.595951	2.506625	-2.028799
30	6	0	3.303215	2.949849	-2.454443
31	6	0	4.784017	2.574298	-2.255358
32	6	0	2.525426	1.825903	-3.165217
33	6	0	-4.051161	1.916377	-0.023472
34	6	0	-4.964676	2.987808	0.047702
35	6	0	-5.654048	3.270343	1.225371
36	6	0	-5.444597	2.483999	2.359929
37	6	0	-4.539544	1.420170	2.305613
38	6	0	-3.847273	1.135552	1.130673
39	6	0	-3.805423	-4.569751	-0.143795
40	16	0	-2.919506	-3.255716	0.708667
41	8	0	-3.900966	-2.277688	1.193483
42	8	0	-1.956433	-3.874302	1.621063
43	6	0	-0.692576	-3.056857	-0.813810
44	6	0	2.181034	-2.139018	3.041706
45	6	0	0.804046	-1.446604	3.022964
46	6	0	3.249552	-1.261091	3.718900
47	6	0	3.952282	-1.972495	-1.877592
48	6	0	5.408193	-2.405727	-2.145148
49	6	0	3.077014	-2.173311	-3.129567
50	6	0	1.642346	2.781097	2.498797
51	6	0	2.457497	3.554048	3.555752
52	6	0	0.172777	2.629079	2.935645
53	1	0	-1.564794	1.510122	-2.410039
54	1	0	5.274278	-0.586257	1.301324
55	1	0	4.973777	2.146494	0.915045
56	1	0	0.698108	5.196098	1.760783
57	1	0	0.905007	6.362356	-0.409056
58	1	0	2.110953	5.292189	-2.276559
59	1	0	3.471898	-4.613931	-1.630313
60	1	0	2.610863	-5.873700	0.315938
61	1	0	2.054505	-4.688624	2.406318
62	1	0	-7.052677	0.168354	-0.129119
63	1	0	-7.419545	-1.138855	-1.290058
64	1	0	-6.045124	-1.301539	-0.150385
65	1	0	-5.572097	1.350839	-3.369952
66	1	0	-7.149378	0.549139	-3.192334
67	1	0	-6.694567	1.863111	-2.078386
68	1	0	3.308803	3.797313	-3.149895
69	1	0	5.327117	3.359547	-1.719601

70	1	0	5.261580	2.451120	-3.232813
71	1	0	4.911945	1.635830	-1.711082
72	1	0	1.499737	2.137628	-3.386954
73	1	0	3.014082	1.576019	-4.113273
74	1	0	2.473914	0.916231	-2.562277
75	1	0	-5.114003	3.619743	-0.824431
76	1	0	-6.344969	4.107249	1.258754
77	1	0	-5.978935	2.699898	3.280050
78	1	0	-4.372353	0.801130	3.181530
79	1	0	-3.161865	0.298037	1.116624
80	1	0	-3.082619	-5.241591	-0.608234
81	1	0	-4.385428	-5.104982	0.610380
82	1	0	-4.455285	-4.115326	-0.891266
83	1	0	-0.364483	-2.671402	-1.779428
84	1	0	-0.764366	-4.145470	-0.879984
85	1	0	0.041952	-2.804869	-0.047638
86	1	0	2.067770	-3.013807	3.692480
87	1	0	0.527896	-1.144146	4.039163
88	1	0	0.807165	-0.550750	2.395342
89	1	0	0.027227	-2.121593	2.651368
90	1	0	4.235984	-1.735831	3.694352
91	1	0	2.981160	-1.115098	4.770155
92	1	0	3.333952	-0.270689	3.266013
93	1	0	3.969177	-0.899847	-1.669316
94	1	0	6.045681	-2.230399	-1.272833
95	1	0	5.823806	-1.842992	-2.987272
96	1	0	5.470949	-3.470221	-2.393002
97	1	0	2.053446	-1.824964	-2.957393
98	1	0	3.489393	-1.610265	-3.973044
99	1	0	3.031468	-3.225661	-3.427969
100	1	0	2.062284	1.773939	2.440482
101	1	0	3.512290	3.630584	3.273184
102	1	0	2.402231	3.046808	4.524386
103	1	0	2.075583	4.571285	3.690234
104	1	0	-0.314785	3.600736	3.064731
105	1	0	-0.402953	2.058070	2.200608
106	1	0	0.118471	2.103907	3.894757

Sum of electronic and zero-point Energies= -2590.608193
Sum of electronic and thermal Energies= -2590.552825
Sum of electronic and thermal Enthalpies= -2590.551881
Sum of electronic and thermal Free Energies= -2590.703645

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.496267	1.597435	-0.380301
2	6	0	1.121248	2.023718	-0.463312
3	6	0	2.845791	0.258657	-0.038014
4	7	0	0.834031	3.297137	-0.788150
5	6	0	4.173312	-0.134475	-0.023907
6	79	0	-0.365669	0.554450	-0.205729
7	6	0	-1.751402	-0.971418	0.026195
8	7	0	-2.587674	-1.150197	1.092045
9	6	0	-3.347158	-2.302470	0.932312
10	6	0	-2.972742	-2.862609	-0.242616
11	7	0	-2.003842	-2.033617	-0.796812

12	6	0	-2.810251	-0.212719	2.183256
13	6	0	-1.298982	-2.378950	-2.021395
14	6	0	-0.159541	-3.205432	-1.899121
15	6	0	0.514843	-3.567772	-3.072059
16	6	0	0.071147	-3.140438	-4.317179
17	6	0	-1.075198	-2.358223	-4.410119
18	6	0	-1.801319	-1.963774	-3.276783
19	6	0	-2.081224	-0.330587	3.388948
20	6	0	-2.365082	0.608926	4.390588
21	6	0	-3.331332	1.595760	4.225092
22	6	0	-4.060405	1.656838	3.044487
23	6	0	-3.822059	0.756110	1.999598
24	7	0	3.531548	2.492328	-0.390079
25	6	0	4.686607	2.174592	0.028423
26	7	0	5.903465	2.543452	-0.296527
27	6	0	6.241941	3.139980	-1.598699
28	6	0	7.022571	2.291244	0.616412
29	1	0	4.808610	0.226605	-0.829044
30	6	0	-3.067475	-1.139622	-3.541273
31	6	0	-4.376364	-1.736773	-2.990494
32	6	0	-2.918109	0.343512	-3.159376
33	6	0	-4.701151	0.815175	0.751705
34	6	0	-6.076129	0.168680	1.025766
35	6	0	-4.880583	2.246336	0.212344
36	6	0	-1.038031	-1.399015	3.739221
37	6	0	-1.562570	-2.847748	3.702112
38	6	0	0.290497	-1.262841	2.974403
39	6	0	0.316955	-3.771144	-0.563142
40	6	0	-0.159320	-5.229745	-0.390994
41	6	0	1.843428	-3.684660	-0.389066
42	6	0	4.718272	-1.271918	0.721422
43	6	0	4.153943	-1.697437	1.939512
44	6	0	4.690798	-2.781056	2.630014
45	6	0	5.808015	-3.454335	2.126835
46	6	0	6.388845	-3.033166	0.928216
47	6	0	5.852151	-1.950304	0.235843
48	6	0	-1.601252	3.683211	-2.099185
49	16	0	-0.812013	3.958715	-0.507467
50	8	0	-0.604792	5.389761	-0.316535
51	8	0	-1.462676	3.147693	0.515365
52	6	0	1.753745	4.337506	-1.317390
53	1	0	2.067801	-0.387988	0.354342
54	1	0	-4.072457	-2.610808	1.666871
55	1	0	-3.306000	-3.757765	-0.740822
56	1	0	1.392077	-4.202212	-3.006091
57	1	0	0.604402	-3.432298	-5.216971
58	1	0	-1.432298	-2.051282	-5.388879
59	1	0	-1.818406	0.551329	5.327287
60	1	0	-3.525733	2.305016	5.023864
61	1	0	-4.829451	2.413005	2.929902
62	1	0	6.778626	4.080793	-1.441656
63	1	0	6.882982	2.461746	-2.172827
64	1	0	5.325151	3.335014	-2.153389
65	1	0	7.528768	3.232767	0.852669
66	1	0	6.640406	1.842823	1.532446
67	1	0	7.744524	1.610239	0.152843
68	1	0	-3.175431	-1.158053	-4.631900
69	1	0	-4.462824	-2.800255	-3.235027
70	1	0	-5.229243	-1.223532	-3.446473

71	1	0	-4.470092	-1.624531	-1.908123
72	1	0	-2.036703	0.775674	-3.644923
73	1	0	-3.798859	0.906424	-3.487855
74	1	0	-2.813261	0.475673	-2.079250
75	1	0	-4.216225	0.235155	-0.038559
76	1	0	-5.981567	-0.872298	1.349804
77	1	0	-6.694703	0.185667	0.122277
78	1	0	-6.612673	0.712192	1.810412
79	1	0	-3.916240	2.744484	0.088293
80	1	0	-5.395065	2.216410	-0.754111
81	1	0	-5.492023	2.860605	0.880852
82	1	0	-0.797330	-1.201139	4.790139
83	1	0	-2.515505	-2.939802	4.232831
84	1	0	-0.843811	-3.510395	4.195438
85	1	0	-1.699618	-3.218256	2.683184
86	1	0	0.683425	-0.243774	3.046165
87	1	0	1.032352	-1.948002	3.399738
88	1	0	0.180002	-1.507345	1.915115
89	1	0	-0.132542	-3.180824	0.240129
90	1	0	-1.248935	-5.313412	-0.444679
91	1	0	0.161362	-5.624177	0.578780
92	1	0	0.261975	-5.872104	-1.171410
93	1	0	2.216532	-2.675774	-0.583021
94	1	0	2.122144	-3.959262	0.632526
95	1	0	2.370667	-4.370178	-1.060148
96	1	0	3.308112	-1.157187	2.353910
97	1	0	4.248796	-3.092745	3.571913
98	1	0	6.229376	-4.293867	2.671239
99	1	0	7.259834	-3.548450	0.534577
100	1	0	6.304648	-1.630548	-0.699889
101	1	0	-1.642662	2.611553	-2.288186
102	1	0	-2.605884	4.103667	-2.019946
103	1	0	-1.032934	4.208012	-2.868068
104	1	0	2.464297	3.858863	-1.987464
105	1	0	2.293417	4.835090	-0.512960
106	1	0	1.169141	5.080801	-1.857475

Sum of electronic and zero-point Energies= -2590.612537
Sum of electronic and thermal Energies= -2590.557222
Sum of electronic and thermal Enthalpies= -2590.556278
Sum of electronic and thermal Free Energies= -2590.707648

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.637703	0.220533	-0.232866
2	6	0	-2.613536	-0.876764	-0.368239
3	6	0	-2.226717	1.437621	-0.337353
4	7	0	-2.387994	-2.098910	0.175919
5	6	0	-3.691956	1.678808	-0.623887
6	79	0	0.434944	0.124917	-0.080381
7	6	0	2.496325	0.146418	0.002035
8	7	0	3.330090	-0.848324	0.425398
9	6	0	4.659884	-0.455589	0.314570
10	6	0	4.656475	0.813689	-0.160813
11	7	0	3.326377	1.166440	-0.362604
12	6	0	2.919626	-2.191196	0.795707

13	6	0	2.905308	2.500708	-0.755364
14	6	0	2.667769	3.430682	0.280265
15	6	0	2.275513	4.726464	-0.080389
16	6	0	2.134240	5.088080	-1.414012
17	6	0	2.394561	4.155660	-2.413928
18	6	0	2.790405	2.842075	-2.123522
19	6	0	2.780337	-3.132387	-0.248423
20	6	0	2.385180	-4.433478	0.090090
21	6	0	2.148432	-4.790374	1.411856
22	6	0	2.318823	-3.848557	2.422490
23	6	0	2.713187	-2.529142	2.154283
24	7	0	-3.769747	-0.759722	-1.051203
25	6	0	-4.313445	0.436896	-1.222130
26	7	0	-5.461493	0.515566	-1.906317
27	6	0	-6.054471	-0.706398	-2.466211
28	6	0	-6.123625	1.790176	-2.199427
29	1	0	-3.737141	2.478047	-1.374045
30	6	0	3.046092	1.929048	-3.329206
31	6	0	4.458636	1.319332	-3.410353
32	6	0	1.956035	0.858771	-3.525671
33	6	0	-4.426614	2.186417	0.629213
34	6	0	-4.518470	3.565456	0.857598
35	6	0	-5.134985	4.051279	2.011957
36	6	0	-5.667517	3.162591	2.946697
37	6	0	-5.580485	1.786983	2.722310
38	6	0	-4.961326	1.297238	1.571798
39	6	0	-3.681133	-3.796174	-1.646586
40	16	0	-3.660712	-3.374297	0.100295
41	8	0	-4.937755	-2.807269	0.519597
42	8	0	-3.075248	-4.497143	0.826476
43	6	0	-1.229344	-2.411683	1.033551
44	6	0	2.870623	-1.608483	3.371542
45	6	0	1.733621	-0.578174	3.507317
46	6	0	4.253354	-0.947979	3.530259
47	6	0	3.073263	-2.810051	-1.712257
48	6	0	4.297483	-3.600343	-2.217979
49	6	0	1.846737	-3.055437	-2.611823
50	6	0	2.848329	3.103716	1.760913
51	6	0	4.015256	3.909357	2.367675
52	6	0	1.549051	3.324224	2.559132
53	1	0	-1.642727	2.344179	-0.203893
54	1	0	5.471706	-1.108987	0.588770
55	1	0	5.464702	1.492692	-0.377430
56	1	0	2.090380	5.460530	0.697369
57	1	0	1.836031	6.098481	-1.677748
58	1	0	2.297364	4.450495	-3.454773
59	1	0	2.274954	-5.176179	-0.693750
60	1	0	1.846843	-5.803827	1.659042
61	1	0	2.151369	-4.140719	3.455102
62	1	0	-7.090627	-0.500293	-2.733428
63	1	0	-5.516078	-1.029478	-3.363877
64	1	0	-6.018871	-1.500678	-1.720026
65	1	0	-5.991685	2.495212	-1.380239
66	1	0	-5.745467	2.229427	-3.130604
67	1	0	-7.192852	1.608843	-2.313681
68	1	0	2.968320	2.599649	-4.193010
69	1	0	5.231395	2.074988	-3.235836
70	1	0	4.619553	0.908344	-4.412326
71	1	0	4.607604	0.504850	-2.697696

72	1	0	0.959887	1.311247	-3.553292
73	1	0	2.116997	0.333824	-4.473774
74	1	0	1.959892	0.117318	-2.723494
75	1	0	-4.106554	4.263199	0.132080
76	1	0	-5.201858	5.122512	2.175933
77	1	0	-6.151176	3.538997	3.842680
78	1	0	-5.997656	1.089921	3.442665
79	1	0	-4.910206	0.223660	1.410691
80	1	0	-2.701904	-4.199772	-1.904937
81	1	0	-4.450337	-4.564006	-1.755377
82	1	0	-3.922866	-2.903739	-2.218743
83	1	0	-0.322699	-2.507363	0.433470
84	1	0	-1.429067	-3.355243	1.536415
85	1	0	-1.095843	-1.622567	1.772801
86	1	0	2.770074	-2.282410	4.230300
87	1	0	1.840635	-0.027005	4.447803
88	1	0	1.733087	0.145337	2.688723
89	1	0	0.755928	-1.070272	3.518818
90	1	0	5.061924	-1.672948	3.391400
91	1	0	4.345443	-0.541644	4.542624
92	1	0	4.409111	-0.121346	2.833504
93	1	0	3.319865	-1.748565	-1.792128
94	1	0	5.183081	-3.402174	-1.606126
95	1	0	4.529885	-3.321328	-3.250785
96	1	0	4.115192	-4.679662	-2.197644
97	1	0	0.989826	-2.458893	-2.281729
98	1	0	2.075161	-2.777425	-3.645746
99	1	0	1.549984	-4.109437	-2.612516
100	1	0	3.104831	2.045618	1.854625
101	1	0	4.951293	3.727526	1.830111
102	1	0	4.166214	3.629491	3.415285
103	1	0	3.818518	4.985870	2.336225
104	1	0	1.239409	4.374254	2.546815
105	1	0	0.728301	2.724180	2.153428
106	1	0	1.695758	3.037441	3.605461

Sum of electronic and zero-point Energies= -2590.682825
Sum of electronic and thermal Energies= -2590.627776
Sum of electronic and thermal Enthalpies= -2590.626831
Sum of electronic and thermal Free Energies= -2590.779397

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.300463	-1.783446	0.323698
2	6	0	0.874881	-2.135004	0.374172
3	6	0	2.737242	-0.526224	0.630154
4	7	0	0.498320	-3.401985	0.487485
5	6	0	4.244006	-0.532645	0.582696
6	79	0	-0.452756	-0.523288	0.184172
7	6	0	-1.666947	1.138082	-0.030032
8	7	0	-2.789038	1.281735	-0.792698
9	6	0	-3.307165	2.564736	-0.661921
10	6	0	-2.489832	3.239648	0.182553
11	7	0	-1.494371	2.351825	0.572371
12	6	0	-3.475268	0.238613	-1.541058
13	6	0	-0.335675	2.745451	1.353740

14	6	0	0.754874	3.295533	0.643838
15	6	0	1.892729	3.660966	1.375633
16	6	0	1.937878	3.503179	2.755805
17	6	0	0.831480	2.996984	3.432238
18	6	0	-0.338563	2.611877	2.761416
19	6	0	-3.153582	-0.000542	-2.896772
20	6	0	-3.883415	-1.006012	-3.547175
21	6	0	-4.889986	-1.721162	-2.906908
22	6	0	-5.203926	-1.437084	-1.584182
23	6	0	-4.507389	-0.454143	-0.871446
24	7	0	3.362360	-2.671117	0.035948
25	6	0	4.478227	-1.990480	0.165065
26	7	0	5.691463	-2.529634	-0.071656
27	6	0	5.780118	-3.937058	-0.455181
28	6	0	6.940273	-1.893019	0.331644
29	1	0	4.636245	-0.379943	1.599162
30	6	0	-1.498329	2.122891	3.638182
31	6	0	-2.796257	2.942679	3.504379
32	6	0	-1.775075	0.611308	3.533686
33	6	0	-4.922870	-0.146453	0.565738
34	6	0	-6.251520	0.637340	0.599492
35	6	0	-5.021625	-1.416553	1.431027
36	6	0	-2.107566	0.732413	-3.746242
37	6	0	-2.281979	2.260851	-3.825114
38	6	0	-0.654657	0.342429	-3.415134
39	6	0	0.718550	3.568465	-0.858784
40	6	0	0.632505	5.085683	-1.128329
41	6	0	1.910525	2.946400	-1.606388
42	6	0	4.836855	0.536753	-0.330175
43	6	0	4.774019	0.402463	-1.724193
44	6	0	5.307934	1.389911	-2.552312
45	6	0	5.906825	2.524540	-1.999205
46	6	0	5.967685	2.667770	-0.611964
47	6	0	5.434153	1.678916	0.217742
48	6	0	-1.546054	-3.384932	2.383797
49	16	0	-1.270754	-3.813851	0.656888
50	8	0	-1.324224	-5.262668	0.508128
51	8	0	-2.043167	-2.931978	-0.211065
52	6	0	1.334248	-4.627827	0.587252
53	1	0	2.137386	0.336872	0.882406
54	1	0	-4.196838	2.872170	-1.186311
55	1	0	-2.519265	4.255686	0.540243
56	1	0	2.745718	4.083284	0.854585
57	1	0	2.824098	3.797078	3.310658
58	1	0	0.863966	2.907766	4.514238
59	1	0	-3.658416	-1.220023	-4.587892
60	1	0	-5.437228	-2.489043	-3.445169
61	1	0	-6.003112	-1.983866	-1.094886
62	1	0	4.921847	-4.200755	-1.072275
63	1	0	6.700637	-4.089923	-1.023467
64	1	0	5.795704	-4.593435	0.424513
65	1	0	7.686450	-2.017993	-0.458557
66	1	0	6.799870	-0.826429	0.493604
67	1	0	7.333273	-2.347382	1.251007
68	1	0	-1.147821	2.291187	4.663165
69	1	0	-2.596308	4.017325	3.561911
70	1	0	-3.475221	2.688275	4.324654
71	1	0	-3.324875	2.740680	2.569737
72	1	0	-0.857231	0.034597	3.689035

73	1	0	-2.497770	0.314885	4.301918
74	1	0	-2.186937	0.337149	2.559283
75	1	0	-4.156186	0.487968	1.019342
76	1	0	-6.183747	1.575979	0.040750
77	1	0	-6.529443	0.877993	1.630991
78	1	0	-7.064766	0.049741	0.161180
79	1	0	-4.106270	-2.009012	1.357253
80	1	0	-5.186570	-1.145450	2.479114
81	1	0	-5.857030	-2.054271	1.125807
82	1	0	-2.288768	0.366263	-4.763475
83	1	0	-3.317911	2.533159	-4.051547
84	1	0	-1.653049	2.658446	-4.628388
85	1	0	-1.989493	2.767953	-2.902495
86	1	0	-0.529320	-0.744632	-3.415751
87	1	0	0.023104	0.763203	-4.166228
88	1	0	-0.341367	0.714896	-2.436454
89	1	0	-0.185424	3.114534	-1.271640
90	1	0	-0.238023	5.534944	-0.639876
91	1	0	0.553646	5.277004	-2.203344
92	1	0	1.523370	5.605210	-0.760438
93	1	0	1.963305	1.865704	-1.448804
94	1	0	1.809164	3.125844	-2.681563
95	1	0	2.866130	3.376835	-1.292786
96	1	0	4.316337	-0.479989	-2.163021
97	1	0	5.260368	1.270555	-3.630566
98	1	0	6.328784	3.288174	-2.645347
99	1	0	6.439221	3.542362	-0.173598
100	1	0	5.490514	1.792514	1.297677
101	1	0	-1.383931	-2.315022	2.513957
102	1	0	-2.582489	-3.651866	2.599601
103	1	0	-0.867459	-3.977994	2.998193
104	1	0	2.366280	-4.342286	0.402714
105	1	0	0.988448	-5.350030	-0.151141
106	1	0	1.219430	-5.063915	1.583263

Sum of electronic and zero-point Energies= -2590.668915
Sum of electronic and thermal Energies= -2590.613704
Sum of electronic and thermal Enthalpies= -2590.612760
Sum of electronic and thermal Free Energies= -2590.763656

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.091593	1.120958	0.955213
2	6	0	0.385187	2.485393	0.601135
3	6	0	1.165884	0.490907	1.549453
4	7	0	-0.649937	3.349821	0.192598
5	6	0	2.520136	1.016141	1.621397
6	79	0	-1.602779	0.044480	0.455363
7	6	0	-3.215599	-1.110724	-0.132571
8	7	0	-4.547067	-0.803382	-0.091452
9	6	0	-5.311691	-1.848516	-0.601999
10	6	0	-4.448087	-2.835467	-0.944115
11	7	0	-3.168815	-2.366301	-0.668295
12	6	0	-5.103144	0.486250	0.273952
13	6	0	-1.964424	-3.168101	-0.802483
14	6	0	-1.558330	-3.912776	0.325854

15	6	0	-0.384285	-4.668571	0.224731
16	6	0	0.359685	-4.683035	-0.947664
17	6	0	-0.078654	-3.960977	-2.052597
18	6	0	-1.250839	-3.192252	-2.023255
19	6	0	-5.186937	1.464579	-0.740627
20	6	0	-5.730740	2.712277	-0.407453
21	6	0	-6.182643	2.977206	0.878866
22	6	0	-6.104824	1.988229	1.854811
23	6	0	-5.570080	0.719448	1.588893
24	7	0	1.599538	3.018538	0.578942
25	6	0	2.665813	2.336923	1.017134
26	7	0	3.868397	2.948650	0.854316
27	6	0	3.950378	4.292309	0.284052
28	6	0	5.149254	2.266221	0.978845
29	1	0	2.993651	0.195810	0.455492
30	6	0	-1.609283	-2.456186	-3.320225
31	6	0	-3.010720	-2.755927	-3.885931
32	6	0	-1.331815	-0.942801	-3.258085
33	6	0	3.278404	0.678600	2.890735
34	6	0	3.476213	-0.649602	3.301287
35	6	0	4.094927	-0.940734	4.518079
36	6	0	4.531292	0.084350	5.357376
37	6	0	4.329062	1.409335	4.969449
38	6	0	3.705404	1.701828	3.756664
39	6	0	0.569244	4.198342	-2.116405
40	16	0	-0.298280	4.815422	-0.667564
41	8	0	0.563257	5.738432	0.077784
42	8	0	-1.621164	5.286913	-1.096003
43	6	0	-1.914254	3.416971	0.953135
44	6	0	-5.539096	-0.262595	2.766394
45	6	0	-4.124561	-0.478115	3.336538
46	6	0	-6.265556	-1.601128	2.534461
47	6	0	-4.730764	1.224692	-2.177840
48	6	0	-5.919658	1.296018	-3.157348
49	6	0	-3.610686	2.199789	-2.589242
50	6	0	-2.341893	-3.942314	1.636073
51	6	0	-2.910727	-5.348932	1.911335
52	6	0	-1.492452	-3.445645	2.821552
53	1	0	1.038400	-0.510636	1.950461
54	1	0	-6.385754	-1.790032	-0.665577
55	1	0	-4.617639	-3.814642	-1.360573
56	1	0	-0.044747	-5.240443	1.082502
57	1	0	1.283488	-5.249600	-1.004420
58	1	0	0.511712	-3.974907	-2.963445
59	1	0	-5.798163	3.482101	-1.169570
60	1	0	-6.600680	3.949738	1.121752
61	1	0	-6.467921	2.198700	2.856825
62	1	0	4.782653	4.821809	0.758961
63	1	0	4.139615	4.242451	-0.796166
64	1	0	3.020371	4.831552	0.454029
65	1	0	5.020358	1.195221	1.109625
66	1	0	5.727816	2.433048	0.063706
67	1	0	5.721385	2.648967	1.832331
68	1	0	-0.905305	-2.859758	-4.057446
69	1	0	-3.222549	-3.830876	-3.888766
70	1	0	-3.065276	-2.405343	-4.922209
71	1	0	-3.805918	-2.251591	-3.331896
72	1	0	-0.291624	-0.747677	-2.985862
73	1	0	-1.515700	-0.492987	-4.240950

74	1	0	-1.971854	-0.439231	-2.529856
75	1	0	3.141962	-1.464066	2.670325
76	1	0	4.237217	-1.978784	4.806447
77	1	0	5.015624	-0.144896	6.302201
78	1	0	4.645764	2.222864	5.616643
79	1	0	3.540651	2.739538	3.484044
80	1	0	-0.124354	3.574893	-2.680011
81	1	0	0.840681	5.086994	-2.689675
82	1	0	1.452371	3.638223	-1.816986
83	1	0	-2.740740	3.646156	0.283905
84	1	0	-1.854400	4.182992	1.735944
85	1	0	-2.076321	2.445178	1.414421
86	1	0	-6.109106	0.245628	3.553687
87	1	0	-4.178278	-1.085622	4.247041
88	1	0	-3.468683	-0.986004	2.626492
89	1	0	-3.653353	0.475402	3.593022
90	1	0	-7.258279	-1.447697	2.097779
91	1	0	-6.401013	-2.111009	3.494275
92	1	0	-5.705912	-2.276291	1.883564
93	1	0	-4.318410	0.215415	-2.247311
94	1	0	-6.703895	0.579942	-2.890103
95	1	0	-5.585695	1.068979	-4.175232
96	1	0	-6.370641	2.293806	-3.171020
97	1	0	-2.746216	2.108939	-1.925327
98	1	0	-3.281361	1.982519	-3.610973
99	1	0	-3.943810	3.242026	-2.561105
100	1	0	-3.194032	-3.263684	1.547063
101	1	0	-3.550021	-5.690300	1.090447
102	1	0	-3.508766	-5.346549	2.829087
103	1	0	-2.110972	-6.086279	2.037118
104	1	0	-0.629259	-4.095003	2.999661
105	1	0	-1.119531	-2.433156	2.640065
106	1	0	-2.092220	-3.431415	3.738093
107	7	0	3.382259	-0.491682	-0.578692
108	16	0	3.134854	0.216477	-2.075291
109	16	0	3.554930	-2.148350	-0.393818
110	8	0	2.275526	-0.555959	-2.962620
111	8	0	2.855354	1.622994	-1.791467
112	8	0	3.484422	-2.878669	-1.653359
113	8	0	2.775999	-2.559933	0.771725
114	6	0	5.346959	-2.247721	0.148767
115	6	0	4.833202	0.229465	-2.876407
116	9	0	5.568013	-1.438741	1.189378
117	9	0	5.604743	-3.506052	0.506228
118	9	0	6.152697	-1.897483	-0.854996
119	9	0	5.185879	-0.989829	-3.270568
120	9	0	5.741047	0.698750	-2.012944
121	9	0	4.773961	1.040519	-3.933927

Sum of electronic and zero-point Energies= -4417.898350
Sum of electronic and thermal Energies= -4417.827785
Sum of electronic and thermal Enthalpies= -4417.826841
Sum of electronic and thermal Free Energies= -4418.012307

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

1	6	0	-0.817993	-1.078967	1.769146
2	6	0	0.440221	-1.588964	1.354621
3	6	0	-1.284083	0.194780	1.413816
4	7	0	0.776974	-2.873986	1.669045
5	6	0	-2.674993	0.273797	1.753889
6	79	0	1.778817	-0.307455	0.391923
7	6	0	3.099143	1.043378	-0.455952
8	7	0	4.461824	1.075626	-0.343138
9	6	0	4.988947	2.153393	-1.046235
10	6	0	3.943129	2.817902	-1.592805
11	7	0	2.794072	2.122932	-1.235719
12	6	0	5.308633	0.071592	0.279262
13	6	0	1.460759	2.614769	-1.532728
14	6	0	0.909682	3.549931	-0.629526
15	6	0	-0.364709	4.057702	-0.911638
16	6	0	-1.065838	3.652379	-2.040603
17	6	0	-0.488546	2.743532	-2.921524
18	6	0	0.788588	2.206357	-2.708027
19	6	0	5.695826	0.199177	1.632601
20	6	0	6.547712	-0.792322	2.140311
21	6	0	7.008176	-1.843679	1.355170
22	6	0	6.628805	-1.926577	0.021911
23	6	0	5.773025	-0.975992	-0.545892
24	7	0	-1.834849	-1.811818	2.399258
25	6	0	-2.900015	-1.043939	2.419780
26	7	0	-4.078951	-1.478544	2.996692
27	6	0	-4.079370	-2.843204	3.512185
28	6	0	-5.359590	-1.060598	2.433430
29	1	0	-3.167797	-0.020134	0.376449
30	6	0	1.299797	1.232673	-3.777373
31	6	0	2.690160	1.548674	-4.359339
32	6	0	1.185098	-0.244646	-3.353807
33	6	0	5.418477	-1.083978	-2.027549
34	6	0	6.588039	-0.595563	-2.907842
35	6	0	4.993764	-2.507340	-2.433620
36	6	0	5.291511	1.308281	2.611943
37	6	0	5.613901	2.743367	2.154410
38	6	0	3.839945	1.185769	3.111902
39	6	0	1.646437	4.053517	0.610701
40	6	0	1.993481	5.550244	0.474948
41	6	0	0.856063	3.785483	1.905539
42	6	0	-3.259612	1.578244	2.225766
43	6	0	-3.865232	1.684414	3.489925
44	6	0	-4.334476	2.911696	3.961028
45	6	0	-4.201605	4.064139	3.186595
46	6	0	-3.590696	3.973583	1.934421
47	6	0	-3.123951	2.747741	1.460445
48	6	0	1.065565	-3.764422	-0.925697
49	16	0	1.929081	-3.722023	0.654468
50	8	0	2.000179	-5.085620	1.181407
51	8	0	3.156480	-2.933993	0.513618
52	6	0	0.127462	-3.724823	2.695590
53	1	0	-0.715500	0.966234	0.912178
54	1	0	6.048683	2.344523	-1.078980
55	1	0	3.902937	3.706001	-2.201565
56	1	0	-0.811114	4.776715	-0.231987
57	1	0	-2.064513	4.028467	-2.232395
58	1	0	-1.043078	2.433981	-3.802351
59	1	0	6.857899	-0.727254	3.179375

60	1	0	7.667756	-2.593034	1.782874
61	1	0	6.996050	-2.743698	-0.589841
62	1	0	-3.177946	-3.014195	4.100331
63	1	0	-4.960563	-2.976420	4.146732
64	1	0	-4.105774	-3.590815	2.705394
65	1	0	-6.141277	-1.195437	3.187729
66	1	0	-5.338021	-0.009130	2.159277
67	1	0	-5.629841	-1.648950	1.545562
68	1	0	0.598533	1.360720	-4.610378
69	1	0	2.782558	2.606449	-4.628530
70	1	0	2.841493	0.961495	-5.271368
71	1	0	3.503165	1.298628	-3.674059
72	1	0	0.159278	-0.492946	-3.066228
73	1	0	1.466497	-0.892668	-4.192033
74	1	0	1.841915	-0.474142	-2.509810
75	1	0	4.562824	-0.432311	-2.222590
76	1	0	6.863089	0.439909	-2.683479
77	1	0	6.318787	-0.650402	-3.968192
78	1	0	7.477525	-1.216292	-2.754339
79	1	0	4.218481	-2.887447	-1.765078
80	1	0	4.609850	-2.501388	-3.459446
81	1	0	5.835711	-3.207279	-2.408168
82	1	0	5.926983	1.133195	3.488594
83	1	0	6.641386	2.824106	1.783649
84	1	0	5.513433	3.426946	3.004268
85	1	0	4.939936	3.097489	1.371278
86	1	0	3.641215	0.182595	3.500179
87	1	0	3.661663	1.905742	3.918754
88	1	0	3.113962	1.380229	2.319093
89	1	0	2.590829	3.510714	0.698362
90	1	0	2.590472	5.744987	-0.422165
91	1	0	2.566875	5.889276	1.344337
92	1	0	1.089769	6.165313	0.411503
93	1	0	0.669954	2.716557	2.042552
94	1	0	1.422241	4.143695	2.772084
95	1	0	-0.112865	4.294059	1.908940
96	1	0	-3.961109	0.799082	4.109813
97	1	0	-4.798439	2.964116	4.942429
98	1	0	-4.569494	5.018639	3.552168
99	1	0	-3.486517	4.860222	1.314305
100	1	0	-2.667775	2.696164	0.479531
101	1	0	0.950673	-2.746673	-1.296533
102	1	0	1.684307	-4.363803	-1.596339
103	1	0	0.090053	-4.226328	-0.772506
104	1	0	-0.120959	-3.090220	3.541765
105	1	0	0.837728	-4.494856	2.990194
106	1	0	-0.792446	-4.173293	2.319602
107	7	0	-3.652021	-0.315871	-0.814777
108	16	0	-4.445906	0.842800	-1.740288
109	16	0	-3.063048	-1.713168	-1.529333
110	8	0	-3.847461	2.153986	-1.502731
111	8	0	-4.726646	0.381512	-3.094235
112	8	0	-2.242056	-2.373687	-0.518322
113	8	0	-2.549983	-1.501537	-2.878718
114	6	0	-4.564241	-2.828899	-1.692524
115	6	0	-6.108332	0.897454	-0.878065
116	9	0	-4.147369	-3.987011	-2.210510
117	9	0	-5.085866	-3.056756	-0.481472
118	9	0	-5.496723	-2.302153	-2.479664

119	9	0	-6.621043	-0.332048	-0.772885
120	9	0	-6.926147	1.655451	-1.608289
121	9	0	-5.986839	1.429858	0.340639

Sum of electronic and zero-point Energies= -4417.876601
Sum of electronic and thermal Energies= -4417.805969
Sum of electronic and thermal Enthalpies= -4417.805025
Sum of electronic and thermal Free Energies= -4417.990160

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.708909	-0.316845	0.251631
2	6	0	2.265520	-1.587899	0.049217
3	6	0	2.673863	0.687498	0.461612
4	7	0	1.375982	-2.711176	-0.156014
5	6	0	4.053309	0.449996	0.451306
6	79	0	-0.302864	0.106726	0.148090
7	6	0	-2.312266	0.599395	0.023073
8	7	0	-3.399975	-0.185410	0.289323
9	6	0	-4.583241	0.520202	0.092831
10	6	0	-4.235868	1.759561	-0.329453
11	7	0	-2.844986	1.802441	-0.351300
12	6	0	-3.353829	-1.523463	0.849783
13	6	0	-2.094056	2.935630	-0.859618
14	6	0	-1.773649	2.935038	-2.234393
15	6	0	-1.067371	4.031914	-2.744662
16	6	0	-0.700730	5.092826	-1.927332
17	6	0	-1.041710	5.073886	-0.578464
18	6	0	-1.743374	4.005251	-0.002799
19	6	0	-3.228500	-1.630839	2.252144
20	6	0	-3.191579	-2.913826	2.812445
21	6	0	-3.281895	-4.046814	2.013576
22	6	0	-3.423162	-3.911124	0.636158
23	6	0	-3.469026	-2.656356	0.010811
24	7	0	3.573010	-1.877313	0.084730
25	6	0	4.463575	-0.897214	0.274559
26	7	0	5.831738	-1.254928	0.271693
27	6	0	6.157000	-2.553984	-0.298942
28	6	0	6.579111	-0.993034	1.502114
29	6	0	-2.016556	4.110688	1.502668
30	6	0	-3.490360	3.986574	1.932337
31	6	0	-1.104151	3.191270	2.336838
32	6	0	4.987300	1.604810	0.555912
33	6	0	4.804293	2.577365	1.553620
34	6	0	5.630727	3.700299	1.624217
35	6	0	6.657327	3.874356	0.695900
36	6	0	6.851062	2.914660	-0.301624
37	6	0	6.028539	1.792042	-0.371045
38	6	0	2.947126	-4.782904	-1.215263
39	16	0	1.570170	-3.656128	-1.529823
40	8	0	1.958256	-2.762563	-2.622059
41	8	0	0.364180	-4.493165	-1.633798
42	6	0	0.851003	-3.362988	1.049554
43	6	0	-3.627123	-2.662956	-1.514562
44	6	0	-2.350024	-2.237632	-2.261433
45	6	0	-4.874437	-1.931085	-2.047806

46	6	0	-3.155196	-0.421591	3.181515
47	6	0	-4.383604	-0.359426	4.111499
48	6	0	-1.843496	-0.401305	3.989351
49	6	0	-2.165450	1.808306	-3.186608
50	6	0	-3.140432	2.308294	-4.271564
51	6	0	-0.926253	1.140396	-3.813729
52	1	0	2.346629	1.717587	0.576507
53	1	0	-5.548333	0.072993	0.264372
54	1	0	-4.836507	2.609871	-0.607272
55	1	0	-0.804278	4.048642	-3.797563
56	1	0	-0.153366	5.936268	-2.338107
57	1	0	-0.754949	5.908201	0.055535
58	1	0	-3.093830	-3.020725	3.888435
59	1	0	-3.249940	-5.035918	2.461557
60	1	0	-3.495661	-4.800327	0.017061
61	1	0	7.241466	-2.603742	-0.445021
62	1	0	5.856108	-3.399704	0.340651
63	1	0	5.668552	-2.667234	-1.268375
64	1	0	6.337184	-0.008533	1.900367
65	1	0	6.368390	-1.747286	2.279923
66	1	0	7.652860	-1.015477	1.287731
67	1	0	-1.726310	5.137678	1.756176
68	1	0	-4.142936	4.610207	1.311813
69	1	0	-3.594891	4.327083	2.968188
70	1	0	-3.857713	2.959186	1.888986
71	1	0	-0.050072	3.375411	2.108986
72	1	0	-1.259421	3.379367	3.405482
73	1	0	-1.298404	2.134161	2.142350
74	1	0	4.012893	2.441666	2.285688
75	1	0	5.473217	4.436091	2.408320
76	1	0	7.302296	4.746990	0.749003
77	1	0	7.644643	3.044000	-1.032735
78	1	0	6.186870	1.046632	-1.142630
79	1	0	2.676641	-5.442577	-0.389142
80	1	0	3.101755	-5.363725	-2.126341
81	1	0	3.816423	-4.178189	-0.963563
82	1	0	0.375631	-2.596180	1.665174
83	1	0	1.641274	-3.852531	1.637450
84	1	0	0.094308	-4.092636	0.760349
85	1	0	-3.782481	-3.719938	-1.761762
86	1	0	-2.503815	-2.343197	-3.341534
87	1	0	-2.082878	-1.198140	-2.058569
88	1	0	-1.500884	-2.864800	-1.980525
89	1	0	-5.774127	-2.198659	-1.482201
90	1	0	-5.041566	-2.218382	-3.091370
91	1	0	-4.765137	-0.844396	-2.025510
92	1	0	-3.167482	0.484775	2.571885
93	1	0	-5.317595	-0.335135	3.540503
94	1	0	-4.343803	0.539965	4.735375
95	1	0	-4.425888	-1.225802	4.780088
96	1	0	-0.974576	-0.396972	3.324342
97	1	0	-1.799068	0.496058	4.615911
98	1	0	-1.763373	-1.270602	4.650789
99	1	0	-2.689467	1.038488	-2.615796
100	1	0	-4.040406	2.750707	-3.831263
101	1	0	-3.450169	1.476926	-4.913475
102	1	0	-2.676589	3.066106	-4.911935
103	1	0	-0.361018	1.843912	-4.434435
104	1	0	-0.253885	0.750495	-3.044083

105	1	0	-1.230639	0.304676	-4.452131

Sum of electronic and zero-point Energies= -2590.290693
Sum of electronic and thermal Energies= -2590.236361
Sum of electronic and thermal Enthalpies= -2590.235417
Sum of electronic and thermal Free Energies= -2590.384643

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.205179	1.799545	0.014321
2	6	0	0.843351	2.053410	-0.074934
3	6	0	2.794395	0.476779	-0.003779
4	7	0	0.369003	3.372727	0.023602
5	6	0	4.156489	0.621350	0.095207
6	79	0	-0.497158	0.459059	-0.078892
7	6	0	-1.758158	-1.173326	0.080421
8	7	0	-3.001588	-1.226460	0.648994
9	6	0	-3.514943	-2.518421	0.602189
10	6	0	-2.574554	-3.295916	0.015463
11	7	0	-1.510931	-2.460914	-0.312095
12	6	0	-3.787829	-0.095522	1.111270
13	6	0	-0.261617	-2.964955	-0.848765
14	6	0	0.703370	-3.414252	0.079543
15	6	0	1.900201	-3.941416	-0.422069
16	6	0	2.127444	-4.026768	-1.790152
17	6	0	1.153792	-3.588300	-2.681979
18	6	0	-0.065761	-3.050398	-2.246380
19	6	0	-3.745332	0.301003	2.467240
20	6	0	-4.562671	1.379801	2.834078
21	6	0	-5.388468	2.025457	1.920201
22	6	0	-5.424699	1.596088	0.600157
23	6	0	-4.628804	0.530282	0.165556
24	7	0	3.232791	2.753664	0.090602
25	6	0	4.361865	2.078258	0.131783
26	7	0	5.597854	2.724076	0.231332
27	6	0	5.532175	4.162554	0.460241
28	6	0	6.619042	2.362935	-0.752136
29	6	0	-1.042290	-2.608540	-3.343248
30	6	0	-2.445553	-3.240659	-3.279328
31	6	0	-1.117619	-1.078064	-3.504964
32	6	0	-4.736282	0.065677	-1.285191
33	6	0	-6.032968	-0.741181	-1.505637
34	6	0	-4.640505	1.230448	-2.288051
35	6	0	-2.901171	-0.317668	3.588763
36	6	0	-3.085863	-1.832078	3.801214
37	6	0	-1.411126	0.065285	3.513844
38	6	0	0.481261	-3.391942	1.590683
39	6	0	0.298444	-4.823974	2.134835
40	6	0	1.608819	-2.658174	2.340651
41	6	0	5.138609	-0.464899	0.248824
42	6	0	6.225072	-0.351763	1.138628
43	6	0	7.117124	-1.407778	1.320019
44	6	0	6.949175	-2.604885	0.620276
45	6	0	5.878500	-2.731506	-0.267844
46	6	0	4.987520	-1.675281	-0.454287
47	6	0	-0.506629	3.606268	-2.578937

48	16	0	-1.022931	3.813530	-0.861386
49	8	0	-1.245272	5.242777	-0.622816
50	8	0	-2.117674	2.866110	-0.615412
51	6	0	1.117303	4.496208	0.629252
52	1	0	2.240992	-0.451589	-0.046289
53	1	0	-4.488513	-2.756599	0.997431
54	1	0	-2.559817	-4.350131	-0.206838
55	1	0	2.661472	-4.285489	0.270200
56	1	0	3.059248	-4.441243	-2.164103
57	1	0	1.335680	-3.664875	-3.750269
58	1	0	-4.546919	1.714377	3.867516
59	1	0	-6.006616	2.858993	2.240630
60	1	0	-6.074727	2.097386	-0.109136
61	1	0	4.838714	4.373484	1.274838
62	1	0	6.531445	4.519281	0.731261
63	1	0	5.187950	4.718018	-0.426250
64	1	0	7.600724	2.692567	-0.395678
65	1	0	6.653861	1.284027	-0.894640
66	1	0	6.431641	2.838308	-1.729860
67	1	0	-0.593570	-2.988676	-4.269236
68	1	0	-2.390110	-4.325228	-3.136513
69	1	0	-2.968558	-3.057441	-4.224092
70	1	0	-3.060919	-2.822024	-2.480300
71	1	0	-0.120106	-0.650489	-3.644373
72	1	0	-1.723563	-0.826739	-4.383115
73	1	0	-1.562171	-0.593986	-2.632282
74	1	0	-3.894970	-0.600010	-1.493947
75	1	0	-6.087386	-1.613411	-0.845987
76	1	0	-6.092722	-1.096292	-2.540306
77	1	0	-6.916257	-0.122869	-1.311719
78	1	0	-3.756308	1.841125	-2.092827
79	1	0	-4.586084	0.836271	-3.308945
80	1	0	-5.520334	1.881192	-2.240296
81	1	0	-3.287537	0.152306	4.501509
82	1	0	-4.145895	-2.106501	3.833249
83	1	0	-2.639746	-2.120977	4.759001
84	1	0	-2.602404	-2.428924	3.024698
85	1	0	-1.286886	1.149345	3.438884
86	1	0	-0.893056	-0.276618	4.417323
87	1	0	-0.913959	-0.378721	2.648222
88	1	0	-0.442591	-2.845870	1.795044
89	1	0	-0.532862	-5.339870	1.642899
90	1	0	0.093032	-4.799802	3.210330
91	1	0	1.200773	-5.425368	1.980449
92	1	0	1.719351	-1.629207	1.988759
93	1	0	1.384053	-2.628657	3.412150
94	1	0	2.574835	-3.159038	2.221404
95	1	0	6.356910	0.574758	1.688646
96	1	0	7.944682	-1.296689	2.015858
97	1	0	7.646646	-3.425887	0.760878
98	1	0	5.744946	-3.653521	-0.828656
99	1	0	4.167427	-1.775798	-1.158707
100	1	0	-0.225898	2.564475	-2.734456
101	1	0	-1.359444	3.879836	-3.202868
102	1	0	0.337265	4.271115	-2.767423
103	1	0	1.652546	4.097625	1.488907
104	1	0	0.401775	5.253259	0.945442
105	1	0	1.852297	4.923840	-0.054837

Sum of electronic and zero-point Energies= -2590.263263
Sum of electronic and thermal Energies= -2590.208563
Sum of electronic and thermal Enthalpies= -2590.207619
Sum of electronic and thermal Free Energies= -2590.358657

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.054824	-0.418390	-0.518849
2	6	0	-1.560009	-1.635450	-1.099259
3	6	0	-1.738004	0.734063	-1.016325
4	7	0	-1.098704	-2.902980	-0.717233
5	6	0	-2.782996	0.727949	-1.928682
6	79	0	1.022841	-0.026446	-0.254978
7	6	0	3.039665	0.375264	-0.153311
8	7	0	4.020171	-0.456721	0.310543
9	6	0	5.274839	0.126252	0.167047
10	6	0	5.078251	1.350977	-0.375904
11	7	0	3.708613	1.489947	-0.578737
12	6	0	3.835808	-1.829530	0.743826
13	6	0	3.098732	2.724988	-1.039615
14	6	0	2.827670	3.711485	-0.063883
15	6	0	2.236010	4.906422	-0.490786
16	6	0	1.934219	5.119835	-1.830128
17	6	0	2.245155	4.145635	-2.772693
18	6	0	2.842424	2.927713	-2.415118
19	6	0	3.938320	-2.832914	-0.245499
20	6	0	3.785301	-4.166287	0.153330
21	6	0	3.537621	-4.492264	1.481246
22	6	0	3.457229	-3.484076	2.436424
23	6	0	3.610589	-2.128927	2.107043
24	7	0	-2.487465	-1.664536	-2.060527
25	6	0	-3.100347	-0.551161	-2.485528
26	7	0	-4.055832	-0.734290	-3.463000
27	6	0	-4.570770	-2.070741	-3.732942
28	6	0	-4.281401	0.220368	-4.540904
29	6	0	3.159798	1.969687	-3.571208
30	6	0	4.618748	1.481721	-3.645094
31	6	0	2.166659	0.798688	-3.692801
32	6	0	-3.555475	1.981143	-2.152085
33	6	0	-2.898092	3.185784	-2.453271
34	6	0	-3.611564	4.377610	-2.589433
35	6	0	-4.997726	4.389858	-2.429656
36	6	0	-5.664153	3.199774	-2.126829
37	6	0	-4.952130	2.009644	-1.987702
38	6	0	-1.552898	-4.421618	-3.009096
39	16	0	-1.923255	-4.335802	-1.248102
40	8	0	-3.367923	-4.211394	-1.058273
41	8	0	-1.208449	-5.449187	-0.615517
42	6	0	0.004493	-3.085220	0.235029
43	6	0	3.503559	-1.133096	3.268654
44	6	0	2.144493	-0.408764	3.319498
45	6	0	4.677927	-0.146952	3.410089
46	6	0	4.228430	-2.531042	-1.714669
47	6	0	5.621105	-3.052697	-2.122493
48	6	0	3.136007	-3.088967	-2.647118
49	6	0	3.215158	3.552505	1.405553

50	6	0	4.553492	4.270206	1.686831
51	6	0	2.130392	4.046898	2.378691
52	1	0	-1.476964	1.687667	-0.568441
53	1	0	6.175216	-0.380588	0.472798
54	1	0	5.773946	2.128213	-0.644733
55	1	0	2.010238	5.676437	0.238654
56	1	0	1.471982	6.051545	-2.143352
57	1	0	2.029856	4.329677	-3.821598
58	1	0	3.858630	-4.955750	-0.588084
59	1	0	3.413478	-5.530285	1.775125
60	1	0	3.271152	-3.746795	3.473689
61	1	0	-5.614793	-1.982550	-4.054541
62	1	0	-4.013377	-2.572648	-4.539019
63	1	0	-4.514702	-2.686512	-2.836546
64	1	0	-3.632003	1.086776	-4.440626
65	1	0	-4.064156	-0.262920	-5.503816
66	1	0	-5.320140	0.571735	-4.560447
67	1	0	3.013411	2.582178	-4.469377
68	1	0	5.324879	2.311882	-3.536788
69	1	0	4.797690	1.020137	-4.622145
70	1	0	4.852508	0.733804	-2.884369
71	1	0	1.134435	1.159331	-3.727524
72	1	0	2.363701	0.239055	-4.614560
73	1	0	2.241408	0.107223	-2.850401
74	1	0	-1.819502	3.182872	-2.585391
75	1	0	-3.082160	5.297084	-2.823990
76	1	0	-5.553781	5.316730	-2.536823
77	1	0	-6.741842	3.200087	-1.987916
78	1	0	-5.475395	1.090814	-1.740177
79	1	0	-0.473193	-4.526371	-3.120130
80	1	0	-2.062988	-5.311606	-3.383158
81	1	0	-1.925143	-3.516487	-3.482373
82	1	0	0.930876	-2.681433	-0.182160
83	1	0	0.124672	-4.150137	0.417253
84	1	0	-0.219571	-2.595376	1.180793
85	1	0	3.543513	-1.764720	4.164387
86	1	0	2.065298	0.178776	4.240046
87	1	0	2.011805	0.271512	2.474497
88	1	0	1.315484	-1.121898	3.305838
89	1	0	5.644608	-0.658561	3.345863
90	1	0	4.623955	0.337902	4.390359
91	1	0	4.658448	0.643473	2.656644
92	1	0	4.235890	-1.447046	-1.850865
93	1	0	6.409309	-2.624782	-1.494573
94	1	0	5.837879	-2.791104	-3.163740
95	1	0	5.680946	-4.142471	-2.032551
96	1	0	2.152016	-2.688717	-2.385450
97	1	0	3.350775	-2.813065	-3.685077
98	1	0	3.081563	-4.181587	-2.600179
99	1	0	3.359025	2.487577	1.607201
100	1	0	5.364437	3.897320	1.053351
101	1	0	4.849290	4.127866	2.731639
102	1	0	4.460825	5.347018	1.507622
103	1	0	2.011923	5.135264	2.339068
104	1	0	1.164347	3.583600	2.170834
105	1	0	2.416795	3.793905	3.404718
106	1	0	-1.309200	-0.258578	0.968958
107	7	0	-1.708888	0.017318	2.137185
108	16	0	-2.347195	-1.177571	3.127065

109	16	0	-1.418032	1.570138	2.664443
110	8	0	-1.545124	-2.387181	2.961903
111	8	0	-2.702570	-0.670762	4.445719
112	8	0	-0.938433	1.640308	4.037555
113	8	0	-0.676092	2.215008	1.577958
114	6	0	-3.963950	-1.521235	2.245500
115	6	0	-3.101045	2.402275	2.632262
116	9	0	-2.913412	3.708693	2.834902
117	9	0	-3.668041	2.217133	1.437928
118	9	0	-3.894382	1.915470	3.582141
119	9	0	-3.732749	-1.927790	0.998108
120	9	0	-4.710035	-0.413300	2.217579
121	9	0	-4.609472	-2.474037	2.915692

Sum of electronic and zero-point Energies= -4417.908444
Sum of electronic and thermal Energies= -4417.837750
Sum of electronic and thermal Enthalpies= -4417.836806
Sum of electronic and thermal Free Energies= -4418.024439

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.044328	-0.074383	1.081133
2	6	0	0.860048	-0.800548	1.112891
3	6	0	2.422161	0.788466	-0.044226
4	7	0	0.525304	-1.573249	2.270998
5	6	0	3.616912	1.358619	0.252571
6	79	0	-0.785718	0.305844	0.272083
7	6	0	-2.332479	1.515121	-0.331665
8	7	0	-3.676913	1.314002	-0.206129
9	6	0	-4.384397	2.371435	-0.765823
10	6	0	-3.469288	3.245417	-1.253346
11	7	0	-2.215236	2.721545	-0.960882
12	6	0	-4.292533	0.191866	0.480087
13	6	0	-0.967472	3.352724	-1.357020
14	6	0	-0.444306	3.023105	-2.627103
15	6	0	0.755382	3.628450	-3.021058
16	6	0	1.410894	4.530438	-2.192822
17	6	0	0.862118	4.850910	-0.956092
18	6	0	-0.334605	4.280999	-0.497266
19	6	0	-4.822378	-0.885635	-0.260520
20	6	0	-5.366807	-1.950795	0.474996
21	6	0	-5.402960	-1.944981	1.862914
22	6	0	-4.907208	-0.850045	2.563625
23	6	0	-4.348158	0.243340	1.894352
24	7	0	3.045366	-0.049482	2.038411
25	6	0	3.977353	0.771080	1.575967
26	7	0	5.109917	1.031202	2.292260
27	6	0	5.193476	0.502072	3.648094
28	6	0	6.404755	1.255556	1.655087
29	6	0	-0.774957	4.706068	0.909757
30	6	0	-2.248672	5.112702	1.084498
31	6	0	-0.337397	3.689781	1.983443
32	6	0	-3.901318	1.468485	2.690796
33	6	0	-5.075854	2.461264	2.839173
34	6	0	-3.316288	1.131468	4.073002
35	6	0	-4.962581	-1.004968	-1.783913

36	6	0	-6.331322	-0.451481	-2.239692
37	6	0	-3.834619	-0.457636	-2.669491
38	6	0	-1.124008	2.050110	-3.585057
39	6	0	-1.614034	2.770667	-4.857052
40	6	0	-0.211017	0.860465	-3.937442
41	6	0	4.317134	2.361148	-0.573761
42	6	0	4.519634	2.121058	-1.944319
43	6	0	5.123442	3.084162	-2.753329
44	6	0	5.537986	4.302257	-2.209484
45	6	0	5.345153	4.550902	-0.847550
46	6	0	4.741122	3.590635	-0.036952
47	6	0	1.922700	-1.510325	4.647391
48	16	0	0.457340	-0.861972	3.828532
49	8	0	-0.712211	-1.427467	4.522449
50	8	0	0.585455	0.591267	3.700243
51	6	0	-0.316641	-2.763216	2.062639
52	1	0	1.827539	0.958096	-0.930632
53	1	0	-5.461269	2.401645	-0.760703
54	1	0	-3.587033	4.190133	-1.757885
55	1	0	1.179343	3.382035	-3.989375
56	1	0	2.349964	4.977531	-2.503783
57	1	0	1.377901	5.558301	-0.313049
58	1	0	-5.767239	-2.802418	-0.068136
59	1	0	-5.821866	-2.791039	2.400142
60	1	0	-4.948373	-0.845339	3.646652
61	1	0	5.437839	-0.569646	3.658501
62	1	0	5.977644	1.044636	4.184411
63	1	0	4.239907	0.647021	4.154956
64	1	0	7.009889	0.338288	1.693305
65	1	0	6.284031	1.542413	0.614517
66	1	0	6.950853	2.048714	2.177163
67	1	0	-0.198608	5.619826	1.101491
68	1	0	-2.575611	5.801094	0.297614
69	1	0	-2.364846	5.629005	2.043413
70	1	0	-2.926915	4.257684	1.094723
71	1	0	0.735844	3.489403	1.925399
72	1	0	-0.556791	4.080300	2.983315
73	1	0	-0.846348	2.729143	1.876878
74	1	0	-3.110825	1.970228	2.127400
75	1	0	-5.469183	2.783585	1.869999
76	1	0	-4.753637	3.354390	3.385358
77	1	0	-5.899365	2.003087	3.398140
78	1	0	-2.537330	0.367592	4.021080
79	1	0	-2.874309	2.032594	4.509849
80	1	0	-4.089225	0.785554	4.768570
81	1	0	-4.988427	-2.085678	-1.967565
82	1	0	-7.154755	-0.893164	-1.670287
83	1	0	-6.493727	-0.669876	-3.300794
84	1	0	-6.382976	0.635944	-2.116506
85	1	0	-2.853615	-0.772185	-2.310828
86	1	0	-3.962499	-0.849865	-3.684378
87	1	0	-3.863675	0.632195	-2.743352
88	1	0	-2.002420	1.637531	-3.088318
89	1	0	-2.299772	3.590155	-4.616604
90	1	0	-2.140815	2.068414	-5.511702
91	1	0	-0.778766	3.193037	-5.425891
92	1	0	0.123214	0.338533	-3.036636
93	1	0	-0.747998	0.137102	-4.558543
94	1	0	0.677642	1.179981	-4.492197

95	1	0	4.213453	1.165460	-2.359707
96	1	0	5.279114	2.878023	-3.808710
97	1	0	6.014233	5.048741	-2.838852
98	1	0	5.663611	5.496224	-0.416544
99	1	0	4.584401	3.790499	1.019343
100	1	0	2.771782	-1.228601	4.025562
101	1	0	1.964615	-1.056635	5.639834
102	1	0	1.814847	-2.592883	4.727279
103	1	0	0.278063	-3.543513	1.583216
104	1	0	-1.175186	-2.525642	1.427134
105	1	0	-0.682640	-3.126745	3.020844
106	1	0	0.841327	-1.676568	-0.113345
107	7	0	0.992721	-2.545714	-1.024837
108	16	0	2.554915	-2.875550	-1.542966
109	16	0	-0.360850	-3.040951	-1.869249
110	6	0	3.134235	-3.937801	-0.114958
111	6	0	-0.512771	-4.888609	-1.542504
112	8	0	3.352355	-1.656120	-1.468497
113	8	0	2.571936	-3.730547	-2.722487
114	8	0	-1.497420	-2.460429	-1.152893
115	8	0	-0.226005	-2.891472	-3.312128
116	9	0	4.398107	-4.299151	-0.338539
117	9	0	3.061894	-3.255016	1.028760
118	9	0	2.370385	-5.031146	-0.020672
119	9	0	0.471698	-5.573916	-2.112442
120	9	0	-1.682861	-5.280933	-2.052601
121	9	0	-0.510481	-5.121229	-0.225556

Sum of electronic and zero-point Energies= -4417.878981
Sum of electronic and thermal Energies= -4417.807905
Sum of electronic and thermal Enthalpies= -4417.806961
Sum of electronic and thermal Free Energies= -4417.994665

A-pa

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.293812	-0.968297	-0.205042
2	6	0	0.899976	-1.890634	-0.157300
3	7	0	-2.700043	-1.076937	-0.200214
4	6	0	1.457717	-0.611166	-0.148344
5	7	0	-0.790432	0.267761	-0.283683
6	6	0	0.533114	0.470342	-0.248108
7	7	0	0.954379	1.803324	-0.271991
8	6	0	-0.046056	2.831387	-0.016836
9	6	0	1.954374	2.223074	-1.251761
10	6	0	2.924148	-0.465555	0.060223
11	6	0	3.829503	-1.231060	-0.693310
12	6	0	5.202851	-1.158689	-0.456140
13	6	0	5.698604	-0.318148	0.540155
14	6	0	4.809399	0.449747	1.296460
15	6	0	3.438480	0.378710	1.060529
16	6	0	-3.629650	1.393669	-0.999111
17	16	0	-3.667786	0.235735	0.375917
18	8	0	-3.051789	0.859588	1.546436
19	8	0	-5.027158	-0.307831	0.465110
20	6	0	-3.317536	-2.405697	-0.217759
21	1	0	1.563444	-2.746386	-0.072676

22	1	0	0.472005	3.744378	0.295421
23	1	0	-0.645289	3.072117	-0.909971
24	1	0	-0.724366	2.510881	0.773380
25	1	0	2.656349	1.420940	-1.467140
26	1	0	1.477243	2.533062	-2.195737
27	1	0	2.521505	3.074572	-0.861291
28	1	0	3.451496	-1.878312	-1.479865
29	1	0	5.884191	-1.756794	-1.054582
30	1	0	6.767023	-0.259524	0.725631
31	1	0	5.185375	1.102300	2.079413
32	1	0	2.752800	0.977556	1.650421
33	1	0	-4.097377	0.914024	-1.858948
34	1	0	-4.205428	2.265884	-0.683656
35	1	0	-2.588689	1.646207	-1.190273
36	1	0	-2.970449	-2.948250	-1.101799
37	1	0	-4.397096	-2.287970	-0.271225
38	1	0	-3.070496	-2.984424	0.680298
39	6	0	-0.475725	-2.103987	-0.185322
40	1	0	-0.875749	-3.107297	-0.143211

Sum of electronic and zero-point Energies= -1295.566471
Sum of electronic and thermal Energies= -1295.545950
Sum of electronic and thermal Enthalpies= -1295.545006
Sum of electronic and thermal Free Energies= -1295.615877

A-pb

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.631576	-0.832631	0.303106
2	6	0	0.675840	-1.431667	0.102151
3	7	0	-3.084328	-1.137845	0.581926
4	6	0	1.584914	-0.417597	0.038632
5	7	0	-0.515678	0.558040	0.345729
6	6	0	0.766921	0.815743	0.181591
7	7	0	1.261009	2.104946	0.210661
8	6	0	0.315944	3.152264	0.578784
9	6	0	2.211083	2.524192	-0.821371
10	6	0	3.050110	-0.573373	-0.014959
11	6	0	3.898992	0.189803	0.808009
12	6	0	5.277120	-0.016360	0.795925
13	6	0	5.838338	-0.987603	-0.035796
14	6	0	5.008247	-1.750778	-0.858645
15	6	0	3.629750	-1.544583	-0.850283
16	6	0	-3.501602	1.591242	0.420878
17	16	0	-3.772322	0.065605	-0.483154
18	8	0	-5.212915	-0.212586	-0.499807
19	8	0	-3.001506	0.096533	-1.723337
20	6	0	-4.016631	-2.148867	1.106530
21	1	0	0.886039	-2.493615	0.078854
22	1	0	-0.232012	2.854237	1.473244
23	1	0	0.876173	4.068239	0.788064
24	1	0	-0.411658	3.358945	-0.220088
25	1	0	2.818624	3.353061	-0.444999
26	1	0	2.875673	1.707179	-1.092152
27	1	0	1.686407	2.862326	-1.728098
28	1	0	3.465743	0.939083	1.463106
29	1	0	5.914398	0.579216	1.443492

30	1	0	6.912666	-1.145911	-0.044545
31	1	0	5.435104	-2.503961	-1.514786
32	1	0	2.989271	-2.127966	-1.505173
33	1	0	-2.423568	1.674261	0.573381
34	1	0	-3.891922	2.394250	-0.207489
35	1	0	-4.053718	1.532718	1.359146
36	1	0	-4.065873	-3.031929	0.456697
37	1	0	-5.013307	-1.720253	1.181460
38	1	0	-3.676844	-2.451313	2.100292
39	6	0	-1.771192	-1.568715	0.412030
40	1	0	-1.663236	-2.652215	0.387507

Sum of electronic and zero-point Energies= -1295.533642
Sum of electronic and thermal Energies= -1295.512648
Sum of electronic and thermal Enthalpies= -1295.511704
Sum of electronic and thermal Free Energies= -1295.584324

Cat

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.734241	0.353813	-0.170241
2	7	0	-2.832104	-0.449591	-0.266775
3	6	0	-3.971100	0.312001	-0.501959
4	6	0	-3.573564	1.606020	-0.575971
5	7	0	-2.200339	1.622289	-0.355273
6	6	0	-2.854892	-1.878165	0.003382
7	6	0	-1.385600	2.820748	-0.463282
8	6	0	-0.854006	3.124642	-1.735166
9	6	0	-0.079623	4.284715	-1.861810
10	6	0	0.150994	5.114738	-0.772641
11	6	0	-0.398580	4.797807	0.465416
12	6	0	-1.180639	3.650902	0.663315
13	6	0	-2.973407	-2.274692	1.353003
14	6	0	-3.001751	-3.647104	1.630883
15	6	0	-2.921988	-4.586841	0.611851
16	6	0	-2.821287	-4.165533	-0.710155
17	6	0	-2.785832	-2.808444	-1.059327
18	6	0	-1.698076	3.422949	2.088838
19	6	0	-3.226311	3.288537	2.228904
20	6	0	-0.957929	2.290667	2.825089
21	6	0	-2.666082	-2.494929	-2.555378
22	6	0	-1.314436	-1.875210	-2.954139
23	6	0	-3.850941	-1.707885	-3.148856
24	6	0	-3.091758	-1.289523	2.513395
25	6	0	-4.472025	-1.398156	3.192823
26	6	0	-1.952728	-1.469367	3.535558
27	6	0	-1.089899	2.262295	-2.972392
28	6	0	-1.873541	3.034997	-4.052326
29	6	0	0.233081	1.706642	-3.534460
30	1	0	-4.945650	-0.138193	-0.593103
31	1	0	-4.129424	2.511468	-0.754747
32	1	0	0.344106	4.536410	-2.828889
33	1	0	0.754048	6.010852	-0.886104
34	1	0	-0.216833	5.453121	1.312293
35	1	0	-3.085786	-3.977579	2.661227
36	1	0	-2.939758	-5.647556	0.843986
37	1	0	-2.760035	-4.906312	-1.501884

38	1	0	-1.437988	4.348311	2.616815
39	1	0	-3.752149	4.076015	1.678057
40	1	0	-3.502163	3.382266	3.284566
41	1	0	-3.597530	2.321325	1.882491
42	1	0	0.125615	2.422150	2.779238
43	1	0	-1.255085	2.276777	3.879599
44	1	0	-1.182215	1.309646	2.401272
45	1	0	-2.698375	-3.479689	-3.036443
46	1	0	-1.230566	-1.848948	-4.046668
47	1	0	-1.211047	-0.851366	-2.588615
48	1	0	-0.475964	-2.451474	-2.555800
49	1	0	-4.811423	-2.139130	-2.846618
50	1	0	-3.800771	-1.742126	-4.242444
51	1	0	-3.840415	-0.654539	-2.857672
52	1	0	-3.009375	-0.274043	2.118177
53	1	0	-5.286011	-1.232920	2.479052
54	1	0	-4.562678	-0.652756	3.989956
55	1	0	-4.620482	-2.385337	3.642817
56	1	0	-0.971937	-1.349961	3.066401
57	1	0	-2.039944	-0.722854	4.331833
58	1	0	-1.984222	-2.458160	4.004601
59	1	0	-1.703224	1.404417	-2.686678
60	1	0	-2.830616	3.402793	-3.667920
61	1	0	-2.079256	2.384973	-4.909220
62	1	0	-1.309069	3.898558	-4.419281
63	1	0	0.894436	2.510653	-3.874033
64	1	0	0.770560	1.124051	-2.780527
65	1	0	0.035731	1.054584	-4.391708
66	7	0	2.130850	-0.873476	0.569078
67	16	0	2.986991	-0.112224	1.787886
68	16	0	2.660536	-2.260219	-0.201145
69	8	0	2.074855	0.175449	2.893891
70	8	0	4.302416	-0.697828	2.010270
71	8	0	3.474929	-3.121527	0.643343
72	8	0	1.499120	-2.780588	-0.924126
73	6	0	3.310359	1.563383	1.001190
74	6	0	3.788811	-1.604747	-1.545365
75	9	0	4.144517	-2.621620	-2.332835
76	9	0	3.135546	-0.692651	-2.279212
77	9	0	4.878283	-1.046817	-1.021674
78	9	0	2.166324	2.243564	0.837534
79	9	0	3.900981	1.424181	-0.188144
80	9	0	4.111228	2.255425	1.813262
81	79	0	0.151084	-0.239484	0.177601

Sum of electronic and zero-point Energies= -3122.415365
Sum of electronic and thermal Energies= -3122.366998
Sum of electronic and thermal Enthalpies= -3122.366054
Sum of electronic and thermal Free Energies= -3122.502785

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.348090	-0.644685	-1.936926
2	6	0	2.517644	-0.418790	-1.476803
3	6	0	0.885772	-1.033146	-3.276266
4	7	0	3.666100	-0.293018	-0.912682

5	6	0	0.078311	-2.061421	-3.605903
6	79	0	-0.061430	0.042078	-0.495924
7	7	0	-2.473449	1.680362	0.473678
8	6	0	-3.395923	1.771592	1.508954
9	6	0	-3.021166	0.874440	2.455930
10	7	0	-1.887453	0.231631	1.975626
11	6	0	-2.564280	2.460138	-0.753790
12	6	0	-1.109407	-0.731267	2.735325
13	6	0	-0.029766	-0.229105	3.498514
14	6	0	0.751222	-1.148265	4.209524
15	6	0	0.470217	-2.510364	4.170493
16	6	0	-0.620404	-2.968995	3.441038
17	6	0	-1.452777	-2.100627	2.716633
18	6	0	-3.345331	1.932187	-1.804990
19	6	0	-3.448874	2.681766	-2.984097
20	6	0	-2.812092	3.908644	-3.114116
21	6	0	-2.068729	4.415329	-2.052696
22	6	0	-1.924441	3.719771	-0.843869
23	6	0	-0.476388	-3.124801	-2.763306
24	6	0	-1.641639	-3.786587	-3.200362
25	6	0	-2.205125	-4.815933	-2.452240
26	6	0	-1.602395	-5.223009	-1.257878
27	6	0	-0.434149	-4.593824	-0.823269
28	6	0	0.129089	-3.555267	-1.566040
29	6	0	4.302743	-1.197339	1.673940
30	16	0	4.336419	-1.776905	-0.028094
31	8	0	5.716049	-1.923583	-0.468674
32	8	0	3.322096	-2.799454	-0.238504
33	6	0	-1.078121	4.414208	0.230838
34	6	0	-1.749013	4.599531	1.604417
35	6	0	0.333679	3.811084	0.363686
36	6	0	-4.108014	0.615253	-1.704682
37	6	0	-5.630163	0.862270	-1.665162
38	6	0	-3.735282	-0.358525	-2.838317
39	6	0	0.262307	1.262731	3.645770
40	6	0	1.738212	1.610799	3.383076
41	6	0	-0.175712	1.763040	5.038617
42	6	0	-2.693340	-2.744487	2.086249
43	6	0	-3.151189	-2.244632	0.709312
44	6	0	-3.868418	-2.729527	3.089524
45	1	0	1.246216	-0.386950	-4.073467
46	1	0	-0.186326	-2.127348	-4.659859
47	1	0	-4.214463	2.471944	1.479694
48	1	0	-3.443440	0.641891	3.419781
49	1	0	1.575712	-0.788802	4.817306
50	1	0	1.086274	-3.211862	4.725268
51	1	0	-0.852682	-4.030094	3.439045
52	1	0	-4.045393	2.297308	-3.804957
53	1	0	-2.905106	4.478683	-4.033550
54	1	0	-1.588790	5.384285	-2.154600
55	1	0	-2.103355	-3.485146	-4.137009
56	1	0	-3.102857	-5.313165	-2.807278
57	1	0	-2.027218	-6.042728	-0.685852
58	1	0	0.060083	-4.928369	0.084119
59	1	0	1.070504	-3.125638	-1.244871
60	1	0	4.788634	-1.977887	2.263636
61	1	0	4.869547	-0.267797	1.734979
62	1	0	3.264204	-1.067150	1.979901
63	1	0	-0.933549	5.428259	-0.159191

64	1	0	-2.764236	4.995961	1.502302
65	1	0	-1.173029	5.319776	2.194561
66	1	0	-1.800394	3.673916	2.181965
67	1	0	0.839789	3.783767	-0.606460
68	1	0	0.936327	4.420807	1.046506
69	1	0	0.304329	2.790645	0.754759
70	1	0	-3.833764	0.129276	-0.767224
71	1	0	-5.911484	1.517066	-0.834051
72	1	0	-6.166086	-0.084922	-1.546150
73	1	0	-5.982676	1.330996	-2.589647
74	1	0	-2.657592	-0.544612	-2.865322
75	1	0	-4.241602	-1.317483	-2.689503
76	1	0	-4.037535	0.024134	-3.818595
77	1	0	-0.327827	1.806716	2.904757
78	1	0	2.055716	1.270651	2.391862
79	1	0	1.883698	2.694587	3.431162
80	1	0	2.404377	1.161969	4.126950
81	1	0	0.391319	1.268058	5.833738
82	1	0	-1.237382	1.568469	5.218926
83	1	0	-0.009329	2.841457	5.128106
84	1	0	-2.414275	-3.795583	1.947314
85	1	0	-2.320485	-2.162726	0.004500
86	1	0	-3.868078	-2.959751	0.294139
87	1	0	-3.660902	-1.280735	0.773419
88	1	0	-3.579987	-3.155534	4.054747
89	1	0	-4.706906	-3.313539	2.696616
90	1	0	-4.230570	-1.710700	3.264548
91	6	0	-1.548398	0.717078	0.747716
92	6	0	4.452023	0.930475	-0.930989
93	6	0	3.937719	2.070509	-0.307108
94	6	0	5.694289	0.942713	-1.569355
95	6	0	4.683799	3.248361	-0.330990
96	1	0	2.964778	2.035685	0.172448
97	6	0	6.432139	2.127102	-1.575566
98	1	0	6.072035	0.045806	-2.045176
99	6	0	5.930579	3.276240	-0.960665
100	1	0	4.291145	4.141993	0.143604
101	1	0	7.397951	2.149988	-2.069741
102	1	0	6.509588	4.194179	-0.974575

Sum of electronic and zero-point Energies= -2554.973832
Sum of electronic and thermal Energies= -2554.920534
Sum of electronic and thermal Enthalpies= -2554.919590
Sum of electronic and thermal Free Energies= -2555.068591

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.685469	-0.433904	-0.038640
2	6	0	1.837038	-1.736421	0.072875
3	6	0	2.720252	0.589235	-0.161480
4	7	0	1.168481	-2.889639	0.004677
5	6	0	3.763382	0.537290	-1.019710
6	79	0	-0.284901	0.288632	0.024885
7	6	0	-2.134344	1.189894	0.102275
8	7	0	-3.372489	0.681357	-0.159374
9	6	0	-4.346838	1.660778	0.004569

10	6	0	-3.705970	2.802964	0.352217
11	7	0	-2.351765	2.498326	0.424152
12	6	0	-3.700847	-0.710692	-0.418805
13	6	0	-1.319999	3.493858	0.659114
14	6	0	-0.908945	3.800341	1.977709
15	6	0	0.078993	4.786201	2.115315
16	6	0	0.627959	5.441835	1.017037
17	6	0	0.189689	5.129119	-0.263587
18	6	0	-0.794484	4.154252	-0.472993
19	6	0	-3.942459	-1.532644	0.704749
20	6	0	-4.312903	-2.863595	0.473086
21	6	0	-4.454189	-3.353832	-0.819531
22	6	0	-4.223592	-2.515837	-1.906687
23	6	0	-3.842545	-1.175232	-1.746934
24	7	0	3.660708	-2.258133	0.291805
25	6	0	4.336257	-1.955301	1.211613
26	7	0	5.095502	-1.636698	2.216514
27	6	0	4.893373	-2.272046	3.531546
28	6	0	6.201713	-0.679142	2.046719
29	6	0	-1.417886	3.164525	3.277778
30	6	0	-2.937893	3.251560	3.512405
31	6	0	-0.892909	1.732849	3.499263
32	6	0	-1.266162	3.879520	-1.899115
33	6	0	-2.000502	5.103190	-2.484152
34	6	0	-0.106024	3.440007	-2.812776
35	6	0	1.835663	-5.340406	1.132623
36	16	0	0.948264	-3.815561	1.492457
37	8	0	-0.473078	-4.121517	1.630680
38	8	0	1.663726	-3.067201	2.527887
39	6	0	4.799377	1.556364	-1.216774
40	6	0	5.873134	1.263569	-2.080039
41	6	0	6.901130	2.181174	-2.290567
42	6	0	6.876180	3.417422	-1.643991
43	6	0	5.813543	3.728188	-0.788464
44	6	0	4.787910	2.812615	-0.576371
45	6	0	-3.614866	-0.376369	-3.036309
46	6	0	-4.462461	0.900693	-3.189527
47	6	0	-2.125186	-0.107151	-3.322776
48	6	0	-3.876310	-1.020900	2.141903
49	6	0	-5.296480	-0.817889	2.711218
50	6	0	-3.046462	-1.937672	3.059541
51	1	0	2.557175	1.482357	0.437119
52	1	0	3.863475	-0.347620	-1.645273
53	1	0	-5.392554	1.451758	-0.149406
54	1	0	-4.079018	3.792320	0.559848
55	1	0	0.415773	5.047434	3.114424
56	1	0	1.385408	6.206266	1.163742
57	1	0	0.607341	5.653340	-1.117201
58	1	0	-4.503940	-3.516133	1.318246
59	1	0	-4.757256	-4.384231	-0.981394
60	1	0	-4.350719	-2.901588	-2.914183
61	1	0	3.946220	-2.811602	3.526843
62	1	0	5.720295	-2.954833	3.750713
63	1	0	4.856128	-1.491306	4.296181
64	1	0	6.146348	-0.225948	1.056786
65	1	0	6.114741	0.104037	2.804793
66	1	0	7.161289	-1.192249	2.163626
67	1	0	-0.966141	3.776128	4.067742
68	1	0	-3.316231	4.260543	3.318427

69	1	0	-3.156585	3.012882	4.558277
70	1	0	-3.501385	2.548535	2.894986
71	1	0	0.198359	1.696382	3.424099
72	1	0	-1.174582	1.383141	4.498472
73	1	0	-1.297731	1.027855	2.769280
74	1	0	-1.982533	3.054687	-1.875302
75	1	0	-2.852248	5.396482	-1.862162
76	1	0	-2.375597	4.877305	-3.487593
77	1	0	-1.335018	5.968821	-2.564957
78	1	0	0.398339	2.553924	-2.414993
79	1	0	-0.484668	3.198217	-3.811200
80	1	0	0.641801	4.231206	-2.927989
81	1	0	1.740244	-5.964363	2.023323
82	1	0	1.370867	-5.826503	0.275225
83	1	0	2.878614	-5.094694	0.932166
84	1	0	5.893843	0.304684	-2.592164
85	1	0	7.717385	1.932872	-2.962327
86	1	0	7.672295	4.137040	-1.808620
87	1	0	5.784419	4.692641	-0.289790
88	1	0	3.965387	3.081248	0.079660
89	1	0	-3.957480	-1.049387	-3.831243
90	1	0	-5.515363	0.714144	-2.954009
91	1	0	-4.412853	1.245041	-4.227645
92	1	0	-4.110058	1.719929	-2.558876
93	1	0	-2.012199	0.341116	-4.316055
94	1	0	-1.683825	0.575751	-2.592552
95	1	0	-1.546839	-1.035595	-3.301521
96	1	0	-3.383551	-0.045471	2.137179
97	1	0	-5.882754	-0.120896	2.103859
98	1	0	-5.245541	-0.418420	3.729403
99	1	0	-5.843625	-1.765665	2.750213
100	1	0	-2.054024	-2.135432	2.646874
101	1	0	-2.927187	-1.468068	4.041400
102	1	0	-3.535560	-2.903616	3.221244
103	6	0	0.800203	-3.496615	-1.258053
104	6	0	1.791279	-3.729007	-2.218629
105	6	0	-0.533978	-3.835671	-1.501047
106	6	0	1.436634	-4.298157	-3.441166
107	1	0	2.820579	-3.462367	-2.004159
108	6	0	-0.869353	-4.421499	-2.723507
109	1	0	-1.289934	-3.643049	-0.749246
110	6	0	0.108340	-4.650330	-3.693505
111	1	0	2.200334	-4.474719	-4.192293
112	1	0	-1.903813	-4.686590	-2.917163
113	1	0	-0.162727	-5.100267	-4.643561

Sum of electronic and zero-point Energies= -2782.291758
Sum of electronic and thermal Energies= -2782.231433
Sum of electronic and thermal Enthalpies= -2782.230489
Sum of electronic and thermal Free Energies= -2782.396553

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.315438	-0.752268	-0.928032
2	6	0	1.317036	-1.383474	-0.378341
3	6	0	2.897757	0.467433	-1.372606

4	7	0	1.293028	-2.738115	0.054313
5	6	0	3.286076	1.437376	-0.504504
6	79	0	-0.367202	-0.151487	-0.097663
7	6	0	-2.068048	0.958603	0.262864
8	7	0	-2.517362	1.417480	1.466656
9	6	0	-3.708484	2.116655	1.309671
10	6	0	-4.019000	2.076272	-0.009070
11	7	0	-2.999496	1.375082	-0.643116
12	6	0	-1.796245	1.353337	2.727320
13	6	0	-3.043819	1.009113	-2.048710
14	6	0	-2.473554	1.854829	-3.028140
15	6	0	-2.571753	1.429752	-4.360762
16	6	0	-3.210126	0.244381	-4.713257
17	6	0	-3.785328	-0.548975	-3.728818
18	6	0	-3.720104	-0.185777	-2.377524
19	6	0	-0.917124	2.420278	3.015128
20	6	0	-0.217657	2.383124	4.227614
21	6	0	-0.388325	1.333147	5.121222
22	6	0	-1.282583	0.310298	4.822627
23	6	0	-2.019678	0.288130	3.629637
24	7	0	3.778504	-2.094336	-1.281857
25	6	0	4.875762	-1.886111	-0.900255
26	7	0	6.080122	-1.655172	-0.456642
27	6	0	6.435038	-1.996095	0.932792
28	6	0	7.143452	-1.199124	-1.363639
29	6	0	-1.765363	3.194516	-2.792388
30	6	0	-2.608266	4.264448	-2.072291
31	6	0	-0.370818	3.050598	-2.155274
32	6	0	-4.417463	-1.063987	-1.341276
33	6	0	-5.950409	-0.963761	-1.483730
34	6	0	-3.951520	-2.529329	-1.410873
35	6	0	-2.983811	-0.890810	3.450457
36	6	0	-4.451356	-0.509684	3.179165
37	6	0	-2.475754	-1.946898	2.451278
38	6	0	-0.727489	3.621291	2.091178
39	6	0	0.747025	3.813368	1.692453
40	6	0	-1.300098	4.904326	2.727343
41	6	0	3.905907	2.716294	-0.829463
42	6	0	4.338263	3.537956	0.230774
43	6	0	4.954091	4.762103	-0.017477
44	6	0	5.144022	5.191493	-1.332298
45	6	0	4.713856	4.391158	-2.397300
46	6	0	4.101587	3.167737	-2.151649
47	6	0	2.830407	-4.721462	1.124057
48	16	0	2.087439	-3.129585	1.523372
49	8	0	1.120295	-3.332550	2.606607
50	8	0	3.152604	-2.134884	1.701784
51	1	0	3.070124	0.565739	-2.442513
52	1	0	3.122288	1.245896	0.554442
53	1	0	-4.217853	2.565715	2.146361
54	1	0	-4.857115	2.477677	-0.554596
55	1	0	-2.142918	2.055062	-5.138543
56	1	0	-3.271561	-0.049648	-5.756862
57	1	0	-4.301513	-1.461568	-4.008639
58	1	0	0.461615	3.192922	4.474730
59	1	0	0.161660	1.317045	6.057369
60	1	0	-1.423430	-0.497890	5.534079
61	1	0	5.522328	-2.186010	1.498053
62	1	0	7.085558	-2.876931	0.950474

63	1	0	6.965652	-1.149034	1.376466
64	1	0	6.718250	-0.966244	-2.339905
65	1	0	7.611738	-0.301264	-0.950240
66	1	0	7.901095	-1.981232	-1.477559
67	1	0	-1.595344	3.587477	-3.801796
68	1	0	-2.120682	5.239842	-2.171543
69	1	0	-2.719424	4.064121	-1.004071
70	1	0	-3.607412	4.348323	-2.511896
71	1	0	-0.424317	2.700889	-1.121803
72	1	0	0.244775	2.338597	-2.713550
73	1	0	0.141637	4.018996	-2.157871
74	1	0	-4.159473	-0.696774	-0.344799
75	1	0	-6.298867	0.069592	-1.387161
76	1	0	-6.444742	-1.561200	-0.710785
77	1	0	-6.283790	-1.336018	-2.458042
78	1	0	-2.867132	-2.611321	-1.300116
79	1	0	-4.420743	-3.108819	-0.609278
80	1	0	-4.229332	-3.000255	-2.359330
81	1	0	-2.986381	-1.382237	4.430476
82	1	0	-4.800615	0.263365	3.871672
83	1	0	-5.086132	-1.390429	3.321012
84	1	0	-4.613773	-0.155023	2.158626
85	1	0	-3.125258	-2.828896	2.484300
86	1	0	-2.474993	-1.572248	1.424284
87	1	0	-1.457312	-2.262958	2.693995
88	1	0	-1.284322	3.442512	1.167918
89	1	0	1.143797	2.912233	1.215858
90	1	0	0.844600	4.643908	0.985905
91	1	0	1.374381	4.043252	2.559952
92	1	0	-2.360789	4.791749	2.973051
93	1	0	-1.200009	5.749774	2.038722
94	1	0	-0.772214	5.161752	3.651389
95	1	0	4.189265	3.204179	1.254160
96	1	0	5.283390	5.380779	0.811533
97	1	0	5.620889	6.146707	-1.529673
98	1	0	4.855070	4.727820	-3.419778
99	1	0	3.763657	2.565426	-2.989121
100	1	0	3.518285	-4.579287	0.291135
101	1	0	3.352006	-5.046720	2.026093
102	1	0	2.044643	-5.430501	0.865649
103	6	0	0.328772	-3.636419	-0.522005
104	6	0	0.272816	-3.698710	-1.922812
105	6	0	-0.506686	-4.459701	0.246072
106	6	0	-0.610408	-4.576620	-2.547372
107	1	0	0.932877	-3.068437	-2.508530
108	6	0	-1.366496	-5.355608	-0.394625
109	1	0	-0.488381	-4.398884	1.326961
110	6	0	-1.426377	-5.417888	-1.786774
111	1	0	-0.644921	-4.616301	-3.632020
112	1	0	-2.002953	-5.997838	0.206867
113	1	0	-2.101674	-6.113553	-2.274984

Sum of electronic and zero-point Energies= -2782.275726
Sum of electronic and thermal Energies= -2782.215250
Sum of electronic and thermal Enthalpies= -2782.214306
Sum of electronic and thermal Free Energies= -2782.380815

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.904469	0.378685	-0.319252
2	6	0	2.784225	-0.649003	-0.008592
3	6	0	2.487523	1.662352	-0.642880
4	7	0	2.427061	-2.024102	0.048485
5	6	0	1.793547	2.689265	-1.201280
6	79	0	-0.151341	0.185067	-0.099911
7	6	0	-2.197814	0.205894	0.294785
8	7	0	-3.225736	-0.482379	-0.286509
9	6	0	-4.446943	-0.103254	0.261574
10	6	0	-4.184352	0.842726	1.193365
11	7	0	-2.806022	1.018192	1.212343
12	6	0	-3.120393	-1.595696	-1.213664
13	6	0	-2.160010	2.043234	2.015654
14	6	0	-1.668390	1.737357	3.305464
15	6	0	-1.062669	2.787040	4.012269
16	6	0	-0.968560	4.072847	3.490484
17	6	0	-1.502051	4.350817	2.237676
18	6	0	-2.112081	3.348072	1.474329
19	6	0	-3.149608	-2.894114	-0.654951
20	6	0	-3.093766	-3.983611	-1.533677
21	6	0	-3.017990	-3.794300	-2.908253
22	6	0	-3.021982	-2.504778	-3.430008
23	6	0	-3.090366	-1.369477	-2.609154
24	7	0	4.114972	-0.379370	0.233368
25	6	0	5.216746	-0.649780	0.578642
26	7	0	6.318909	-0.819172	1.229742
27	6	0	6.328120	-0.743042	2.711925
28	6	0	7.606317	-1.030604	0.541839
29	6	0	-1.757258	0.390215	4.033839
30	6	0	-3.193065	-0.131388	4.238616
31	6	0	-0.833987	-0.701592	3.465775
32	6	0	-2.753812	3.713696	0.136804
33	6	0	-4.131901	4.374303	0.356743
34	6	0	-1.864331	4.624686	-0.727462
35	6	0	3.298391	-4.320508	1.296489
36	16	0	2.382576	-2.792138	1.576105
37	8	0	1.016896	-3.162397	1.952021
38	8	0	3.168637	-1.922034	2.462273
39	6	0	2.334395	3.979073	-1.618891
40	6	0	1.590585	4.769521	-2.517651
41	6	0	2.072858	5.998245	-2.961646
42	6	0	3.304513	6.470478	-2.504251
43	6	0	4.049976	5.705764	-1.600112
44	6	0	3.573553	4.474933	-1.162967
45	6	0	-3.175007	-0.017711	-3.330329
46	6	0	-4.402123	0.837525	-2.961130
47	6	0	-1.876260	0.807886	-3.277576
48	6	0	-3.332326	-3.159555	0.839870
49	6	0	-4.765237	-3.661977	1.120998
50	6	0	-2.296339	-4.142839	1.413258
51	1	0	3.562196	1.784606	-0.511610
52	1	0	0.737046	2.524609	-1.404297
53	1	0	-5.375635	-0.540603	-0.065424
54	1	0	-4.837492	1.396749	1.846827
55	1	0	-0.668959	2.584527	5.004065
56	1	0	-0.497642	4.861429	4.069960

57	1	0	-1.451803	5.361720	1.847474
58	1	0	-3.128867	-4.991237	-1.131949
59	1	0	-2.983090	-4.649717	-3.576760
60	1	0	-2.993717	-2.365957	-4.506835
61	1	0	5.303903	-0.813834	3.075975
62	1	0	6.908524	-1.585277	3.097168
63	1	0	6.790512	0.195715	3.030225
64	1	0	7.443607	-1.063782	-0.535193
65	1	0	8.288073	-0.209264	0.780936
66	1	0	8.047258	-1.974080	0.875107
67	1	0	-1.380280	0.608267	5.040231
68	1	0	-3.851345	0.649750	4.633065
69	1	0	-3.181835	-0.952573	4.962736
70	1	0	-3.634177	-0.518179	3.316708
71	1	0	0.196198	-0.346216	3.374317
72	1	0	-0.829635	-1.569695	4.133018
73	1	0	-1.151804	-1.045963	2.479879
74	1	0	-2.913274	2.792621	-0.431011
75	1	0	-4.813103	3.724990	0.914345
76	1	0	-4.602022	4.609454	-0.603926
77	1	0	-4.029623	5.308291	0.919275
78	1	0	-0.856884	4.216477	-0.837913
79	1	0	-2.303800	4.736378	-1.724137
80	1	0	-1.770575	5.629446	-0.303480
81	1	0	3.275941	-4.859505	2.245179
82	1	0	2.804170	-4.901425	0.518509
83	1	0	4.321912	-4.075613	1.012629
84	1	0	0.633257	4.402780	-2.877272
85	1	0	1.488449	6.588075	-3.661181
86	1	0	3.680241	7.431145	-2.843088
87	1	0	5.001677	6.077513	-1.232234
88	1	0	4.151935	3.903029	-0.444010
89	1	0	-3.313639	-0.288421	-4.383759
90	1	0	-5.324268	0.248193	-2.992040
91	1	0	-4.507230	1.653717	-3.683469
92	1	0	-4.317976	1.288416	-1.969528
93	1	0	-1.955737	1.662954	-3.958522
94	1	0	-1.676687	1.191047	-2.273648
95	1	0	-1.012439	0.209257	-3.581777
96	1	0	-3.202906	-2.217573	1.378768
97	1	0	-5.523398	-2.961159	0.757689
98	1	0	-4.917219	-3.796549	2.196817
99	1	0	-4.947284	-4.625741	0.633950
100	1	0	-1.276676	-3.766272	1.307997
101	1	0	-2.481789	-4.290709	2.482152
102	1	0	-2.357277	-5.127053	0.937037
103	6	0	2.080789	-2.731318	-1.155664
104	6	0	2.889930	-2.559698	-2.288775
105	6	0	0.978601	-3.591687	-1.212915
106	6	0	2.592579	-3.237458	-3.468708
107	1	0	3.744108	-1.891584	-2.246031
108	6	0	0.709316	-4.289279	-2.392977
109	1	0	0.333709	-3.704061	-0.350692
110	6	0	1.506711	-4.114755	-3.523308
111	1	0	3.221025	-3.090625	-4.342011
112	1	0	-0.148654	-4.952421	-2.427530
113	1	0	1.284014	-4.652030	-4.439754

Sum of electronic and zero-point Energies= -2782.306485

Sum of electronic and thermal Energies= -2782.246496
Sum of electronic and thermal Enthalpies= -2782.245552
Sum of electronic and thermal Free Energies= -2782.409040

B-b1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.644657	-0.565839	-0.551400
2	6	0	1.439441	-1.194393	-0.308537
3	6	0	2.811260	0.870297	-0.756707
4	7	0	1.491404	-2.619862	-0.081183
5	6	0	3.985238	1.532958	-0.819610
6	79	0	-0.354596	-0.193779	-0.078700
7	6	0	-2.102704	0.855506	0.326081
8	7	0	-2.459721	1.360438	1.543408
9	6	0	-3.660398	2.054589	1.456180
10	6	0	-4.074296	1.964793	0.169012
11	7	0	-3.106497	1.238746	-0.517402
12	6	0	-1.654079	1.322032	2.753714
13	6	0	-3.274668	0.811655	-1.896147
14	6	0	-2.792187	1.608049	-2.960165
15	6	0	-2.997992	1.119149	-4.258230
16	6	0	-3.663985	-0.078603	-4.499257
17	6	0	-4.164270	-0.815991	-3.433681
18	6	0	-3.987833	-0.388066	-2.111677
19	6	0	-0.741762	2.381340	2.952704
20	6	0	0.026897	2.371687	4.123272
21	6	0	-0.105468	1.353879	5.059251
22	6	0	-1.027089	0.334001	4.845573
23	6	0	-1.834045	0.286216	3.699703
24	7	0	3.795889	-1.337230	-0.609153
25	6	0	4.946103	-1.574296	-0.633475
26	7	0	6.165308	-1.977915	-0.487977
27	6	0	6.666101	-2.312120	0.867240
28	6	0	7.107727	-2.040415	-1.621525
29	6	0	-2.093008	2.967913	-2.849536
30	6	0	-2.914973	4.063263	-2.142831
31	6	0	-0.661173	2.890838	-2.290775
32	6	0	-4.626525	-1.192244	-0.981537
33	6	0	-6.159482	-1.014516	-0.990979
34	6	0	-4.247360	-2.682478	-1.029512
35	6	0	-2.823094	-0.882960	3.615235
36	6	0	-4.304833	-0.477637	3.495487
37	6	0	-2.436391	-1.945704	2.570069
38	6	0	-0.591868	3.548999	1.980287
39	6	0	0.875808	3.792697	1.583527
40	6	0	-1.222319	4.831321	2.562116
41	6	0	4.181980	2.962704	-1.071872
42	6	0	5.436456	3.535606	-0.791725
43	6	0	5.673265	4.892172	-1.003356
44	6	0	4.660241	5.706788	-1.511418
45	6	0	3.412338	5.150537	-1.809510
46	6	0	3.174968	3.795905	-1.596341
47	6	0	2.695823	-4.844984	0.985630
48	16	0	2.092825	-3.205592	1.434870
49	8	0	1.008588	-3.367185	2.408092
50	8	0	3.246152	-2.373069	1.797928

51	1	0	1.870415	1.401952	-0.858913
52	1	0	4.909546	0.982957	-0.644201
53	1	0	-4.103845	2.533598	2.313493
54	1	0	-4.955113	2.343915	-0.322338
55	1	0	-2.635130	1.704965	-5.097836
56	1	0	-3.809700	-0.423347	-5.518705
57	1	0	-4.710226	-1.733775	-3.626195
58	1	0	0.732752	3.176168	4.302277
59	1	0	0.498761	1.359359	5.961508
60	1	0	-1.134373	-0.450761	5.588477
61	1	0	5.828851	-2.310317	1.565778
62	1	0	7.119831	-3.306290	0.836424
63	1	0	7.415730	-1.576742	1.172782
64	1	0	6.592628	-1.765745	-2.541872
65	1	0	7.936596	-1.348553	-1.447589
66	1	0	7.496527	-3.058403	-1.711415
67	1	0	-1.991179	3.301882	-3.888799
68	1	0	-2.457222	5.040503	-2.328643
69	1	0	-2.955873	3.923825	-1.059995
70	1	0	-3.940403	4.100559	-2.524274
71	1	0	-0.647137	2.603130	-1.236894
72	1	0	-0.062261	2.162067	-2.846130
73	1	0	-0.179369	3.870954	-2.380625
74	1	0	-4.259749	-0.803319	-0.028566
75	1	0	-6.445549	0.038646	-0.905381
76	1	0	-6.611638	-1.556726	-0.154071
77	1	0	-6.596938	-1.402055	-1.917039
78	1	0	-3.163291	-2.819765	-1.017734
79	1	0	-4.667450	-3.201314	-0.161538
80	1	0	-4.640635	-3.175361	-1.924616
81	1	0	-2.733926	-1.376770	4.589939
82	1	0	-4.569520	0.294410	4.225554
83	1	0	-4.937190	-1.349510	3.692900
84	1	0	-4.561956	-0.109682	2.499333
85	1	0	-3.094922	-2.816123	2.670580
86	1	0	-2.533245	-1.570452	1.548319
87	1	0	-1.404434	-2.279782	2.708336
88	1	0	-1.134759	3.306951	1.062798
89	1	0	1.341425	2.881926	1.196327
90	1	0	0.936019	4.564075	0.809297
91	1	0	1.475502	4.138453	2.431446
92	1	0	-2.282131	4.689869	2.796788
93	1	0	-1.141450	5.656563	1.846842
94	1	0	-0.716709	5.136444	3.484220
95	1	0	6.229602	2.907686	-0.392579
96	1	0	6.647873	5.312658	-0.774127
97	1	0	4.842352	6.763224	-1.683031
98	1	0	2.625410	5.775824	-2.221457
99	1	0	2.209700	3.375803	-1.859055
100	1	0	3.480859	-4.738542	0.237438
101	1	0	3.089755	-5.272549	1.909620
102	1	0	1.874615	-5.451415	0.607272
103	6	0	0.514666	-3.418360	-0.782051
104	6	0	0.564972	-3.366011	-2.183738
105	6	0	-0.425878	-4.246822	-0.153289
106	6	0	-0.308410	-4.136937	-2.947856
107	1	0	1.297167	-2.725383	-2.664086
108	6	0	-1.273998	-5.039188	-0.931025
109	1	0	-0.500073	-4.267902	0.926745

110	6	0	-1.222665	-4.988885	-2.324469
111	1	0	-0.259566	-4.084863	-4.031294
112	1	0	-1.990704	-5.687891	-0.436369
113	1	0	-1.890086	-5.604894	-2.918896

Sum of electronic and zero-point Energies= -2782.305407
Sum of electronic and thermal Energies= -2782.245438
Sum of electronic and thermal Enthalpies= -2782.244494
Sum of electronic and thermal Free Energies= -2782.408124

B-tsa2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.618502	-0.010360	-0.826852
2	6	0	-2.375277	-1.135841	-0.586995
3	6	0	-2.231190	1.044127	-1.548033
4	7	0	-1.810885	-2.321955	-0.035581
5	6	0	-3.475263	1.644559	-1.332254
6	79	0	0.383970	0.255155	-0.362764
7	6	0	2.305555	0.778007	0.196635
8	7	0	3.268261	0.070256	0.854354
9	6	0	4.388488	0.862472	1.082270
10	6	0	4.115597	2.089852	0.577234
11	7	0	2.842792	2.022130	0.024236
12	6	0	3.261066	-1.353498	1.148066
13	6	0	2.145178	3.177648	-0.512654
14	6	0	1.391536	3.952865	0.395744
15	6	0	0.726788	5.081068	-0.102055
16	6	0	0.811562	5.429306	-1.444322
17	6	0	1.576645	4.655933	-2.312595
18	6	0	2.269485	3.515675	-1.880557
19	6	0	3.808525	-2.207515	0.165410
20	6	0	3.883882	-3.575323	0.456559
21	6	0	3.430234	-4.075920	1.670887
22	6	0	2.900062	-3.209032	2.621850
23	6	0	2.809281	-1.826347	2.402101
24	7	0	-3.674869	-1.265017	-1.033197
25	6	0	-4.449711	-0.381125	-1.458187
26	7	0	-5.748499	-0.204244	-1.449032
27	6	0	-6.576303	-0.736677	-0.350256
28	6	0	-6.432387	0.617277	-2.448892
29	1	0	-3.789608	2.295797	-2.147274
30	6	0	3.080362	2.768551	-2.947021
31	6	0	4.584253	2.618166	-2.647972
32	6	0	2.450741	1.426933	-3.368213
33	6	0	-4.147907	1.990874	-0.059237
34	6	0	-5.118118	3.012262	-0.110121
35	6	0	-5.784244	3.429803	1.040454
36	6	0	-5.494161	2.830788	2.267974
37	6	0	-4.532349	1.818575	2.333552
38	6	0	-3.861335	1.400124	1.186496
39	6	0	-3.585296	-4.301157	0.834236
40	16	0	-2.569094	-2.918085	1.386493
41	8	0	-3.446257	-1.831708	1.841803
42	8	0	-1.530460	-3.452446	2.265813
43	6	0	2.232926	-0.994558	3.554704
44	6	0	0.781904	-0.540980	3.305249

45	6	0	3.117163	0.167275	4.044818
46	6	0	4.354373	-1.706342	-1.170107
47	6	0	5.888357	-1.855124	-1.232333
48	6	0	3.683694	-2.405997	-2.367471
49	6	0	1.302538	3.642335	1.888289
50	6	0	2.056206	4.703959	2.715641
51	6	0	-0.154914	3.502525	2.366659
52	1	0	-1.698696	1.379025	-2.440036
53	1	0	5.261241	0.478313	1.584059
54	1	0	4.700183	2.994735	0.552821
55	1	0	0.145159	5.696809	0.576493
56	1	0	0.295879	6.310920	-1.813594
57	1	0	1.651953	4.944716	-3.357017
58	1	0	4.313971	-4.250356	-0.276532
59	1	0	3.501719	-5.138145	1.886017
60	1	0	2.557020	-3.606539	3.572344
61	1	0	-7.052327	0.096217	0.176429
62	1	0	-7.347916	-1.394760	-0.761782
63	1	0	-5.941446	-1.285764	0.343437
64	1	0	-5.733145	0.894556	-3.236775
65	1	0	-7.251790	0.039149	-2.886657
66	1	0	-6.842325	1.518805	-1.983306
67	1	0	3.022236	3.417071	-3.829131
68	1	0	5.023053	3.565586	-2.318585
69	1	0	5.106672	2.311905	-3.560088
70	1	0	4.789303	1.861845	-1.886959
71	1	0	1.405710	1.558851	-3.666135
72	1	0	2.994967	1.013234	-4.224179
73	1	0	2.476072	0.688014	-2.563913
74	1	0	-5.330871	3.499629	-1.058515
75	1	0	-6.519861	4.226039	0.979498
76	1	0	-6.009948	3.152803	3.167456
77	1	0	-4.301853	1.345163	3.282800
78	1	0	-3.131278	0.605145	1.269717
79	1	0	-2.938589	-5.049367	0.375606
80	1	0	-4.067362	-4.708346	1.724668
81	1	0	-4.321976	-3.927939	0.122891
82	1	0	2.186519	-1.698991	4.393423
83	1	0	0.379724	-0.073851	4.211284
84	1	0	0.717839	0.189761	2.493838
85	1	0	0.141546	-1.389542	3.048725
86	1	0	4.154377	-0.150797	4.193544
87	1	0	2.740912	0.524532	5.008913
88	1	0	3.115117	1.018755	3.360444
89	1	0	4.128761	-0.640752	-1.258654
90	1	0	6.379269	-1.319587	-0.413463
91	1	0	6.272277	-1.454994	-2.176425
92	1	0	6.189764	-2.905798	-1.168627
93	1	0	2.595322	-2.303683	-2.332613
94	1	0	4.041613	-1.968672	-3.305329
95	1	0	3.917721	-3.475072	-2.395436
96	1	0	1.789372	2.681619	2.072478
97	1	0	3.106193	4.777954	2.415060
98	1	0	2.026035	4.449482	3.780051
99	1	0	1.606602	5.695213	2.596347
100	1	0	-0.707512	4.442618	2.269949
101	1	0	-0.688956	2.736582	1.796279
102	1	0	-0.176128	3.217274	3.423457
103	6	0	-1.065560	-3.236811	-0.865166

104	6	0	-1.460481	-3.454314	-2.193584
105	6	0	0.037918	-3.920211	-0.340959
106	6	0	-0.744988	-4.343027	-2.994846
107	1	0	-2.325079	-2.935630	-2.593582
108	6	0	0.724878	-4.831469	-1.144985
109	1	0	0.346731	-3.740397	0.681145
110	6	0	0.343918	-5.042935	-2.470845
111	1	0	-1.052211	-4.501165	-4.024314
112	1	0	1.575168	-5.362919	-0.730304
113	1	0	0.890140	-5.746223	-3.091773

Sum of electronic and zero-point Energies= -2782.292569
Sum of electronic and thermal Energies= -2782.234080
Sum of electronic and thermal Enthalpies= -2782.233136
Sum of electronic and thermal Free Energies= -2782.391820

B-tsb2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.594753	-0.341035	-0.126547
2	6	0	1.467289	-1.228879	-0.048871
3	6	0	2.450571	1.074722	-0.144329
4	7	0	1.699819	-2.558431	0.044383
5	6	0	3.576720	1.883843	-0.139603
6	79	0	-0.451444	-0.378338	0.026337
7	6	0	-2.296014	0.564896	0.126213
8	7	0	-3.235222	0.613193	-0.865016
9	6	0	-4.330295	1.370373	-0.467632
10	6	0	-4.069512	1.814847	0.784829
11	7	0	-2.826535	1.306026	1.144984
12	6	0	-3.213632	-0.142016	-2.109172
13	6	0	-2.178237	1.659660	2.397560
14	6	0	-1.425871	2.855469	2.420142
15	6	0	-0.817252	3.222938	3.626892
16	6	0	-0.958189	2.444391	4.768848
17	6	0	-1.734018	1.290767	4.726188
18	6	0	-2.375417	0.867821	3.552624
19	6	0	-2.674520	0.429493	-3.284565
20	6	0	-2.694206	-0.367486	-4.438288
21	6	0	-3.236943	-1.648245	-4.441552
22	6	0	-3.799779	-2.162752	-3.280525
23	6	0	-3.806594	-1.424585	-2.090983
24	7	0	3.849045	-0.810680	-0.411394
25	6	0	4.768905	-0.028941	-0.787570
26	7	0	6.075516	-0.021857	-0.666237
27	6	0	6.778615	-0.768098	0.390473
28	6	0	6.897213	0.831210	-1.529060
29	1	0	4.387396	1.599884	0.527904
30	6	0	-3.225944	-0.403012	3.670792
31	6	0	-4.699355	-0.264694	3.244121
32	6	0	-2.563509	-1.634317	3.026725
33	6	0	-4.511213	-1.997830	-0.862523
34	6	0	-6.040544	-1.826391	-0.989325
35	6	0	-4.159480	-3.473314	-0.597983
36	6	0	-2.104288	1.844011	-3.448180
37	6	0	-3.093244	2.979516	-3.119775
38	6	0	-0.747163	2.064288	-2.756421

39	6	0	-1.308799	3.785990	1.214956
40	6	0	-2.282967	4.976115	1.351154
41	6	0	0.126071	4.295295	0.991811
42	6	0	3.631520	3.269952	-0.612334
43	6	0	2.807089	3.727400	-1.658418
44	6	0	2.878494	5.048641	-2.092953
45	6	0	3.781862	5.937351	-1.502650
46	6	0	4.617835	5.493721	-0.475136
47	6	0	4.546035	4.173115	-0.038165
48	6	0	-0.163493	-4.113085	1.455873
49	16	0	0.360714	-3.748015	-0.224607
50	8	0	1.004597	-4.928291	-0.785944
51	8	0	-0.706270	-3.060091	-0.945703
52	1	0	1.460374	1.486981	-0.308901
53	1	0	-5.180735	1.520465	-1.111725
54	1	0	-4.647657	2.428426	1.455546
55	1	0	-0.234831	4.136857	3.671599
56	1	0	-0.481844	2.745114	5.697216
57	1	0	-1.862729	0.701924	5.629810
58	1	0	-2.282201	0.038414	-5.357602
59	1	0	-3.236321	-2.236063	-5.354475
60	1	0	-4.244583	-3.151776	-3.295086
61	1	0	7.613108	-1.319469	-0.053158
62	1	0	7.175464	-0.079215	1.145080
63	1	0	6.088285	-1.471142	0.855042
64	1	0	7.636551	0.221674	-2.058528
65	1	0	6.254542	1.333698	-2.250793
66	1	0	7.424457	1.582058	-0.930384
67	1	0	-3.253103	-0.606823	4.747532
68	1	0	-5.157260	0.630214	3.677448
69	1	0	-5.263541	-1.130821	3.605037
70	1	0	-4.825004	-0.223603	2.160079
71	1	0	-1.552726	-1.774061	3.424940
72	1	0	-3.146245	-2.534667	3.251038
73	1	0	-2.491641	-1.536553	1.940210
74	1	0	-4.187086	-1.431393	0.015131
75	1	0	-6.326731	-0.777772	-1.115906
76	1	0	-6.544302	-2.207761	-0.094900
77	1	0	-6.423720	-2.380471	-1.852580
78	1	0	-3.077951	-3.623541	-0.571159
79	1	0	-4.586381	-3.788083	0.360305
80	1	0	-4.574384	-4.135530	-1.364534
81	1	0	-1.907273	1.928585	-4.523194
82	1	0	-4.063747	2.813456	-3.598128
83	1	0	-2.697866	3.929278	-3.494920
84	1	0	-3.255275	3.096914	-2.045430
85	1	0	-0.031039	1.285240	-3.035861
86	1	0	-0.334218	3.033953	-3.056687
87	1	0	-0.837831	2.062151	-1.667488
88	1	0	-1.594613	3.226617	0.319803
89	1	0	-3.321679	4.645835	1.446472
90	1	0	-2.215726	5.627016	0.473273
91	1	0	-2.043134	5.577057	2.234637
92	1	0	0.848390	3.475312	0.967481
93	1	0	0.191260	4.832894	0.041318
94	1	0	0.439202	4.992016	1.775888
95	1	0	2.128179	3.033532	-2.145107
96	1	0	2.240425	5.384117	-2.905431
97	1	0	3.841202	6.964719	-1.848687

98	1	0	5.325223	6.177336	-0.015284
99	1	0	5.194750	3.835355	0.766652
100	1	0	-0.573263	-3.207897	1.901984
101	1	0	-0.929013	-4.887251	1.372753
102	1	0	0.697749	-4.488646	2.008806
103	6	0	2.927843	-3.210200	0.471403
104	6	0	3.696762	-3.960711	-0.421256
105	6	0	3.279187	-3.125664	1.822936
106	6	0	4.835504	-4.614249	0.044686
107	1	0	3.403627	-4.025997	-1.461525
108	6	0	4.427403	-3.776116	2.277786
109	1	0	2.668279	-2.540825	2.504397
110	6	0	5.205181	-4.522863	1.389931
111	1	0	5.434117	-5.200460	-0.645477
112	1	0	4.703767	-3.709044	3.325640
113	1	0	6.090727	-5.040078	1.746407

Sum of electronic and zero-point Energies= -2782.297401
Sum of electronic and thermal Energies= -2782.238806
Sum of electronic and thermal Enthalpies= -2782.237862
Sum of electronic and thermal Free Energies= -2782.396832

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.602539	0.293644	-0.270346
2	6	0	-2.525645	-0.844761	-0.389545
3	6	0	-2.229043	1.472906	-0.498800
4	7	0	-2.327166	-1.988639	0.317485
5	6	0	-3.684148	1.607101	-0.905225
6	79	0	0.470554	0.240465	-0.129663
7	6	0	2.525772	0.431498	-0.221237
8	7	0	3.499931	-0.522174	-0.307251
9	6	0	4.758842	0.063928	-0.377977
10	6	0	4.572080	1.405480	-0.323507
11	7	0	3.200774	1.619856	-0.251562
12	6	0	3.277814	-1.951918	-0.407832
13	6	0	2.606929	2.943465	-0.142116
14	6	0	2.384204	3.453242	1.155946
15	6	0	1.836307	4.737195	1.273431
16	6	0	1.531751	5.493499	0.149412
17	6	0	1.777621	4.973621	-1.117473
18	6	0	2.319905	3.694069	-1.308076
19	6	0	2.873652	-2.465503	-1.661525
20	6	0	2.647987	-3.843804	-1.763023
21	6	0	2.835193	-4.685923	-0.672731
22	6	0	3.269017	-4.157271	0.537990
23	6	0	3.509428	-2.784860	0.709721
24	7	0	-3.586185	-0.847593	-1.218244
25	6	0	-4.157595	0.309447	-1.525084
26	7	0	-5.208649	0.295334	-2.352940
27	6	0	-5.651054	-0.981102	-2.930482
28	6	0	-5.915050	1.515556	-2.755286
29	1	0	-3.721629	2.386911	-1.674857
30	6	0	2.498266	3.259699	-2.769502
31	6	0	3.883904	2.723249	-3.171424
32	6	0	1.371867	2.318347	-3.239544

33	6	0	-4.566766	2.076253	0.264551
34	6	0	-4.708730	3.450187	0.499489
35	6	0	-5.457155	3.909658	1.584245
36	6	0	-6.075445	2.999964	2.443213
37	6	0	-5.942585	1.629762	2.210670
38	6	0	-5.191633	1.165796	1.129050
39	6	0	-3.323607	-3.927054	-1.465759
40	16	0	-3.542194	-3.346847	0.221836
41	8	0	-4.884633	-2.804547	0.417120
42	8	0	-3.003559	-4.350777	1.128376
43	6	0	4.066346	-2.380656	2.081570
44	6	0	3.592719	-1.050379	2.686353
45	6	0	5.608101	-2.475918	2.103425
46	6	0	2.738885	-1.607670	-2.917408
47	6	0	3.828157	-1.973478	-3.946964
48	6	0	1.333838	-1.703949	-3.540756
49	6	0	2.731243	2.688019	2.428817
50	6	0	3.845110	3.400802	3.221970
51	6	0	1.488095	2.447979	3.307169
52	1	0	-1.692242	2.413178	-0.407887
53	1	0	5.656866	-0.523701	-0.471964
54	1	0	5.275529	2.221338	-0.348189
55	1	0	1.658700	5.148538	2.261973
56	1	0	1.116660	6.491288	0.256909
57	1	0	1.549764	5.575439	-1.992645
58	1	0	2.339613	-4.261931	-2.716056
59	1	0	2.660328	-5.753461	-0.768983
60	1	0	3.438895	-4.822952	1.379983
61	1	0	-6.630201	-0.838242	-3.386319
62	1	0	-4.950896	-1.328581	-3.697340
63	1	0	-5.718585	-1.731841	-2.141593
64	1	0	-5.945002	2.234807	-1.937811
65	1	0	-5.448217	1.974887	-3.634935
66	1	0	-6.943405	1.255157	-3.007528
67	1	0	2.373219	4.188173	-3.338974
68	1	0	4.688050	3.364635	-2.796618
69	1	0	3.958895	2.707957	-4.263637
70	1	0	4.065183	1.705507	-2.819980
71	1	0	0.388977	2.769497	-3.070527
72	1	0	1.473092	2.118057	-4.312029
73	1	0	1.390920	1.362939	-2.709112
74	1	0	-4.231479	4.164969	-0.166865
75	1	0	-5.560058	4.977347	1.752832
76	1	0	-6.662132	3.356117	3.284258
77	1	0	-6.429211	0.915617	2.868134
78	1	0	-5.113423	0.095201	0.959049
79	1	0	-2.302601	-4.295995	-1.563160
80	1	0	-4.038300	-4.743651	-1.590280
81	1	0	-3.531270	-3.106067	-2.147717
82	1	0	3.706346	-3.164915	2.758873
83	1	0	3.840105	-1.037472	3.753115
84	1	0	4.094929	-0.192962	2.233582
85	1	0	2.512451	-0.917702	2.588716
86	1	0	5.955521	-3.446502	1.737945
87	1	0	5.978598	-2.345014	3.125409
88	1	0	6.068152	-1.697688	1.486388
89	1	0	2.894332	-0.562566	-2.641663
90	1	0	4.831664	-1.870467	-3.522297
91	1	0	3.760952	-1.317063	-4.820700

92	1	0	3.720065	-3.005466	-4.296361
93	1	0	0.565576	-1.399974	-2.822420
94	1	0	1.263676	-1.047409	-4.414216
95	1	0	1.108297	-2.721673	-3.876407
96	1	0	3.112990	1.706399	2.146025
97	1	0	4.744443	3.541589	2.613784
98	1	0	4.120720	2.811125	4.102346
99	1	0	3.523287	4.387259	3.571306
100	1	0	1.054844	3.388762	3.662569
101	1	0	0.714710	1.904357	2.755502
102	1	0	1.759267	1.856764	4.188138
103	6	0	-1.501914	-2.041094	1.500018
104	6	0	-1.880317	-1.288525	2.617263
105	6	0	-0.415294	-2.915612	1.559921
106	6	0	-1.150246	-1.400303	3.799051
107	1	0	-2.742203	-0.631701	2.559095
108	6	0	0.299057	-3.031049	2.751011
109	1	0	-0.140121	-3.503202	0.691495
110	6	0	-0.065199	-2.276752	3.868956
111	1	0	-1.441908	-0.819073	4.668051
112	1	0	1.135353	-3.719550	2.804684
113	1	0	0.489099	-2.379790	4.796824

Sum of electronic and zero-point Energies= -2782.362471
Sum of electronic and thermal Energies= -2782.304285
Sum of electronic and thermal Enthalpies= -2782.303341
Sum of electronic and thermal Free Energies= -2782.462557

B-b2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.478804	-0.560606	-0.052349
2	6	0	-1.261468	-1.369819	-0.121236
3	6	0	-2.538029	0.728654	-0.498438
4	7	0	-1.399006	-2.693997	-0.172361
5	6	0	-3.966574	1.191871	-0.352536
6	79	0	0.542890	-0.329758	-0.083036
7	6	0	2.261817	0.821892	-0.073398
8	7	0	3.386174	0.668319	0.683348
9	6	0	4.312775	1.661529	0.388448
10	6	0	3.754527	2.457991	-0.555410
11	7	0	2.501970	1.926777	-0.839132
12	6	0	3.686622	-0.439139	1.578352
13	6	0	1.529122	2.584369	-1.693079
14	6	0	0.714937	3.569898	-1.091608
15	6	0	-0.245740	4.201192	-1.892915
16	6	0	-0.380540	3.878978	-3.238222
17	6	0	0.463382	2.932190	-3.811826
18	6	0	1.445968	2.263022	-3.067452
19	6	0	3.344113	-0.366547	2.948028
20	6	0	3.694649	-1.468016	3.742090
21	6	0	4.364557	-2.570840	3.222763
22	6	0	4.714779	-2.595737	1.878963
23	6	0	4.385962	-1.534854	1.026958
24	7	0	-3.709600	-1.042882	0.429778
25	6	0	-4.576531	-0.069738	0.280242
26	7	0	-5.865876	-0.177360	0.669786

27	6	0	-6.331965	-1.450121	1.215489
28	6	0	-6.900820	0.763381	0.260413
29	1	0	-4.403582	1.346420	-1.350222
30	6	0	2.335119	1.280430	-3.840077
31	6	0	3.844509	1.582954	-3.775618
32	6	0	2.045167	-0.201328	-3.533846
33	6	0	4.834998	-1.589392	-0.431872
34	6	0	6.353998	-1.345965	-0.550054
35	6	0	4.442756	-2.912661	-1.115380
36	6	0	2.644832	0.792273	3.669828
37	6	0	3.335036	2.162773	3.535848
38	6	0	1.135837	0.884338	3.373671
39	6	0	0.883705	4.018260	0.358967
40	6	0	1.510789	5.427380	0.416590
41	6	0	-0.431849	3.972203	1.155335
42	6	0	-4.106678	2.486001	0.443245
43	6	0	-3.936359	2.491940	1.834914
44	6	0	-4.046673	3.682224	2.553822
45	6	0	-4.323646	4.881339	1.892419
46	6	0	-4.489591	4.884014	0.506473
47	6	0	-4.380637	3.692273	-0.213677
48	6	0	0.475122	-3.828702	-1.919590
49	16	0	0.085044	-3.778028	-0.163110
50	8	0	-0.403841	-5.081412	0.262608
51	8	0	1.139381	-3.083446	0.568072
52	1	0	-1.733013	1.329603	-0.897878
53	1	0	5.269198	1.708724	0.882509
54	1	0	4.123804	3.341894	-1.048868
55	1	0	-0.884824	4.961396	-1.455599
56	1	0	-1.125776	4.381066	-3.848202
57	1	0	0.371821	2.709611	-4.871018
58	1	0	3.441963	-1.447879	4.798163
59	1	0	4.624315	-3.402851	3.870195
60	1	0	5.254152	-3.449504	1.482366
61	1	0	-5.516237	-1.933715	1.750550
62	1	0	-7.164251	-1.258985	1.897772
63	1	0	-6.671504	-2.126346	0.420069
64	1	0	-7.594173	0.926529	1.090828
65	1	0	-6.469549	1.725649	-0.008418
66	1	0	-7.474157	0.375592	-0.593116
67	1	0	2.049761	1.429506	-4.888024
68	1	0	4.047656	2.640341	-3.972843
69	1	0	4.366758	0.998063	-4.539660
70	1	0	4.283937	1.322835	-2.809771
71	1	0	0.978387	-0.421559	-3.646125
72	1	0	2.600499	-0.837813	-4.231713
73	1	0	2.341018	-0.474464	-2.517841
74	1	0	4.331272	-0.787835	-0.979341
75	1	0	6.644641	-0.380671	-0.123828
76	1	0	6.664339	-1.358508	-1.600139
77	1	0	6.918309	-2.122976	-0.024116
78	1	0	3.378218	-3.120068	-0.980068
79	1	0	4.661827	-2.860813	-2.187122
80	1	0	5.002582	-3.761763	-0.710927
81	1	0	2.723958	0.529567	4.731190
82	1	0	4.409121	2.090197	3.735113
83	1	0	2.909868	2.857473	4.267622
84	1	0	3.200426	2.609522	2.547891
85	1	0	0.644605	-0.080847	3.530349

86	1	0	0.669850	1.615716	4.043367
87	1	0	0.936258	1.197606	2.345596
88	1	0	1.577039	3.334155	0.854157
89	1	0	2.471843	5.464746	-0.106132
90	1	0	1.679009	5.726713	1.456115
91	1	0	0.854053	6.172529	-0.044268
92	1	0	-0.870509	2.970779	1.150336
93	1	0	-0.245213	4.252939	2.196849
94	1	0	-1.179832	4.666469	0.760812
95	1	0	-3.727835	1.562580	2.357843
96	1	0	-3.920939	3.672234	3.632420
97	1	0	-4.416039	5.805550	2.454605
98	1	0	-4.713515	5.810071	-0.014808
99	1	0	-4.517388	3.699530	-1.292429
100	1	0	0.745543	-2.824985	-2.248248
101	1	0	1.318807	-4.513896	-2.023745
102	1	0	-0.396087	-4.214772	-2.449400
103	6	0	-2.617777	-3.438580	-0.435932
104	6	0	-3.166647	-3.379877	-1.719417
105	6	0	-3.181139	-4.244992	0.554367
106	6	0	-4.313482	-4.120355	-2.006488
107	1	0	-2.711751	-2.747678	-2.476386
108	6	0	-4.324220	-4.982006	0.255964
109	1	0	-2.731526	-4.286286	1.539025
110	6	0	-4.892275	-4.920751	-1.020235
111	1	0	-4.748765	-4.074651	-2.999908
112	1	0	-4.769526	-5.610860	1.020385
113	1	0	-5.779601	-5.503763	-1.246959

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.134235	-1.015307	0.715141
2	6	0	-0.355060	-2.367652	0.292398
3	6	0	-1.239219	-0.489047	1.358627
4	7	0	0.761298	-3.143900	-0.135933
5	6	0	-2.555107	-1.109162	1.424781
6	79	0	1.509477	0.172270	0.308589
7	6	0	2.967546	1.567620	-0.181018
8	7	0	4.294859	1.435516	-0.487435
9	6	0	4.858998	2.670634	-0.796525
10	6	0	3.880670	3.596218	-0.656678
11	7	0	2.727171	2.910714	-0.296596
12	6	0	5.046480	0.202563	-0.632353
13	6	0	1.482898	3.576700	0.048472
14	6	0	1.279884	3.897014	1.407957
15	6	0	0.084796	4.536902	1.759646
16	6	0	-0.870668	4.846806	0.801513
17	6	0	-0.633170	4.542397	-0.535018
18	6	0	0.545270	3.911416	-0.957183
19	6	0	4.990506	-0.449246	-1.883331
20	6	0	5.774299	-1.596708	-2.063497
21	6	0	6.604164	-2.063879	-1.052515
22	6	0	6.647962	-1.395142	0.167319
23	6	0	5.872072	-0.255068	0.421326
24	7	0	-1.525056	-2.983312	0.255861

25	6	0	-2.631496	-2.397358	0.739273
26	7	0	-3.791674	-3.073596	0.545225
27	6	0	-3.798917	-4.368826	-0.135129
28	6	0	-5.113216	-2.507798	0.779993
29	1	0	-3.138770	-0.261177	0.344311
30	6	0	0.681226	3.669610	-2.465986
31	6	0	1.847183	4.429427	-3.130456
32	6	0	0.664931	2.187354	-2.876588
33	6	0	-3.293446	-0.913886	2.736461
34	6	0	-3.579060	0.364077	3.242413
35	6	0	-4.175687	0.523138	4.494247
36	6	0	-4.501660	-0.586785	5.273599
37	6	0	-4.211274	-1.862903	4.789749
38	6	0	-3.609429	-2.023293	3.541772
39	6	0	-0.346187	-3.658517	-2.595746
40	16	0	0.502167	-4.485384	-1.243235
41	8	0	-0.349461	-5.543276	-0.689194
42	8	0	1.849942	-4.839263	-1.699231
43	6	0	5.987910	0.346921	1.827020
44	6	0	4.707551	0.168599	2.664443
45	6	0	6.512372	1.794626	1.888670
46	6	0	4.129616	0.039791	-3.044365
47	6	0	4.981886	0.365146	-4.286818
48	6	0	3.017918	-0.974171	-3.378818
49	6	0	2.303805	3.602397	2.501633
50	6	0	2.853027	4.906891	3.113707
51	6	0	1.727560	2.677122	3.590413
52	1	0	-1.167155	0.488971	1.826663
53	1	0	5.895079	2.766713	-1.076079
54	1	0	3.892700	4.666739	-0.776968
55	1	0	-0.096765	4.787065	2.800352
56	1	0	-1.803465	5.319950	1.091011
57	1	0	-1.389285	4.781739	-1.276466
58	1	0	5.738529	-2.119942	-3.013733
59	1	0	7.216302	-2.946802	-1.212165
60	1	0	7.298030	-1.765508	0.955021
61	1	0	-4.557369	-5.004973	0.332442
62	1	0	-4.053623	-4.240888	-1.194827
63	1	0	-2.820068	-4.838758	-0.063636
64	1	0	-5.061764	-1.441080	0.979373
65	1	0	-5.724462	-2.661529	-0.115243
66	1	0	-5.606280	-2.992249	1.631212
67	1	0	-0.231265	4.105313	-2.888792
68	1	0	1.881818	5.475482	-2.806927
69	1	0	1.714218	4.421938	-4.217663
70	1	0	2.817155	3.971820	-2.920189
71	1	0	-0.234849	1.685738	-2.514250
72	1	0	0.670308	2.110393	-3.969987
73	1	0	1.531938	1.644910	-2.495367
74	1	0	-3.332692	1.242191	2.658477
75	1	0	-4.388354	1.525046	4.857341
76	1	0	-4.969037	-0.459973	6.245833
77	1	0	-4.441697	-2.740201	5.388237
78	1	0	-3.374817	-3.024463	3.193403
79	1	0	0.313621	-2.882381	-2.982837
80	1	0	-0.505209	-4.435467	-3.346138
81	1	0	-1.291885	-3.241418	-2.257019
82	1	0	6.757855	-0.261965	2.316531
83	1	0	4.887339	0.504100	3.692280

84	1	0	3.870396	0.742563	2.262039
85	1	0	4.399809	-0.880030	2.695437
86	1	0	7.404814	1.925139	1.266961
87	1	0	6.789180	2.035761	2.920630
88	1	0	5.765566	2.526085	1.572509
89	1	0	3.638933	0.967646	-2.743519
90	1	0	5.758717	1.102368	-4.058660
91	1	0	4.348714	0.774709	-5.080758
92	1	0	5.475800	-0.526855	-4.686001
93	1	0	2.385212	-1.159879	-2.505528
94	1	0	2.385541	-0.588449	-4.185669
95	1	0	3.433941	-1.933079	-3.705736
96	1	0	3.150784	3.077907	2.053001
97	1	0	3.299822	5.551099	2.349185
98	1	0	3.622018	4.683301	3.861031
99	1	0	2.063486	5.480553	3.610438
100	1	0	0.885692	3.144091	4.112264
101	1	0	1.378245	1.734253	3.158859
102	1	0	2.494832	2.447725	4.337736
103	7	0	-3.643167	0.449365	-0.630972
104	16	0	-3.358446	-0.124461	-2.178332
105	16	0	-3.999289	2.059202	-0.332145
106	8	0	-2.611896	0.796425	-3.024391
107	8	0	-2.916981	-1.506353	-1.995645
108	8	0	-4.038468	2.873211	-1.540595
109	8	0	-3.245250	2.481495	0.845635
110	6	0	-5.775949	1.919902	0.248386
111	6	0	-5.063312	-0.277454	-2.951354
112	9	0	-5.870248	1.047618	1.257169
113	9	0	-6.172771	3.121614	0.667186
114	9	0	-6.560547	1.516759	-0.752141
115	9	0	-5.562758	0.917283	-3.249588
116	9	0	-5.890831	-0.909223	-2.110811
117	9	0	-4.935906	-0.999298	-4.065711
118	6	0	1.772129	-3.420864	0.860395
119	6	0	1.378253	-3.807595	2.148532
120	6	0	3.128572	-3.357416	0.531209
121	6	0	2.339980	-4.102887	3.112789
122	1	0	0.322045	-3.882680	2.384087
123	6	0	4.084193	-3.681378	1.494822
124	1	0	3.422004	-3.072146	-0.470677
125	6	0	3.696436	-4.046352	2.786018
126	1	0	2.028205	-4.396406	4.110905
127	1	0	5.135892	-3.640532	1.231952
128	1	0	4.447149	-4.293178	3.531494

Sum of electronic and zero-point Energies= -4609.578135
Sum of electronic and thermal Energies= -4609.504414
Sum of electronic and thermal Enthalpies= -4609.503470
Sum of electronic and thermal Free Energies= -4609.696688

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.810259	1.235790	1.186672
2	6	0	-0.418073	1.666908	0.621228
3	6	0	1.203396	-0.111453	1.220902

4	7	0	-0.659591	3.003524	0.464067
5	6	0	2.573188	-0.165829	1.640269
6	79	0	-1.837688	0.201049	0.153827
7	6	0	-3.200852	-1.309915	-0.225679
8	7	0	-4.557116	-1.295660	-0.045357
9	6	0	-5.116933	-2.512702	-0.419483
10	6	0	-4.098553	-3.308612	-0.822771
11	7	0	-2.933705	-2.559435	-0.710640
12	6	0	-5.378234	-0.161470	0.344744
13	6	0	-1.616799	-3.135864	-0.914884
14	6	0	-1.047441	-3.823864	0.179583
15	6	0	0.211375	-4.409755	-0.000767
16	6	0	0.881117	-4.315773	-1.214879
17	6	0	0.284373	-3.650654	-2.280823
18	6	0	-0.979607	-3.053114	-2.174016
19	6	0	-5.688013	0.065242	1.705150
20	6	0	-6.526018	1.153550	1.987978
21	6	0	-7.047554	1.964790	0.986311
22	6	0	-6.743775	1.700542	-0.342674
23	6	0	-5.904077	0.637568	-0.693875
24	7	0	1.842595	2.057265	1.649231
25	6	0	2.853965	1.271471	1.937667
26	7	0	4.028606	1.784632	2.455784
27	6	0	4.091950	3.235792	2.596516
28	6	0	5.304439	1.169645	2.105514
29	1	0	3.141896	-0.306245	0.253454
30	6	0	-1.511170	-2.371842	-3.441214
31	6	0	-2.946895	-2.741221	-3.855955
32	6	0	-1.300776	-0.844985	-3.429268
33	6	0	-5.627695	0.364615	-2.170791
34	6	0	-6.829418	-0.337695	-2.836712
35	6	0	-5.251942	1.641317	-2.945450
36	6	0	-5.215034	-0.753409	2.912917
37	6	0	-5.554975	-2.255010	2.863557
38	6	0	-3.737206	-0.516678	3.275942
39	6	0	-1.752608	-3.986994	1.525357
40	6	0	-2.135355	-5.461188	1.769544
41	6	0	-0.917331	-3.434076	2.695288
42	6	0	3.056262	-1.315905	2.482900
43	6	0	3.581835	-1.098454	3.768880
44	6	0	3.960782	-2.168448	4.580950
45	6	0	3.816234	-3.481954	4.133856
46	6	0	3.284649	-3.711233	2.863482
47	6	0	2.906962	-2.642965	2.049727
48	6	0	-1.479041	3.202600	-2.175244
49	16	0	-2.050270	3.546895	-0.500697
50	8	0	-2.131360	4.992727	-0.318850
51	8	0	-3.214081	2.706621	-0.206515
52	1	0	0.601584	-0.961912	0.929008
53	1	0	-6.176731	-2.693436	-0.350303
54	1	0	-4.087176	-4.324952	-1.180280
55	1	0	0.671269	-4.942127	0.825694
56	1	0	1.869763	-4.745324	-1.331304
57	1	0	0.811584	-3.586508	-3.228155
58	1	0	-6.776525	1.359225	3.024781
59	1	0	-7.695237	2.797780	1.243457
60	1	0	-7.158658	2.330692	-1.122217
61	1	0	3.159258	3.605316	3.020485
62	1	0	4.926368	3.485723	3.259224

63	1	0	4.241483	3.738263	1.629776
64	1	0	6.057209	1.465700	2.843155
65	1	0	5.230455	0.085350	2.120816
66	1	0	5.653352	1.483507	1.111314
67	1	0	-0.867478	-2.757905	-4.240587
68	1	0	-3.107096	-3.824457	-3.831211
69	1	0	-3.123037	-2.405131	-4.883353
70	1	0	-3.704490	-2.270021	-3.225955
71	1	0	-0.250230	-0.594074	-3.255300
72	1	0	-1.595510	-0.421758	-4.396731
73	1	0	-1.897872	-0.365632	-2.647643
74	1	0	-4.770055	-0.309771	-2.238732
75	1	0	-7.071363	-1.285389	-2.345609
76	1	0	-6.614799	-0.549601	-3.889774
77	1	0	-7.722563	0.295290	-2.796269
78	1	0	-4.460584	2.188102	-2.428443
79	1	0	-4.907170	1.379195	-3.951500
80	1	0	-6.107355	2.314970	-3.062327
81	1	0	-5.797696	-0.351367	3.750675
82	1	0	-6.604273	-2.418917	2.595462
83	1	0	-5.392222	-2.697362	3.852219
84	1	0	-4.932323	-2.805279	2.154820
85	1	0	-3.522562	0.551485	3.373411
86	1	0	-3.506738	-0.999931	4.232167
87	1	0	-3.057681	-0.920007	2.521838
88	1	0	-2.681821	-3.412754	1.501743
89	1	0	-2.766485	-5.852338	0.964637
90	1	0	-2.685536	-5.561532	2.711256
91	1	0	-1.246931	-6.098139	1.833093
92	1	0	-0.694417	-2.372240	2.558709
93	1	0	-1.469618	-3.545225	3.634669
94	1	0	0.035655	-3.959553	2.806974
95	1	0	3.688642	-0.082355	4.134045
96	1	0	4.364088	-1.970133	5.570519
97	1	0	4.115147	-4.314473	4.764478
98	1	0	3.174451	-4.727951	2.494894
99	1	0	2.510498	-2.842250	1.061952
100	1	0	-1.280062	2.135318	-2.270500
101	1	0	-2.279565	3.515619	-2.848066
102	1	0	-0.577549	3.789228	-2.351096
103	7	0	3.682416	-0.391965	-0.937019
104	16	0	4.471691	-1.786526	-1.453713
105	16	0	3.194843	0.761962	-2.051014
106	8	0	3.800963	-2.963813	-0.908101
107	8	0	4.847798	-1.723336	-2.860519
108	8	0	2.346607	1.699176	-1.319941
109	8	0	2.750204	0.193986	-3.318531
110	6	0	4.749577	1.750041	-2.412871
111	6	0	6.080782	-1.649504	-0.504163
112	9	0	4.409851	2.740351	-3.242858
113	9	0	5.218822	2.277271	-1.276393
114	9	0	5.696268	1.006300	-2.975676
115	9	0	6.641793	-0.454188	-0.708836
116	9	0	6.900534	-2.603121	-0.946108
117	9	0	5.871218	-1.821059	0.803063
118	6	0	0.172970	4.120813	0.879338
119	6	0	1.198991	4.581296	0.052274
120	6	0	-0.134068	4.773896	2.071530
121	6	0	1.926925	5.706242	0.432951

122	1	0	1.453923	4.031629	-0.847017
123	6	0	0.605886	5.894092	2.450358
124	1	0	-0.946333	4.406088	2.689704
125	6	0	1.632393	6.364812	1.629992
126	1	0	2.730370	6.065769	-0.203346
127	1	0	0.371328	6.404417	3.379844
128	1	0	2.201423	7.243068	1.921247

Sum of electronic and zero-point Energies= -4609.555854
Sum of electronic and thermal Energies= -4609.481883
Sum of electronic and thermal Enthalpies= -4609.480939
Sum of electronic and thermal Free Energies= -4609.674581

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.645698	-0.234236	-0.150826
2	6	0	-2.169073	-1.491402	0.173524
3	6	0	-2.642196	0.732271	-0.402936
4	7	0	-1.253823	-2.585751	0.441809
5	6	0	-4.014283	0.474776	-0.315908
6	79	0	0.340992	0.304530	-0.093820
7	6	0	2.275641	1.039369	0.035222
8	7	0	3.477676	0.398609	0.152493
9	6	0	4.524069	1.313253	0.236272
10	6	0	3.971544	2.548742	0.198169
11	7	0	2.599199	2.369977	0.058004
12	6	0	3.711004	-1.030475	0.052157
13	6	0	1.649868	3.466605	0.101137
14	6	0	1.134056	3.825815	1.365241
15	6	0	0.233996	4.897407	1.426716
16	6	0	-0.135295	5.591148	0.281806
17	6	0	0.398551	5.223777	-0.949605
18	6	0	1.301551	4.159381	-1.081887
19	6	0	3.879463	-1.564914	-1.243341
20	6	0	4.177045	-2.928523	-1.357956
21	6	0	4.305277	-3.730704	-0.231161
22	6	0	4.133995	-3.177257	1.033970
23	6	0	3.838318	-1.818798	1.219787
24	7	0	-3.472732	-1.801763	0.231687
25	6	0	-4.390710	-0.858388	-0.003335
26	7	0	-5.748925	-1.237985	0.095243
27	6	0	-6.017228	-2.491267	0.786508
28	6	0	-6.556582	-1.096220	-1.116900
29	6	0	1.783658	3.853626	-2.505337
30	6	0	3.309438	3.883420	-2.715919
31	6	0	1.156928	2.573303	-3.089294
32	6	0	-4.974379	1.601068	-0.479354
33	6	0	-4.853016	2.484698	-1.565192
34	6	0	-5.703876	3.583622	-1.696586
35	6	0	-6.692867	3.822361	-0.742126
36	6	0	-6.824738	2.951424	0.343053
37	6	0	-5.978202	1.852278	0.473342
38	6	0	-2.592933	-4.468479	2.002491
39	16	0	-1.281581	-3.228059	2.016705
40	8	0	-1.678459	-2.137664	2.907970
41	8	0	-0.017052	-3.941534	2.239039

42	6	0	3.663186	-1.355737	2.671167
43	6	0	2.190451	-1.095470	3.039021
44	6	0	4.579452	-0.201647	3.120443
45	6	0	3.759336	-0.729611	-2.515348
46	6	0	5.081326	-0.712156	-3.308052
47	6	0	2.587204	-1.211501	-3.392192
48	6	0	1.520030	3.116202	2.660625
49	6	0	2.294760	4.061197	3.601222
50	6	0	0.292055	2.508937	3.365979
51	1	0	-2.340839	1.754496	-0.616235
52	1	0	5.549832	0.995445	0.324023
53	1	0	4.416531	3.528628	0.250912
54	1	0	-0.179668	5.187204	2.387454
55	1	0	-0.834854	6.419544	0.346008
56	1	0	0.108779	5.772649	-1.841271
57	1	0	4.310143	-3.360916	-2.344700
58	1	0	4.540237	-4.786315	-0.334254
59	1	0	4.228483	-3.811137	1.910618
60	1	0	-7.093586	-2.553531	0.979209
61	1	0	-5.716363	-3.381074	0.210267
62	1	0	-5.489641	-2.509254	1.741794
63	1	0	-6.355512	-0.144885	-1.607664
64	1	0	-6.363296	-1.909840	-1.837361
65	1	0	-7.618734	-1.121345	-0.851649
66	1	0	1.391463	4.684258	-3.104955
67	1	0	3.758623	4.776293	-2.267682
68	1	0	3.526648	3.906708	-3.789288
69	1	0	3.808748	3.004825	-2.302001
70	1	0	0.065111	2.608981	-3.032035
71	1	0	1.439795	2.466477	-4.142845
72	1	0	1.479760	1.676863	-2.555775
73	1	0	-4.090809	2.297852	-2.316634
74	1	0	-5.594872	4.249879	-2.548168
75	1	0	-7.356705	4.676490	-0.842514
76	1	0	-7.588680	3.132006	1.094568
77	1	0	-6.088726	1.174935	1.313036
78	1	0	-2.322878	-5.245325	1.286056
79	1	0	-2.658633	-4.881217	3.010636
80	1	0	-3.513100	-3.966481	1.706571
81	1	0	3.975502	-2.222191	3.266713
82	1	0	2.110407	-0.867527	4.108124
83	1	0	1.770250	-0.254485	2.481680
84	1	0	1.571305	-1.971844	2.833322
85	1	0	5.620314	-0.370998	2.822483
86	1	0	4.555914	-0.129426	4.213058
87	1	0	4.263952	0.766333	2.725156
88	1	0	3.543119	0.303023	-2.231711
89	1	0	5.910610	-0.339120	-2.697869
90	1	0	4.988227	-0.064190	-4.186168
91	1	0	5.353227	-1.711911	-3.662802
92	1	0	1.643815	-1.179369	-2.839755
93	1	0	2.490671	-0.574013	-4.277879
94	1	0	2.738708	-2.239963	-3.736196
95	1	0	2.187650	2.287206	2.415749
96	1	0	3.191788	4.463427	3.118435
97	1	0	2.606744	3.525422	4.503943
98	1	0	1.677607	4.909749	3.915391
99	1	0	-0.417179	3.282312	3.679834
100	1	0	-0.234043	1.809775	2.709744

101	1	0	0.604851	1.962897	4.262040
102	6	0	-0.866829	-3.439768	-0.647994
103	6	0	0.433988	-3.960718	-0.704907
104	6	0	-1.776381	-3.740408	-1.674293
105	6	0	0.805752	-4.784678	-1.766949
106	1	0	1.135938	-3.722289	0.083047
107	6	0	-1.384074	-4.544860	-2.744082
108	1	0	-2.783576	-3.343880	-1.623190
109	6	0	-0.094647	-5.077199	-2.793217
110	1	0	1.815123	-5.184642	-1.796272
111	1	0	-2.096124	-4.764458	-3.534983
112	1	0	0.205611	-5.710568	-3.623182

Sum of electronic and zero-point Energies= -2781.975964
Sum of electronic and thermal Energies= -2781.918451
Sum of electronic and thermal Enthalpies= -2781.917507
Sum of electronic and thermal Free Energies= -2782.074208

B-b3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.340120	-0.920063	-0.436211
2	6	0	-1.050518	-1.410980	-0.495239
3	6	0	-2.701404	0.467663	-0.209703
4	7	0	-0.914669	-2.825577	-0.620694
5	6	0	-4.069075	0.540837	-0.176270
6	79	0	0.583113	-0.164792	-0.223729
7	6	0	2.148313	1.134886	0.170275
8	7	0	3.362322	0.864941	0.740067
9	6	0	4.123357	2.023258	0.860359
10	6	0	3.371257	3.041983	0.380809
11	7	0	2.171730	2.485482	-0.051464
12	6	0	3.896192	-0.448495	1.058247
13	6	0	1.057301	3.289004	-0.515698
14	6	0	0.169826	3.786598	0.463812
15	6	0	-0.896700	4.587848	0.036366
16	6	0	-1.071211	4.890445	-1.308469
17	6	0	-0.172214	4.399553	-2.250097
18	6	0	0.916190	3.592337	-1.889452
19	6	0	3.750282	-0.985914	2.357356
20	6	0	4.333394	-2.239643	2.590372
21	6	0	5.033576	-2.923865	1.602754
22	6	0	5.175882	-2.359556	0.342137
23	6	0	4.612854	-1.114406	0.040567
24	7	0	-3.504466	-1.681779	-0.583635
25	6	0	-4.510493	-0.847697	-0.440915
26	7	0	-5.830425	-1.283759	-0.507216
27	6	0	-6.009224	-2.729540	-0.593936
28	6	0	-6.754541	-0.548661	-1.369326
29	6	0	1.824165	3.127044	-3.034514
30	6	0	3.315073	3.485244	-2.886564
31	6	0	1.632907	1.641693	-3.396324
32	6	0	4.829452	-0.517967	-1.348189
33	6	0	6.261078	0.040148	-1.488425
34	6	0	4.521224	-1.522545	-2.474162
35	6	0	3.013303	-0.354496	3.545098
36	6	0	3.465867	1.064509	3.937020

37	6	0	1.480693	-0.446544	3.421645
38	6	0	0.346377	3.527697	1.958795
39	6	0	0.762748	4.820723	2.690118
40	6	0	-0.910680	2.911794	2.601094
41	6	0	-4.865391	1.728259	0.175322
42	6	0	-5.992094	1.633049	1.015562
43	6	0	-6.703188	2.771265	1.393074
44	6	0	-6.308782	4.033628	0.943877
45	6	0	-5.194710	4.144179	0.108519
46	6	0	-4.484283	3.007031	-0.273845
47	6	0	0.189794	-2.789852	-3.105189
48	16	0	0.450246	-3.450289	-1.448262
49	8	0	0.296602	-4.905616	-1.492052
50	8	0	1.710743	-2.882775	-0.941181
51	1	0	-2.002421	1.275856	-0.041444
52	1	0	5.114311	2.009168	1.282982
53	1	0	3.571873	4.097446	0.298420
54	1	0	-1.596857	4.976280	0.768723
55	1	0	-1.901382	5.515570	-1.624554
56	1	0	-0.309988	4.647605	-3.298721
57	1	0	4.231905	-2.683689	3.576629
58	1	0	5.469940	-3.894514	1.819243
59	1	0	5.725722	-2.893823	-0.425388
60	1	0	-5.368452	-3.224339	0.135552
61	1	0	-7.058715	-2.963715	-0.386209
62	1	0	-5.749382	-3.124446	-1.588264
63	1	0	-7.785210	-0.768158	-1.071098
64	1	0	-6.596105	0.524796	-1.283443
65	1	0	-6.636141	-0.835199	-2.427683
66	1	0	1.471969	3.697162	-3.902920
67	1	0	3.448449	4.534264	-2.601059
68	1	0	3.820523	3.336546	-3.846801
69	1	0	3.826738	2.862581	-2.149674
70	1	0	0.578833	1.417797	-3.585889
71	1	0	2.202044	1.404340	-4.302513
72	1	0	1.970177	0.977884	-2.596919
73	1	0	4.136698	0.318206	-1.472487
74	1	0	6.474972	0.807005	-0.736697
75	1	0	6.402845	0.488784	-2.477801
76	1	0	7.004535	-0.755917	-1.371521
77	1	0	3.538977	-1.978487	-2.330646
78	1	0	4.543071	-1.011781	-3.443268
79	1	0	5.264551	-2.325972	-2.516383
80	1	0	3.286114	-0.990675	4.395995
81	1	0	4.557197	1.134078	4.000844
82	1	0	3.059968	1.314854	4.923134
83	1	0	3.116094	1.827685	3.238518
84	1	0	1.166630	-1.476909	3.230881
85	1	0	1.009502	-0.112379	4.353214
86	1	0	1.095273	0.168042	2.604541
87	1	0	1.155250	2.805356	2.090211
88	1	0	1.682614	5.242565	2.271692
89	1	0	0.935407	4.618909	3.752620
90	1	0	-0.016800	5.586733	2.618198
91	1	0	-1.184604	1.970416	2.117601
92	1	0	-0.725168	2.707874	3.661038
93	1	0	-1.773142	3.583333	2.541661
94	1	0	-6.297891	0.654830	1.373478
95	1	0	-7.566262	2.671971	2.046127

96	1	0	-6.865436	4.919278	1.237064
97	1	0	-4.885614	5.120362	-0.257245
98	1	0	-3.628705	3.098380	-0.936307
99	1	0	0.156600	-1.701749	-3.051491
100	1	0	1.034947	-3.124746	-3.709396
101	1	0	-0.748002	-3.190135	-3.490324
102	6	0	-1.628985	-3.744241	0.234275
103	6	0	-2.409121	-4.773446	-0.298806
104	6	0	-1.526379	-3.591723	1.620599
105	6	0	-3.079675	-5.646923	0.554529
106	1	0	-2.490246	-4.878422	-1.373573
107	6	0	-2.216175	-4.456615	2.470085
108	1	0	-0.914862	-2.789759	2.021043
109	6	0	-2.991293	-5.489290	1.940428
110	1	0	-3.681560	-6.448224	0.135119
111	1	0	-2.137778	-4.328743	3.546171
112	1	0	-3.522162	-6.168329	2.601698

Sum of electronic and zero-point Energies= -2781.942976
Sum of electronic and thermal Energies= -2781.884960
Sum of electronic and thermal Enthalpies= -2781.884015
Sum of electronic and thermal Free Energies= -2782.042481

B-tsa4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.018593	0.732752	0.297190
2	6	0	-1.124982	2.150115	0.459047
3	6	0	-1.903608	0.027736	1.162973
4	7	0	-0.292984	3.024461	-0.300401
5	6	0	-2.760254	0.615183	2.084603
6	79	0	0.919744	-0.153427	0.254960
7	6	0	2.759567	-1.016896	0.605994
8	7	0	4.015037	-0.568952	0.298475
9	6	0	4.984384	-1.439486	0.785993
10	6	0	4.331971	-2.456551	1.397356
11	7	0	2.972871	-2.178932	1.298557
12	6	0	4.337025	0.719974	-0.289176
13	6	0	1.941682	-3.088602	1.761985
14	6	0	1.538243	-4.109416	0.874194
15	6	0	0.521050	-4.978103	1.290061
16	6	0	-0.058623	-4.853386	2.545841
17	6	0	0.394202	-3.869471	3.419706
18	6	0	1.406271	-2.964776	3.066149
19	6	0	4.426449	1.822735	0.591398
20	6	0	4.716614	3.076616	0.040252
21	6	0	4.940187	3.225251	-1.323077
22	6	0	4.896452	2.112847	-2.157276
23	6	0	4.597092	0.830034	-1.673766
24	7	0	-1.929995	2.758683	1.323106
25	6	0	-2.682539	2.039858	2.177327
26	7	0	-3.395222	2.769817	3.105857
27	6	0	-3.462552	4.218603	2.958635
28	6	0	-3.571976	2.309926	4.481349
29	6	0	1.819018	-1.961256	4.152057
30	6	0	3.324532	-1.915462	4.474073
31	6	0	1.246031	-0.547390	3.939705

32	6	0	-3.766233	-0.229435	2.785810
33	6	0	-3.384446	-1.414729	3.435926
34	6	0	-4.336257	-2.243878	4.032073
35	6	0	-5.689061	-1.905173	3.990189
36	6	0	-6.083007	-0.732147	3.340842
37	6	0	-5.134116	0.095547	2.743857
38	6	0	-1.073650	5.657994	0.204689
39	16	0	0.279162	4.485904	0.402150
40	8	0	1.377091	4.945261	-0.450988
41	8	0	0.511300	4.252820	1.828754
42	6	0	4.629621	-0.310403	-2.698342
43	6	0	3.310991	-1.080502	-2.866780
44	6	0	5.823941	-1.268262	-2.506881
45	6	0	4.313290	1.677647	2.108020
46	6	0	5.723322	1.589528	2.733166
47	6	0	3.500587	2.797561	2.778929
48	6	0	2.184386	-4.335010	-0.490556
49	6	0	2.915231	-5.692889	-0.531598
50	6	0	1.167817	-4.211651	-1.638254
51	1	0	-1.959643	-1.051977	1.052196
52	1	0	6.036363	-1.248100	0.655840
53	1	0	4.697741	-3.338103	1.897347
54	1	0	0.187582	-5.763390	0.619071
55	1	0	-0.847399	-5.533558	2.854035
56	1	0	-0.038933	-3.799443	4.413737
57	1	0	4.763885	3.944726	0.687722
58	1	0	5.153152	4.206790	-1.735476
59	1	0	5.096237	2.233462	-3.218330
60	1	0	-4.253122	4.590423	3.617061
61	1	0	-2.516949	4.710599	3.223720
62	1	0	-3.716056	4.479378	1.930536
63	1	0	-3.216200	1.290164	4.602312
64	1	0	-2.998173	2.955379	5.160585
65	1	0	-4.626437	2.342407	4.778995
66	1	0	1.340408	-2.346393	5.060984
67	1	0	3.739710	-2.921538	4.597659
68	1	0	3.475888	-1.376813	5.415576
69	1	0	3.904255	-1.397608	3.707355
70	1	0	0.160095	-0.574018	3.811636
71	1	0	1.469828	0.077945	4.811386
72	1	0	1.662787	-0.060302	3.055706
73	1	0	-2.332567	-1.684727	3.476065
74	1	0	-4.018196	-3.154173	4.533149
75	1	0	-6.430032	-2.548770	4.455528
76	1	0	-7.135256	-0.465957	3.290126
77	1	0	-5.447564	0.998407	2.228932
78	1	0	-1.930993	5.267406	0.747676
79	1	0	-0.732630	6.611196	0.613116
80	1	0	-1.282874	5.752616	-0.861642
81	1	0	4.808082	0.195158	-3.655343
82	1	0	3.385339	-1.746647	-3.733708
83	1	0	3.077287	-1.697433	-1.997428
84	1	0	2.463496	-0.412407	-3.028370
85	1	0	6.762915	-0.719791	-2.376772
86	1	0	5.928310	-1.907531	-3.390219
87	1	0	5.687144	-1.927358	-1.645278
88	1	0	3.798714	0.738245	2.324548
89	1	0	6.305615	0.760232	2.318773
90	1	0	5.652271	1.444354	3.816626

91	1	0	6.285300	2.512557	2.553597
92	1	0	2.508775	2.916184	2.338089
93	1	0	3.376626	2.569851	3.843316
94	1	0	4.009527	3.765271	2.717622
95	1	0	2.939827	-3.561738	-0.648577
96	1	0	3.662764	-5.773810	0.264814
97	1	0	3.427146	-5.817397	-1.491588
98	1	0	2.217132	-6.528923	-0.417204
99	1	0	0.365864	-4.952229	-1.551751
100	1	0	0.717389	-3.217772	-1.657940
101	1	0	1.664856	-4.373083	-2.600466
102	1	0	-1.501288	0.209970	-1.016928
103	7	0	-2.176874	-0.225933	-1.996505
104	16	0	-3.735091	0.370217	-2.122816
105	16	0	-1.322443	-0.920010	-3.255536
106	8	0	-3.840596	1.480404	-1.178279
107	8	0	-4.200126	0.484135	-3.498631
108	8	0	-1.627506	-0.374129	-4.569338
109	8	0	0.050771	-1.019900	-2.765696
110	6	0	-4.773687	-0.990453	-1.352399
111	6	0	-1.934000	-2.698998	-3.303457
112	9	0	-0.996428	-3.437455	-3.905746
113	9	0	-2.126775	-3.165962	-2.064213
114	9	0	-3.068590	-2.787669	-3.992962
115	9	0	-4.264706	-1.376110	-0.181135
116	9	0	-4.840464	-2.045461	-2.166718
117	9	0	-6.001540	-0.504496	-1.160810
118	6	0	-0.151646	2.888890	-1.727021
119	6	0	1.101661	2.640114	-2.293808
120	6	0	-1.274864	3.060407	-2.546171
121	6	0	1.224855	2.561527	-3.680743
122	1	0	1.964253	2.527086	-1.650012
123	6	0	-1.145613	2.960676	-3.931579
124	1	0	-2.243564	3.243905	-2.093699
125	6	0	0.105503	2.716098	-4.500743
126	1	0	2.200169	2.371970	-4.119071
127	1	0	-2.023178	3.063990	-4.561736
128	1	0	0.204155	2.636158	-5.579064

Sum of electronic and zero-point Energies= -4609.590233
Sum of electronic and thermal Energies= -4609.516405
Sum of electronic and thermal Enthalpies= -4609.515460
Sum of electronic and thermal Free Energies= -4609.708545

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.960717	-0.167411	-1.245181
2	6	0	0.859706	0.639763	-1.009535
3	6	0	2.393124	-1.245511	-0.342780
4	7	0	0.499995	1.612892	-2.035350
5	6	0	3.493827	-1.822284	-0.887141
6	79	0	-0.840291	-0.417627	-0.222795
7	6	0	-2.521818	-1.457370	0.341649
8	7	0	-3.822354	-1.079144	0.165913
9	6	0	-4.686441	-2.009128	0.727805
10	6	0	-3.917054	-2.986740	1.266173

11	7	0	-2.592525	-2.650278	1.004518
12	6	0	-4.252382	0.081733	-0.593253
13	6	0	-1.476430	-3.461336	1.461511
14	6	0	-0.953161	-3.189859	2.745856
15	6	0	0.068069	-4.019331	3.226200
16	6	0	0.549074	-5.078737	2.467581
17	6	0	0.020012	-5.319526	1.203573
18	6	0	-1.000776	-4.525345	0.659147
19	6	0	-4.563943	1.286981	0.068177
20	6	0	-4.891883	2.384128	-0.744387
21	6	0	-4.936203	2.287447	-2.128986
22	6	0	-4.684540	1.066893	-2.747389
23	6	0	-4.347382	-0.063922	-1.998113
24	7	0	2.816596	-0.099403	-2.335128
25	6	0	3.705178	-1.066925	-2.163176
26	7	0	4.713367	-1.270380	-3.055362
27	6	0	4.883906	-0.305859	-4.136076
28	6	0	5.240706	-2.600202	-3.352269
29	6	0	-1.448855	-4.891748	-0.761833
30	6	0	-2.953343	-5.158431	-0.953718
31	6	0	-0.903134	-3.917330	-1.824202
32	6	0	-4.197492	-1.416522	-2.692814
33	6	0	-5.584192	-2.079811	-2.848695
34	6	0	-3.483059	-1.344854	-4.052279
35	6	0	-4.701509	1.522318	1.577419
36	6	0	-6.169212	1.297257	2.006295
37	6	0	-3.748710	0.790161	2.530913
38	6	0	-1.474847	-2.061894	3.630918
39	6	0	-2.487505	-2.599829	4.663954
40	6	0	-0.346517	-1.285317	4.334780
41	6	0	4.355003	-2.826870	-0.233660
42	6	0	5.748178	-2.646995	-0.146471
43	6	0	6.544269	-3.566694	0.533356
44	6	0	5.966912	-4.684438	1.140422
45	6	0	4.585700	-4.871459	1.064831
46	6	0	3.786106	-3.953174	0.384912
47	6	0	1.283364	1.481804	-4.710518
48	16	0	-0.054098	1.107269	-3.560518
49	8	0	-1.192089	1.950692	-3.947556
50	8	0	-0.224676	-0.350089	-3.498348
51	1	0	1.962765	-1.451709	0.626288
52	1	0	-5.756290	-1.887556	0.689944
53	1	0	-4.179666	-3.892620	1.786774
54	1	0	0.487030	-3.827784	4.207939
55	1	0	1.334898	-5.717932	2.860124
56	1	0	0.401153	-6.148773	0.613923
57	1	0	-5.114919	3.333312	-0.264879
58	1	0	-5.176882	3.160727	-2.728246
59	1	0	-4.739557	0.993410	-3.827259
60	1	0	4.692829	0.699605	-3.763794
61	1	0	5.912163	-0.372610	-4.503903
62	1	0	4.199405	-0.506144	-4.972253
63	1	0	6.332882	-2.569869	-3.427305
64	1	0	4.964165	-3.311409	-2.579309
65	1	0	4.838137	-2.953958	-4.311867
66	1	0	-0.959262	-5.854457	-0.954272
67	1	0	-3.345141	-5.826254	-0.178831
68	1	0	-3.111074	-5.646235	-1.921606
69	1	0	-3.550244	-4.244721	-0.950390

70	1	0	0.183791	-3.819620	-1.747282
71	1	0	-1.139559	-4.287668	-2.827952
72	1	0	-1.324422	-2.914437	-1.727888
73	1	0	-3.592500	-2.063952	-2.052927
74	1	0	-6.091863	-2.203800	-1.886676
75	1	0	-5.485927	-3.069333	-3.308594
76	1	0	-6.232747	-1.472913	-3.490079
77	1	0	-2.506856	-0.864108	-3.968357
78	1	0	-3.333221	-2.359715	-4.437061
79	1	0	-4.076638	-0.805535	-4.798412
80	1	0	-4.494283	2.591048	1.707308
81	1	0	-6.863487	1.880769	1.394120
82	1	0	-6.307966	1.587984	3.053340
83	1	0	-6.449848	0.241365	1.916845
84	1	0	-2.712754	0.867643	2.202633
85	1	0	-3.812411	1.254143	3.520540
86	1	0	-4.012823	-0.263724	2.651894
87	1	0	-1.998673	-1.348530	2.993004
88	1	0	-3.341056	-3.090827	4.185238
89	1	0	-2.872350	-1.779841	5.279208
90	1	0	-2.014220	-3.328362	5.331847
91	1	0	0.441236	-0.992080	3.636724
92	1	0	-0.749190	-0.372731	4.782867
93	1	0	0.113936	-1.871559	5.137933
94	1	0	6.200659	-1.770910	-0.601680
95	1	0	7.616702	-3.405347	0.597302
96	1	0	6.588377	-5.400838	1.669741
97	1	0	4.127644	-5.737349	1.534835
98	1	0	2.712532	-4.104492	0.327317
99	1	0	2.153100	0.919742	-4.374792
100	1	0	0.940259	1.172663	-5.699516
101	1	0	1.464576	2.556977	-4.688208
102	1	0	0.925421	1.264703	0.361117
103	7	0	1.120919	1.925075	1.437648
104	16	0	2.394865	1.527090	2.441396
105	16	0	-0.231207	2.700525	2.056546
106	6	0	3.846322	2.203734	1.468465
107	6	0	0.305116	4.495701	2.342340
108	8	0	2.599094	0.079303	2.461637
109	8	0	2.358032	2.310042	3.672863
110	8	0	-1.184252	2.746869	0.949725
111	8	0	-0.631914	2.194189	3.366081
112	9	0	4.950612	1.974231	2.182116
113	9	0	3.956537	1.586525	0.286172
114	9	0	3.712675	3.513740	1.270308
115	9	0	-0.764116	5.262559	2.111764
116	9	0	1.282308	4.833468	1.502993
117	9	0	0.708208	4.669891	3.594358
118	6	0	0.752931	3.016866	-1.866802
119	6	0	-0.294355	3.947071	-1.895665
120	6	0	2.074257	3.458052	-1.704362
121	6	0	-0.011914	5.307782	-1.776348
122	1	0	-1.310498	3.593735	-2.012260
123	6	0	2.344445	4.818967	-1.566003
124	1	0	2.874990	2.727324	-1.690795
125	6	0	1.302975	5.748005	-1.610023
126	1	0	-0.826678	6.025754	-1.800451
127	1	0	3.369303	5.152400	-1.429668
128	1	0	1.514047	6.808764	-1.508154

Sum of electronic and zero-point Energies= -4609.558049
Sum of electronic and thermal Energies= -4609.484033
Sum of electronic and thermal Enthalpies= -4609.483089
Sum of electronic and thermal Free Energies= -4609.676227

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.741282	0.567612	-0.372629
2	6	0	-1.935943	1.870277	-0.408520
3	6	0	-2.727712	-0.498378	-0.487179
4	7	0	-1.289584	3.020397	-0.599924
5	6	0	-3.731158	-0.536826	-1.397840
6	79	0	0.252440	-0.039195	-0.110681
7	6	0	2.162903	-0.773075	0.108349
8	7	0	3.310807	-0.338936	-0.486595
9	6	0	4.388262	-1.130057	-0.102582
10	6	0	3.901190	-2.084666	0.727542
11	7	0	2.537857	-1.846616	0.860450
12	6	0	3.447347	0.872933	-1.276893
13	6	0	1.636563	-2.728684	1.582185
14	6	0	1.376149	-2.515975	2.956064
15	6	0	0.505451	-3.422258	3.578310
16	6	0	-0.071091	-4.485652	2.890019
17	6	0	0.220526	-4.676999	1.545367
18	6	0	1.081356	-3.808656	0.861700
19	6	0	3.734872	2.065197	-0.575046
20	6	0	3.869538	3.244238	-1.319441
21	6	0	3.734584	3.238322	-2.702534
22	6	0	3.479944	2.043124	-3.368670
23	6	0	3.336918	0.825775	-2.686152
24	7	0	-3.778206	2.357085	-0.382455
25	6	0	-4.508947	2.135773	0.518947
26	7	0	-5.322905	1.912647	1.506344
27	6	0	-5.174368	2.654168	2.772632
28	6	0	-6.414969	0.933062	1.375391
29	6	0	1.938022	-1.396410	3.841267
30	6	0	3.474897	-1.318299	3.913479
31	6	0	1.313282	-0.017677	3.552974
32	6	0	1.396647	-4.089063	-0.605994
33	6	0	2.191469	-5.401798	-0.760340
34	6	0	0.123284	-4.107874	-1.473116
35	6	0	-0.652502	3.360754	-1.887670
36	6	0	-2.354431	5.497282	0.031893
37	16	0	-1.268785	4.211060	0.673640
38	8	0	0.088056	4.748167	0.740759
39	8	0	-1.909685	3.576627	1.825590
40	6	0	3.091518	-0.414037	-3.556207
41	6	0	4.099246	-1.563610	-3.366011
42	6	0	1.639020	-0.924552	-3.507678
43	6	0	3.968206	2.106445	0.933871
44	6	0	5.478283	2.200009	1.241183
45	6	0	3.201630	3.245904	1.628998
46	1	0	-2.571355	-1.354057	0.166994
47	1	0	-3.833507	0.290482	-2.097221
48	1	0	5.387382	-0.942380	-0.459612

49	1	0	4.388895	-2.899234	1.237285
50	1	0	0.284055	-3.288204	4.633169
51	1	0	-0.736168	-5.170654	3.407541
52	1	0	-0.217317	-5.516772	1.015237
53	1	0	4.091610	4.173530	-0.805778
54	1	0	3.848341	4.160034	-3.265769
55	1	0	3.402243	2.043046	-4.452179
56	1	0	-4.238840	3.213758	2.753508
57	1	0	-6.021036	3.333948	2.909719
58	1	0	-5.146863	1.938301	3.598875
59	1	0	-6.335963	0.422229	0.415612
60	1	0	-6.336394	0.197559	2.180784
61	1	0	-7.380812	1.443198	1.441631
62	1	0	1.612317	-1.667924	4.852362
63	1	0	3.918212	-2.303950	4.088999
64	1	0	3.766118	-0.672058	4.747870
65	1	0	3.919087	-0.898352	3.008135
66	1	0	0.220329	-0.065246	3.579653
67	1	0	1.638828	0.703847	4.310159
68	1	0	1.603441	0.370437	2.573708
69	1	0	2.029214	-3.282846	-0.986052
70	1	0	3.118921	-5.380987	-0.179243
71	1	0	2.453148	-5.566914	-1.810540
72	1	0	1.608261	-6.264811	-0.423102
73	1	0	-0.426081	-3.164761	-1.391995
74	1	0	0.385914	-4.260017	-2.525063
75	1	0	-0.553138	-4.918175	-1.182936
76	1	0	-1.399295	3.676910	-2.622905
77	1	0	-0.121756	2.478675	-2.249868
78	1	0	0.075273	4.155649	-1.718923
79	1	0	-2.413188	6.267526	0.803523
80	1	0	-1.915732	5.912210	-0.876231
81	1	0	-3.332534	5.058997	-0.165595
82	1	0	3.249131	-0.055098	-4.580141
83	1	0	5.130608	-1.196326	-3.368137
84	1	0	3.999985	-2.273273	-4.193755
85	1	0	3.934727	-2.119962	-2.440396
86	1	0	1.497424	-1.714523	-4.253331
87	1	0	1.378486	-1.334241	-2.528913
88	1	0	0.930059	-0.120975	-3.730926
89	1	0	3.604640	1.169670	1.364086
90	1	0	6.036024	1.364960	0.805378
91	1	0	5.648283	2.192163	2.322747
92	1	0	5.903056	3.126876	0.841610
93	1	0	2.134691	3.226992	1.393977
94	1	0	3.315909	3.158765	2.714316
95	1	0	3.585866	4.230637	1.344179
96	6	0	-4.709423	-1.586371	-1.570030
97	6	0	-5.717673	-1.614521	-2.516087
98	16	0	-4.789178	-3.024291	-0.563342
99	6	0	-6.542934	-2.769687	-2.439528
100	1	0	-5.848524	-0.825001	-3.248447
101	6	0	-6.164542	-3.620026	-1.435320
102	1	0	-7.377647	-2.963953	-3.102617
103	1	0	-6.607208	-4.566344	-1.156116

Sum of electronic and zero-point Energies= -2911.392540
Sum of electronic and thermal Energies= -2911.335501
Sum of electronic and thermal Enthalpies= -2911.334557

Sum of electronic and thermal Free Energies= -2911.493796

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.359044	-0.612074	-1.135374
2	6	0	1.397847	-1.437256	-0.823675
3	6	0	2.875837	0.707974	-1.172102
4	7	0	1.478281	-2.853584	-0.802590
5	6	0	3.156733	1.409567	-0.038244
6	79	0	-0.380381	-0.432284	-0.297021
7	6	0	-2.188160	0.404490	0.241850
8	7	0	-2.680484	0.582570	1.501889
9	6	0	-3.947784	1.151979	1.455531
10	6	0	-4.261131	1.311518	0.146355
11	7	0	-3.170347	0.860677	-0.588394
12	6	0	-1.943035	0.379216	2.738087
13	6	0	-3.177993	0.753498	-2.037936
14	6	0	-2.703064	1.818658	-2.837450
15	6	0	-2.754802	1.634501	-4.226760
16	6	0	-3.262356	0.472731	-4.800045
17	6	0	-3.749939	-0.542385	-3.986477
18	6	0	-3.722703	-0.426570	-2.590917
19	6	0	-1.187623	1.471842	3.217432
20	6	0	-0.467323	1.298063	4.405787
21	6	0	-0.500109	0.091362	5.093531
22	6	0	-1.279102	-0.956647	4.613589
23	6	0	-2.031570	-0.848101	3.435002
24	7	0	3.922057	-1.708401	-1.796696
25	6	0	5.005388	-1.541746	-1.360350
26	7	0	6.194437	-1.366092	-0.852230
27	6	0	6.568183	-2.044853	0.401146
28	6	0	7.229725	-0.629722	-1.591253
29	6	0	-2.145637	3.161934	-2.350619
30	6	0	-3.096783	3.981151	-1.457454
31	6	0	-0.738311	3.058169	-1.733790
32	6	0	-4.327234	-1.543763	-1.742841
33	6	0	-5.866714	-1.535355	-1.848027
34	6	0	-3.764104	-2.930058	-2.106158
35	6	0	-2.878961	-2.069341	3.056454
36	6	0	-4.389457	-1.795384	2.923011
37	6	0	-2.337059	-2.855213	1.848424
38	6	0	-1.165278	2.837024	2.532930
39	6	0	0.265626	3.307915	2.217072
40	6	0	-1.916527	3.885852	3.378818
41	6	0	0.251966	-3.576331	-1.191853
42	6	0	3.170742	-4.914554	-0.227883
43	16	0	2.281434	-3.557217	0.554548
44	8	0	1.290353	-4.127432	1.472631
45	8	0	3.268769	-2.587518	1.046150
46	1	0	3.098599	1.128340	-2.152186
47	1	0	2.952284	0.931759	0.918145
48	1	0	-4.500336	1.382719	2.351406
49	1	0	-5.144373	1.704122	-0.329997
50	1	0	-2.394850	2.432089	-4.870169
51	1	0	-3.291519	0.368112	-5.880488
52	1	0	-4.167224	-1.436619	-4.437797

53	1	0	0.116903	2.123928	4.799279
54	1	0	0.065027	-0.029614	6.012842
55	1	0	-1.316580	-1.889156	5.168702
56	1	0	5.667712	-2.428916	0.881323
57	1	0	7.268028	-2.861745	0.194928
58	1	0	7.049268	-1.319265	1.063064
59	1	0	6.789855	-0.164320	-2.473345
60	1	0	7.652019	0.146492	-0.946570
61	1	0	8.027220	-1.312003	-1.903397
62	1	0	-2.028101	3.750015	-3.268422
63	1	0	-2.721202	5.005897	-1.369542
64	1	0	-3.177547	3.576865	-0.445698
65	1	0	-4.102257	4.033731	-1.887389
66	1	0	-0.744784	2.520276	-0.782976
67	1	0	-0.051546	2.535402	-2.406473
68	1	0	-0.337461	4.061399	-1.551423
69	1	0	-4.070544	-1.362141	-0.696022
70	1	0	-6.287360	-0.572589	-1.541069
71	1	0	-6.298003	-2.312159	-1.208260
72	1	0	-6.193595	-1.727058	-2.875331
73	1	0	-2.672447	-2.944683	-2.039741
74	1	0	-4.158630	-3.685838	-1.419487
75	1	0	-4.044031	-3.233374	-3.119863
76	1	0	-2.778025	-2.739900	3.917656
77	1	0	-4.767697	-1.211866	3.768806
78	1	0	-4.931275	-2.746668	2.909555
79	1	0	-4.641239	-1.266313	2.000582
80	1	0	-2.906800	-3.783641	1.728808
81	1	0	-2.428272	-2.285102	0.919886
82	1	0	-1.284388	-3.119751	1.984459
83	1	0	-1.689097	2.756496	1.577152
84	1	0	0.792267	2.580357	1.592969
85	1	0	0.239593	4.260746	1.678574
86	1	0	0.852546	3.462686	3.128434
87	1	0	-2.950652	3.582309	3.569926
88	1	0	-1.937016	4.850843	2.861794
89	1	0	-1.431586	4.035975	4.348958
90	1	0	0.469047	-4.642827	-1.277718
91	1	0	-0.044208	-3.211596	-2.176333
92	1	0	-0.565849	-3.435539	-0.479409
93	1	0	3.829799	-4.497987	-0.988635
94	1	0	3.734214	-5.410697	0.564766
95	1	0	2.459667	-5.614039	-0.667013
96	6	0	3.703016	2.734370	0.042890
97	6	0	4.011541	3.416813	1.209571
98	16	0	4.099245	3.718396	-1.357161
99	6	0	4.560025	4.704113	0.986070
100	1	0	3.845091	2.989017	2.192102
101	6	0	4.667141	5.002925	-0.349433
102	1	0	4.862589	5.382599	1.774551
103	1	0	5.045085	5.910321	-0.800952

Sum of electronic and zero-point Energies= -2911.379138
Sum of electronic and thermal Energies= -2911.322300
Sum of electronic and thermal Enthalpies= -2911.321356
Sum of electronic and thermal Free Energies= -2911.479140

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.983324	-0.019835	-0.371447
2	6	0	2.754375	-1.172986	-0.434748
3	6	0	2.688035	1.235688	-0.477242
4	7	0	2.300408	-2.530574	-0.470424
5	6	0	2.124870	2.463286	-0.291478
6	79	0	-0.083229	-0.008503	-0.142400
7	6	0	-2.149431	0.134773	0.028023
8	7	0	-3.113938	-0.724687	-0.418363
9	6	0	-4.383451	-0.223055	-0.152211
10	6	0	-4.214464	0.974767	0.456556
11	7	0	-2.843768	1.177577	0.571474
12	6	0	-2.892065	-2.057574	-0.951708
13	6	0	-2.279820	2.422697	1.061066
14	6	0	-1.956182	2.572260	2.430068
15	6	0	-1.459113	3.822660	2.825787
16	6	0	-1.311172	4.877112	1.929408
17	6	0	-1.659365	4.703754	0.594773
18	6	0	-2.148293	3.475600	0.128865
19	6	0	-2.906444	-3.127722	-0.027118
20	6	0	-2.689436	-4.419589	-0.523223
21	6	0	-2.482152	-4.642616	-1.879386
22	6	0	-2.516286	-3.574102	-2.770414
23	6	0	-2.734445	-2.255328	-2.343432
24	7	0	4.129783	-1.076372	-0.431353
25	6	0	5.218059	-1.545344	-0.391949
26	7	0	6.394872	-1.956831	-0.062020
27	6	0	6.745117	-2.147065	1.367637
28	6	0	7.444594	-2.202840	-1.068556
29	6	0	-2.110557	1.518951	3.534433
30	6	0	-3.547025	0.996933	3.731989
31	6	0	-1.094756	0.364329	3.446253
32	6	0	-2.556074	3.351091	-1.338196
33	6	0	-3.811788	4.197009	-1.633943
34	6	0	-1.407347	3.720338	-2.295934
35	6	0	1.173737	-2.876590	-1.356343
36	6	0	2.639414	-5.028584	0.618545
37	16	0	2.303986	-3.313837	1.062666
38	8	0	0.985603	-3.270342	1.701688
39	8	0	3.480422	-2.790705	1.771362
40	6	0	-2.816334	-1.191139	-3.446818
41	6	0	-4.117965	-0.366879	-3.459375
42	6	0	-1.575453	-0.284236	-3.542481
43	6	0	-3.232365	-2.940698	1.454367
44	6	0	-4.710020	-3.302717	1.722450
45	6	0	-2.310660	-3.741807	2.390853
46	1	0	3.755700	1.204341	-0.696853
47	1	0	1.063069	2.520007	-0.058734
48	1	0	-5.276282	-0.759878	-0.426310
49	1	0	-4.928879	1.694211	0.821501
50	1	0	-1.198835	3.971331	3.869572
51	1	0	-0.940760	5.836796	2.277906
52	1	0	-1.568069	5.535207	-0.097322
53	1	0	-2.696076	-5.258972	0.163720
54	1	0	-2.321730	-5.651645	-2.248304
55	1	0	-2.390838	-3.761927	-3.832986
56	1	0	5.831136	-2.135328	1.959943

57	1	0	7.236532	-3.117273	1.476850
58	1	0	7.426313	-1.353284	1.687162
59	1	0	7.043732	-2.021846	-2.065583
60	1	0	8.287886	-1.530045	-0.887937
61	1	0	7.786012	-3.238867	-0.992996
62	1	0	-1.867556	2.062070	4.455347
63	1	0	-4.268960	1.818726	3.781146
64	1	0	-3.606472	0.447289	4.676928
65	1	0	-3.858821	0.313515	2.938620
66	1	0	-0.070864	0.740715	3.362587
67	1	0	-1.155121	-0.249451	4.351403
68	1	0	-1.278380	-0.287271	2.589065
69	1	0	-2.812095	2.307813	-1.538595
70	1	0	-4.650675	3.911969	-0.991192
71	1	0	-4.123334	4.065513	-2.675226
72	1	0	-3.620274	5.263323	-1.475211
73	1	0	-0.520925	3.105344	-2.113878
74	1	0	-1.720192	3.564659	-3.333413
75	1	0	-1.115510	4.770950	-2.197978
76	1	0	1.330810	-2.354744	-2.301219
77	1	0	0.200097	-2.593521	-0.947596
78	1	0	1.184231	-3.951173	-1.556194
79	1	0	2.739665	-5.562446	1.565414
80	1	0	1.804359	-5.439038	0.051683
81	1	0	3.567714	-5.074596	0.049749
82	1	0	-2.832385	-1.774153	-4.375346
83	1	0	-4.999482	-1.009860	-3.369518
84	1	0	-4.197214	0.171591	-4.409358
85	1	0	-4.153382	0.376888	-2.660062
86	1	0	-1.647048	0.347879	-4.434410
87	1	0	-1.471727	0.368634	-2.672668
88	1	0	-0.658118	-0.875537	-3.623606
89	1	0	-3.098380	-1.884623	1.704327
90	1	0	-5.398704	-2.711293	1.111465
91	1	0	-4.958763	-3.129555	2.774487
92	1	0	-4.897347	-4.359163	1.502826
93	1	0	-1.256435	-3.528691	2.205792
94	1	0	-2.536033	-3.484447	3.430878
95	1	0	-2.467201	-4.821249	2.290390
96	6	0	2.801597	3.728553	-0.355024
97	6	0	2.236290	4.971315	-0.120323
98	16	0	4.504752	3.909039	-0.754278
99	6	0	3.148496	6.048257	-0.256853
100	1	0	1.192534	5.084315	0.149718
101	6	0	4.409696	5.629136	-0.596695
102	1	0	2.887262	7.089681	-0.111041
103	1	0	5.290551	6.233345	-0.766211

Sum of electronic and zero-point Energies= -2911.414820
Sum of electronic and thermal Energies= -2911.358374
Sum of electronic and thermal Enthalpies= -2911.357429
Sum of electronic and thermal Free Energies= -2911.513473

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.717325	-0.397439	-0.720190

2	6	0	1.554834	-1.144970	-0.759285
3	6	0	2.786985	1.030824	-0.430783
4	7	0	1.687725	-2.542825	-1.038455
5	6	0	3.919917	1.749311	-0.261653
6	79	0	-0.318354	-0.379225	-0.310994
7	6	0	-2.204055	0.287878	0.247834
8	7	0	-2.737900	0.250742	1.503319
9	6	0	-4.021958	0.782474	1.506764
10	6	0	-4.306491	1.134178	0.229079
11	7	0	-3.180755	0.837839	-0.531879
12	6	0	-2.039782	-0.148605	2.715459
13	6	0	-3.152271	0.951376	-1.980689
14	6	0	-2.723736	2.149250	-2.597677
15	6	0	-2.733022	2.175357	-3.999834
16	6	0	-3.159431	1.088377	-4.756432
17	6	0	-3.608459	-0.061527	-4.119220
18	6	0	-3.620334	-0.156464	-2.721766
19	6	0	-1.302062	0.848689	3.389710
20	6	0	-0.635451	0.486666	4.567050
21	6	0	-0.701876	-0.810643	5.058350
22	6	0	-1.455686	-1.766649	4.385012
23	6	0	-2.152788	-1.471309	3.204675
24	7	0	3.919284	-1.035342	-0.976021
25	6	0	5.082395	-1.187017	-1.048982
26	7	0	6.322557	-1.549612	-0.995999
27	6	0	6.831960	-2.236042	0.215846
28	6	0	7.279492	-1.217918	-2.069092
29	6	0	-2.262119	3.432530	-1.897452
30	6	0	-3.296049	4.065865	-0.946500
31	6	0	-0.881062	3.309638	-1.229501
32	6	0	-4.189489	-1.415889	-2.072003
33	6	0	-5.722141	-1.471495	-2.242455
34	6	0	-3.534474	-2.702286	-2.607637
35	6	0	-2.962311	-2.621105	2.591748
36	6	0	-4.472909	-2.353280	2.447693
37	6	0	-2.357915	-3.179494	1.290300
38	6	0	-1.235192	2.300313	2.922028
39	6	0	0.215074	2.796767	2.777226
40	6	0	-2.039760	3.218460	3.865268
41	6	0	0.508669	-3.161972	-1.685571
42	6	0	3.199370	-4.832467	-0.766756
43	16	0	2.337231	-3.578711	0.203401
44	8	0	1.235930	-4.237970	0.909225
45	8	0	3.348120	-2.823821	0.952853
46	1	0	1.815158	1.512392	-0.368467
47	1	0	4.882572	1.240109	-0.285862
48	1	0	-4.606141	0.852116	2.409509
49	1	0	-5.191119	1.566661	-0.208498
50	1	0	-2.405158	3.079484	-4.504510
51	1	0	-3.157654	1.146923	-5.840780
52	1	0	-3.966606	-0.897173	-4.711743
53	1	0	-0.063557	1.235486	5.105376
54	1	0	-0.178487	-1.076659	5.971816
55	1	0	-1.514590	-2.775072	4.783570
56	1	0	5.989434	-2.498487	0.856359
57	1	0	7.358775	-3.143188	-0.091934
58	1	0	7.521455	-1.576266	0.750170
59	1	0	6.755914	-0.721469	-2.885915
60	1	0	8.055996	-0.554923	-1.677123

61	1	0	7.740416	-2.138205	-2.438048
62	1	0	-2.136769	4.152543	-2.714661
63	1	0	-2.984668	5.085695	-0.697836
64	1	0	-3.393656	3.517943	-0.006402
65	1	0	-4.284227	4.126711	-1.413885
66	1	0	-0.900160	2.637326	-0.368403
67	1	0	-0.135061	2.931596	-1.935315
68	1	0	-0.547743	4.292810	-0.881344
69	1	0	-3.983092	-1.377107	-0.999705
70	1	0	-6.207093	-0.586309	-1.819032
71	1	0	-6.130862	-2.354049	-1.739615
72	1	0	-6.001335	-1.528360	-3.299713
73	1	0	-2.447131	-2.670667	-2.492354
74	1	0	-3.911075	-3.571392	-2.058858
75	1	0	-3.756422	-2.864058	-3.667205
76	1	0	-2.878198	-3.427783	3.329105
77	1	0	-4.893995	-1.929496	3.365320
78	1	0	-4.992233	-3.297005	2.251204
79	1	0	-4.703923	-1.677881	1.620418
80	1	0	-2.902801	-4.081195	0.988378
81	1	0	-2.423705	-2.458907	0.470889
82	1	0	-1.305850	-3.447408	1.423533
83	1	0	-1.695843	2.368358	1.933125
84	1	0	0.795441	2.145921	2.116536
85	1	0	0.228352	3.807445	2.357540
86	1	0	0.730166	2.837361	3.742258
87	1	0	-3.086377	2.905528	3.936380
88	1	0	-2.019175	4.251450	3.502578
89	1	0	-1.622272	3.210899	4.877472
90	1	0	0.763947	-4.165486	-2.032776
91	1	0	0.259761	-2.558278	-2.558209
92	1	0	-0.353568	-3.222019	-1.016226
93	1	0	3.956690	-4.347020	-1.381470
94	1	0	3.657324	-5.506314	-0.039891
95	1	0	2.490469	-5.384307	-1.382750
96	6	0	4.044651	3.170929	-0.033672
97	6	0	5.219186	3.850320	0.227978
98	16	0	2.698733	4.294810	-0.069761
99	6	0	5.045805	5.249907	0.406517
100	1	0	6.178916	3.348744	0.294015
101	6	0	3.739801	5.637750	0.275432
102	1	0	5.854069	5.938847	0.621698
103	1	0	3.323639	6.632344	0.357292

Sum of electronic and zero-point Energies= -2911.408262
Sum of electronic and thermal Energies= -2911.351782
Sum of electronic and thermal Enthalpies= -2911.350838
Sum of electronic and thermal Free Energies= -2911.506561

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.638758	-0.270758	-0.480096
2	6	0	2.606454	0.712755	-0.599064
3	6	0	1.993308	-1.602704	-0.850997
4	7	0	2.482919	2.067366	-0.253925
5	6	0	3.055069	-2.372240	-0.395984

6	79	0	-0.422459	-0.103089	-0.200143
7	6	0	-2.469685	-0.078866	0.048361
8	7	0	-3.255394	0.953977	0.470597
9	6	0	-4.593176	0.574436	0.494366
10	6	0	-4.641507	-0.722735	0.104241
11	7	0	-3.336158	-1.107984	-0.181186
12	6	0	-2.806344	2.313707	0.714518
13	6	0	-2.962015	-2.470454	-0.520763
14	6	0	-2.647579	-3.336380	0.549293
15	6	0	-2.299201	-4.658003	0.241369
16	6	0	-2.273071	-5.105153	-1.073425
17	6	0	-2.606788	-4.234006	-2.106366
18	6	0	-2.964566	-2.898895	-1.869216
19	6	0	-2.752761	3.182184	-0.398178
20	6	0	-2.328327	4.499597	-0.180662
21	6	0	-1.979778	4.940496	1.089926
22	6	0	-2.065215	4.068500	2.171494
23	6	0	-2.484411	2.737796	2.025475
24	7	0	3.764845	0.458148	-1.316974
25	6	0	4.301069	-0.622845	-1.603456
26	7	0	5.504944	-1.097950	-1.757454
27	6	0	6.662895	-0.476965	-1.076867
28	6	0	5.762007	-2.323284	-2.518462
29	1	0	3.177676	-3.336284	-0.888262
30	6	0	-3.309888	-2.060033	-3.106211
31	6	0	-4.712174	-1.422144	-3.106196
32	6	0	-2.221261	-1.031741	-3.467375
33	6	0	4.180638	3.567627	-1.857072
34	16	0	3.913121	3.056158	-0.153722
35	8	0	5.047484	2.235572	0.282177
36	8	0	3.523653	4.235869	0.614388
37	6	0	1.310741	2.531890	0.496049
38	6	0	-2.542149	1.900126	3.309580
39	6	0	-1.405887	0.865562	3.415649
40	6	0	-3.911282	1.270081	3.629125
41	6	0	-3.166858	2.766096	-1.808174
42	6	0	-4.434638	3.521670	-2.256566
43	6	0	-2.023399	2.954181	-2.823581
44	6	0	-2.699177	-2.912959	2.015410
45	6	0	-3.813999	-3.665139	2.770508
46	6	0	-1.336843	-3.095493	2.711718
47	1	0	1.348970	-2.096593	-1.579264
48	1	0	-5.373106	1.256709	0.789930
49	1	0	-5.471461	-1.401754	-0.001936
50	1	0	-2.056428	-5.343955	1.046670
51	1	0	-2.007933	-6.134637	-1.295430
52	1	0	-2.600255	-4.595637	-3.130576
53	1	0	-2.281988	5.187862	-1.018637
54	1	0	-1.656229	5.965655	1.243361
55	1	0	-1.808733	4.426256	3.164391
56	1	0	7.047638	-1.169531	-0.321813
57	1	0	7.443237	-0.275557	-1.816697
58	1	0	6.345466	0.450636	-0.601330
59	1	0	4.839000	-2.661244	-2.987598
60	1	0	6.508000	-2.119541	-3.292292
61	1	0	6.145912	-3.103523	-1.853724
62	1	0	-3.320965	-2.786875	-3.926881
63	1	0	-5.480568	-2.144973	-2.813439
64	1	0	-4.952966	-1.075943	-4.116556

65	1	0	-4.782542	-0.557993	-2.441701
66	1	0	-1.242007	-1.511911	-3.561044
67	1	0	-2.458347	-0.559542	-4.427032
68	1	0	-2.133725	-0.244014	-2.715486
69	1	0	3.301793	4.121569	-2.187646
70	1	0	5.059665	4.215556	-1.847970
71	1	0	4.350283	2.684787	-2.471036
72	1	0	0.418019	2.445759	-0.128086
73	1	0	1.463291	3.573653	0.767704
74	1	0	1.169202	1.941239	1.405866
75	1	0	-2.362286	2.627014	4.110204
76	1	0	-1.431138	0.384569	4.399476
77	1	0	-1.486869	0.084647	2.655781
78	1	0	-0.427302	1.342216	3.301378
79	1	0	-4.722914	1.995809	3.514043
80	1	0	-3.918744	0.929562	4.669566
81	1	0	-4.133600	0.403290	3.002644
82	1	0	-3.412856	1.701407	-1.798533
83	1	0	-5.264490	3.361396	-1.561054
84	1	0	-4.751426	3.178876	-3.246880
85	1	0	-4.257627	4.600277	-2.318496
86	1	0	-1.135648	2.383970	-2.531285
87	1	0	-2.337879	2.608570	-3.813633
88	1	0	-1.735302	4.006085	-2.919172
89	1	0	-2.941434	-1.848354	2.061577
90	1	0	-4.791754	-3.508085	2.304041
91	1	0	-3.872984	-3.316596	3.806660
92	1	0	-3.626523	-4.743537	2.792796
93	1	0	-1.035586	-4.147643	2.741459
94	1	0	-0.550966	-2.532918	2.197919
95	1	0	-1.391306	-2.739811	3.745720
96	6	0	3.854422	-2.264916	0.803940
97	6	0	4.793501	-3.207903	1.198060
98	16	0	3.740315	-0.993714	2.007345
99	6	0	5.415875	-2.913672	2.437351
100	1	0	5.003251	-4.097589	0.613160
101	6	0	4.946180	-1.748802	2.989335
102	1	0	6.167154	-3.538635	2.905049
103	1	0	5.235758	-1.289861	3.925152

Sum of electronic and zero-point Energies= -2911.393830
Sum of electronic and thermal Energies= -2911.338808
Sum of electronic and thermal Enthalpies= -2911.337864
Sum of electronic and thermal Free Energies= -2911.489651

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.448088	1.579529	-0.126245
2	6	0	1.064631	2.050709	-0.084843
3	6	0	2.804730	0.311199	0.389057
4	7	0	0.825892	3.364098	-0.062895
5	6	0	4.117464	-0.143615	0.258153
6	79	0	-0.397900	0.555796	-0.128577
7	6	0	-1.748569	-1.016081	-0.137310
8	7	0	-2.728772	-1.256299	0.782170
9	6	0	-3.413350	-2.424873	0.474195

10	6	0	-2.845219	-2.932728	-0.646158
11	7	0	-1.833140	-2.056236	-1.019420
12	6	0	-3.141214	-0.366614	1.858029
13	6	0	-0.924098	-2.334911	-2.118987
14	6	0	0.203702	-3.136717	-1.833348
15	6	0	1.079789	-3.430332	-2.885953
16	6	0	0.842161	-2.958339	-4.170972
17	6	0	-0.295104	-2.199944	-4.429374
18	6	0	-1.216865	-1.874283	-3.423554
19	6	0	-2.580802	-0.497501	3.149445
20	6	0	-3.043802	0.393839	4.128215
21	6	0	-4.020680	1.346342	3.857276
22	6	0	-4.578635	1.421866	2.587483
23	6	0	-4.156829	0.569216	1.560497
24	7	0	3.456150	2.374666	-0.564144
25	6	0	4.678878	2.032732	-0.378134
26	7	0	5.742093	2.244899	-1.125726
27	6	0	5.669791	2.604041	-2.550344
28	6	0	7.083363	2.076261	-0.562759
29	1	0	4.583435	-0.059409	-0.719486
30	6	0	-2.446396	-1.071589	-3.867354
31	6	0	-3.808207	-1.723357	-3.560753
32	6	0	-2.411862	0.400451	-3.418126
33	6	0	-4.849052	0.642203	0.200519
34	6	0	-6.225896	-0.054029	0.253964
35	6	0	-4.997754	2.084095	-0.319509
36	6	0	-1.540991	-1.527590	3.609500
37	6	0	-1.952012	-2.999630	3.414057
38	6	0	-0.119321	-1.264493	3.079827
39	6	0	0.461025	-3.748019	-0.457450
40	6	0	0.034294	-5.231656	-0.436505
41	6	0	1.924515	-3.605770	-0.003049
42	6	0	-1.210004	3.717570	-1.939001
43	16	0	-0.878339	3.969741	-0.190056
44	8	0	-0.795747	5.403427	0.068016
45	8	0	-1.735303	3.107980	0.617061
46	6	0	1.822452	4.440610	0.158734
47	1	0	2.098867	-0.207086	1.031076
48	1	0	-4.228764	-2.781695	1.081282
49	1	0	-3.066607	-3.820412	-1.215108
50	1	0	1.951637	-4.046950	-2.695064
51	1	0	1.529534	-3.198168	-4.976777
52	1	0	-0.488869	-1.858866	-5.442233
53	1	0	-2.630870	0.325276	5.130410
54	1	0	-4.356653	2.017818	4.641589
55	1	0	-5.355539	2.151856	2.387553
56	1	0	6.254984	3.511389	-2.730792
57	1	0	6.078290	1.796750	-3.168760
58	1	0	4.629817	2.783898	-2.819517
59	1	0	7.642453	3.015129	-0.636508
60	1	0	6.995519	1.786874	0.483826
61	1	0	7.631262	1.301181	-1.110185
62	1	0	-2.371914	-1.051988	-4.960827
63	1	0	-3.819678	-2.778448	-3.852132
64	1	0	-4.590941	-1.214949	-4.133022
65	1	0	-4.081207	-1.655460	-2.505330
66	1	0	-1.475052	0.875142	-3.728856
67	1	0	-3.240459	0.951071	-3.877038
68	1	0	-2.500804	0.496869	-2.332841

69	1	0	-4.235432	0.103435	-0.527213
70	1	0	-6.143204	-1.101513	0.559892
71	1	0	-6.707746	-0.026792	-0.729015
72	1	0	-6.888712	0.447413	0.966816
73	1	0	-4.042345	2.613458	-0.295369
74	1	0	-5.372307	2.070223	-1.348602
75	1	0	-5.714766	2.659936	0.274088
76	1	0	-1.485098	-1.381428	4.694436
77	1	0	-2.968416	-3.181661	3.777664
78	1	0	-1.276487	-3.645918	3.984064
79	1	0	-1.899655	-3.316324	2.369489
80	1	0	0.185529	-0.230605	3.269300
81	1	0	0.594415	-1.926777	3.581873
82	1	0	-0.044642	-1.446784	2.004501
83	1	0	-0.153626	-3.217892	0.275105
84	1	0	-1.021160	-5.356957	-0.696496
85	1	0	0.189180	-5.659539	0.559328
86	1	0	0.623294	-5.817734	-1.149793
87	1	0	2.267074	-2.569704	-0.063162
88	1	0	2.027138	-3.939878	1.034054
89	1	0	2.601694	-4.218977	-0.606161
90	1	0	-1.136128	2.655227	-2.167680
91	1	0	-2.225612	4.082164	-2.106827
92	1	0	-0.493695	4.308999	-2.510414
93	1	0	2.389257	4.630060	-0.753549
94	1	0	2.507251	4.122372	0.942675
95	1	0	1.292495	5.336986	0.471284
96	6	0	4.762092	-1.097026	1.132570
97	6	0	5.838089	-1.914411	0.838050
98	16	0	4.265518	-1.330225	2.799178
99	6	0	6.245030	-2.732618	1.925173
100	1	0	6.311340	-1.927479	-0.138141
101	6	0	5.486885	-2.531047	3.049403
102	1	0	7.064207	-3.440469	1.878466
103	1	0	5.577931	-3.013863	4.012695

Sum of electronic and zero-point Energies= -2911.398421
Sum of electronic and thermal Energies= -2911.343462
Sum of electronic and thermal Enthalpies= -2911.342518
Sum of electronic and thermal Free Energies= -2911.492958

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.621880	-0.227751	-0.193490
2	6	0	2.592812	0.868430	-0.373503
3	6	0	2.222826	-1.441633	-0.231141
4	7	0	2.387107	2.094145	0.165764
5	6	0	3.698851	-1.666680	-0.502762
6	79	0	-0.451029	-0.122128	-0.067125
7	6	0	-2.513205	-0.134005	-0.006255
8	7	0	-3.346830	0.864778	0.407426
9	6	0	-4.676967	0.476670	0.285151
10	6	0	-4.673821	-0.793615	-0.187758
11	7	0	-3.343328	-1.151698	-0.376530
12	6	0	-2.934344	2.206740	0.778825
13	6	0	-2.922614	-2.488118	-0.762886

14	6	0	-2.698225	-3.416987	0.276633
15	6	0	-2.304428	-4.713975	-0.077963
16	6	0	-2.149364	-5.077730	-1.409456
17	6	0	-2.397608	-4.146425	-2.413477
18	6	0	-2.794034	-2.831697	-2.129250
19	6	0	-2.783365	3.145674	-0.265709
20	6	0	-2.385939	4.445816	0.073778
21	6	0	-2.158044	4.803920	1.396791
22	6	0	-2.339710	3.864359	2.407564
23	6	0	-2.737078	2.546032	2.138425
24	7	0	3.724727	0.735511	-1.093524
25	6	0	4.273756	-0.462988	-1.221575
26	7	0	5.380714	-0.580324	-1.962212
27	6	0	5.916541	0.606785	-2.642485
28	6	0	6.066867	-1.861075	-2.162229
29	1	0	3.770227	-2.533511	-1.171057
30	6	0	-3.035439	-1.920003	-3.338870
31	6	0	-4.445874	-1.307670	-3.435447
32	6	0	-1.941249	-0.852247	-3.525954
33	6	0	3.681319	3.781804	-1.665403
34	16	0	3.681903	3.347596	0.078264
35	8	0	4.953204	2.748375	0.469944
36	8	0	3.131725	4.474499	0.824745
37	6	0	1.244625	2.419144	1.041140
38	6	0	-2.907406	1.627922	3.355835
39	6	0	-1.775689	0.593191	3.501647
40	6	0	-4.294018	0.973383	3.505012
41	6	0	-3.066393	2.822067	-1.731202
42	6	0	-4.284506	3.615186	-2.247133
43	6	0	-1.832562	3.062593	-2.622028
44	6	0	-2.894199	-3.087633	1.754793
45	6	0	-4.068062	-3.891601	2.350311
46	6	0	-1.603601	-3.307935	2.567008
47	1	0	1.651480	-2.348788	-0.055211
48	1	0	-5.488900	1.133490	0.550739
49	1	0	-5.482524	-1.470099	-0.410422
50	1	0	-2.128509	-5.447205	0.702689
51	1	0	-1.849518	-6.088849	-1.668417
52	1	0	-2.289771	-4.443013	-3.452770
53	1	0	-2.267227	5.186928	-0.710336
54	1	0	-1.854937	5.816744	1.644761
55	1	0	-2.179213	4.157550	3.440986
56	1	0	6.905729	0.369785	-3.032172
57	1	0	5.270599	0.906096	-3.474147
58	1	0	5.989527	1.431617	-1.931738
59	1	0	6.013996	-2.473752	-1.263011
60	1	0	5.644965	-2.411099	-3.011834
61	1	0	7.119087	-1.663159	-2.367922
62	1	0	-2.950121	-2.592086	-4.200793
63	1	0	-5.221781	-2.061683	-3.267991
64	1	0	-4.595699	-0.897638	-4.439535
65	1	0	-4.600755	-0.491996	-2.725384
66	1	0	-0.945798	-1.306829	-3.541815
67	1	0	-2.090974	-0.329055	-4.476876
68	1	0	-1.952391	-0.108947	-2.725520
69	1	0	2.706991	4.208991	-1.903634
70	1	0	4.465857	4.532644	-1.783152
71	1	0	3.892436	2.887485	-2.246776
72	1	0	0.325945	2.491164	0.456436

73	1	0	1.447423	3.376623	1.515644
74	1	0	1.132706	1.648188	1.803109
75	1	0	-2.810525	2.302776	4.214287
76	1	0	-1.890256	0.046050	4.443578
77	1	0	-1.774147	-0.133517	2.685920
78	1	0	-0.795820	1.080864	3.516328
79	1	0	-5.098504	1.701591	3.359549
80	1	0	-4.395242	0.568390	4.517033
81	1	0	-4.448109	0.146728	2.807905
82	1	0	-3.315439	1.761185	-1.811428
83	1	0	-5.175200	3.420354	-1.641658
84	1	0	-4.510001	3.335465	-3.281273
85	1	0	-4.099260	4.694003	-2.226795
86	1	0	-0.979724	2.464456	-2.284321
87	1	0	-2.053919	2.783158	-3.657092
88	1	0	-1.533078	4.115825	-2.622519
89	1	0	-3.151073	-2.029221	1.844355
90	1	0	-4.998111	-3.710200	1.802300
91	1	0	-4.230171	-3.609850	3.395744
92	1	0	-3.871572	-4.968249	2.322846
93	1	0	-1.294034	-4.357977	2.558756
94	1	0	-0.778342	-2.708532	2.169519
95	1	0	-1.761257	-3.020155	3.611469
96	6	0	4.477772	-1.971841	0.770028
97	6	0	5.126307	-1.098951	1.607926
98	16	0	4.556286	-3.604908	1.386421
99	6	0	5.693650	-1.742922	2.749694
100	1	0	5.206064	-0.032769	1.420927
101	6	0	5.468397	-3.090647	2.769033
102	1	0	6.250482	-1.220862	3.518888
103	1	0	5.785329	-3.817381	3.504024

Sum of electronic and zero-point Energies= -2911.464288
Sum of electronic and thermal Energies= -2911.409477
Sum of electronic and thermal Enthalpies= -2911.408533
Sum of electronic and thermal Free Energies= -2911.560928

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.275934	1.790455	-0.309085
2	6	0	0.849594	2.128843	-0.413405
3	6	0	2.738246	0.538888	-0.595761
4	7	0	0.472376	3.387526	-0.591067
5	6	0	4.245152	0.569209	-0.492868
6	79	0	-0.473082	0.519589	-0.188669
7	6	0	-1.688754	-1.134733	0.067213
8	7	0	-2.813761	-1.253316	0.829914
9	6	0	-3.333615	-2.538786	0.735852
10	6	0	-2.514544	-3.239891	-0.085305
11	7	0	-1.516257	-2.365864	-0.498220
12	6	0	-3.499669	-0.187000	1.545178
13	6	0	-0.355906	-2.785195	-1.263835
14	6	0	0.732073	-3.313834	-0.533899
15	6	0	1.869850	-3.706777	-1.251147
16	6	0	1.918646	-3.593859	-2.635659
17	6	0	0.815118	-3.106896	-3.330451

18	6	0	-0.355519	-2.697537	-2.675019
19	6	0	-3.180452	0.091786	2.893918
20	6	0	-3.909444	1.117867	3.512358
21	6	0	-4.912985	1.815716	2.848719
22	6	0	-5.224679	1.492975	1.534322
23	6	0	-4.528793	0.487781	0.852697
24	7	0	3.312111	2.693501	0.021822
25	6	0	4.442255	2.031133	-0.059103
26	7	0	5.636854	2.584285	0.228070
27	6	0	5.691534	3.988142	0.631340
28	6	0	6.912724	1.969058	-0.120955
29	1	0	4.677625	0.433509	-1.495771
30	6	0	-1.511663	-2.233033	-3.569601
31	6	0	-2.813683	-3.042129	-3.412473
32	6	0	-1.781507	-0.717660	-3.514276
33	6	0	-4.942161	0.137314	-0.575367
34	6	0	-6.264963	-0.657151	-0.586458
35	6	0	-5.052111	1.381444	-1.476450
36	6	0	-2.138201	-0.617817	3.767605
37	6	0	-2.313285	-2.143426	3.888290
38	6	0	-0.683758	-0.237205	3.431991
39	6	0	0.691484	-3.535815	0.976965
40	6	0	0.572641	-5.041069	1.296782
41	6	0	1.897623	-2.916949	1.704519
42	6	0	-1.544878	3.276457	-2.516567
43	16	0	-1.295640	3.785141	-0.807526
44	8	0	-1.354987	5.239052	-0.726530
45	8	0	-2.075757	2.940868	0.090223
46	6	0	1.308432	4.608132	-0.739837
47	1	0	2.161921	-0.334756	-0.865485
48	1	0	-4.225241	-2.829210	1.266564
49	1	0	-2.544751	-4.265992	-0.412882
50	1	0	2.720893	-4.114573	-0.715964
51	1	0	2.806346	-3.906268	-3.177620
52	1	0	0.850320	-3.052309	-4.414675
53	1	0	-3.686390	1.362269	4.546786
54	1	0	-5.459795	2.600448	3.362567
55	1	0	-6.021500	2.026732	1.027206
56	1	0	4.795271	4.239380	1.197293
57	1	0	6.575008	4.140808	1.255952
58	1	0	5.756749	4.653019	-0.239520
59	1	0	7.602499	2.043989	0.725188
60	1	0	6.787438	0.915246	-0.359422
61	1	0	7.365574	2.479260	-0.981125
62	1	0	-1.159845	-2.435858	-4.587838
63	1	0	-2.618276	-4.118944	-3.433189
64	1	0	-3.488920	-2.812633	-4.243111
65	1	0	-3.344538	-2.806586	-2.486964
66	1	0	-0.860578	-0.151026	-3.687719
67	1	0	-2.502486	-0.442424	-4.291952
68	1	0	-2.192255	-0.410524	-2.549226
69	1	0	-4.170609	-0.503682	-1.011276
70	1	0	-6.190176	-1.579628	-0.002349
71	1	0	-6.541788	-0.927988	-1.610744
72	1	0	-7.082057	-0.063510	-0.163699
73	1	0	-4.143967	1.986541	-1.417541
74	1	0	-5.211437	1.078613	-2.516693
75	1	0	-5.895659	2.018018	-1.191949
76	1	0	-2.323438	-0.223552	4.773542

77	1	0	-3.350262	-2.409064	4.117828
78	1	0	-1.687963	-2.518450	4.705116
79	1	0	-2.017125	-2.676262	2.981517
80	1	0	-0.558031	0.849482	3.404353
81	1	0	-0.009144	-0.637974	4.196749
82	1	0	-0.366643	-0.635599	2.464753
83	1	0	-0.201675	-3.048210	1.374735
84	1	0	-0.309647	-5.486647	0.826492
85	1	0	0.494196	-5.195611	2.377763
86	1	0	1.450264	-5.591607	0.942341
87	1	0	1.985128	-1.846194	1.500349
88	1	0	1.785453	-3.046693	2.785790
89	1	0	2.841110	-3.390365	1.416935
90	1	0	-1.373979	2.203013	-2.596596
91	1	0	-2.580221	3.525791	-2.757326
92	1	0	-0.862417	3.846610	-3.148131
93	1	0	2.334901	4.339774	-0.505908
94	1	0	0.939702	5.372503	-0.057357
95	1	0	1.222519	4.981811	-1.763873
96	6	0	4.820984	-0.466092	0.446379
97	6	0	4.859158	-0.443703	1.817885
98	16	0	5.537916	-1.935165	-0.167654
99	6	0	5.468648	-1.605340	2.381994
100	1	0	4.477059	0.382443	2.407558
101	6	0	5.885837	-2.499394	1.435043
102	1	0	5.597737	-1.761961	3.446574
103	1	0	6.384707	-3.448028	1.577324

Sum of electronic and zero-point Energies= -2911.450662
Sum of electronic and thermal Energies= -2911.395741
Sum of electronic and thermal Enthalpies= -2911.394797
Sum of electronic and thermal Free Energies= -2911.544987

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.119487	1.035283	1.087711
2	6	0	0.480097	2.431135	0.997752
3	6	0	1.161231	0.257290	1.549490
4	7	0	-0.477493	3.417923	0.771261
5	6	0	2.539217	0.694867	1.721790
6	79	0	-1.596205	0.060560	0.453594
7	6	0	-3.217100	-1.028096	-0.225701
8	7	0	-4.500557	-0.605730	-0.438017
9	6	0	-5.293413	-1.647816	-0.910220
10	6	0	-4.502235	-2.746145	-0.969055
11	7	0	-3.231788	-2.351696	-0.564505
12	6	0	-4.962323	0.766426	-0.349821
13	6	0	-2.121255	-3.272661	-0.392781
14	6	0	-1.964166	-3.860336	0.880951
15	6	0	-0.894539	-4.744595	1.067327
16	6	0	-0.015429	-5.033291	0.032055
17	6	0	-0.207932	-4.457360	-1.219144
18	6	0	-1.262909	-3.570771	-1.476764
19	6	0	-4.795464	1.578277	-1.493368
20	6	0	-5.243675	2.904063	-1.429360
21	6	0	-5.842837	3.403945	-0.280289

22	6	0	-6.013160	2.575710	0.824910
23	6	0	-5.585835	1.239852	0.828378
24	7	0	1.724061	2.898423	1.091392
25	6	0	2.749618	2.107034	1.409627
26	7	0	3.979767	2.687024	1.404811
27	6	0	4.118416	4.117754	1.140076
28	6	0	5.226018	1.936678	1.310311
29	1	0	2.981094	0.145595	0.416454
30	6	0	-1.351728	-3.021394	-2.906088
31	6	0	-2.684162	-3.289292	-3.632727
32	6	0	-0.926158	-1.546792	-3.024180
33	6	0	0.890428	4.745749	-1.232865
34	16	0	-0.010867	5.031087	0.297965
35	8	0	0.858052	5.674902	1.283906
36	8	0	-1.281566	5.677956	-0.049331
37	6	0	-1.903429	3.231443	1.079735
38	6	0	-5.827531	0.455493	2.124102
39	6	0	-4.542632	0.251875	2.949204
40	6	0	-6.617203	-0.858579	1.975220
41	6	0	-4.171408	1.075468	-2.793097
42	6	0	-5.202591	1.075929	-3.939693
43	6	0	-2.915819	1.882895	-3.174762
44	6	0	-2.911661	-3.596005	2.048850
45	6	0	-3.691550	-4.870802	2.429333
46	6	0	-2.170606	-3.013993	3.267692
47	1	0	0.989966	-0.797745	1.740920
48	1	0	-6.334888	-1.507979	-1.148512
49	1	0	-4.715857	-3.760184	-1.263904
50	1	0	-0.748960	-5.204534	2.039801
51	1	0	0.820754	-5.705927	0.196403
52	1	0	0.487444	-4.682307	-2.021926
53	1	0	-5.119415	3.548836	-2.293561
54	1	0	-6.182122	4.434944	-0.245150
55	1	0	-6.491100	2.969938	1.717291
56	1	0	4.989341	4.487851	1.690486
57	1	0	4.278826	4.301345	0.069559
58	1	0	3.223841	4.649682	1.458578
59	1	0	5.045825	0.868868	1.224662
60	1	0	5.768672	2.265217	0.416325
61	1	0	5.857255	2.107707	2.189997
62	1	0	-0.598744	-3.595181	-3.458774
63	1	0	-3.009606	-4.328205	-3.509039
64	1	0	-2.553295	-3.108998	-4.705103
65	1	0	-3.489634	-2.634866	-3.291086
66	1	0	0.088007	-1.394284	-2.648866
67	1	0	-0.937212	-1.241885	-4.076834
68	1	0	-1.592812	-0.880883	-2.471089
69	1	0	0.186115	4.342346	-1.960452
70	1	0	1.246765	5.728374	-1.548520
71	1	0	1.718074	4.061748	-1.057894
72	1	0	-2.445877	2.780249	0.245880
73	1	0	-2.341539	4.205081	1.293303
74	1	0	-1.990929	2.587621	1.955023
75	1	0	-6.470054	1.115006	2.720134
76	1	0	-4.785036	-0.217843	3.909131
77	1	0	-3.818377	-0.381131	2.431700
78	1	0	-4.053387	1.208463	3.156164
79	1	0	-7.508845	-0.722664	1.353795
80	1	0	-6.950487	-1.193506	2.963266

81	1	0	-6.018829	-1.663646	1.543701
82	1	0	-3.852544	0.040987	-2.647846
83	1	0	-6.080998	0.471823	-3.689698
84	1	0	-4.756260	0.664506	-4.851059
85	1	0	-5.549971	2.089212	-4.167583
86	1	0	-2.163815	1.838743	-2.381301
87	1	0	-2.467858	1.474771	-4.086517
88	1	0	-3.153280	2.935401	-3.362261
89	1	0	-3.647533	-2.850425	1.737586
90	1	0	-4.254375	-5.265721	1.577051
91	1	0	-4.401536	-4.658084	3.235905
92	1	0	-3.019300	-5.661943	2.777754
93	1	0	-1.432751	-3.717893	3.666172
94	1	0	-1.647070	-2.089938	3.005044
95	1	0	-2.881000	-2.789419	4.070739
96	7	0	3.330208	-0.331464	-0.745164
97	16	0	3.163013	0.686937	-2.061058
98	16	0	3.279467	-1.999578	-0.865924
99	8	0	2.188280	0.235477	-3.045304
100	8	0	3.091870	2.033643	-1.494065
101	8	0	3.013620	-2.477297	-2.218245
102	8	0	2.528740	-2.495372	0.284103
103	6	0	5.070622	-2.433946	-0.510984
104	6	0	4.833556	0.629036	-2.914970
105	9	0	5.504082	-1.793985	0.578278
106	9	0	5.147072	-3.750011	-0.311134
107	9	0	5.841084	-2.098405	-1.547575
108	9	0	4.986227	-0.510456	-3.582823
109	9	0	5.812592	0.753309	-2.012172
110	9	0	4.889183	1.654771	-3.766284
111	6	0	3.282765	0.103940	2.882234
112	6	0	3.834580	0.783812	3.944808
113	16	0	3.425551	-1.626048	3.150125
114	6	0	4.374500	-0.062129	4.958060
115	1	0	3.837822	1.865890	4.004572
116	6	0	4.220471	-1.388839	4.672465
117	1	0	4.845753	0.307700	5.861985
118	1	0	4.528204	-2.244832	5.257125

Sum of electronic and zero-point Energies= -4738.682154
Sum of electronic and thermal Energies= -4738.611707
Sum of electronic and thermal Enthalpies= -4738.610763
Sum of electronic and thermal Free Energies= -4738.797093

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.954113	-0.427579	-2.187001
2	6	0	-0.355799	-0.994054	-2.110898
3	6	0	1.357466	0.647442	-1.384656
4	7	0	-0.733686	-2.021089	-2.912342
5	6	0	2.762014	0.860199	-1.599454
6	79	0	-1.643953	-0.176282	-0.674551
7	6	0	-2.896230	0.673430	0.726136
8	7	0	-3.777424	0.047061	1.562535
9	6	0	-4.468868	0.976847	2.330134
10	6	0	-4.031866	2.204331	1.951815

11	7	0	-3.060196	2.005196	0.980094
12	6	0	-3.965086	-1.388782	1.684728
13	6	0	-2.340042	3.081237	0.319299
14	6	0	-2.750301	3.453276	-0.981945
15	6	0	-2.046074	4.479381	-1.622476
16	6	0	-0.979906	5.117676	-1.001336
17	6	0	-0.614107	4.747819	0.286884
18	6	0	-1.279563	3.732238	0.990660
19	6	0	-5.100826	-2.001894	1.104693
20	6	0	-5.232384	-3.388887	1.277730
21	6	0	-4.304353	-4.136133	1.994373
22	6	0	-3.207075	-3.503006	2.565080
23	6	0	-3.011999	-2.122145	2.430290
24	7	0	2.025002	-0.864450	-2.983792
25	6	0	3.068316	-0.128690	-2.672037
26	7	0	4.290919	-0.303324	-3.282420
27	6	0	4.359930	-1.352451	-4.294919
28	6	0	5.516566	-0.173226	-2.492239
29	1	0	3.154893	0.050716	-0.447320
30	6	0	-0.798126	3.518474	2.432679
31	6	0	-1.538960	4.466581	3.401690
32	6	0	-0.767315	2.087246	2.984863
33	6	0	-1.819932	-1.484155	3.136952
34	6	0	-2.037457	-1.481686	4.664588
35	6	0	-0.485038	-2.157625	2.769984
36	6	0	-6.257199	-1.328195	0.352584
37	6	0	-7.381015	-0.902499	1.323009
38	6	0	-5.912482	-0.194414	-0.623309
39	6	0	-3.950634	2.837570	-1.694008
40	6	0	-5.115000	3.847512	-1.761890
41	6	0	-3.597839	2.303690	-3.094629
42	6	0	-2.220482	-3.659848	-1.230739
43	16	0	-2.351347	-2.721601	-2.760599
44	8	0	-2.468771	-3.664740	-3.871516
45	8	0	-3.343599	-1.654675	-2.604642
46	6	0	0.053719	-2.675940	-3.989534
47	1	0	0.744512	1.193272	-0.680976
48	1	0	-5.193263	0.678813	3.069500
49	1	0	-4.314168	3.190211	2.281600
50	1	0	-2.341344	4.778205	-2.623052
51	1	0	-0.433950	5.901201	-1.518284
52	1	0	0.217853	5.250610	0.770711
53	1	0	-6.093655	-3.884838	0.838278
54	1	0	-4.439684	-5.207788	2.110203
55	1	0	-2.487343	-4.082801	3.133467
56	1	0	3.527332	-1.247118	-4.991467
57	1	0	5.301888	-1.245766	-4.841062
58	1	0	4.313791	-2.354902	-3.847959
59	1	0	6.343897	0.108128	-3.152170
60	1	0	5.409353	0.602363	-1.736105
61	1	0	5.767344	-1.117883	-1.992196
62	1	0	0.246960	3.848531	2.416241
63	1	0	-1.503048	5.503969	3.055356
64	1	0	-1.080504	4.422680	4.395457
65	1	0	-2.591591	4.185524	3.514080
66	1	0	-0.295231	1.395590	2.285081
67	1	0	-0.169010	2.076253	3.901587
68	1	0	-1.763056	1.721559	3.246245
69	1	0	-1.748555	-0.445058	2.818094

70	1	0	-2.960718	-0.960945	4.941120
71	1	0	-1.201353	-0.980552	5.162711
72	1	0	-2.099025	-2.501395	5.060134
73	1	0	-0.310530	-2.140913	1.690485
74	1	0	0.350264	-1.635304	3.244057
75	1	0	-0.444156	-3.200694	3.101013
76	1	0	-6.677334	-2.133065	-0.262665
77	1	0	-7.675341	-1.724343	1.982858
78	1	0	-8.264549	-0.586259	0.758177
79	1	0	-7.074245	-0.058521	1.948760
80	1	0	-5.065257	-0.453728	-1.262008
81	1	0	-6.777845	-0.008656	-1.268892
82	1	0	-5.697697	0.741607	-0.102762
83	1	0	-4.295188	1.984086	-1.111136
84	1	0	-5.404509	4.195588	-0.764593
85	1	0	-5.992202	3.386549	-2.228390
86	1	0	-4.844817	4.727965	-2.354900
87	1	0	-2.792842	1.565506	-3.043095
88	1	0	-4.471789	1.816983	-3.539619
89	1	0	-3.285929	3.105594	-3.772133
90	1	0	-2.003999	-2.980627	-0.406663
91	1	0	-3.187095	-4.143947	-1.082877
92	1	0	-1.429456	-4.400197	-1.356463
93	1	0	-0.413242	-2.475707	-4.955685
94	1	0	0.072911	-3.755178	-3.828470
95	1	0	1.059095	-2.262534	-3.945271
96	7	0	3.500442	-0.667198	0.604008
97	16	0	3.169895	0.072169	2.058988
98	16	0	3.572911	-2.330801	0.419449
99	8	0	2.244475	1.174483	1.793271
100	8	0	2.935913	-0.858344	3.158952
101	8	0	3.769151	-2.553867	-1.010000
102	8	0	2.540626	-3.047162	1.160180
103	6	0	5.211958	-2.813542	1.197086
104	6	0	4.822035	0.884922	2.422035
105	9	0	5.473352	-4.072046	0.837667
106	9	0	6.181900	-2.015051	0.739427
107	9	0	5.161783	-2.734680	2.523907
108	9	0	5.711678	-0.039231	2.790712
109	9	0	4.649380	1.754270	3.419608
110	9	0	5.280440	1.526784	1.346794
111	6	0	3.376156	2.215241	-1.566346
112	6	0	4.152829	2.802941	-2.539981
113	16	0	3.067860	3.369483	-0.279121
114	6	0	4.503300	4.157121	-2.262122
115	1	0	4.440838	2.275608	-3.441056
116	6	0	3.982000	4.605394	-1.081808
117	1	0	5.112272	4.767198	-2.920179
118	1	0	4.092313	5.578479	-0.623059

Sum of electronic and zero-point Energies= -4738.664479
Sum of electronic and thermal Energies= -4738.594299
Sum of electronic and thermal Enthalpies= -4738.593354
Sum of electronic and thermal Free Energies= -4738.777628

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

1	6	0	1.720823	-0.292617	0.215117
2	6	0	2.296626	-1.558099	0.025810
3	6	0	2.668094	0.731465	0.391285
4	7	0	1.426499	-2.699144	-0.151441
5	6	0	4.055196	0.520623	0.368232
6	79	0	-0.299162	0.097254	0.129688
7	6	0	-2.317191	0.554997	0.019844
8	7	0	-3.389082	-0.245188	0.303222
9	6	0	-4.585520	0.439050	0.111104
10	6	0	-4.262406	1.680004	-0.325647
11	7	0	-2.872757	1.745490	-0.360755
12	6	0	-3.315884	-1.576902	0.875800
13	6	0	-2.144640	2.885803	-0.886419
14	6	0	-1.837392	2.877467	-2.264163
15	6	0	-1.152953	3.980309	-2.791026
16	6	0	-0.794486	5.053809	-1.986605
17	6	0	-1.122136	5.041882	-0.634369
18	6	0	-1.802226	3.968215	-0.042426
19	6	0	-3.180624	-1.668773	2.278357
20	6	0	-3.117987	-2.945612	2.850346
21	6	0	-3.192909	-4.087494	2.062603
22	6	0	-3.344307	-3.967320	0.684797
23	6	0	-3.415881	-2.719480	0.048079
24	7	0	3.609456	-1.820765	0.048303
25	6	0	4.486844	-0.825825	0.212594
26	7	0	5.860497	-1.165064	0.199271
27	6	0	6.194725	-2.456109	-0.386373
28	6	0	6.591079	-0.925731	1.445933
29	6	0	-2.064372	4.083742	1.464260
30	6	0	-3.533846	3.947551	1.905207
31	6	0	-1.136126	3.182199	2.300359
32	6	0	3.022718	-4.778555	-1.155378
33	16	0	1.634151	-3.675800	-1.501344
34	8	0	2.014697	-2.805183	-2.614376
35	8	0	0.437580	-4.528079	-1.585866
36	6	0	0.895757	-3.322182	1.066886
37	6	0	-3.582480	-2.743365	-1.476236
38	6	0	-2.315121	-2.308493	-2.234239
39	6	0	-4.842202	-2.033679	-2.010121
40	6	0	-3.123293	-0.449674	3.195931
41	6	0	-4.348524	-0.399225	4.130829
42	6	0	-1.808729	-0.399793	3.997816
43	6	0	-2.221049	1.736389	-3.202591
44	6	0	-3.215688	2.211385	-4.280897
45	6	0	-0.978030	1.083399	-3.837764
46	1	0	2.318932	1.755945	0.487522
47	1	0	-5.541474	-0.022508	0.295356
48	1	0	-4.879437	2.517726	-0.605773
49	1	0	-0.900372	3.991629	-3.846573
50	1	0	-0.263686	5.901557	-2.410035
51	1	0	-0.841521	5.885829	-0.010515
52	1	0	-3.012309	-3.040612	3.926693
53	1	0	-3.141173	-5.071617	2.519612
54	1	0	-3.404792	-4.863462	0.074476
55	1	0	7.278602	-2.492943	-0.540658
56	1	0	5.908062	-3.310679	0.247702
57	1	0	5.699830	-2.564895	-1.353053
58	1	0	6.343457	0.052489	1.856253

59	1	0	6.368315	-1.694266	2.205557
60	1	0	7.667763	-0.945342	1.246319
61	1	0	-1.783508	5.116035	1.706398
62	1	0	-4.197424	4.558841	1.284030
63	1	0	-3.634983	4.295495	2.938906
64	1	0	-3.890237	2.915850	1.872990
65	1	0	-0.085666	3.373198	2.062123
66	1	0	-1.284196	3.380839	3.368079
67	1	0	-1.322733	2.121260	2.119817
68	1	0	2.759796	-5.416754	-0.310148
69	1	0	3.182559	-5.384085	-2.049319
70	1	0	3.886184	-4.157927	-0.923129
71	1	0	0.409002	-2.543232	1.657734
72	1	0	1.684756	-3.789590	1.674168
73	1	0	0.147410	-4.065294	0.790875
74	1	0	-3.724904	-3.804760	-1.712058
75	1	0	-2.472628	-2.428118	-3.312322
76	1	0	-2.061590	-1.263173	-2.044098
77	1	0	-1.455893	-2.920596	-1.950714
78	1	0	-5.735387	-2.308407	-1.437706
79	1	0	-5.010304	-2.333048	-3.050124
80	1	0	-4.748000	-0.945420	-1.998432
81	1	0	-3.153357	0.450589	2.577939
82	1	0	-5.285303	-0.395657	3.563902
83	1	0	-4.320858	0.506423	4.746211
84	1	0	-4.373453	-1.259989	4.807495
85	1	0	-0.942515	-0.387392	3.329416
86	1	0	-1.776478	0.504295	4.615284
87	1	0	-1.711330	-1.261030	4.667420
88	1	0	-2.726104	0.962842	-2.619803
89	1	0	-4.118063	2.642494	-3.834361
90	1	0	-3.518534	1.369960	-4.912933
91	1	0	-2.771223	2.971622	-4.932056
92	1	0	-0.431313	1.790416	-4.470910
93	1	0	-0.290836	0.711791	-3.072161
94	1	0	-1.275537	0.237042	-4.465326
95	6	0	4.972418	1.669892	0.434357
96	6	0	6.159094	1.890401	-0.228770
97	16	0	4.573674	3.073082	1.418142
98	6	0	6.735125	3.167451	0.032020
99	1	0	6.594547	1.146564	-0.883699
100	6	0	5.995004	3.920208	0.902252
101	1	0	7.662269	3.510670	-0.413833
102	1	0	6.198697	4.914722	1.274293

Sum of electronic and zero-point Energies= -2911.076114
Sum of electronic and thermal Energies= -2911.022076
Sum of electronic and thermal Enthalpies= -2911.021132
Sum of electronic and thermal Free Energies= -2911.169990

C-b3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.272132	1.724116	0.065906
2	6	0	0.913575	1.992112	-0.037896
3	6	0	2.857742	0.401751	0.098173
4	7	0	0.466358	3.322766	0.046042

5	6	0	4.222182	0.553873	0.189294
6	79	0	-0.472309	0.439366	-0.058836
7	6	0	-1.814529	-1.132338	0.077396
8	7	0	-3.066500	-1.122229	0.630237
9	6	0	-3.647295	-2.384589	0.568307
10	6	0	-2.743010	-3.207010	-0.013830
11	7	0	-1.632555	-2.428033	-0.322374
12	6	0	-3.799393	0.046321	1.086633
13	6	0	-0.404928	-2.995285	-0.845422
14	6	0	0.516723	-3.508261	0.093343
15	6	0	1.691757	-4.093174	-0.394519
16	6	0	1.941194	-4.169941	-1.759005
17	6	0	1.008105	-3.670027	-2.661470
18	6	0	-0.189698	-3.075026	-2.240292
19	6	0	-3.743082	0.444680	2.441506
20	6	0	-4.504338	1.566346	2.800616
21	6	0	-5.291809	2.250144	1.880733
22	6	0	-5.347413	1.815934	0.562881
23	6	0	-4.606360	0.708482	0.135663
24	7	0	3.299466	2.681325	0.106187
25	6	0	4.429362	2.012154	0.161516
26	7	0	5.668208	2.657917	0.225969
27	6	0	5.602483	4.097866	0.449579
28	6	0	6.646875	2.302832	-0.804160
29	6	0	-1.124573	-2.573073	-3.347386
30	6	0	-2.556283	-3.140543	-3.314288
31	6	0	-1.126936	-1.039001	-3.490492
32	6	0	-4.738980	0.238248	-1.311449
33	6	0	-6.069948	-0.514641	-1.519780
34	6	0	-4.600580	1.388506	-2.325870
35	6	0	-2.943254	-0.217279	3.570867
36	6	0	-3.206104	-1.721084	3.776063
37	6	0	-1.435196	0.090946	3.515807
38	6	0	0.270492	-3.488668	1.600795
39	6	0	0.020888	-4.915239	2.132205
40	6	0	1.414573	-2.805711	2.373198
41	6	0	-0.301431	3.596684	-2.583689
42	16	0	-0.880597	3.801983	-0.886245
43	8	0	-1.079087	5.233737	-0.642541
44	8	0	-2.004993	2.877789	-0.691346
45	6	0	1.206764	4.424303	0.700504
46	1	0	2.304049	-0.527566	0.090045
47	1	0	-4.636552	-2.573039	0.951137
48	1	0	-2.781451	-4.258973	-0.243836
49	1	0	2.419562	-4.487748	0.306583
50	1	0	2.859738	-4.621756	-2.121267
51	1	0	1.206061	-3.741072	-3.727278
52	1	0	-4.476087	1.903299	3.833040
53	1	0	-5.866750	3.116283	2.195107
54	1	0	-5.969660	2.345954	-0.150383
55	1	0	4.937023	4.309739	1.287229
56	1	0	6.608623	4.460536	0.684823
57	1	0	5.225681	4.647323	-0.427159
58	1	0	7.640956	2.641039	-0.492922
59	1	0	6.682401	1.223559	-0.944521
60	1	0	6.410383	2.776250	-1.771889
61	1	0	-0.678013	-2.962026	-4.270733
62	1	0	-2.552708	-4.228462	-3.187025
63	1	0	-3.056138	-2.919665	-4.263551

64	1	0	-3.163791	-2.705622	-2.517827
65	1	0	-0.108080	-0.655713	-3.601346
66	1	0	-1.700534	-0.749596	-4.378628
67	1	0	-1.569642	-0.545834	-2.622009
68	1	0	-3.927381	-0.464079	-1.518226
69	1	0	-6.159438	-1.378454	-0.853053
70	1	0	-6.149255	-0.875072	-2.551283
71	1	0	-6.924875	0.142816	-1.327456
72	1	0	-3.690589	1.963430	-2.142063
73	1	0	-4.568795	0.982170	-3.342932
74	1	0	-5.452575	2.075485	-2.280244
75	1	0	-3.316892	0.268981	4.480410
76	1	0	-4.278902	-1.941724	3.796023
77	1	0	-2.785293	-2.035075	4.737397
78	1	0	-2.745307	-2.339160	3.002412
79	1	0	-1.256214	1.167792	3.447452
80	1	0	-0.946175	-0.279799	4.424092
81	1	0	-0.950093	-0.373954	2.654340
82	1	0	-0.633448	-2.906758	1.795168
83	1	0	-0.822452	-5.393691	1.623212
84	1	0	-0.201086	-4.889548	3.204411
85	1	0	0.900175	-5.552304	1.988484
86	1	0	1.568064	-1.778540	2.032090
87	1	0	1.177258	-2.776634	3.442065
88	1	0	2.362405	-3.341529	2.260520
89	1	0	-0.040477	2.549646	-2.738669
90	1	0	-1.121575	3.897044	-3.238380
91	1	0	0.565784	4.241405	-2.731705
92	1	0	1.718905	3.997057	1.560672
93	1	0	0.487565	5.175276	1.023598
94	1	0	1.958600	4.869165	0.046924
95	6	0	5.226193	-0.480684	0.387212
96	6	0	6.406703	-0.417616	1.097721
97	16	0	5.017571	-2.098155	-0.271134
98	6	0	7.128879	-1.646468	1.126070
99	1	0	6.724787	0.490371	1.595905
100	6	0	6.505286	-2.649259	0.436460
101	1	0	8.071927	-1.777446	1.645636
102	1	0	6.828291	-3.671676	0.297020

Sum of electronic and zero-point Energies= -2911.048988
Sum of electronic and thermal Energies= -2910.994575
Sum of electronic and thermal Enthalpies= -2910.993630
Sum of electronic and thermal Free Energies= -2911.144361

C-tsa4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.045373	0.407175	-0.498913
2	6	0	1.563419	1.628480	-1.061015
3	6	0	1.715677	-0.743812	-1.012409
4	7	0	1.111684	2.892696	-0.663314
5	6	0	2.755485	-0.732833	-1.932890
6	79	0	-1.039860	0.029505	-0.256171
7	6	0	-3.060247	-0.353882	-0.175354
8	7	0	-4.034361	0.475957	0.304911
9	6	0	-5.293943	-0.090486	0.140422

10	6	0	-5.106812	-1.302874	-0.432919
11	7	0	-3.737675	-1.450408	-0.632709
12	6	0	-3.837413	1.834861	0.775114
13	6	0	-3.136639	-2.679076	-1.121562
14	6	0	-2.879000	-3.691955	-0.169549
15	6	0	-2.294403	-4.880463	-0.623290
16	6	0	-1.986995	-5.062563	-1.965986
17	6	0	-2.285230	-4.062561	-2.885415
18	6	0	-2.874532	-2.849146	-2.500382
19	6	0	-3.923087	2.865048	-0.187978
20	6	0	-3.756712	4.185560	0.246690
21	6	0	-3.512337	4.473500	1.583987
22	6	0	-3.448744	3.439668	2.512626
23	6	0	-3.615954	2.095514	2.146895
24	7	0	2.494433	1.663366	-2.019941
25	6	0	3.094692	0.551915	-2.465059
26	7	0	4.069985	0.737432	-3.422574
27	6	0	4.599647	2.075258	-3.656905
28	6	0	4.239981	-0.165932	-4.555042
29	6	0	-3.178439	-1.859708	-3.633390
30	6	0	-4.634081	-1.361348	-3.703492
31	6	0	-2.177882	-0.691806	-3.718630
32	6	0	1.593079	4.444278	-2.928634
33	16	0	1.953626	4.327922	-1.167569
34	8	0	3.395419	4.186260	-0.970666
35	8	0	1.244460	5.436555	-0.520780
36	6	0	0.012836	3.070547	0.295151
37	6	0	-3.526477	1.068522	3.282592
38	6	0	-2.175979	0.327535	3.322106
39	6	0	-4.712807	0.092724	3.392639
40	6	0	-4.209300	2.605677	-1.666042
41	6	0	-5.594392	3.153138	-2.065858
42	6	0	-3.106815	3.176739	-2.578532
43	6	0	-3.273925	-3.567142	1.301194
44	6	0	-4.618311	-4.283235	1.556716
45	6	0	-2.197940	-4.092422	2.267935
46	1	0	1.449119	-1.703140	-0.581841
47	1	0	-6.190786	0.417337	0.454795
48	1	0	-5.808846	-2.066029	-0.724650
49	1	0	-2.078757	-5.670327	0.087757
50	1	0	-1.530511	-5.989828	-2.300138
51	1	0	-2.065992	-4.222049	-3.937525
52	1	0	-3.816967	4.995097	-0.473963
53	1	0	-3.377758	5.501889	1.905798
54	1	0	-3.265017	3.672820	3.557336
55	1	0	5.637789	1.980263	-3.993962
56	1	0	4.039705	2.609603	-4.440160
57	1	0	4.562777	2.663926	-2.741615
58	1	0	3.689862	-1.091909	-4.406358
59	1	0	3.869993	0.315615	-5.472743
60	1	0	5.297732	-0.412287	-4.699578
61	1	0	-3.029821	-2.449676	-4.546136
62	1	0	-5.345588	-2.189900	-3.621308
63	1	0	-4.804303	-0.873225	-4.669127
64	1	0	-4.868212	-0.632287	-2.924761
65	1	0	-1.147460	-1.057399	-3.755123
66	1	0	-2.365202	-0.108188	-4.627441
67	1	0	-2.255028	-0.021010	-2.859896
68	1	0	0.514759	4.558547	-3.043490

69	1	0	2.111488	5.336644	-3.285198
70	1	0	1.961770	3.544523	-3.414644
71	1	0	-0.914230	2.666133	-0.119861
72	1	0	-0.108852	4.134853	0.479856
73	1	0	0.240664	2.578560	1.239067
74	1	0	-3.564025	1.677191	4.194158
75	1	0	-2.108308	-0.282508	4.228866
76	1	0	-2.047162	-0.334522	2.462102
77	1	0	-1.338742	1.031041	3.329214
78	1	0	-5.673248	0.616861	3.336325
79	1	0	-4.669840	-0.417350	4.360570
80	1	0	-4.698126	-0.678714	2.619613
81	1	0	-4.227663	1.525874	-1.831429
82	1	0	-6.390070	2.717319	-1.453007
83	1	0	-5.809166	2.921816	-3.114651
84	1	0	-5.642835	4.240701	-1.947033
85	1	0	-2.128144	2.759391	-2.323640
86	1	0	-3.319841	2.931037	-3.624402
87	1	0	-3.041125	4.267051	-2.502089
88	1	0	-3.412738	-2.506711	1.528503
89	1	0	-5.423092	-3.890074	0.927601
90	1	0	-4.919695	-4.164614	2.602877
91	1	0	-4.531077	-5.355903	1.351823
92	1	0	-2.085565	-5.180111	2.201319
93	1	0	-1.227735	-3.630079	2.077929
94	1	0	-2.489225	-3.863950	3.298324
95	1	0	1.277616	0.216562	0.983635
96	7	0	1.661225	-0.090962	2.155010
97	16	0	2.284745	1.074864	3.188178
98	16	0	1.377005	-1.660947	2.631923
99	8	0	1.473481	2.283176	3.058233
100	8	0	2.635758	0.528566	4.492126
101	8	0	0.897185	-1.777600	4.001733
102	8	0	0.637200	-2.274242	1.525573
103	6	0	3.904060	1.460353	2.328807
104	6	0	3.064336	-2.483214	2.572676
105	9	0	2.883967	-3.796952	2.728827
106	9	0	3.631885	-2.252511	1.386377
107	9	0	3.853054	-2.025255	3.540396
108	9	0	3.675251	1.912315	1.096431
109	9	0	4.656280	0.359029	2.263524
110	9	0	4.539701	2.391804	3.037309
111	6	0	3.477112	-1.990722	-2.197266
112	6	0	2.944429	-3.213802	-2.532579
113	16	0	5.207001	-2.145447	-1.926061
114	6	0	3.907755	-4.266073	-2.588582
115	1	0	1.887985	-3.348410	-2.738252
116	6	0	5.172211	-3.841263	-2.291009
117	1	0	3.666929	-5.291288	-2.846581
118	1	0	6.086982	-4.417515	-2.269293

Sum of electronic and zero-point Energies= -4738.693323
Sum of electronic and thermal Energies= -4738.623014
Sum of electronic and thermal Enthalpies= -4738.622070
Sum of electronic and thermal Free Energies= -4738.808726

C-tsb4

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-2.065939	-0.023571	1.028912
2	6	0	-0.906447	0.742393	1.079073
3	6	0	-2.383689	-0.914504	-0.089545
4	7	0	-0.607558	1.532743	2.231737
5	6	0	-3.564176	-1.526953	0.193679
6	79	0	0.798023	-0.303777	0.273981
7	6	0	2.417718	-1.442470	-0.273455
8	7	0	3.743820	-1.129213	-0.194597
9	6	0	4.522719	-2.169712	-0.686577
10	6	0	3.670816	-3.147612	-1.083351
11	7	0	2.384598	-2.700130	-0.803875
12	6	0	4.278106	0.086142	0.393723
13	6	0	1.181278	-3.450669	-1.121220
14	6	0	0.611880	-3.258709	-2.399439
15	6	0	-0.553719	-3.968744	-2.712560
16	6	0	-1.129657	-4.842667	-1.799390
17	6	0	-0.532695	-5.030593	-0.557622
18	6	0	0.632622	-4.349435	-0.176387
19	6	0	4.693196	1.150107	-0.433959
20	6	0	5.157980	2.307567	0.211106
21	6	0	5.227235	2.402503	1.594572
22	6	0	4.847498	1.320510	2.382742
23	6	0	4.371310	0.138871	1.805846
24	7	0	-3.088737	-0.067240	1.962292
25	6	0	-3.983399	-0.922354	1.493835
26	7	0	-5.126115	-1.206300	2.185983
27	6	0	-5.249518	-0.662130	3.533227
28	6	0	-6.405018	-1.430515	1.514813
29	6	0	1.136668	-4.638026	1.243789
30	6	0	2.636303	-4.948586	1.396306
31	6	0	0.674439	-3.568995	2.253671
32	6	0	4.054883	-1.062128	2.695752
33	6	0	5.325407	-1.916504	2.902577
34	6	0	3.443067	-0.684166	4.055596
35	6	0	4.788480	1.172191	-1.965069
36	6	0	6.195289	0.719410	-2.416249
37	6	0	3.703135	0.455001	-2.779633
38	6	0	1.204271	-2.323093	-3.448662
39	6	0	1.646863	-3.099018	-4.705313
40	6	0	0.231536	-1.184825	-3.812123
41	6	0	-2.105093	1.511727	4.550350
42	16	0	-0.598482	0.862880	3.810931
43	8	0	0.532962	1.466054	4.535298
44	8	0	-0.698680	-0.594570	3.715177
45	6	0	0.223877	2.731478	2.026296
46	1	0	-1.759834	-1.079967	-0.956443
47	1	0	5.598599	-2.115945	-0.704715
48	1	0	3.853807	-4.117289	-1.516032
49	1	0	-1.015563	-3.826468	-3.684258
50	1	0	-2.044079	-5.371496	-2.050390
51	1	0	-0.983335	-5.719847	0.150874
52	1	0	5.468173	3.150488	-0.400270
53	1	0	5.582711	3.317267	2.060187
54	1	0	4.916687	1.394481	3.461997
55	1	0	-5.514840	0.404699	3.525219
56	1	0	-6.035122	-1.213410	4.058458
57	1	0	-4.304724	-0.782690	4.062564

58	1	0	-6.998848	-0.505084	1.509680
59	1	0	-6.255069	-1.751255	0.488040
60	1	0	-6.975405	-2.201574	2.043681
61	1	0	0.620178	-5.564849	1.523221
62	1	0	2.977949	-5.674699	0.650578
63	1	0	2.811782	-5.384472	2.385619
64	1	0	3.264075	-4.058888	1.320240
65	1	0	-0.409551	-3.432102	2.221277
66	1	0	0.947874	-3.869594	3.271133
67	1	0	1.123560	-2.592756	2.058078
68	1	0	3.318608	-1.683131	2.179818
69	1	0	5.746272	-2.265111	1.954195
70	1	0	5.098316	-2.796504	3.514004
71	1	0	6.099750	-1.338068	3.418598
72	1	0	2.584369	-0.015972	3.957300
73	1	0	3.104902	-1.591129	4.566897
74	1	0	4.176051	-0.202679	4.712517
75	1	0	4.704133	2.234028	-2.224809
76	1	0	6.983272	1.280117	-1.904371
77	1	0	6.314114	0.869920	-3.494768
78	1	0	6.354981	-0.345466	-2.213125
79	1	0	2.703566	0.695891	-2.415823
80	1	0	3.769892	0.785613	-3.821891
81	1	0	3.840326	-0.629143	-2.779791
82	1	0	2.096022	-1.856713	-3.028727
83	1	0	2.365405	-3.887855	-4.458448
84	1	0	2.121029	-2.419826	-5.421565
85	1	0	0.796325	-3.570381	-5.209011
86	1	0	-0.043012	-0.603042	-2.927508
87	1	0	0.695444	-0.499836	-4.528775
88	1	0	-0.689802	-1.567301	-4.263993
89	1	0	-2.925210	1.195565	3.906735
90	1	0	-2.178269	1.089291	5.554710
91	1	0	-2.017054	2.597888	4.599027
92	1	0	-0.375713	3.510747	1.551459
93	1	0	1.080761	2.499486	1.386571
94	1	0	0.591907	3.091369	2.984882
95	1	0	-0.912092	1.609347	-0.129158
96	7	0	-1.100535	2.491065	-1.035601
97	16	0	-2.682839	2.808396	-1.496417
98	16	0	0.219117	2.991979	-1.925039
99	6	0	-3.215009	3.881618	-0.058316
100	6	0	0.373007	4.840033	-1.605321
101	8	0	-3.468467	1.585847	-1.375383
102	8	0	-2.750526	3.652424	-2.681965
103	8	0	1.382378	2.418837	-1.245229
104	8	0	0.040447	2.840398	-3.362776
105	9	0	-4.485398	4.242183	-0.242548
106	9	0	-3.106706	3.205708	1.087759
107	9	0	-2.449068	4.975978	0.007087
108	9	0	-0.635365	5.519639	-2.139540
109	9	0	1.521747	5.239534	-2.157395
110	9	0	0.417443	5.073929	-0.289035
111	6	0	-4.208210	-2.576542	-0.589454
112	6	0	-4.727685	-3.782339	-0.169442
113	16	0	-4.334284	-2.440917	-2.333105
114	6	0	-5.212648	-4.596168	-1.234297
115	1	0	-4.739731	-4.076667	0.873943
116	6	0	-5.062519	-4.007631	-2.462183

117	1	0	-5.653390	-5.576623	-1.091493
118	1	0	-5.352279	-4.393892	-3.429833

Sum of electronic and zero-point Energies= -4738.663232
Sum of electronic and thermal Energies= -4738.592485
Sum of electronic and thermal Enthalpies= -4738.591541
Sum of electronic and thermal Free Energies= -4738.778853