Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

DFT study on the reaction mechanisms and stereoselectivities of NHC-catalyzed [2 + 2] cycloaddition between arylalkylketenes and electron-deficient benzaldehydes

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1. The complete reference of Gaussian 09.

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A., Jr. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, *GAUSSIAN 09 (Revision C.01),* Gaussian, Inc., Wallingford, CT, 2010.

2. Computed Energies of All Stationary Points.

Table S1. Single-point energies (E) calculated at the M06-2X/6-311+G(d, p) level, zero-point vibrational energy (ZPVE) and correction for Gibbs free energy calculated at the M06-2X/6-31G(d, p) level, E+ZPVE, and Gibbs free energies (G) (Unit: Hartree)

	E	ZPVE	E+ZPVE	The Correction of G	G
NHC	-1693.044159	0.591381	-1692.452778	0.526528	-1692.517631
R1	-462.205629	0.173389	-462.032240	0.137049	-462.0685798
R2	-549.986527	0.113871	-549.872656	0.081482	-549.9050454
M01(E)	-2155.261726	0.766264	-2154.495462	0.688436	-2154.578012
M01(Z)	-2155.266448	0.766558	-2154.499890	0.686962	-2154.574764
TS1(E)	-2155.257013	0.766922	-2154.490091	0.689479	-2154.569962
TS1(Z)	-2155.259441	0.765900	-2154.493541	0.691095	-2154.565918
M1(E)	-2155.290762	0.769569	-2154.521193	0.693926	-2154.595371

M1(Z)	-2155.289297	0.769449	-2154.519848	0.692638	-2154.598124
M02(SS)	-2705.307255	0.885090	-2704.422165	0.799569	-2704.507686
M02(RR)	-2705.301940	0.886891	-2704.415049	0.798296	-2704.503644
M02(SR)	-2705.309222	0.886017	-2704.423205	0.799700	-2704.509522
M02(RS)	-2705.287105	0.884859	-2704.402246	0.795747	-2704.491358
TS2(SS)	-2705.283554	0.886690	-2704.396864	0.803425	-2704.480129
TS2(RR)	-2705.269735	0.886050	-2704.383685	0.799798	-2704.469937
TS2(SR)	-2705.288324	0.886766	-2704.401558	0.802677	-2704.485647
TS2(RS)	-2705.260670	0.885630	-2704.375040	0.79935	-2704.46132
M2(SS)	-2705.300670	0.888495	-2704.412175	0.804976	-2704.495694
M2(RR)	-2705.286120	0.889506	-2704.396614	0.806255	-2704.479865
M2(SR)	-2705.299484	0.889543	-2704.409941	0.805396	-2704.494088
M2(RS)	-2705.296368	0.888982	-2704.407386	0.805155	-2704.491213
TS3(SS)	-2705.280971	0.886373	-2704.394598	0.801554	-2704.479417
TS3(RR)	-2705.272504	0.886593	-2704.385911	0.800534	-2704.47197
TS3(SR)	-2705.290320	0.888188	-2704.402132	0.806375	-2704.483945
TS3(RS)	-2705.285304	0.887554	-2704.397750	0.801883	-2704.483421
M01'(Re)	-2243.071668	0.708905	-2242.362763	0.633889	-2242.437779
M01'(Si)	-2243.057733	0.707484	-2242.350249	0.630734	-2242.426999
TS1'(Re)	-2243.048143	0.708320	-2242.339823	0.632939	-2242.415204
TS1'(Si)	-2243.034074	0.708477	-2242.325597	0.635451	-2242.398623
M1'(Re)	-2243.062639	0.710974	-2242.351665	0.637372	-2242.425267

M1'(Si)	-2243.049395	0.710731	-2242.338664	0.638174	-2242.411221
M02'(SS)	-2705.282523	0.886760	-2704.395763	0.800840	-2704.481683
M02'(RR)	-2705.283340	0.885502	-2704.397838	0.797749	-2704.485591
M02'(SR)	-2705.294902	0.884949	-2704.409953	0.793795	-2704.501107
M02'(RS)	-2705.281962	0.885378	-2704.396584	0.797252	-2704.48471
TS2'(SS)	-2705.280627	0.885049	-2704.395578	0.799942	-2704.468264
TS2'(RR)	-2705.280627	0.885049	-2704.395578	0.799203	-2704.481424
TS2'(SR)	-2705.278673	0.884933	-2704.393740	0.797985	-2704.480688
TS2'(RS)	-2705.270554	0.885951	-2704.384603	0.799481	-2704.471073
M2'(SS)	-2705.295915	0.888197	-2704.407718	0.802914	-2704.493001
M2'(RR)	-2705.293889	0.887918	-2704.405971	0.803565	-2704.490324
M2'(SR)	-2705.292988	0.887551	-2704.405437	0.801408	-2704.49158
M2'(RS)	-2705.289595	0.888504	-2704.401091	0.802539	-2704.487056
TS3'(SS)	-2705.241309	0.884922	-2704.356387	0.797334	-2704.443975
TS3'(RR)	-2705.243832	0.885169	-2704.358663	0.799252	-2704.44458
TS3'(SR)	-2705.244877	0.884771	-2704.360106	0.797595	-2704.447282
TS3'(RS)	-2705.242732	0.884770	-2704.357962	0.798183	-2704.444549
P(SS)	-1012.259020	0.294274	-1011.964746	0.247331	-1012.011689
P(RR)	-1012.259020	0.294274	-1011.964746	0.247331	-1012.011689
P(SR)	-1012.263042	0.294043	-1011.968999	0.247306	-1012.015736
P(RS)	-1012.263042	0.294043	-1011.968999	0.247306	-1012.015736
M02X(SS)	-2705.294388	0.886276	-2704.408112	0.799753	-2704.494635
M02X(RR)	-2705.306553	0.886382	-2704.420171	0.801421	-2704.505132

M02X(SR)	-2705.317893	0.886172	-2704.431721	0.798882	-2704.519011
M02X(RS)	-2705.294253	0.885102	-2704.409151	0.796847	-2704.497406
TS2X(SS)	-2705.181241	0.883702	-2704.297539	0.799760	-2704.381481
TS2X(RR)	-2705.162864	0.883429	-2704.279435	0.800712	-2704.362152
TS2X(SR)	-2705.187875	0.884592	-2704.303283	0.800187	-2704.387688
TS2X(RS)	-2705.177824	0.882291	-2704.295533	0.800812	-2704.377012
M2X(SS)	-2705.256268	0.887952	-2704.368316	0.805534	-2704.450734
M2X(RR)	-2705.255769	0.88866	-2704.367109	0.807963	-2704.447806
M2X(SR)	-2705.279037	0.888464	-2704.390573	0.804556	-2704.474481
M2X(RS)	-2705.269347	0.888161	-2704.381186	0.805677	-2704.46367

3. Figures S1-S6

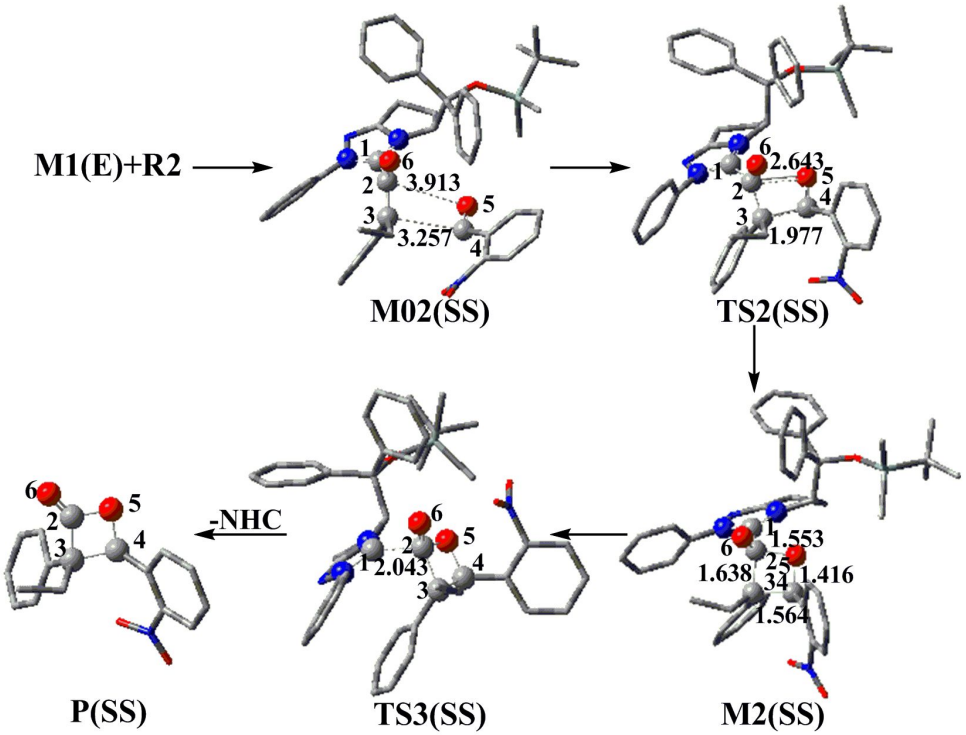

Figure S1. Optimized structures for **M02(SS), TS2(SS), M2(SS), TS3(SS)** and **P(SS)** (distance in Å)

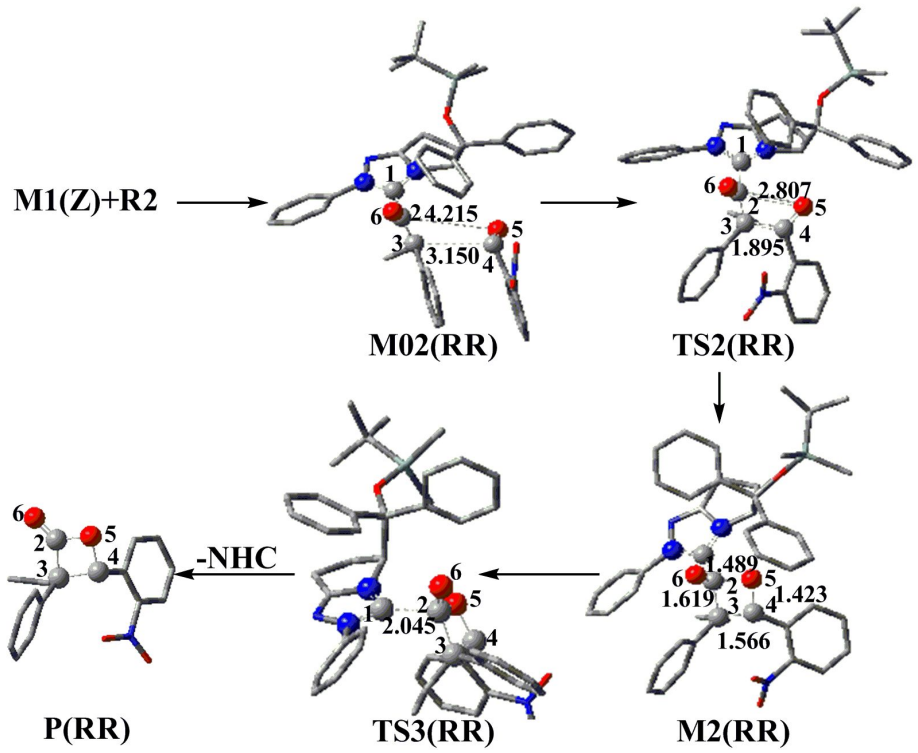

Figure S2. Optimized structures for **M02(RR), TS2(RR), M2(RR), TS3(RR)** and **P(RR)** (distance in Å)

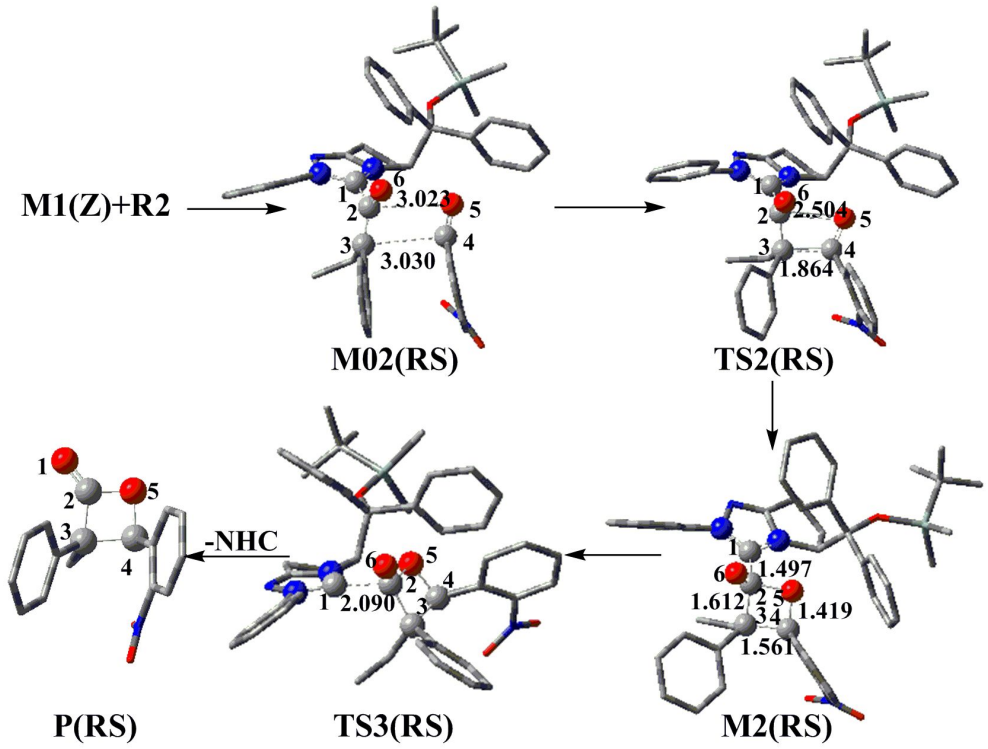

Figure S3. Optimized structures for **M02(RS), TS2(RS), M2(RS), TS3(RS)** and **P(RS)** (distance in Å)

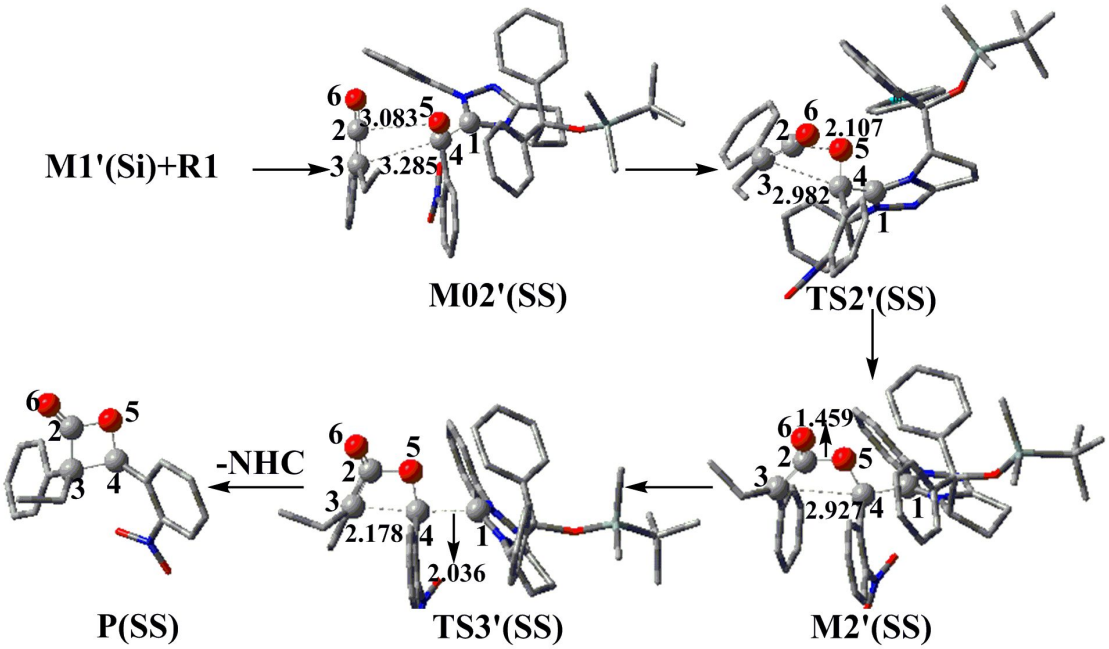

Figure S4. Optimized structures for **M02'(SS), TS2'(SS), M2'(SS), TS3'(SS)** and **P(SS)** (distance in Å)

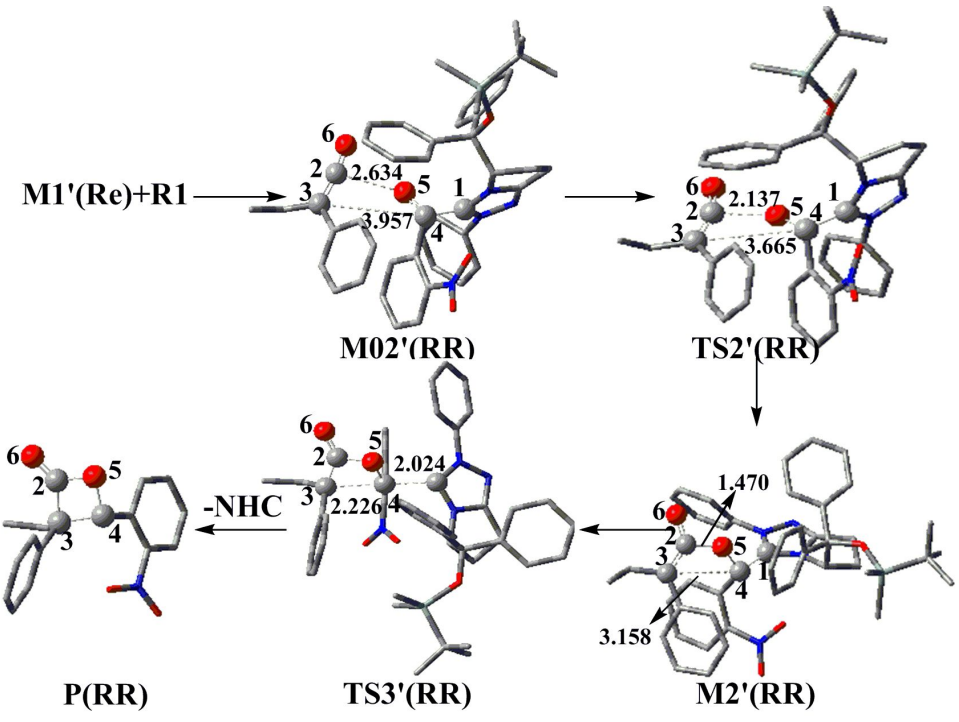

Figure S5. Optimized structures for **M02'(RR), TS2'(RR), M2'(RR), TS3'(RR)** and **P(RR)** (distance in Å)

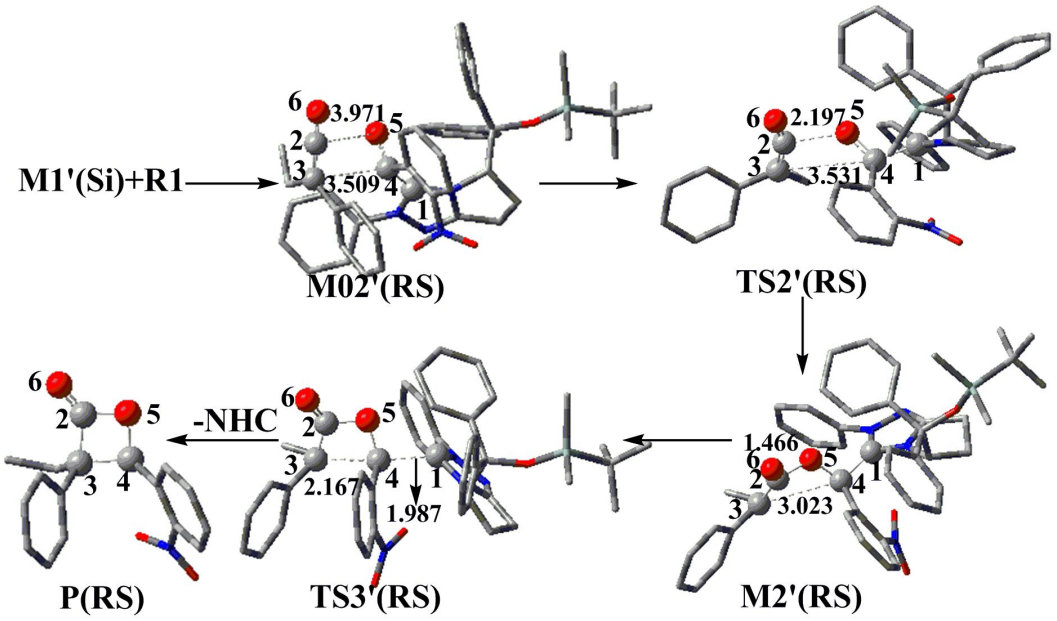

Figure S6. Optimized structures for **M02'(RS), TS2'(RS), M2'(RS), TS3'(RS)** and **P(RS)** (distance in Å)

4. Cartesian coordinates of all the stationary points.

NHC

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-3.411680	0.736859	-0.691809
2	8	0	-2.258842	-0.282482	-0.006094
3	7	0	3.358863	-0.269817	-0.840479
4	7	0	3.112134	-1.627685	-0.982143
5	7	0	1.298308	-0.391545	-1.037129
6	6	0	4.962939	1.520201	-0.471262
7	1	0	4.128990	2.209213	-0.415599
8	6	0	6.277172	1.947341	-0.327012
9	1	0	6.476610	2.999993	-0.153705
10	6	0	7.331764	1.038830	-0.399578
11	1	0	8.355478	1.379148	-0.285002
12	6	0	7.059783	-0.308082	-0.619359
13	1	0	7.872056	-1.025507	-0.678436
14	6	0	5.749055	-0.752800	-0.767964
15	1	0	5.526825	-1.798217	-0.939797
16	6	0	4.705171	0.166931	-0.693454

17	6	0	2.272914	0.547424	-0.871332
18	6	0	1.825364	-1.657010	-1.097939
19	6	0	0.760786	-2.686503	-1.272991
20	1	0	0.597500	-3.214773	-0.328215
21	1	0	1.010908	-3.418126	-2.042434
22	6	0	-0.455052	-1.801836	-1.656564
23	1	0	-1.396095	-2.181167	-1.257562
24	1	0	-0.543084	-1.754855	-2.745120
25	6	0	-0.159657	-0.374177	-1.119881
26	1	0	-0.478580	0.384525	-1.836723
27	6	0	-0.874195	-0.095917	0.241540
28	6	0	-2.865589	1.383718	-2.371298
29	1	0	-2.005824	2.055054	-2.283658
30	1	0	-3.681933	1.961064	-2.817951
31	1	0	-2.608365	0.576173	-3.064635
32	6	0	-3.851483	2.186114	0.414046
33	1	0	-3.057884	2.939688	0.424235
34	1	0	-4.018486	1.861251	1.444702
35	1	0	-4.770244	2.661659	0.052683
36	6	0	-4.892238	-0.429176	-0.879719
37	6	0	-5.961617	0.224557	-1.766241
38	1	0	-6.852576	-0.414692	-1.817003
39	1	0	-5.601927	0.371526	-2.790348
40	1	0	-6.279964	1.198670	-1.376603
41	6	0	-5.489770	-0.724958	0.503357
42	1	0	-6.303428	-1.457192	0.417177
43	1	0	-5.904196	0.177873	0.964992
44	1	0	-4.737896	-1.138164	1.185289
45	6	0	-4.440769	-1.747007	-1.523160
46	1	0	-5.306151	-2.398133	-1.704521
47	1	0	-3.744172	-2.285079	-0.872397
48	1	0	-3.942725	-1.582577	-2.486410
49	6	0	-0.432488	-1.151733	1.253857
50	6	0	0.836506	-1.069104	1.838382
51	6	0	-1.249316	-2.241766	1.556127
52	6	0	1.294902	-2.080814	2.674629
53	1	0	1.466921	-0.207976	1.630629
54	6	0	-0.792540	-3.250316	2.403915
55	1	0	-2.242465	-2.293021	1.122730
56	6	0	0.483370	-3.179112	2.955249
57	1	0	-1.437138	-4.093501	2.632178
58	6	0	-0.652852	1.316346	0.789345
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60	6	0	-1.086108	1.574870	2.095120

61	6	0	-0.125568	3.666855	0.547530
62	1	0	0.227796	2.205079	-0.973513
63	6	0	-1.046036	2.860077	2.619536
64	1	0	-1.468820	0.754384	2.696053
65	6	0	-0.568645	3.914540	1.841757
66	1	0	-1.390502	3.041008	3.632780
67	1	0	2.286342	-2.008258	3.109818
68	1	0	0.840703	-3.968023	3.609323
69	1	0	-0.534811	4.920839	2.247090
70	1	0	0.262535	4.477716	-0.060471

R1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.182232	0.122717	-0.238219
2	6	0	1.809280	1.283818	-0.165806
3	8	0	2.373064	2.303901	-0.110447
4	6	0	-0.290036	0.081305	-0.119010
5	6	0	-0.989656	-1.092583	-0.424549
6	6	0	-1.025716	1.204244	0.291992
7	6	0	-2.378068	-1.138952	-0.326103
8	1	0	-0.451171	-1.978662	-0.744731
9	6	0	-2.409735	1.156402	0.380717
10	1	0	-0.505227	2.124169	0.548419
11	6	0	-3.096843	-0.017946	0.074385
12	1	0	-2.897613	-2.061100	-0.567081
13	1	0	-2.955224	2.039543	0.698217
14	1	0	-4.178260	-0.056605	0.150502
15	6	0	2.027616	-1.127840	-0.417381
16	6	0	2.035454	-2.014982	0.829415
17	1	0	3.052322	-0.842008	-0.671761
18	1	0	1.648253	-1.683845	-1.282771
19	1	0	2.599571	-2.933552	0.647037
20	1	0	2.495979	-1.486762	1.667893
21	1	0	1.019683	-2.289479	1.125198

R2

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

1	6	0	0.229144	0.893368	0.000144
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3	6	0	1.118305	-1.384924	-0.000097
4	6	0	2.423534	-0.903698	0.000003
5	6	0	2.645511	0.465168	0.000193
6	6	0	1.558592	1.332692	0.000239
7	1	0	0.913902	-2.447001	-0.000230
8	1	0	3.253224	-1.601571	-0.000052
9	1	0	3.654565	0.862159	0.000281
10	1	0	1.743448	2.402773	0.000309
11	7	0	-1.286294	-1.157926	0.000095
12	6	0	-0.734003	2.063658	-0.000131
13	8	0	-1.933449	2.096393	-0.000664
14	1	0	-0.160287	3.013010	0.000211
15	8	0	-1.310380	-2.378164	-0.001208
16	8	0	-2.270151	-0.453742	0.001464

M01(E)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.607737	-2.681652	1.077153
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3	6	0	-1.918343	-3.285164	0.119097
4	6	0	-1.762946	-2.658542	-1.208181
5	6	0	-0.648840	-2.956262	-2.003799
6	6	0	-2.731826	-1.781757	-1.722332
7	6	0	-0.492898	-2.369543	-3.258517
8	1	0	0.105995	-3.647622	-1.641722
9	6	0	-2.566408	-1.184542	-2.965876
10	1	0	-3.622669	-1.567018	-1.136514
11	6	0	-1.442221	-1.472389	-3.741235
12	1	0	0.379253	-2.616330	-3.857393
13	1	0	-3.322158	-0.495889	-3.331220
14	1	0	-1.316486	-1.013480	-4.716965
15	6	0	-1.339732	-4.655690	0.460207
16	6	0	0.085473	-4.639415	1.017335
17	1	0	-1.380909	-5.257879	-0.454241
18	1	0	-1.996734	-5.152793	1.180894

19	1	0	0.150459	-4.000205	1.902657
20	1	0	0.397378	-5.648666	1.301188
21	1	0	0.804559	-4.263115	0.286307
22	14	0	3.665211	-0.748268	0.129220
23	8	0	2.764681	0.666304	0.001921
24	7	0	-2.898706	1.094069	-0.355399
25	7	0	-2.562651	1.832568	-1.478654
26	7	0	-0.884492	0.693198	-0.637480
27	6	0	-4.559250	0.569934	1.336646
28	1	0	-3.754912	0.213773	1.969049
29	6	0	-5.886408	0.524416	1.746421
30	1	0	-6.124113	0.125828	2.727493
31	6	0	-6.902752	0.990628	0.914252
32	1	0	-7.936439	0.956277	1.242026
33	6	0	-6.581781	1.502334	-0.339730
34	1	0	-7.365178	1.868135	-0.995742
35	6	0	-5.258611	1.545641	-0.770384
36	1	0	-4.995412	1.937672	-1.745132
37	6	0	-4.253314	1.076651	0.073180
38	6	0	-1.902610	0.356668	0.202652
39	6	0	-1.305258	1.557768	-1.612512
40	6	0	-0.195476	1.928798	-2.535364
41	1	0	0.142337	2.948128	-2.320372
42	1	0	-0.495833	1.873954	-3.583200
43	6	0	0.881167	0.875872	-2.164441
44	1	0	1.890401	1.288215	-2.180236
45	1	0	0.836889	0.044772	-2.872084
46	6	0	0.525639	0.334658	-0.753240
47	1	0	0.619343	-0.752792	-0.729477
48	6	0	1.422023	0.948625	0.366163
49	6	0	2.746189	-2.204208	-0.627780
50	1	0	1.861023	-2.437177	-0.027269
51	1	0	3.382876	-3.095270	-0.631949
52	1	0	2.419339	-2.007851	-1.654978
53	6	0	4.110968	-1.162075	1.903832
54	1	0	3.240861	-1.526413	2.459615
55	1	0	4.498911	-0.284968	2.429487
56	1	0	4.881126	-1.941310	1.924799
57	6	0	5.215221	-0.323148	-0.873289
58	6	0	6.068613	-1.582450	-1.074942
59	1	0	6.991515	-1.331528	-1.613844
60	1	0	5.539001	-2.339413	-1.663605
61	1	0	6.359963	-2.037884	-0.121462
62	6	0	6.033430	0.733354	-0.117771

63	1	0	6.904485	1.038005	-0.712842
64	1	0	6.404140	0.347352	0.837970
65	1	0	5.436774	1.629165	0.088040
66	6	0	4.811838	0.238353	-2.242969
67	1	0	5.705246	0.441214	-2.848318
68	1	0	4.256114	1.175709	-2.137428
69	1	0	4.184879	-0.464851	-2.804557
70	6	0	1.248943	2.467425	0.352843
71	6	0	0.100698	3.049646	0.902421
72	6	0	2.190827	3.287009	-0.270455
73	6	0	-0.114532	4.419701	0.799188
74	1	0	-0.628794	2.422517	1.408522
75	6	0	1.977569	4.661572	-0.366178
76	1	0	3.092627	2.841051	-0.675833
77	6	0	0.821444	5.230409	0.159299
78	1	0	2.719317	5.287444	-0.852758
79	6	0	1.148696	0.367376	1.755429
80	6	0	0.422947	-0.805183	1.969916
81	6	0	1.758106	0.993431	2.848956
82	6	0	0.308467	-1.335470	3.255737
83	1	0	-0.091918	-1.303922	1.154785
84	6	0	1.654042	0.459522	4.126976
85	1	0	2.325073	1.905913	2.683706
86	6	0	0.926066	-0.711606	4.334378
87	1	0	2.138284	0.956745	4.961388
88	1	0	0.653140	6.299653	0.079497
89	1	0	-1.015209	4.853634	1.221193
90	1	0	0.833250	-1.128488	5.332161
91	1	0	-0.283857	-2.232221	3.412920

M01(Z)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-3.755199	1.542657	-0.703625
2	8	0	-3.168306	0.138435	0.012968
3	7	0	1.638918	-2.769929	-0.707071
4	7	0	0.715884	-3.778310	-0.936319
5	7	0	-0.151001	-1.758656	-0.988755
6	6	0	3.755990	-2.475896	0.457844
7	1	0	3.295820	-1.693556	1.049353
8	6	0	5.086307	-2.837207	0.645957

9	1	0	5.683129	-2.307227	1.380919
10	6	0	5.641797	-3.882104	-0.088075
11	1	0	6.677658	-4.165275	0.066543
12	6	0	4.859575	-4.569734	-1.013674
13	1	0	5.285079	-5.389798	-1.582916
14	6	0	3.533030	-4.207067	-1.222402
15	1	0	2.910011	-4.728255	-1.940174
16	6	0	2.992634	-3.152564	-0.490263
17	6	0	1.164724	-1.495815	-0.728785
18	6	0	-0.378041	-3.107923	-1.092417
19	6	0	-1.819113	-3.414485	-1.313041
20	1	0	-2.255580	-3.801862	-0.386930
21	1	0	-1.975141	-4.148232	-2.104806
22	6	0	-2.377370	-2.013889	-1.667327
23	1	0	-3.376926	-1.846008	-1.267763
24	1	0	-2.426568	-1.903944	-2.753825
25	6	0	-1.375255	-0.965917	-1.107817
26	1	0	-1.228611	-0.164617	-1.833713
27	6	0	-1.849954	-0.335308	0.241467
28	6	0	-3.052762	1.784575	-2.432444
29	1	0	-1.986785	2.030070	-2.406426
30	1	0	-3.563653	2.620240	-2.921948
31	1	0	-3.188006	0.896845	-3.059459
32	6	0	-3.433422	3.067143	0.337995
33	1	0	-2.383635	3.373198	0.298680
34	1	0	-3.688862	2.882468	1.385464
35	1	0	-4.046285	3.901837	-0.019906
36	6	0	-5.615423	1.187523	-0.789356
37	6	0	-6.314797	2.253961	-1.643856
38	1	0	-7.399649	2.085745	-1.642836
39	1	0	-5.978552	2.224013	-2.685799
40	1	0	-6.141126	3.266296	-1.260757
41	6	0	-6.201173	1.211111	0.629758
42	1	0	-7.268071	0.952575	0.605624
43	1	0	-6.110944	2.202607	1.086768
44	1	0	-5.695501	0.490972	1.283062
45	6	0	-5.861100	-0.194635	-1.408151
46	1	0	-6.938454	-0.376327	-1.517864
47	1	0	-5.450033	-0.988074	-0.775463
48	1	0	-5.407909	-0.285991	-2.402796
49	6	0	-1.930392	-1.438149	1.296046
50	6	0	-0.767349	-1.899674	1.923894
51	6	0	-3.150367	-2.045056	1.596146
52	6	0	-0.823212	-2.975213	2.803850

53	1	0	0.182608	-1.409424	1.721600
54	6	0	-3.205198	-3.117640	2.485492
55	1	0	-4.055741	-1.669077	1.131891
56	6	0	-2.041679	-3.592417	3.082800
57	1	0	-4.161099	-3.580939	2.709652
58	6	0	-0.985450	0.840622	0.707483
59	6	0	-0.175937	1.577592	-0.156635
60	6	0	-1.150906	1.296561	2.020937
61	6	0	0.435507	2.756205	0.271540
62	1	0	0.010241	1.241715	-1.170221
63	6	0	-0.533550	2.462455	2.454831
64	1	0	-1.782078	0.731750	2.700973
65	6	0	0.256107	3.203631	1.575898
66	1	0	-0.676454	2.800068	3.476476
67	6	0	3.458807	1.348906	-0.205933
68	6	0	2.753685	0.791484	0.767715
69	8	0	2.183095	0.365227	1.691198
70	6	0	3.900578	2.744023	0.002334
71	6	0	4.572328	3.433047	-1.017433
72	6	0	3.667824	3.425460	1.210869
73	6	0	4.992570	4.748420	-0.835371
74	1	0	4.771038	2.941951	-1.963855
75	6	0	4.086358	4.736730	1.386357
76	1	0	3.151280	2.919707	2.023191
77	6	0	4.753104	5.411182	0.363150
78	1	0	5.511059	5.255511	-1.643382
79	1	0	3.894721	5.234395	2.332323
80	1	0	5.081349	6.435760	0.501901
81	6	0	3.711543	0.605947	-1.503431
82	6	0	2.760213	1.025337	-2.625243
83	1	0	3.605278	-0.467026	-1.334401
84	1	0	4.755391	0.778895	-1.789365
85	1	0	3.077260	0.605616	-3.584663
86	1	0	1.761766	0.643743	-2.396873
87	1	0	2.705792	2.113562	-2.727375
88	1	0	1.070803	3.312028	-0.412096
89	1	0	0.736763	4.119952	1.905294
90	1	0	0.088188	-3.329490	3.274711
91	1	0	-2.083085	-4.431958	3.769350

TS1(E)

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	-2.269935	-1.984774	1.250295
2	8	0	-2.572977	-1.736623	2.360861
3	6	0	-1.914624	-2.804915	0.251216
4	6	0	-1.798415	-2.476847	-1.179826
5	6	0	-0.706241	-2.948912	-1.923371
6	6	0	-2.781171	-1.736729	-1.854129
7	6	0	-0.575972	-2.649797	-3.277431
8	1	0	0.056302	-3.544642	-1.427855
9	6	0	-2.633392	-1.405576	-3.197001
10	1	0	-3.667469	-1.421889	-1.310514
11	6	0	-1.528129	-1.857838	-3.916560
12	1	0	0.281193	-3.024322	-3.829899
13	1	0	-3.397930	-0.809988	-3.687038
14	1	0	-1.419836	-1.612371	-4.968270
15	6	0	-1.654804	-4.234035	0.742146
16	6	0	-0.270047	-4.447127	1.357303
17	1	0	-1.793436	-4.904385	-0.112659
18	1	0	-2.417769	-4.510956	1.477923
19	1	0	-0.107902	-3.753359	2.189104
20	1	0	-0.160947	-5.465985	1.741070
21	1	0	0.524443	-4.277579	0.624608
22	14	0	3.679087	-0.785833	0.257475
23	8	0	2.755708	0.579432	-0.086250
24	7	0	-2.921918	0.922567	-0.310163
25	7	0	-2.596745	1.634824	-1.448233
26	7	0	-0.909172	0.496750	-0.619023
27	6	0	-4.533541	0.604954	1.477807
28	1	0	-3.712545	0.358413	2.141503
29	6	0	-5.852386	0.592697	1.918024
30	1	0	-6.065087	0.334121	2.950049
31	6	0	-6.891644	0.921599	1.049966
32	1	0	-7.917634	0.917266	1.402528
33	6	0	-6.607935	1.259290	-0.270819
34	1	0	-7.412408	1.516073	-0.952184
35	6	0	-5.295031	1.263728	-0.731946
36	1	0	-5.056266	1.519091	-1.757478
37	6	0	-4.267719	0.934625	0.149642
38	6	0	-1.927464	0.170971	0.218232
39	6	0	-1.345388	1.339885	-1.606360
40	6	0	-0.270086	1.633209	-2.595967
41	1	0	0.097110	2.656497	-2.470683
42	1	0	-0.627234	1.509349	-3.619870

43	6	0	0.796530	0.574232	-2.207708
44	1	0	1.816059	0.946052	-2.311543
45	1	0	0.680552	-0.306766	-2.843860
46	6	0	0.507967	0.160092	-0.740872
47	1	0	0.634906	-0.916042	-0.606904
48	6	0	1.427248	0.920747	0.272784
49	6	0	2.782790	-2.361189	-0.246304
50	1	0	1.904713	-2.525943	0.387691
51	1	0	3.444443	-3.224197	-0.116146
52	1	0	2.454381	-2.337068	-1.291259
53	6	0	4.161205	-0.892267	2.066502
54	1	0	3.314286	-1.189784	2.692340
55	1	0	4.527114	0.070846	2.433536
56	1	0	4.958906	-1.632023	2.196423
57	6	0	5.206998	-0.497376	-0.823076
58	6	0	6.080987	-1.759463	-0.848037
59	1	0	6.996934	-1.572271	-1.423484
60	1	0	5.563027	-2.602113	-1.318826
61	1	0	6.385097	-2.068500	0.158780
62	6	0	6.018317	0.672293	-0.248351
63	1	0	6.876184	0.895792	-0.896339
64	1	0	6.408134	0.441756	0.749041
65	1	0	5.410267	1.580780	-0.171528
66	6	0	4.776036	-0.152134	-2.254687
67	1	0	5.657373	-0.037863	-2.899746
68	1	0	4.214134	0.787059	-2.281119
69	1	0	4.144998	-0.935044	-2.692299
70	6	0	1.260390	2.424908	0.053672
71	6	0	0.117929	3.080870	0.525467
72	6	0	2.203761	3.148376	-0.676653
73	6	0	-0.094519	4.424561	0.236103
74	1	0	-0.607560	2.533702	1.122372
75	6	0	1.994985	4.497729	-0.958005
76	1	0	3.099728	2.644856	-1.023440
77	6	0	0.841076	5.136220	-0.512934
78	1	0	2.737230	5.048748	-1.527116
79	6	0	1.185161	0.548808	1.736232
80	6	0	0.529217	-0.619366	2.121357
81	6	0	1.755712	1.358630	2.725757
82	6	0	0.431085	-0.965900	3.469434
83	1	0	0.076496	-1.271255	1.381630
84	6	0	1.673181	1.007450	4.066882
85	1	0	2.276569	2.266030	2.433203
86	6	0	1.006052	-0.158304	4.443744

87	1	0	2.125747	1.644679	4.820032
88	1	0	0.674922	6.184908	-0.737642
89	1	0	-0.991641	4.915839	0.598660
90	1	0	0.929489	-0.428506	5.492145
91	1	0	-0.118394	-1.858747	3.750290

TS1(Z)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-3.822572	1.299169	-0.657172
2	8	0	-3.119737	-0.076534	0.010074
3	7	0	2.003634	-2.463912	-0.635225
4	7	0	1.191370	-3.535557	-0.960351
5	7	0	0.124818	-1.610732	-0.919378
6	6	0	4.072742	-2.070374	0.597033
7	1	0	3.534380	-1.416586	1.273038
8	6	0	5.434591	-2.306881	0.760596
9	1	0	5.969005	-1.803021	1.558935
10	6	0	6.102177	-3.194765	-0.078443
11	1	0	7.162498	-3.379387	0.058228
12	6	0	5.402876	-3.853767	-1.087859
13	1	0	5.916501	-4.551947	-1.740537
14	6	0	4.045514	-3.614830	-1.272978
15	1	0	3.485541	-4.113938	-2.055650
16	6	0	3.392638	-2.716657	-0.432060
17	6	0	1.399885	-1.251884	-0.600122
18	6	0	0.040547	-2.967305	-1.114955
19	6	0	-1.350455	-3.399593	-1.422586
20	1	0	-1.784835	-3.884784	-0.543380
21	1	0	-1.394139	-4.095300	-2.261424
22	6	0	-2.031323	-2.042947	-1.727146
23	1	0	-3.058803	-1.999795	-1.367726
24	1	0	-2.045034	-1.875261	-2.807055
25	6	0	-1.168333	-0.932848	-1.064513
26	1	0	-1.064756	-0.087564	-1.746854
27	6	0	-1.771140	-0.419201	0.284804
28	6	0	-3.088202	1.679915	-2.346853
29	1	0	-2.058259	2.040470	-2.267778
30	1	0	-3.669869	2.468233	-2.835965
31	1	0	-3.099597	0.801126	-3.000287
32	6	0	-3.691701	2.794729	0.465878

33	1	0	-2.680157	3.211095	0.471654
34	1	0	-3.950275	2.531015	1.495272
35	1	0	-4.382211	3.576509	0.130705
36	6	0	-5.632861	0.763787	-0.825196
37	6	0	-6.419458	1.816863	-1.618185
38	1	0	-7.483071	1.547265	-1.652005
39	1	0	-6.066010	1.891771	-2.652255
40	1	0	-6.348236	2.811619	-1.163548
41	6	0	-6.247265	0.615962	0.574230
42	1	0	-7.276399	0.240331	0.499817
43	1	0	-6.282396	1.574749	1.102558
44	1	0	-5.675745	-0.087996	1.189649
45	6	0	-5.721646	-0.583405	-1.553976
46	1	0	-6.772137	-0.865058	-1.705899
47	1	0	-5.243165	-1.379324	-0.973907
48	1	0	-5.244388	-0.548105	-2.540807
49	6	0	-1.782461	-1.579904	1.278821
50	6	0	-0.611130	-1.948638	1.951040
51	6	0	-2.940812	-2.334060	1.468448
52	6	0	-0.594250	-3.076901	2.764878
53	1	0	0.284587	-1.340044	1.842769
54	6	0	-2.923755	-3.459368	2.291660
55	1	0	-3.854734	-2.032261	0.968069
56	6	0	-1.748621	-3.840031	2.932177
57	1	0	-3.832508	-4.036689	2.431268
58	6	0	-1.056914	0.816500	0.840417
59	6	0	-0.343068	1.701484	0.032119
60	6	0	-1.272874	1.162859	2.179373
61	6	0	0.147454	2.901775	0.546054
62	1	0	-0.124690	1.466411	-1.003229
63	6	0	-0.777393	2.352685	2.697491
64	1	0	-1.840592	0.491036	2.816486
65	6	0	-0.063484	3.228482	1.880392
66	1	0	-0.951330	2.598228	3.740361
67	6	0	3.044945	1.338954	-0.464553
68	6	0	2.431042	0.685680	0.528284
69	8	0	2.059500	0.441987	1.617024
70	6	0	3.461374	2.718627	-0.115968
71	6	0	3.895341	3.599383	-1.121817
72	6	0	3.416917	3.217673	1.200546
73	6	0	4.267676	4.908217	-0.825954
74	1	0	3.939069	3.267502	-2.153382
75	6	0	3.787157	4.524122	1.488885
76	1	0	3.082955	2.575014	2.008744

77	6	0	4.217036	5.384330	0.479414
78	1	0	4.596549	5.558685	-1.631058
79	1	0	3.741943	4.871903	2.516857
80	1	0	4.505976	6.404741	0.708213
81	6	0	3.244386	0.800271	-1.860463
82	6	0	2.111113	1.156471	-2.825523
83	1	0	3.362101	-0.283594	-1.819374
84	1	0	4.195368	1.191511	-2.236975
85	1	0	2.366481	0.896526	-3.857196
86	1	0	1.209287	0.601160	-2.548677
87	1	0	1.877247	2.225475	-2.787406
88	1	0	0.719549	3.566145	-0.094648
89	1	0	0.334794	4.155521	2.280991
90	1	0	0.322527	-3.356676	3.273829
91	1	0	-1.733458	-4.719767	3.567522

M1(E)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.068877	-1.214687	-0.566553
2	8	0	3.205344	0.189401	-0.215484
3	7	0	-2.441746	1.412553	-0.485097
4	7	0	-1.914433	2.373493	-1.305624
5	7	0	-0.408679	0.861730	-0.725159
6	6	0	-4.233537	1.236799	1.146394
7	1	0	-3.478876	1.120803	1.919567
8	6	0	-5.595523	1.191684	1.425554
9	1	0	-5.924803	1.050255	2.449587
10	6	0	-6.528940	1.325256	0.399205
11	1	0	-7.589443	1.290970	0.626160
12	6	0	-6.107420	1.499152	-0.917397
13	1	0	-6.835109	1.594761	-1.715905
14	6	0	-4.749537	1.535249	-1.216405
15	1	0	-4.391225	1.642583	-2.234255
16	6	0	-3.838864	1.406517	-0.175221
17	6	0	-1.554360	0.477142	-0.132359
18	6	0	-0.673740	2.014407	-1.420664
19	6	0	0.539463	2.521556	-2.114055
20	1	0	0.982049	3.328582	-1.521370
21	1	0	0.319485	2.896003	-3.113786
22	6	0	1.432256	1.259504	-2.116833

23	1	0	2.489444	1.494861	-2.007381
24	1	0	1.299413	0.720192	-3.058051
25	6	0	0.957945	0.345910	-0.949373
26	1	0	0.890190	-0.688596	-1.290705
27	6	0	1.901316	0.408697	0.295931
28	6	0	3.136293	-2.273604	-1.810070
29	6	0	4.494070	-2.212906	0.961784
30	1	0	3.625959	-2.758603	1.342991
31	1	0	4.858407	-1.562260	1.761644
32	1	0	5.281283	-2.938248	0.727568
33	6	0	5.643199	-0.507213	-1.350097
34	6	0	6.460509	-1.638180	-1.989790
35	1	0	7.406709	-1.244980	-2.383459
36	1	0	5.924522	-2.103137	-2.824226
37	1	0	6.708678	-2.424538	-1.267693
38	6	0	6.484645	0.177770	-0.264037
39	1	0	7.369222	0.650968	-0.710463
40	1	0	6.836169	-0.539509	0.485226
41	1	0	5.913633	0.955861	0.255237
42	6	0	5.281985	0.523550	-2.427182
43	1	0	6.190942	0.892095	-2.920870
44	1	0	4.765388	1.384581	-1.990496
45	1	0	4.635645	0.096598	-3.203842
46	6	0	1.849587	1.828761	0.858157
47	6	0	0.756921	2.233499	1.635704
48	6	0	2.843948	2.753203	0.535514
49	6	0	0.653817	3.558372	2.049701
50	1	0	-0.002795	1.504260	1.922534
51	6	0	2.737444	4.077247	0.959873
52	1	0	3.701667	2.429086	-0.044087
53	6	0	1.637624	4.485227	1.708706
54	1	0	3.517843	4.787811	0.705358
55	6	0	1.598118	-0.661319	1.347501
56	6	0	0.954951	-1.860566	1.041159
57	6	0	2.134396	-0.497506	2.628302
58	6	0	0.838022	-2.869416	1.994725
59	1	0	0.487495	-2.025600	0.076409
60	6	0	2.022818	-1.502971	3.580389
61	1	0	2.647284	0.427511	2.874829
62	6	0	1.374102	-2.695651	3.265964
63	1	0	2.443583	-1.355939	4.569972
64	6	0	-2.574540	-1.671319	0.586867
65	6	0	-1.811189	-0.580899	0.923659
66	8	0	-1.368965	-0.210988	2.055073

67	6	0	-3.190938	-1.810520	-0.737980
68	6	0	-4.543022	-2.189106	-0.855647
69	6	0	-2.504211	-1.538945	-1.936508
70	6	0	-5.180006	-2.236521	-2.088771
71	1	0	-5.104292	-2.420412	0.045175
72	6	0	-3.145981	-1.566261	-3.171225
73	1	0	-1.436073	-1.337972	-1.901793
74	6	0	-4.492310	-1.909280	-3.257536
75	1	0	-6.227742	-2.519196	-2.137731
76	1	0	-2.581812	-1.345730	-4.073081
77	1	0	-4.992692	-1.942451	-4.219851
78	6	0	-2.975021	-2.579055	1.727341
79	6	0	-3.984258	-1.947122	2.694550
80	1	0	-2.070962	-2.824655	2.299052
81	1	0	-3.370662	-3.520940	1.329674
82	1	0	-4.228676	-2.627919	3.516328
83	1	0	-3.552243	-1.036250	3.118010
84	1	0	-4.915087	-1.677594	2.184960
85	1	0	0.316078	-3.786019	1.738879
86	1	0	1.280798	-3.479892	4.010276
87	1	0	-0.198349	3.864945	2.648056
88	1	0	1.552560	5.516795	2.035540
89	1	0	2.852450	-1.697983	-2.697749
90	1	0	3.769614	-3.103594	-2.140063
91	1	0	2.232852	-2.710466	-1.374948

M1(Z)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-3.933673	1.064448	-0.684795
2	8	0	-3.075050	-0.267959	-0.113778
3	7	0	2.358400	-2.101822	-0.489693
4	7	0	1.649438	-3.211393	-0.873554
5	7	0	0.380634	-1.406122	-0.810963
6	6	0	4.369577	-1.477044	0.753001
7	1	0	3.762462	-0.850490	1.399410
8	6	0	5.748230	-1.583234	0.914810
9	1	0	6.233184	-1.017688	1.703032
10	6	0	6.499228	-2.411479	0.084904
11	1	0	7.572632	-2.487800	0.222939
12	6	0	5.873538	-3.146637	-0.920156

13	1	0	6.455927	-3.794613	-1.566224
14	6	0	4.499906	-3.046259	-1.107009
15	1	0	3.991252	-3.602019	-1.886282
16	6	0	3.770557	-2.206956	-0.269495
17	6	0	1.608432	-0.992063	-0.453495
18	6	0	0.450115	-2.753693	-1.053337
19	6	0	-0.872006	-3.303597	-1.457256
20	1	0	-1.319985	-3.833421	-0.610775
21	1	0	-0.791072	-3.989420	-2.300922
22	6	0	-1.644348	-2.006180	-1.800185
23	1	0	-2.700761	-2.066009	-1.543750
24	1	0	-1.564007	-1.807101	-2.871679
25	6	0	-0.965528	-0.839431	-1.026976
26	1	0	-0.880509	0.042843	-1.663094
27	6	0	-1.730424	-0.457969	0.289366
28	6	0	-3.178689	1.698166	-2.286270
29	6	0	-4.082400	2.438211	0.579503
30	1	0	-3.141935	2.980918	0.709388
31	1	0	-4.376030	2.036760	1.553789
32	1	0	-4.850998	3.152033	0.262180
33	6	0	-5.636144	0.300021	-1.022158
34	6	0	-6.492818	1.281245	-1.834651
35	1	0	-7.504089	0.876661	-1.971055
36	1	0	-6.070611	1.456220	-2.830045
37	1	0	-6.592935	2.251524	-1.334419
38	6	0	-6.334891	0.000141	0.312237
39	1	0	-7.292888	-0.506037	0.134347
40	1	0	-6.544834	0.917425	0.872472
41	1	0	-5.724272	-0.650714	0.948517
42	6	0	-5.485613	-1.006843	-1.811201
43	1	0	-6.473571	-1.411850	-2.067745
44	1	0	-4.956756	-1.764475	-1.223782
45	1	0	-4.935459	-0.859236	-2.748413
46	6	0	-1.689197	-1.666668	1.225694
47	6	0	-0.525512	-1.961138	1.948600
48	6	0	-2.782017	-2.530766	1.305757
49	6	0	-0.452775	-3.129659	2.701944
50	1	0	0.315953	-1.266859	1.930030
51	6	0	-2.705588	-3.695748	2.068159
52	1	0	-3.690790	-2.284627	0.767735
53	6	0	-1.536881	-4.004359	2.757690
54	1	0	-3.562608	-4.359935	2.121852
55	6	0	-1.219282	0.823444	0.953040
56	6	0	-0.619117	1.856228	0.230005

57	6	0	-1.515878	1.037025	2.302589
58	6	0	-0.292894	3.062003	0.847570
59	1	0	-0.352451	1.737586	-0.813910
60	6	0	-1.200926	2.241957	2.919169
61	1	0	-2.000588	0.250244	2.872301
62	6	0	-0.582969	3.257769	2.193466
63	1	0	-1.434840	2.385983	3.969200
64	6	0	2.478493	1.309780	-0.724377
65	6	0	2.018214	0.344780	0.140848
66	8	0	1.859269	0.298994	1.401367
67	6	0	2.850388	2.648777	-0.246474
68	6	0	3.129280	3.689167	-1.156827
69	6	0	2.911199	2.973629	1.127037
70	6	0	3.427779	4.978137	-0.727570
71	1	0	3.108578	3.496100	-2.224328
72	6	0	3.213812	4.263110	1.548793
73	1	0	2.692592	2.199152	1.849991
74	6	0	3.470577	5.279829	0.630899
75	1	0	3.628338	5.750959	-1.464410
76	1	0	3.245743	4.475609	2.614109
77	1	0	3.703875	6.285372	0.966630
78	6	0	2.616678	1.002272	-2.199786
79	6	0	4.075585	0.836467	-2.646460
80	1	0	4.658065	1.730366	-2.406833
81	1	0	4.536829	-0.005148	-2.119765
82	1	0	4.150479	0.655967	-3.723400
83	1	0	0.210325	3.836457	0.277380
84	1	0	-0.318836	4.194013	2.675109
85	1	0	0.454973	-3.353198	3.253394
86	1	0	-1.474955	-4.913821	3.346862
87	1	0	-3.061798	0.893729	-3.020533
88	1	0	-3.826456	2.462080	-2.728536
89	1	0	-2.201663	2.159395	-2.119523
90	1	0	2.072877	0.082937	-2.451005
91	1	0	2.135825	1.784327	-2.802742

M02(SS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.192175	-1.798121	-0.417191
2	8	0	3.823229	-0.155862	-0.300726

3	7	0	-1.123709	2.783010	-0.511932
4	7	0	-0.397779	3.325324	-1.537992
5	7	0	0.523145	1.468822	-0.764720
6	6	0	-2.690247	3.438229	1.226652
7	1	0	-1.967524	3.108643	1.968306
8	6	0	-3.940379	3.933431	1.582868
9	1	0	-4.203501	4.007939	2.632689
10	6	0	-4.847258	4.327859	0.601356
11	1	0	-5.820328	4.712206	0.888851
12	6	0	-4.512273	4.226439	-0.747320
13	1	0	-5.221938	4.526426	-1.510673
14	6	0	-3.270804	3.725120	-1.122717
15	1	0	-2.992459	3.609160	-2.164116
16	6	0	-2.382279	3.341563	-0.125796
17	6	0	-0.601758	1.641505	-0.054916
18	6	0	0.601092	2.505058	-1.660592
19	6	0	1.791896	2.371476	-2.541849
20	1	0	2.576359	3.055961	-2.206707
21	1	0	1.553928	2.590229	-3.583063
22	6	0	2.171435	0.889600	-2.304224
23	1	0	3.245791	0.722099	-2.345782
24	1	0	1.697340	0.266354	-3.067347
25	6	0	1.605218	0.471024	-0.917111
26	1	0	1.158640	-0.523208	-0.973245
27	6	0	2.686173	0.512898	0.220721
28	6	0	2.833776	-2.728113	-1.320589
29	6	0	4.524842	-2.596275	1.246956
30	1	0	3.602138	-2.755836	1.812473
31	1	0	5.188867	-1.977329	1.856780
32	1	0	5.008147	-3.568609	1.098713
33	6	0	5.786567	-1.764523	-1.444719
34	6	0	6.150385	-3.189993	-1.882899
35	1	0	7.109352	-3.188597	-2.417366
36	1	0	5.397381	-3.610678	-2.557995
37	1	0	6.254207	-3.867790	-1.027685
38	6	0	6.925939	-1.185307	-0.594879
39	1	0	7.842693	-1.100867	-1.193428
40	1	0	7.150984	-1.823076	0.266616
41	1	0	6.676217	-0.186269	-0.219492
42	6	0	5.596258	-0.887712	-2.688294
43	1	0	6.492615	-0.922923	-3.321695
44	1	0	5.426017	0.157560	-2.409325
45	1	0	4.747288	-1.219662	-3.298503
46	6	0	3.073414	1.970720	0.466684

47	6	0	2.239811	2.792734	1.235944
48	6	0	4.219850	2.509072	-0.117420
49	6	0	2.537929	4.144080	1.379604
50	1	0	1.364605	2.363314	1.726149
51	6	0	4.518204	3.862758	0.037523
52	1	0	4.875730	1.861583	-0.690166
53	6	0	3.673248	4.684724	0.776726
54	1	0	5.414428	4.271881	-0.418499
55	6	0	2.267028	-0.190536	1.514507
56	6	0	1.242249	-1.133594	1.586289
57	6	0	3.059503	0.031218	2.645804
58	6	0	1.016704	-1.833935	2.771329
59	1	0	0.573430	-1.313475	0.748638
60	6	0	2.837891	-0.670072	3.823455
61	1	0	3.864987	0.758251	2.592738
62	6	0	1.812544	-1.611321	3.888961
63	1	0	3.464117	-0.481478	4.689634
64	6	0	-2.254145	0.056614	0.903739
65	6	0	-1.137506	0.841485	1.103495
66	8	0	-0.507009	1.087894	2.175678
67	6	0	-3.070304	0.092367	-0.315409
68	6	0	-4.474649	-0.024376	-0.220218
69	6	0	-2.553191	0.252698	-1.621594
70	6	0	-5.299886	0.071314	-1.334157
71	1	0	-4.928970	-0.176355	0.753800
72	6	0	-3.381132	0.360444	-2.735071
73	1	0	-1.479884	0.239447	-1.784250
74	6	0	-4.764107	0.275783	-2.604143
75	1	0	-6.373847	-0.027091	-1.207397
76	1	0	-2.933247	0.479378	-3.717929
77	1	0	-5.408598	0.338560	-3.474243
78	6	0	-2.796774	-0.587878	2.159275
79	6	0	-3.487367	0.409079	3.098696
80	1	0	-1.952860	-1.036416	2.698009
81	1	0	-3.477972	-1.407151	1.898810
82	1	0	-3.889326	-0.086600	3.988402
83	1	0	-2.758218	1.157263	3.420698
84	1	0	-4.307292	0.931544	2.595204
85	1	0	0.194728	-2.541711	2.823112
86	1	0	1.628349	-2.156519	4.809214
87	1	0	1.884683	4.775737	1.973310
88	1	0	3.902928	5.739006	0.894304
89	1	0	2.609238	-2.286966	-2.297988
90	1	0	3.145062	-3.765149	-1.486299

91	1	0	1.902097	-2.751623	-0.747349
92	6	0	-2.313176	-3.150023	-0.320110
93	6	0	-3.697112	-3.372382	-0.253543
94	6	0	-4.296561	-3.950697	0.857675
95	6	0	-3.509734	-4.342822	1.935111
96	6	0	-2.133977	-4.140548	1.896863
97	6	0	-1.553306	-3.541681	0.784741
98	1	0	-5.370160	-4.086806	0.862251
99	1	0	-3.975562	-4.805087	2.798220
100	1	0	-1.514377	-4.447812	2.732996
101	1	0	-0.482640	-3.368239	0.741571
102	7	0	-4.611348	-3.035188	-1.363032
103	6	0	-1.553653	-2.494088	-1.439855
104	8	0	-0.398434	-2.152651	-1.282827
105	1	0	-2.065317	-2.346207	-2.393850
106	8	0	-4.139148	-2.888797	-2.475919
107	8	0	-5.797789	-2.956035	-1.108455

M02(RR)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.703588	-1.436439	0.084272
2	8	0	3.175584	-0.739371	-0.062594
3	7	0	1.050729	3.137866	-0.548053
4	7	0	2.117473	3.008382	-1.401778
5	7	0	1.189496	1.063912	-0.956670
6	6	0	0.026694	4.635569	1.096103
7	1	0	-0.167011	3.781990	1.739919
8	6	0	-0.349926	5.927117	1.455840
9	1	0	-0.845906	6.084549	2.407501
10	6	0	-0.087353	7.006045	0.616996
11	1	0	-0.381520	8.007974	0.911371
12	6	0	0.555551	6.798841	-0.601948
13	1	0	0.762940	7.635378	-1.260637
14	6	0	0.929940	5.517520	-0.987413
15	1	0	1.425347	5.335018	-1.933305
16	6	0	0.656729	4.452586	-0.130884
17	6	0	0.442984	1.966037	-0.301652
18	6	0	2.159444	1.733848	-1.644734
19	6	0	2.871480	0.833715	-2.594044

20	1	0	3.873104	0.602313	-2.236354
21	1	0	2.945646	1.289277	-3.582482
22	6	0	1.962439	-0.418763	-2.568360
23	1	0	2.556607	-1.328545	-2.642527
24	1	0	1.260690	-0.393277	-3.406961
25	6	0	1.153811	-0.379724	-1.237046
26	1	0	0.111184	-0.688883	-1.359821
27	6	0	1.830577	-1.200535	-0.105150
28	6	0	5.087284	-2.336381	-1.519498
29	6	0	4.916440	-2.593430	1.554506
30	1	0	4.672257	-3.629465	1.313156
31	1	0	4.303037	-2.278872	2.405241
32	1	0	5.962635	-2.562937	1.876660
33	6	0	5.913972	0.006765	0.378338
34	6	0	7.341943	-0.528944	0.175602
35	1	0	8.069656	0.262565	0.395989
36	1	0	7.509722	-0.853166	-0.857109
37	1	0	7.570820	-1.373124	0.835233
38	6	0	5.777748	0.527774	1.817487
39	1	0	6.528584	1.306760	2.003632
40	1	0	5.928855	-0.260920	2.561284
41	1	0	4.794508	0.976406	1.992637
42	6	0	5.703307	1.182594	-0.579925
43	1	0	6.437376	1.971772	-0.370531
44	1	0	4.706402	1.621858	-0.467262
45	1	0	5.844779	0.884412	-1.625595
46	6	0	1.161832	-0.933376	1.245748
47	6	0	-0.076859	-1.515268	1.531672
48	6	0	1.784455	-0.154275	2.216628
49	6	0	-0.682146	-1.321757	2.767201
50	1	0	-0.548172	-2.169547	0.802800
51	6	0	1.189737	0.019628	3.465771
52	1	0	2.741123	0.304606	1.995522
53	6	0	-0.041018	-0.560173	3.743081
54	1	0	1.691328	0.620207	4.218200
55	6	0	1.711169	-2.704093	-0.423370
56	6	0	1.167348	-3.220756	-1.603588
57	6	0	2.121140	-3.611404	0.559929
58	6	0	1.114418	-4.597730	-1.821587
59	1	0	0.746763	-2.572434	-2.363290
60	6	0	2.086170	-4.982580	0.339986
61	1	0	2.441691	-3.232594	1.523633
62	6	0	1.594068	-5.482819	-0.863744
63	1	0	2.422030	-5.659952	1.118861

64	6	0	-1.970806	1.555816	-0.306434
65	6	0	-0.844574	1.720216	0.487941
66	8	0	-0.682171	1.743224	1.735969
67	6	0	-3.280455	1.302267	0.308310
68	6	0	-4.477580	1.458791	-0.423359
69	6	0	-3.407110	0.826784	1.634554
70	6	0	-5.719612	1.167449	0.130937
71	1	0	-4.443043	1.813268	-1.448737
72	6	0	-4.652149	0.535537	2.180586
73	1	0	-2.507024	0.699652	2.223656
74	6	0	-5.821375	0.703815	1.439693
75	1	0	-6.614575	1.298448	-0.471880
76	1	0	-4.707736	0.159445	3.198406
77	1	0	-6.789266	0.469257	1.872101
78	6	0	-1.915776	1.758821	-1.809054
79	6	0	-2.168810	3.207139	-2.252168
80	1	0	-3.115383	3.579362	-1.850360
81	1	0	-1.381895	3.869353	-1.876441
82	1	0	-2.198670	3.296662	-3.343300
83	1	0	0.687268	-4.972662	-2.745940
84	1	0	1.557557	-6.552977	-1.039279
85	1	0	-1.644129	-1.786214	2.962354
86	1	0	-0.504481	-0.418968	4.714381
87	1	0	5.133081	-1.647816	-2.370628
88	1	0	6.047322	-2.858318	-1.459157
89	1	0	4.312580	-3.083071	-1.726291
90	6	0	-4.013150	-1.745033	-1.095370
91	6	0	-4.804867	-2.153163	-0.019623
92	6	0	-6.182902	-2.277917	-0.113736
93	6	0	-6.798772	-2.004749	-1.329422
94	6	0	-6.033261	-1.617615	-2.427707
95	6	0	-4.654519	-1.486826	-2.307284
96	1	0	-6.745739	-2.592173	0.756448
97	1	0	-7.875107	-2.102191	-1.418713
98	1	0	-6.514028	-1.411742	-3.378123
99	1	0	-4.044609	-1.165333	-3.145363
100	7	0	-4.181322	-2.542330	1.249840
101	6	0	-2.544859	-1.459019	-1.015001
102	8	0	-1.838479	-1.533083	-2.000747
103	1	0	-2.155180	-1.117541	-0.049293
104	8	0	-2.998404	-2.850932	1.222985
105	8	0	-4.874361	-2.570222	2.246764
106	1	0	-0.952060	1.432158	-2.220565
107	1	0	-2.648373	1.098407	-2.290099

M02(SR)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.222774	-1.794480	-0.590952
2	8	0	3.825112	-0.179276	-0.311738
3	7	0	-1.078868	2.828864	-0.299028
4	7	0	-0.309738	3.504016	-1.207714
5	7	0	0.566434	1.543895	-0.678809
6	6	0	-2.729782	3.260611	1.438611
7	1	0	-2.047075	2.835380	2.168856
8	6	0	-3.999268	3.705763	1.792251
9	1	0	-4.316571	3.642072	2.827649
10	6	0	-4.854672	4.235517	0.827337
11	1	0	-5.842713	4.580733	1.113573
12	6	0	-4.446562	4.323326	-0.501294
13	1	0	-5.115167	4.729792	-1.252406
14	6	0	-3.185952	3.870437	-0.876093
15	1	0	-2.854036	3.893723	-1.907872
16	6	0	-2.351748	3.345034	0.102243
17	6	0	-0.584353	1.624365	0.007333
18	6	0	0.686348	2.698260	-1.411004
19	6	0	1.913639	2.686754	-2.250935
20	1	0	2.681641	3.312803	-1.787469
21	1	0	1.720199	3.054336	-3.259014
22	6	0	2.287558	1.185267	-2.212081
23	1	0	3.363707	1.022069	-2.218062
24	1	0	1.859842	0.680429	-3.082017
25	6	0	1.654499	0.575641	-0.928347
26	1	0	1.210912	-0.398778	-1.145880
27	6	0	2.686033	0.448721	0.250062
28	6	0	2.950971	-2.607379	-1.709347
29	6	0	4.471790	-2.760482	0.994558
30	1	0	3.526756	-2.985456	1.495812
31	1	0	5.095211	-2.194519	1.692886
32	1	0	4.979023	-3.707530	0.779077
33	6	0	5.880489	-1.622479	-1.498885
34	6	0	6.288451	-2.976727	-2.095960
35	1	0	7.278757	-2.899969	-2.563629
36	1	0	5.584594	-3.308159	-2.867061
37	1	0	6.347591	-3.760894	-1.332282

38	6	0	6.958065	-1.159368	-0.507928
39	1	0	7.909421	-0.991820	-1.030176
40	1	0	7.136303	-1.907474	0.271821
41	1	0	6.674768	-0.221305	-0.016772
42	6	0	5.765121	-0.591049	-2.628295
43	1	0	6.702845	-0.543866	-3.197889
44	1	0	5.566037	0.409608	-2.230549
45	1	0	4.963265	-0.842262	-3.333040
46	6	0	3.097659	1.856534	0.681644
47	6	0	2.245304	2.624335	1.486145
48	6	0	4.292692	2.412842	0.224600
49	6	0	2.575112	3.942018	1.788957
50	1	0	1.332263	2.179329	1.883148
51	6	0	4.621806	3.731463	0.537748
52	1	0	4.962358	1.805458	-0.374521
53	6	0	3.758925	4.502355	1.310467
54	1	0	5.555143	4.152460	0.176925
55	6	0	2.186668	-0.401128	1.422066
56	6	0	1.261266	-1.430882	1.249272
57	6	0	2.812137	-0.264245	2.664089
58	6	0	0.964642	-2.303572	2.293852
59	1	0	0.758106	-1.566224	0.298650
60	6	0	2.508370	-1.125736	3.711964
61	1	0	3.547732	0.520660	2.809359
62	6	0	1.583290	-2.151007	3.530342
63	1	0	2.999989	-0.999538	4.671350
64	6	0	-2.358339	0.076827	0.817982
65	6	0	-1.165902	0.728952	1.084512
66	8	0	-0.524057	0.878431	2.163615
67	6	0	-3.087031	0.317831	-0.438427
68	6	0	-4.488758	0.475392	-0.421585
69	6	0	-2.461073	0.434983	-1.698967
70	6	0	-5.205772	0.776507	-1.573500
71	1	0	-5.021469	0.395575	0.520244
72	6	0	-3.176491	0.762054	-2.846662
73	1	0	-1.401943	0.211318	-1.795590
74	6	0	-4.557051	0.938865	-2.796577
75	1	0	-6.283104	0.902673	-1.509786
76	1	0	-2.650456	0.845882	-3.794147
77	1	0	-5.116918	1.184669	-3.693225
78	6	0	-3.128874	-0.487568	1.998141
79	6	0	-2.326812	-1.293632	3.023274
80	1	0	-1.819183	-2.141728	2.554525
81	1	0	-1.559201	-0.679463	3.491617

82	1	0	-2.999579	-1.697414	3.785801
83	1	0	0.249900	-3.108068	2.141560
84	1	0	1.347344	-2.827291	4.345590
85	1	0	1.906859	4.531608	2.408650
86	1	0	4.011541	5.530262	1.550804
87	1	0	2.830929	-2.044712	-2.642112
88	1	0	3.281815	-3.617507	-1.972757
89	1	0	1.964963	-2.698532	-1.244701
90	6	0	-2.815872	-2.875180	-0.927080
91	6	0	-3.744799	-3.361058	-0.001220
92	6	0	-5.099497	-3.455239	-0.282971
93	6	0	-5.546876	-3.086096	-1.547386
94	6	0	-4.641253	-2.638120	-2.506041
95	6	0	-3.291417	-2.529445	-2.192165
96	1	0	-5.775712	-3.827662	0.476618
97	1	0	-6.603216	-3.157254	-1.782075
98	1	0	-4.989638	-2.347653	-3.491034
99	1	0	-2.578256	-2.136206	-2.906879
100	7	0	-3.307710	-3.851852	1.311416
101	6	0	-1.398942	-2.531353	-0.603542
102	8	0	-0.611887	-2.197949	-1.468469
103	1	0	-1.113994	-2.537495	0.454595
104	8	0	-2.180974	-4.317680	1.392195
105	8	0	-4.098617	-3.793407	2.232994
106	1	0	-3.628119	0.342502	2.527841
107	1	0	-3.942172	-1.120737	1.620524

M02(RS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	5.192194	-0.929908	-0.427309
2	8	0	3.737970	-0.081942	-0.322976
3	7	0	-0.527195	2.887696	-0.647926
4	7	0	0.537879	3.223965	-1.441243
5	7	0	0.600792	1.107116	-0.832963
6	6	0	-2.177976	3.852659	0.877503
7	1	0	-1.964729	3.067078	1.596669
8	6	0	-3.126907	4.837731	1.136696
9	1	0	-3.668316	4.815799	2.076353
10	6	0	-3.374812	5.846400	0.209776
11	1	0	-4.113432	6.611622	0.423806

12	6	0	-2.672727	5.874455	-0.993383
13	1	0	-2.860155	6.658985	-1.718497
14	6	0	-1.731901	4.892169	-1.278069
15	1	0	-1.179452	4.891987	-2.210184
16	6	0	-1.504388	3.889076	-0.339440
17	6	0	-0.536914	1.588418	-0.302745
18	6	0	1.194683	2.110980	-1.549258
19	6	0	2.336674	1.580163	-2.351349
20	1	0	3.288927	1.786698	-1.858478
21	1	0	2.349141	1.997725	-3.358336
22	6	0	2.014683	0.063961	-2.307939
23	1	0	2.897474	-0.554871	-2.453260
24	1	0	1.273520	-0.176007	-3.076511
25	6	0	1.369663	-0.150541	-0.919973
26	1	0	0.671150	-0.981303	-0.874156
27	6	0	2.460425	-0.318071	0.248933
28	6	0	5.211526	-1.939996	-2.015006
29	6	0	5.561733	-2.043460	1.033474
30	1	0	4.968298	-2.961676	1.013282
31	1	0	5.374172	-1.537458	1.984800
32	1	0	6.622205	-2.320541	1.003117
33	6	0	6.526245	0.419744	-0.534459
34	6	0	7.795133	-0.189460	-1.153053
35	1	0	8.610730	0.544840	-1.133867
36	1	0	7.637539	-0.483042	-2.196022
37	1	0	8.137897	-1.073014	-0.601461
38	6	0	6.866297	0.944154	0.868811
39	1	0	7.594315	1.763168	0.799632
40	1	0	7.309889	0.161004	1.492797
41	1	0	5.983681	1.326338	1.393482
42	6	0	6.061516	1.587087	-1.414076
43	1	0	6.881566	2.301978	-1.562267
44	1	0	5.231603	2.131341	-0.952149
45	1	0	5.735439	1.249563	-2.405900
46	6	0	2.227285	0.734594	1.330290
47	6	0	1.099834	0.669185	2.151022
48	6	0	3.081109	1.834033	1.434497
49	6	0	0.840198	1.684486	3.067869
50	1	0	0.390923	-0.146981	2.048711
51	6	0	2.830277	2.839438	2.365528
52	1	0	3.940809	1.900560	0.779110
53	6	0	1.709975	2.765690	3.188038
54	1	0	3.508098	3.684323	2.437840
55	6	0	2.387648	-1.761398	0.760652

56	6	0	2.301072	-2.799824	-0.173640
57	6	0	2.500472	-2.088012	2.110522
58	6	0	2.329866	-4.130074	0.226841
59	1	0	2.206226	-2.573739	-1.233537
60	6	0	2.518067	-3.420945	2.517142
61	1	0	2.581913	-1.302023	2.852631
62	6	0	2.436915	-4.445529	1.580373
63	1	0	2.601736	-3.655229	3.573511
64	6	0	-2.767289	0.600123	-0.537164
65	6	0	-1.757729	0.911469	0.362355
66	8	0	-1.724295	0.822276	1.618398
67	6	0	-4.128966	0.317682	-0.047499
68	6	0	-5.068161	-0.343020	-0.863919
69	6	0	-4.575027	0.729288	1.226343
70	6	0	-6.365565	-0.594982	-0.431666
71	1	0	-4.774780	-0.683567	-1.852973
72	6	0	-5.876563	0.488318	1.648828
73	1	0	-3.874314	1.225797	1.885457
74	6	0	-6.783959	-0.181836	0.830324
75	1	0	-7.052479	-1.121845	-1.088640
76	1	0	-6.184874	0.825609	2.634926
77	1	0	-7.797376	-0.375809	1.167927
78	6	0	-2.552190	0.615875	-2.039188
79	6	0	-3.325414	1.718364	-2.773017
80	1	0	-4.397510	1.635091	-2.576950
81	1	0	-3.006294	2.706848	-2.429442
82	1	0	-3.169631	1.660206	-3.854611
83	1	0	2.259604	-4.918751	-0.515517
84	1	0	2.451889	-5.482462	1.899933
85	1	0	-0.060758	1.627668	3.668874
86	1	0	1.508275	3.553180	3.907398
87	1	0	5.128802	-1.309404	-2.906794
88	1	0	6.154233	-2.491881	-2.088042
89	1	0	4.400521	-2.672885	-2.034260
90	6	0	-2.805444	-2.591317	0.264789
91	6	0	-3.650996	-3.375076	-0.531072
92	6	0	-4.882646	-3.830165	-0.080298
93	6	0	-5.318837	-3.455254	1.184502
94	6	0	-4.511490	-2.655435	1.988734
95	6	0	-3.261066	-2.247908	1.540059
96	1	0	-5.487235	-4.450869	-0.729644
97	1	0	-6.294086	-3.777651	1.532170
98	1	0	-4.862493	-2.334876	2.963564
99	1	0	-2.626770	-1.599189	2.137284

100	7	0	-3.292847	-3.752398	-1.903745
101	6	0	-1.443060	-2.088271	-0.087748
102	8	0	-0.626077	-1.860362	0.781916
103	1	0	-1.208624	-1.947292	-1.152586
104	8	0	-2.552684	-3.011834	-2.534288
105	8	0	-3.771698	-4.776407	-2.354321
106	1	0	-1.485911	0.716896	-2.275022
107	1	0	-2.825824	-0.361562	-2.460149

TS2(SS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-4.081585	1.763363	-0.450971
2	8	0	-3.777667	0.097044	-0.399261
3	7	0	1.337055	-2.550327	-0.027484
4	7	0	0.622333	-3.320574	-0.895251
5	7	0	-0.349135	-1.358090	-0.535555
6	6	0	2.633336	-3.134735	1.944334
7	1	0	1.813333	-2.783322	2.562769
8	6	0	3.796423	-3.653710	2.505279
9	1	0	3.890348	-3.715925	3.583887
10	6	0	4.833555	-4.087105	1.682287
11	1	0	5.739516	-4.489492	2.123433
12	6	0	4.718036	-4.002575	0.294421
13	1	0	5.533829	-4.326389	-0.342851
14	6	0	3.562576	-3.487582	-0.282015
15	1	0	3.452476	-3.383994	-1.357454
16	6	0	2.540787	-3.061114	0.558767
17	6	0	0.810023	-1.333936	0.149052
18	6	0	-0.385911	-2.560407	-1.202392
19	6	0	-1.499403	-2.619953	-2.188960
20	1	0	-2.283884	-3.302668	-1.853562
21	1	0	-1.131111	-2.961166	-3.157919
22	6	0	-1.951632	-1.135986	-2.204726
23	1	0	-3.021462	-1.020379	-2.373829
24	1	0	-1.417828	-0.600163	-2.994429
25	6	0	-1.546009	-0.522773	-0.840505
26	1	0	-1.213811	0.509052	-0.931550
27	6	0	-2.725681	-0.636419	0.202613
28	6	0	-2.650469	2.719943	-1.197423
29	6	0	-4.532962	2.457612	1.233089

30	1	0	-3.659163	2.547754	1.884444
31	1	0	-5.264924	1.822687	1.740224
32	1	0	-4.973213	3.453922	1.112527
33	6	0	-5.594355	1.822401	-1.599005
34	6	0	-5.892661	3.279728	-1.981958
35	1	0	-6.795380	3.331300	-2.604826
36	1	0	-5.070840	3.724803	-2.553296
37	1	0	-6.068524	3.906446	-1.099787
38	6	0	-6.812223	1.227437	-0.876665
39	1	0	-7.681980	1.207234	-1.546902
40	1	0	-7.088164	1.817874	0.003702
41	1	0	-6.620133	0.200429	-0.545318
42	6	0	-5.322487	1.011282	-2.872918
43	1	0	-6.174465	1.085086	-3.562013
44	1	0	-5.169512	-0.047858	-2.640853
45	1	0	-4.434989	1.371525	-3.406440
46	6	0	-3.180420	-2.092743	0.312914
47	6	0	-2.412079	-3.013697	1.034307
48	6	0	-4.328099	-2.538174	-0.344339
49	6	0	-2.754213	-4.362182	1.051951
50	1	0	-1.544651	-2.670858	1.594407
51	6	0	-4.677761	-3.887773	-0.316991
52	1	0	-4.938564	-1.820118	-0.880463
53	6	0	-3.884681	-4.805457	0.367143
54	1	0	-5.571685	-4.221178	-0.835018
55	6	0	-2.440636	-0.061966	1.589244
56	6	0	-1.417523	0.850604	1.823797
57	6	0	-3.334923	-0.366883	2.625955
58	6	0	-1.271697	1.430942	3.087147
59	1	0	-0.720873	1.116706	1.032720
60	6	0	-3.203595	0.229448	3.872140
61	1	0	-4.144742	-1.067695	2.444798
62	6	0	-2.162957	1.130269	4.108519
63	1	0	-3.908575	-0.009485	4.662249
64	6	0	2.754046	0.386934	0.113182
65	6	0	1.642246	-0.239174	0.856211
66	8	0	1.329191	0.034616	1.998111
67	6	0	3.290186	-0.319657	-1.099985
68	6	0	4.658478	-0.582443	-1.270260
69	6	0	2.438704	-0.674459	-2.162740
70	6	0	5.138748	-1.227812	-2.405572
71	1	0	5.367686	-0.274260	-0.511204
72	6	0	2.912535	-1.338217	-3.290637
73	1	0	1.392709	-0.378752	-2.119280

74	6	0	4.268645	-1.632324	-3.415376
75	1	0	6.204423	-1.414471	-2.499761
76	1	0	2.221604	-1.600605	-4.086792
77	1	0	4.644406	-2.139587	-4.298185
78	6	0	3.799051	0.892405	1.114086
79	6	0	4.437561	-0.195026	1.988088
80	1	0	3.324098	1.618002	1.778770
81	1	0	4.566267	1.433770	0.554067
82	1	0	5.275118	0.216755	2.560061
83	1	0	3.708350	-0.586193	2.701711
84	1	0	4.809384	-1.041770	1.401663
85	1	0	-0.442068	2.108179	3.267460
86	1	0	-2.048716	1.586715	5.086851
87	1	0	-2.140155	-5.065611	1.605028
88	1	0	-4.152661	-5.857043	0.380273
89	1	0	-2.476063	2.431889	-2.240266
90	1	0	-2.899364	3.787198	-1.189364
91	1	0	-1.698927	2.597321	-0.667823
92	6	0	2.124362	3.059682	0.114767
93	6	0	3.234277	3.886409	-0.109632
94	6	0	3.501982	5.021237	0.654801
95	6	0	2.658089	5.350672	1.703549
96	6	0	1.530432	4.564930	1.942852
97	6	0	1.266294	3.458377	1.146604
98	1	0	4.367867	5.623542	0.410545
99	1	0	2.869861	6.220294	2.315882
100	1	0	0.847472	4.826442	2.745595
101	1	0	0.364138	2.873922	1.282470
102	7	0	4.187314	3.626829	-1.197669
103	6	0	1.706572	1.830273	-0.683633
104	8	0	0.450571	1.546833	-0.652742
105	1	0	2.220767	1.779013	-1.652229
106	8	0	4.318386	2.480383	-1.598762
107	8	0	4.811343	4.577542	-1.643223

TS(RR)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	5.235232	-0.647113	-0.407416
2	8	0	3.669832	-0.041008	-0.252634
3	7	0	-0.284403	2.756754	-0.691629

4	7	0	0.738106	3.012285	-1.561637
5	7	0	0.673719	0.885967	-0.976213
6	6	0	-1.401534	4.112528	1.002333
7	1	0	-0.910614	3.523415	1.768942
8	6	0	-2.264474	5.157828	1.315778
9	1	0	-2.454812	5.398199	2.355885
10	6	0	-2.873407	5.895333	0.303456
11	1	0	-3.542369	6.710714	0.557470
12	6	0	-2.624893	5.594525	-1.034611
13	1	0	-3.098367	6.170602	-1.821893
14	6	0	-1.772264	4.548117	-1.366169
15	1	0	-1.559605	4.294642	-2.399267
16	6	0	-1.182115	3.819312	-0.338871
17	6	0	-0.367009	1.458693	-0.359451
18	6	0	1.299070	1.848509	-1.717813
19	6	0	2.379960	1.252834	-2.558128
20	1	0	3.362433	1.498492	-2.153875
21	1	0	2.314804	1.602937	-3.589123
22	6	0	2.064301	-0.257256	-2.398912
23	1	0	2.958441	-0.868940	-2.490807
24	1	0	1.345329	-0.563139	-3.165829
25	6	0	1.391261	-0.407821	-1.014477
26	1	0	0.648683	-1.202454	-0.930448
27	6	0	2.415703	-0.548657	0.188932
28	6	0	5.450520	-1.417174	-2.111157
29	6	0	5.757322	-1.907847	0.875865
30	1	0	5.310801	-2.888432	0.690060
31	1	0	5.498249	-1.603750	1.893172
32	1	0	6.847139	-2.015743	0.822945
33	6	0	6.338428	0.889152	-0.243717
34	6	0	7.746450	0.560175	-0.763797
35	1	0	8.415879	1.414866	-0.601382
36	1	0	7.740762	0.344158	-1.837406
37	1	0	8.187915	-0.300721	-0.248477
38	6	0	6.432193	1.295626	1.234857
39	1	0	7.016394	2.219678	1.336456
40	1	0	6.928627	0.523572	1.832331
41	1	0	5.444033	1.474084	1.673928
42	6	0	5.779276	2.063606	-1.055635
43	1	0	6.455449	2.926269	-0.991260
44	1	0	4.800058	2.382910	-0.683083
45	1	0	5.675247	1.810532	-2.118222
46	6	0	1.956980	0.312559	1.369514
47	6	0	0.916239	-0.099953	2.207263

48	6	0	2.534536	1.569509	1.570428
49	6	0	0.499494	0.717654	3.254850
50	1	0	0.413125	-1.042868	2.008521
51	6	0	2.103736	2.389977	2.610350
52	1	0	3.328017	1.900766	0.910397
53	6	0	1.091787	1.959916	3.465014
54	1	0	2.566363	3.361636	2.754107
55	6	0	2.546264	-2.034433	0.549815
56	6	0	2.514781	-3.009328	-0.452780
57	6	0	2.814134	-2.441265	1.858819
58	6	0	2.750574	-4.349033	-0.158488
59	1	0	2.297803	-2.737061	-1.481347
60	6	0	3.036051	-3.782104	2.159219
61	1	0	2.858816	-1.704634	2.653194
62	6	0	3.010271	-4.741307	1.151988
63	1	0	3.238130	-4.073197	3.185001
64	6	0	-2.516134	0.033096	-0.454519
65	6	0	-1.622758	0.900911	0.334033
66	8	0	-1.788369	1.261887	1.483552
67	6	0	-3.984854	0.300768	-0.246889
68	6	0	-4.905291	0.038255	-1.278623
69	6	0	-4.517685	0.763649	0.971166
70	6	0	-6.270485	0.255225	-1.118188
71	1	0	-4.563605	-0.338997	-2.235596
72	6	0	-5.882295	0.983453	1.126624
73	1	0	-3.861157	0.936744	1.810753
74	6	0	-6.770999	0.741102	0.083805
75	1	0	-6.941736	0.039214	-1.943958
76	1	0	-6.252034	1.334663	2.085103
77	1	0	-7.835495	0.907235	0.213700
78	6	0	-2.100238	-0.207261	-1.903575
79	6	0	-2.184191	0.989345	-2.859157
80	1	0	-3.137868	1.514047	-2.751195
81	1	0	-1.386702	1.720991	-2.692367
82	1	0	-2.096789	0.657912	-3.898176
83	1	0	2.717506	-5.086997	-0.953586
84	1	0	3.185783	-5.786492	1.385036
85	1	0	-0.314287	0.387969	3.892165
86	1	0	0.760897	2.592308	4.283108
87	1	0	5.266468	-0.704398	-2.922136
88	1	0	6.475728	-1.786213	-2.218848
89	1	0	4.781530	-2.273954	-2.243532
90	6	0	-2.956878	-2.613209	-0.154289
91	6	0	-4.296342	-2.879732	0.155559

92	6	0	-5.067545	-3.801558	-0.548288
93	6	0	-4.495558	-4.520499	-1.587526
94	6	0	-3.153586	-4.313412	-1.899432
95	6	0	-2.410721	-3.376527	-1.192351
96	1	0	-6.100352	-3.948191	-0.257619
97	1	0	-5.087823	-5.246847	-2.133331
98	1	0	-2.685609	-4.885046	-2.695012
99	1	0	-1.361881	-3.201593	-1.407822
100	7	0	-4.974500	-2.267189	1.312091
101	6	0	-2.019135	-1.557209	0.447329
102	8	0	-0.767440	-1.771379	0.244375
103	1	0	-2.343438	-1.209410	1.439148
104	8	0	-4.302210	-1.968553	2.283760
105	8	0	-6.185088	-2.144110	1.256194
106	1	0	-1.092184	-0.632436	-1.906544
107	1	0	-2.724833	-1.013319	-2.296673

TS2(SR)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.286150	-1.661714	-0.685443
2	8	0	3.873565	-0.075227	-0.273561
3	7	0	-1.162781	2.713165	-0.214017
4	7	0	-0.378569	3.449334	-1.052194
5	7	0	0.513885	1.467762	-0.622254
6	6	0	-2.832349	3.004985	1.534220
7	1	0	-2.152747	2.553664	2.250170
8	6	0	-4.112182	3.402853	1.909780
9	1	0	-4.437919	3.253423	2.933459
10	6	0	-4.961503	3.998853	0.980744
11	1	0	-5.958155	4.305508	1.279775
12	6	0	-4.535471	4.204757	-0.329978
13	1	0	-5.200677	4.661249	-1.054854
14	6	0	-3.266421	3.800593	-0.726479
15	1	0	-2.924260	3.913344	-1.748552
16	6	0	-2.439585	3.198150	0.213817
17	6	0	-0.659622	1.498739	0.018745
18	6	0	0.631387	2.664353	-1.283347
19	6	0	1.858361	2.710290	-2.121118
20	1	0	2.613568	3.338255	-1.641240
21	1	0	1.648826	3.109077	-3.114269

22	6	0	2.258439	1.214158	-2.138711
23	1	0	3.336771	1.073628	-2.168348
24	1	0	1.823193	0.734424	-3.019279
25	6	0	1.652021	0.546481	-0.871891
26	1	0	1.224235	-0.431651	-1.091764
27	6	0	2.695701	0.454540	0.309487
28	6	0	2.995363	-2.420299	-1.821635
29	6	0	4.602181	-2.734861	0.818359
30	1	0	3.674916	-3.054033	1.300815
31	1	0	5.196130	-2.191303	1.558896
32	1	0	5.162724	-3.629213	0.524613
33	6	0	5.916612	-1.396940	-1.621103
34	6	0	6.327013	-2.700403	-2.320969
35	1	0	7.303168	-2.576437	-2.807756
36	1	0	5.606313	-2.988448	-3.094017
37	1	0	6.417493	-3.534840	-1.615764
38	6	0	7.011531	-0.988067	-0.625014
39	1	0	7.949356	-0.775645	-1.155493
40	1	0	7.214667	-1.783169	0.100235
41	1	0	6.729574	-0.087497	-0.067438
42	6	0	5.764510	-0.290607	-2.672501
43	1	0	6.689387	-0.191966	-3.256281
44	1	0	5.564072	0.677310	-2.200805
45	1	0	4.951300	-0.502296	-3.377229
46	6	0	3.011325	1.869861	0.790435
47	6	0	2.102660	2.544420	1.615051
48	6	0	4.167729	2.527188	0.371435
49	6	0	2.325457	3.870569	1.969776
50	1	0	1.227820	2.014861	1.989588
51	6	0	4.394168	3.854158	0.736742
52	1	0	4.885403	1.991516	-0.240723
53	6	0	3.468845	4.532514	1.523832
54	1	0	5.297732	4.356295	0.405003
55	6	0	2.283127	-0.461191	1.466352
56	6	0	1.384757	-1.514529	1.302490
57	6	0	2.964651	-0.339992	2.682940
58	6	0	1.146159	-2.411661	2.344538
59	1	0	0.835984	-1.635261	0.373251
60	6	0	2.736221	-1.239801	3.717403
61	1	0	3.684826	0.461860	2.817055
62	6	0	1.820195	-2.278064	3.552955
63	1	0	3.272783	-1.129351	4.654550
64	6	0	-2.500529	-0.238532	0.500008
65	6	0	-1.305115	0.473706	0.939205

66	8	0	-0.698781	0.337725	1.993079
67	6	0	-3.237865	0.344236	-0.675415
68	6	0	-4.622533	0.571338	-0.630806
69	6	0	-2.584296	0.640732	-1.888557
70	6	0	-5.310739	1.097523	-1.720746
71	1	0	-5.185895	0.344059	0.265543
72	6	0	-3.273073	1.167129	-2.976295
73	1	0	-1.534672	0.387278	-1.997682
74	6	0	-4.642442	1.408975	-2.899444
75	1	0	-6.380509	1.266804	-1.639936
76	1	0	-2.733823	1.376895	-3.895837
77	1	0	-5.179404	1.822177	-3.747592
78	6	0	-3.414841	-0.652361	1.662561
79	6	0	-2.807092	-1.206274	2.958606
80	1	0	-2.039902	-1.964240	2.789353
81	1	0	-2.347172	-0.417389	3.552363
82	1	0	-3.606794	-1.665463	3.546332
83	1	0	0.422334	-3.209909	2.203692
84	1	0	1.633637	-2.975780	4.363206
85	1	0	1.609958	4.385611	2.602911
86	1	0	3.643186	5.567043	1.801599
87	1	0	2.871395	-1.824001	-2.732673
88	1	0	3.322281	-3.420645	-2.124645
89	1	0	2.010775	-2.527408	-1.355910
90	6	0	-2.669831	-2.627838	-0.750216
91	6	0	-3.482078	-3.504184	-0.025664
92	6	0	-4.591821	-4.146057	-0.566633
93	6	0	-4.887362	-3.956760	-1.909289
94	6	0	-4.065047	-3.137455	-2.681568
95	6	0	-2.979181	-2.488851	-2.106941
96	1	0	-5.186925	-4.796900	0.063218
97	1	0	-5.740906	-4.458864	-2.351305
98	1	0	-4.274655	-3.001389	-3.737719
99	1	0	-2.329509	-1.849751	-2.692132
100	7	0	-3.168890	-3.863204	1.364866
101	6	0	-1.540511	-1.768009	-0.200443
102	8	0	-0.656574	-1.392732	-1.055013
103	1	0	-1.202857	-2.092310	0.795804
104	8	0	-2.004136	-4.090491	1.646711
105	8	0	-4.097459	-3.956935	2.149125
106	1	0	-4.016496	0.225534	1.940111
107	1	0	-4.136638	-1.378985	1.268047

TS2(RS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	5.098736	-0.947904	-0.397913
2	8	0	3.637187	-0.110226	-0.333503
3	7	0	-0.435393	2.900648	-0.641098
4	7	0	0.603846	3.206025	-1.476551
5	7	0	0.555776	1.057451	-0.978409
6	6	0	-1.645828	4.030258	1.148523
7	1	0	-1.238892	3.313141	1.852984
8	6	0	-2.501000	5.050794	1.554300
9	1	0	-2.776082	5.129612	2.600340
10	6	0	-2.986344	5.972570	0.630343
11	1	0	-3.649124	6.767066	0.956287
12	6	0	-2.616775	5.883973	-0.710796
13	1	0	-2.989613	6.605715	-1.429023
14	6	0	-1.774027	4.864666	-1.137090
15	1	0	-1.470065	4.775216	-2.174349
16	6	0	-1.312932	3.944708	-0.199495
17	6	0	-0.503864	1.590743	-0.359012
18	6	0	1.183546	2.057512	-1.667039
19	6	0	2.310364	1.508897	-2.479713
20	1	0	3.268408	1.732493	-2.005138
21	1	0	2.308233	1.912044	-3.492989
22	6	0	1.994617	-0.007978	-2.410491
23	1	0	2.886596	-0.621379	-2.516272
24	1	0	1.284092	-0.271448	-3.200046
25	6	0	1.305403	-0.216109	-1.044917
26	1	0	0.588249	-1.031444	-0.987942
27	6	0	2.335318	-0.369124	0.176647
28	6	0	5.188060	-1.940856	-1.993114
29	6	0	5.438926	-2.077834	1.056705
30	1	0	4.860084	-3.004010	1.003306
31	1	0	5.215573	-1.592091	2.010522
32	1	0	6.503749	-2.339109	1.052375
33	6	0	6.412504	0.422540	-0.431843
34	6	0	7.739639	-0.169296	-0.933487
35	1	0	8.534694	0.584714	-0.867255
36	1	0	7.673099	-0.488470	-1.979023
37	1	0	8.058029	-1.032449	-0.337037
38	6	0	6.623235	0.982944	0.983040
39	1	0	7.337744	1.816458	0.957164
40	1	0	7.028322	0.223471	1.660082

41	1	0	5.690685	1.356801	1.420773
42	6	0	5.996354	1.562550	-1.369038
43	1	0	6.811643	2.291057	-1.469412
44	1	0	5.124034	2.098122	-0.980655
45	1	0	5.752578	1.199743	-2.375459
46	6	0	2.045208	0.684628	1.249145
47	6	0	0.951406	0.563427	2.111372
48	6	0	2.819462	1.847433	1.296858
49	6	0	0.668964	1.577500	3.025150
50	1	0	0.295171	-0.299453	2.028226
51	6	0	2.528987	2.861479	2.206162
52	1	0	3.652817	1.955740	0.612783
53	6	0	1.455596	2.725808	3.081708
54	1	0	3.143416	3.756101	2.226563
55	6	0	2.263097	-1.813149	0.685562
56	6	0	2.202353	-2.852509	-0.248703
57	6	0	2.386735	-2.140108	2.034959
58	6	0	2.263532	-4.182194	0.150781
59	1	0	2.102574	-2.629640	-1.308297
60	6	0	2.435356	-3.472036	2.440967
61	1	0	2.459449	-1.354875	2.778610
62	6	0	2.377669	-4.497323	1.503385
63	1	0	2.526591	-3.704653	3.497145
64	6	0	-2.599730	0.121485	-0.632625
65	6	0	-1.751749	0.929369	0.269206
66	8	0	-1.915166	1.066902	1.460672
67	6	0	-4.078765	0.206329	-0.309532
68	6	0	-4.965022	-0.638073	-0.997992
69	6	0	-4.637855	1.125426	0.588977
70	6	0	-6.335550	-0.596125	-0.771917
71	1	0	-4.571493	-1.349861	-1.716333
72	6	0	-6.012654	1.171413	0.811788
73	1	0	-4.003422	1.817712	1.127712
74	6	0	-6.871544	0.308081	0.141990
75	1	0	-6.986278	-1.273938	-1.316451
76	1	0	-6.410413	1.895971	1.516300
77	1	0	-7.941286	0.342693	0.322039
78	6	0	-2.359633	0.305830	-2.139275
79	6	0	-2.909129	1.604036	-2.731171
80	1	0	-3.993060	1.656490	-2.599797
81	1	0	-2.483073	2.488895	-2.247491
82	1	0	-2.691476	1.668769	-3.801033
83	1	0	2.209727	-4.971140	-0.592574
84	1	0	2.416224	-5.534079	1.821555

85	1	0	-0.190048	1.469639	3.680089
86	1	0	1.228289	3.512449	3.794781
87	1	0	5.148082	-1.304506	-2.883498
88	1	0	6.131304	-2.495777	-2.026296
89	1	0	4.376331	-2.671438	-2.054217
90	6	0	-2.893147	-2.383629	0.374807
91	6	0	-3.555841	-3.462657	-0.212296
92	6	0	-4.482892	-4.253669	0.469968
93	6	0	-4.800204	-3.938380	1.778895
94	6	0	-4.154870	-2.866141	2.401570
95	6	0	-3.202047	-2.129197	1.717534
96	1	0	-4.944127	-5.088574	-0.043205
97	1	0	-5.539937	-4.524433	2.313070
98	1	0	-4.394907	-2.615183	3.429995
99	1	0	-2.668362	-1.313332	2.194283
100	7	0	-3.322208	-3.840678	-1.609545
101	6	0	-1.790457	-1.508094	-0.222549
102	8	0	-0.777313	-1.358596	0.573335
103	1	0	-1.571378	-1.782234	-1.269280
104	8	0	-3.071949	-2.961356	-2.423391
105	8	0	-3.409809	-5.021139	-1.901501
106	1	0	-1.289382	0.211811	-2.360898
107	1	0	-2.820239	-0.546061	-2.647380

M2(SS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-3.946179	1.876961	-0.225900
2	8	0	-3.735244	0.212054	-0.443632
3	7	0	1.334037	-2.469633	0.024908
4	7	0	0.669386	-3.230486	-0.901232
5	7	0	-0.343711	-1.306904	-0.523571
6	6	0	2.587500	-2.998443	2.035354
7	1	0	1.819195	-2.497533	2.615618
8	6	0	3.698435	-3.589449	2.630681
9	1	0	3.789937	-3.588456	3.711373
10	6	0	4.689795	-4.169017	1.843544
11	1	0	5.553068	-4.627700	2.314497
12	6	0	4.583906	-4.159000	0.451890
13	1	0	5.364153	-4.601044	-0.158484
14	6	0	3.478655	-3.579394	-0.159027

15	1	0	3.368017	-3.544140	-1.238742
16	6	0	2.501199	-3.007980	0.648694
17	6	0	0.788699	-1.262848	0.207430
18	6	0	-0.334868	-2.478784	-1.235007
19	6	0	-1.374489	-2.476210	-2.306184
20	1	0	-2.177384	-3.186728	-2.097941
21	1	0	-0.921390	-2.736274	-3.264831
22	6	0	-1.843184	-0.993828	-2.257486
23	1	0	-2.902812	-0.877475	-2.482181
24	1	0	-1.272089	-0.407650	-2.982990
25	6	0	-1.519006	-0.469472	-0.833060
26	1	0	-1.209934	0.573486	-0.821300
27	6	0	-2.768072	-0.655547	0.121450
28	6	0	-2.373325	2.841829	-0.589361
29	6	0	-4.571465	2.296923	1.490367
30	1	0	-3.778187	2.217735	2.239723
31	1	0	-5.383684	1.628533	1.789339
32	1	0	-4.953213	3.324106	1.502590
33	6	0	-5.269774	2.254645	-1.527924
34	6	0	-5.424280	3.773609	-1.687335
35	1	0	-6.226059	3.998499	-2.402702
36	1	0	-4.505874	4.236405	-2.064739
37	1	0	-5.684454	4.260906	-0.740387
38	6	0	-6.609385	1.649821	-1.085306
39	1	0	-7.372974	1.809215	-1.858035
40	1	0	-6.973854	2.108707	-0.159894
41	1	0	-6.524424	0.570351	-0.915577
42	6	0	-4.866982	1.643989	-2.876599
43	1	0	-5.602821	1.907511	-3.647942
44	1	0	-4.818782	0.552011	-2.816134
45	1	0	-3.889532	2.007160	-3.215928
46	6	0	-3.288542	-2.087907	-0.000633
47	6	0	-2.617534	-3.127205	0.653470
48	6	0	-4.392701	-2.387942	-0.798057
49	6	0	-3.008834	-4.448394	0.466055
50	1	0	-1.785818	-2.897828	1.315963
51	6	0	-4.792291	-3.711532	-0.976604
52	1	0	-4.929699	-1.577722	-1.279540
53	6	0	-4.093065	-4.745175	-0.358830
54	1	0	-5.651402	-3.934935	-1.601341
55	6	0	-2.569807	-0.318536	1.598930
56	6	0	-1.497529	0.424081	2.075399
57	6	0	-3.577205	-0.705870	2.496007
58	6	0	-1.407585	0.753509	3.429910

59	1	0	-0.715748	0.764888	1.413221
60	6	0	-3.505609	-0.352273	3.835270
61	1	0	-4.424919	-1.280926	2.134561
62	6	0	-2.412247	0.376101	4.310177
63	1	0	-4.297902	-0.652096	4.513971
64	6	0	2.850514	0.471170	0.043496
65	6	0	1.509827	-0.015883	0.852029
66	8	0	1.515816	0.010738	2.111541
67	6	0	3.268791	-0.303795	-1.194301
68	6	0	4.586140	-0.719597	-1.419444
69	6	0	2.329513	-0.589847	-2.197458
70	6	0	4.934697	-1.436280	-2.562754
71	1	0	5.361456	-0.479158	-0.702053
72	6	0	2.665554	-1.320438	-3.331477
73	1	0	1.312649	-0.217211	-2.094000
74	6	0	3.975207	-1.758998	-3.516684
75	1	0	5.966764	-1.742350	-2.704560
76	1	0	1.906318	-1.530387	-4.079530
77	1	0	4.246187	-2.324793	-4.402162
78	6	0	3.989167	0.789752	1.012133
79	6	0	4.555979	-0.393007	1.798108
80	1	0	3.609525	1.504230	1.744973
81	1	0	4.772747	1.307710	0.444182
82	1	0	5.479556	-0.098620	2.306473
83	1	0	3.826259	-0.697293	2.547870
84	1	0	4.777857	-1.265053	1.176163
85	1	0	-0.530640	1.288922	3.778796
86	1	0	-2.346249	0.635424	5.362218
87	1	0	-2.470357	-5.245754	0.967702
88	1	0	-4.399790	-5.775747	-0.505534
89	1	0	-2.047980	2.715536	-1.627839
90	1	0	-2.571530	3.907823	-0.433268
91	1	0	-1.536046	2.566742	0.061081
92	6	0	2.272101	3.024247	0.321538
93	6	0	3.176287	3.982784	-0.152320
94	6	0	3.387942	5.205390	0.479837
95	6	0	2.695176	5.491482	1.645770
96	6	0	1.796494	4.554382	2.153699
97	6	0	1.585075	3.348184	1.496368
98	1	0	4.094971	5.903686	0.050142
99	1	0	2.859066	6.434878	2.154340
100	1	0	1.254755	4.765624	3.070056
101	1	0	0.895465	2.609461	1.889136
102	7	0	3.970892	3.734254	-1.359976

103	6	0	1.972586	1.701340	-0.358244
104	8	0	0.768725	1.135161	0.125398
105	1	0	1.934849	1.852174	-1.441024
106	8	0	4.122651	2.577490	-1.720951
107	8	0	4.450084	4.694999	-1.937947

M2(RR)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	5.049714	-1.234231	0.400838
2	8	0	3.790805	-0.455270	-0.426198
3	7	0	-0.977272	2.584436	-0.972998
4	7	0	-0.023380	3.234805	-1.712926
5	7	0	0.586509	1.165103	-1.241568
6	6	0	-2.862845	3.036312	0.525727
7	1	0	-2.444397	2.338793	1.244357
8	6	0	-4.083400	3.672626	0.744530
9	1	0	-4.635773	3.443915	1.650692
10	6	0	-4.588090	4.576170	-0.184400
11	1	0	-5.539188	5.067092	-0.006430
12	6	0	-3.867673	4.854711	-1.346903
13	1	0	-4.252455	5.565452	-2.070512
14	6	0	-2.664536	4.208421	-1.597579
15	1	0	-2.104491	4.391913	-2.507071
16	6	0	-2.187161	3.292567	-0.660392
17	6	0	-0.640233	1.311183	-0.704554
18	6	0	0.910851	2.350303	-1.852466
19	6	0	2.232185	2.281550	-2.532432
20	1	0	2.973675	2.850508	-1.966183
21	1	0	2.183858	2.681424	-3.546015
22	6	0	2.499517	0.758485	-2.494784
23	1	0	3.554924	0.512799	-2.404396
24	1	0	2.114589	0.304396	-3.411408
25	6	0	1.698737	0.184403	-1.296266
26	1	0	1.281093	-0.799337	-1.505268
27	6	0	2.563969	0.090198	0.038512
28	6	0	4.924477	-3.083563	0.091711
29	6	0	5.025341	-0.880676	2.240812
30	1	0	4.183166	-1.377805	2.728588
31	1	0	4.958940	0.192269	2.446383

32	1	0	5.951925	-1.253987	2.691592
33	6	0	6.672160	-0.587417	-0.392541
34	6	0	7.684227	-1.743898	-0.477160
35	1	0	8.639816	-1.372257	-0.868927
36	1	0	7.339081	-2.541302	-1.142491
37	1	0	7.883974	-2.187615	0.505519
38	6	0	7.320437	0.525247	0.448026
39	1	0	8.232112	0.882655	-0.048711
40	1	0	7.608249	0.158727	1.438833
41	1	0	6.667141	1.389768	0.598496
42	6	0	6.413044	-0.074750	-1.816978
43	1	0	7.362982	0.192179	-2.298778
44	1	0	5.776045	0.815731	-1.825359
45	1	0	5.927070	-0.835338	-2.439807
46	6	0	2.779120	1.501569	0.592666
47	6	0	1.744641	2.225649	1.204589
48	6	0	4.004540	2.138315	0.388505
49	6	0	1.950266	3.544234	1.601622
50	1	0	0.770453	1.767853	1.377834
51	6	0	4.211943	3.454326	0.796327
52	1	0	4.795165	1.601111	-0.119033
53	6	0	3.181835	4.164812	1.404060
54	1	0	5.177583	3.921946	0.628448
55	6	0	1.923366	-0.917992	1.003515
56	6	0	1.796522	-2.232222	0.537629
57	6	0	1.488069	-0.630255	2.292856
58	6	0	1.210848	-3.221470	1.313347
59	1	0	2.161692	-2.482305	-0.456061
60	6	0	0.898600	-1.621570	3.077881
61	1	0	1.600493	0.362257	2.707784
62	6	0	0.746390	-2.913319	2.591689
63	1	0	0.553010	-1.370384	4.075365
64	6	0	-2.764979	-0.304358	-0.137158
65	6	0	-1.332829	0.332151	0.270456
66	8	0	-1.127165	0.786014	1.457946
67	6	0	-3.968933	0.030272	0.716415
68	6	0	-5.251166	0.145419	0.166205
69	6	0	-3.838551	0.179277	2.107209
70	6	0	-6.357813	0.431104	0.962984
71	1	0	-5.410837	0.001263	-0.896619
72	6	0	-4.941401	0.476965	2.899963
73	1	0	-2.855344	0.079451	2.550637
74	6	0	-6.207994	0.610318	2.332710
75	1	0	-7.339292	0.509651	0.505568

76	1	0	-4.811422	0.593753	3.971968
77	1	0	-7.068732	0.836062	2.954790
78	6	0	-3.039594	-0.322888	-1.651728
79	6	0	-3.471160	0.976851	-2.343744
80	1	0	-4.086127	1.613984	-1.703539
81	1	0	-2.613389	1.568000	-2.672884
82	1	0	-4.053156	0.740858	-3.239198
83	1	0	1.110586	-4.228789	0.919955
84	1	0	0.277349	-3.677798	3.203031
85	1	0	1.134698	4.086907	2.069464
86	1	0	3.334935	5.192351	1.717961
87	1	0	4.805507	-3.298497	-0.975803
88	1	0	5.830684	-3.590613	0.435701
89	1	0	4.074296	-3.514910	0.623710
90	6	0	-2.190168	-2.855963	-0.613879
91	6	0	-3.404823	-3.537433	-0.714053
92	6	0	-3.607698	-4.619640	-1.559287
93	6	0	-2.540701	-5.089510	-2.314882
94	6	0	-1.309488	-4.444561	-2.232044
95	6	0	-1.146122	-3.334942	-1.407240
96	1	0	-4.589559	-5.076222	-1.608772
97	1	0	-2.674643	-5.945157	-2.967191
98	1	0	-0.472379	-4.798272	-2.825328
99	1	0	-0.199376	-2.808525	-1.362320
100	7	0	-4.560753	-3.108384	0.085542
101	6	0	-1.991284	-1.617415	0.224110
102	8	0	-0.734415	-0.998053	-0.022962
103	1	0	-2.102533	-1.859054	1.287400
104	8	0	-5.641493	-3.057956	-0.477204
105	8	0	-4.371820	-2.852495	1.259294
106	1	0	-2.137708	-0.706833	-2.143688
107	1	0	-3.807975	-1.086048	-1.828871

M2(SR)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.765827	-1.336392	-0.095477
2	8	0	3.905280	0.092938	-0.346716
3	7	0	-1.329659	1.947688	-0.817637
4	7	0	-0.668451	2.264841	-1.976663
5	7	0	0.301149	0.594453	-0.906578

6	6	0	-2.689284	3.020507	0.895857
7	1	0	-1.994955	2.650883	1.646867
8	6	0	-3.818797	3.762596	1.231265
9	1	0	-4.007532	3.999346	2.273276
10	6	0	-4.694350	4.204267	0.242352
11	1	0	-5.570500	4.784141	0.513433
12	6	0	-4.444193	3.907132	-1.096181
13	1	0	-5.126410	4.248296	-1.867698
14	6	0	-3.329500	3.157320	-1.451354
15	1	0	-3.122666	2.898765	-2.483086
16	6	0	-2.475737	2.718502	-0.445770
17	6	0	-0.790024	0.899741	-0.183584
18	6	0	0.316357	1.423283	-1.999232
19	6	0	1.435743	1.088727	-2.923014
20	1	0	2.180966	1.885803	-2.926852
21	1	0	1.076676	0.941319	-3.942777
22	6	0	1.962721	-0.219732	-2.280862
23	1	0	3.035646	-0.338203	-2.399278
24	1	0	1.461968	-1.074046	-2.746034
25	6	0	1.550608	-0.187608	-0.783667
26	1	0	1.315319	-1.181049	-0.408060
27	6	0	2.640554	0.508912	0.145345
28	6	0	3.693079	-2.825987	-0.517472
29	6	0	5.440165	-1.501772	1.644212
30	1	0	4.649870	-1.726091	2.366244
31	1	0	5.931155	-0.578109	1.962792
32	1	0	6.178813	-2.310371	1.679377
33	6	0	6.194559	-1.153218	-1.328679
34	6	0	6.968114	-2.475563	-1.431816
35	1	0	7.828885	-2.356830	-2.102671
36	1	0	6.343642	-3.279424	-1.836734
37	1	0	7.354282	-2.803951	-0.460182
38	6	0	7.141957	-0.046376	-0.842643
39	1	0	7.943432	0.113907	-1.575717
40	1	0	7.613243	-0.307424	0.110764
41	1	0	6.613314	0.904341	-0.709795
42	6	0	5.663981	-0.775453	-2.717340
43	1	0	6.491784	-0.711028	-3.435737
44	1	0	5.161941	0.198139	-2.696670
45	1	0	4.955015	-1.519628	-3.100629
46	6	0	2.551620	2.028557	-0.020755
47	6	0	1.548979	2.738958	0.652914
48	6	0	3.437508	2.712689	-0.850463
49	6	0	1.405826	4.106301	0.444892

50	1	0	0.880333	2.213494	1.337920
51	6	0	3.298009	4.087171	-1.045431
52	1	0	4.232964	2.162037	-1.342629
53	6	0	2.275414	4.783869	-0.409531
54	1	0	3.992330	4.611581	-1.694747
55	6	0	2.573480	0.139038	1.634931
56	6	0	1.947136	-0.999032	2.136152
57	6	0	3.340049	0.919313	2.511979
58	6	0	2.068116	-1.340102	3.484063
59	1	0	1.315381	-1.614151	1.511787
60	6	0	3.466706	0.577945	3.851134
61	1	0	3.849516	1.800392	2.133186
62	6	0	2.826972	-0.558161	4.345356
63	1	0	4.066391	1.198429	4.509483
64	6	0	-2.732042	-0.420689	1.141421
65	6	0	-1.229700	0.205337	1.127207
66	8	0	-0.791610	0.874715	2.120935
67	6	0	-3.624800	-0.109445	-0.050394
68	6	0	-4.898091	0.456501	0.093348
69	6	0	-3.190867	-0.376818	-1.360178
70	6	0	-5.706872	0.715825	-1.010466
71	1	0	-5.270383	0.716115	1.076649
72	6	0	-3.991166	-0.114701	-2.465892
73	1	0	-2.205453	-0.806648	-1.522362
74	6	0	-5.263464	0.425884	-2.295679
75	1	0	-6.688266	1.154485	-0.858399
76	1	0	-3.620673	-0.341557	-3.461043
77	1	0	-5.896011	0.625148	-3.154974
78	6	0	-3.392726	-0.111068	2.493647
79	6	0	-2.746483	-0.737859	3.730237
80	1	0	-2.984374	-1.803288	3.804509
81	1	0	-1.664144	-0.598074	3.719061
82	1	0	-3.143625	-0.258490	4.629534
83	1	0	1.553955	-2.220918	3.855578
84	1	0	2.916796	-0.825235	5.393529
85	1	0	0.613941	4.643959	0.957339
86	1	0	2.162331	5.851590	-0.568393
87	1	0	3.264350	-2.758005	-1.523240
88	1	0	4.291804	-3.741473	-0.470578
89	1	0	2.875139	-2.938586	0.200923
90	6	0	-2.261295	-2.813084	-0.013550
91	6	0	-3.508101	-3.371433	-0.312757
92	6	0	-3.713789	-4.267659	-1.354987
93	6	0	-2.631581	-4.671829	-2.123509

94	6	0	-1.368479	-4.158024	-1.840725
95	6	0	-1.194451	-3.239810	-0.810356
96	1	0	-4.716057	-4.633673	-1.540734
97	1	0	-2.774197	-5.381990	-2.930023
98	1	0	-0.511677	-4.468461	-2.430433
99	1	0	-0.214605	-2.820994	-0.609911
100	7	0	-4.689825	-3.016236	0.478252
101	6	0	-1.994787	-1.796044	1.078910
102	8	0	-0.708928	-1.205274	0.941152
103	1	0	-2.073506	-2.323639	2.033692
104	8	0	-4.512305	-2.693089	1.641774
105	8	0	-5.780375	-3.089125	-0.057223
106	1	0	-3.382058	0.979770	2.601431
107	1	0	-4.437096	-0.429133	2.464102

M2(RS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-4.859470	0.652880	-0.430732
2	8	0	-3.567840	-0.419302	-0.282872
3	7	0	1.368390	-2.981897	-0.465103
4	7	0	0.401073	-3.759564	-1.052245
5	7	0	-0.229437	-1.654227	-0.896864
6	6	0	3.123372	-3.504016	1.177972
7	1	0	2.639240	-2.839233	1.881562
8	6	0	4.296666	-4.190461	1.481713
9	1	0	4.725698	-4.091058	2.473014
10	6	0	4.912181	-5.001844	0.532321
11	1	0	5.824190	-5.533645	0.782586
12	6	0	4.356227	-5.136292	-0.738428
13	1	0	4.828854	-5.771255	-1.479825
14	6	0	3.190348	-4.452882	-1.062379
15	1	0	2.735137	-4.546863	-2.042462
16	6	0	2.598333	-3.635060	-0.102835
17	6	0	1.010090	-1.691692	-0.374407
18	6	0	-0.556213	-2.919954	-1.298498
19	6	0	-1.895659	-2.948174	-1.952196
20	1	0	-2.647360	-3.308515	-1.243967
21	1	0	-1.910548	-3.582384	-2.838474
22	6	0	-2.074835	-1.445246	-2.264740
23	1	0	-3.117256	-1.147273	-2.330838

24	1	0	-1.578573	-1.218666	-3.213184
25	6	0	-1.322421	-0.683823	-1.143064
26	1	0	-0.873450	0.232076	-1.517302
27	6	0	-2.220535	-0.355515	0.148185
28	6	0	-4.698319	1.685585	-1.993722
29	6	0	-5.102908	1.762115	1.058821
30	1	0	-4.394555	2.595426	1.069477
31	1	0	-4.986194	1.204821	1.992837
32	1	0	-6.117858	2.175515	1.036927
33	6	0	-6.329633	-0.536858	-0.598066
34	6	0	-7.560022	0.216906	-1.123391
35	1	0	-8.433498	-0.447886	-1.133165
36	1	0	-7.408896	0.577302	-2.146203
37	1	0	-7.814259	1.079343	-0.495623
38	6	0	-6.662975	-1.132101	0.777732
39	1	0	-7.456190	-1.885548	0.683792
40	1	0	-7.019133	-0.362586	1.471307
41	1	0	-5.794139	-1.615801	1.237184
42	6	0	-5.985557	-1.668376	-1.575825
43	1	0	-6.842707	-2.344164	-1.694959
44	1	0	-5.134599	-2.260476	-1.222097
45	1	0	-5.734073	-1.278740	-2.570201
46	6	0	-2.014069	-1.455144	1.199204
47	6	0	-0.859219	-1.496685	1.992202
48	6	0	-2.943350	-2.489784	1.317343
49	6	0	-0.639159	-2.558869	2.862644
50	1	0	-0.118027	-0.705342	1.933268
51	6	0	-2.725525	-3.548691	2.198814
52	1	0	-3.841562	-2.464325	0.710605
53	6	0	-1.569833	-3.590760	2.970710
54	1	0	-3.463636	-4.340895	2.276819
55	6	0	-1.940595	1.062043	0.674240
56	6	0	-1.781546	2.122394	-0.226022
57	6	0	-1.961118	1.356866	2.037364
58	6	0	-1.602367	3.428346	0.218474
59	1	0	-1.793420	1.942802	-1.297550
60	6	0	-1.773689	2.662307	2.488144
61	1	0	-2.117133	0.565288	2.761088
62	6	0	-1.584076	3.702315	1.584954
63	1	0	-1.775684	2.862132	3.555031
64	6	0	2.543486	0.454542	-0.804404
65	6	0	1.792994	-0.490719	0.264127
66	8	0	2.317949	-0.789491	1.385154
67	6	0	3.973849	0.802193	-0.474428

68	6	0	4.499752	2.028105	-0.896786
69	6	0	4.828009	-0.118786	0.140655
70	6	0	5.840865	2.338914	-0.691973
71	1	0	3.849744	2.738755	-1.401548
72	6	0	6.170550	0.193125	0.343179
73	1	0	4.427698	-1.068411	0.476048
74	6	0	6.681525	1.421674	-0.066267
75	1	0	6.228842	3.296486	-1.025897
76	1	0	6.820587	-0.531519	0.824647
77	1	0	7.727957	1.660862	0.096702
78	6	0	2.423024	0.050457	-2.283393
79	6	0	3.368263	-1.065830	-2.716454
80	1	0	4.407723	-0.732478	-2.671259
81	1	0	3.284723	-1.942603	-2.066919
82	1	0	3.152890	-1.380662	-3.741021
83	1	0	-1.454393	4.228063	-0.502324
84	1	0	-1.420706	4.715611	1.937665
85	1	0	0.268474	-2.569852	3.458079
86	1	0	-1.395696	-4.417220	3.652253
87	1	0	-4.448164	1.071997	-2.865420
88	1	0	-5.648645	2.187620	-2.202645
89	1	0	-3.936720	2.461670	-1.889963
90	6	0	1.741489	2.703340	0.379821
91	6	0	1.647027	4.025458	-0.058582
92	6	0	1.794983	5.122805	0.785880
93	6	0	2.095579	4.900441	2.120150
94	6	0	2.221374	3.590889	2.587583
95	6	0	2.031877	2.511141	1.734909
96	1	0	1.681962	6.120845	0.380203
97	1	0	2.234082	5.741236	2.790930
98	1	0	2.459905	3.411259	3.630948
99	1	0	2.097484	1.485603	2.091297
100	7	0	1.355689	4.325934	-1.460337
101	6	0	1.423509	1.485378	-0.458246
102	8	0	0.710921	0.541534	0.326236
103	1	0	0.847047	1.775295	-1.343464
104	8	0	1.787819	3.568026	-2.318111
105	8	0	0.705267	5.328198	-1.707690
106	1	0	1.380953	-0.233996	-2.491938
107	1	0	2.613046	0.948942	-2.883883

TS3(SS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-4.171890	1.221249	-0.322595
2	8	0	-3.645502	-0.381132	-0.378534
3	7	0	1.699231	-2.354186	-0.029992
4	7	0	1.143995	-3.182544	-0.980470
5	7	0	-0.076990	-1.392769	-0.584881
6	6	0	3.356634	-2.130280	1.732503
7	1	0	2.689155	-1.451844	2.256264
8	6	0	4.616157	-2.437727	2.238196
9	1	0	4.927018	-2.001764	3.182392
10	6	0	5.470039	-3.292759	1.546190
11	1	0	6.449584	-3.527298	1.949916
12	6	0	5.059306	-3.851467	0.337933
13	1	0	5.719614	-4.517117	-0.208556
14	6	0	3.807293	-3.553030	-0.186385
15	1	0	3.477001	-3.963997	-1.132082
16	6	0	2.972521	-2.687984	0.515897
17	6	0	1.013914	-1.215892	0.199522
18	6	0	0.058728	-2.553818	-1.304796
19	6	0	-1.034700	-2.712182	-2.306309
20	1	0	-1.719404	-3.512674	-2.014000
21	1	0	-0.632317	-2.943716	-3.294150
22	6	0	-1.694330	-1.307145	-2.246136
23	1	0	-2.772485	-1.338555	-2.400524
24	1	0	-1.256616	-0.667608	-3.018020
25	6	0	-1.350628	-0.710214	-0.855265
26	1	0	-1.175330	0.364823	-0.896061
27	6	0	-2.502558	-1.005718	0.182532
28	6	0	-2.862759	2.400419	-0.974832
29	6	0	-4.744999	1.719671	1.390432
30	1	0	-3.901610	1.909964	2.060322
31	1	0	-5.357014	0.929625	1.835207
32	1	0	-5.351209	2.630554	1.333404
33	6	0	-5.648114	1.174018	-1.514833
34	6	0	-6.098644	2.604967	-1.840269
35	1	0	-6.995888	2.586149	-2.472780
36	1	0	-5.324019	3.158363	-2.382128
37	1	0	-6.348024	3.172450	-0.936002
38	6	0	-6.809069	0.410347	-0.863082
39	1	0	-7.645304	0.314193	-1.568439
40	1	0	-7.183097	0.928427	0.026315
41	1	0	-6.506114	-0.599079	-0.562143

42	6	0	-5.250562	0.462220	-2.814504
43	1	0	-6.084073	0.479991	-3.529474
44	1	0	-4.990671	-0.584166	-2.624147
45	1	0	-4.390611	0.941836	-3.297707
46	6	0	-2.768178	-2.510472	0.218002
47	6	0	-1.876285	-3.362872	0.878002
48	6	0	-3.862083	-3.060833	-0.450210
49	6	0	-2.046328	-4.742129	0.824015
50	1	0	-1.043895	-2.941389	1.437276
51	6	0	-4.039330	-4.442876	-0.494147
52	1	0	-4.567848	-2.397559	-0.938189
53	6	0	-3.125082	-5.287362	0.129498
54	1	0	-4.893858	-4.859186	-1.018600
55	6	0	-2.274208	-0.466195	1.595286
56	6	0	-1.428633	0.606493	1.855770
57	6	0	-3.065593	-0.967427	2.638850
58	6	0	-1.347462	1.163157	3.133025
59	1	0	-0.822718	1.041050	1.075141
60	6	0	-2.999764	-0.407117	3.907327
61	1	0	-3.744415	-1.793476	2.448443
62	6	0	-2.135310	0.660326	4.160088
63	1	0	-3.623478	-0.803678	4.702545
64	6	0	2.984264	0.977233	-0.068395
65	6	0	1.731789	0.581375	0.853113
66	8	0	1.678245	0.606538	2.061990
67	6	0	3.656689	0.001048	-1.024456
68	6	0	5.035633	-0.238876	-0.991858
69	6	0	2.923432	-0.638758	-2.037164
70	6	0	5.646709	-1.098827	-1.902096
71	1	0	5.658528	0.259046	-0.260556
72	6	0	3.526146	-1.502230	-2.943749
73	1	0	1.852061	-0.474055	-2.122667
74	6	0	4.896800	-1.740326	-2.880110
75	1	0	6.718075	-1.262414	-1.840405
76	1	0	2.920175	-1.987285	-3.703051
77	1	0	5.371277	-2.412562	-3.587944
78	6	0	3.957730	1.804800	0.789843
79	6	0	4.640248	1.078524	1.953808
80	1	0	3.393608	2.635948	1.221293
81	1	0	4.703545	2.249653	0.118170
82	1	0	5.358278	1.754524	2.427380
83	1	0	3.893792	0.791552	2.694953
84	1	0	5.173405	0.176514	1.650486
85	1	0	-0.659526	1.987081	3.293818

86	1	0	-2.078577	1.091053	5.155004
87	1	0	-1.336848	-5.390711	1.327573
88	1	0	-3.258609	-6.363587	0.087707
89	1	0	-2.572613	2.143333	-1.999890
90	1	0	-3.269499	3.417464	-0.990630
91	1	0	-1.962498	2.431358	-0.353460
92	6	0	2.064134	3.349823	-0.820141
93	6	0	1.437640	4.229655	0.057028
94	6	0	1.550827	5.610462	-0.050915
95	6	0	2.350214	6.145717	-1.052342
96	6	0	3.010343	5.293878	-1.935962
97	6	0	2.853676	3.918418	-1.824742
98	1	0	1.021275	6.246685	0.650285
99	1	0	2.453262	7.221267	-1.142783
100	1	0	3.636092	5.703351	-2.721627
101	1	0	3.345406	3.254284	-2.531461
102	7	0	0.626033	3.754406	1.196455
103	6	0	1.909467	1.851419	-0.798980
104	8	0	0.850005	1.406711	0.039002
105	1	0	1.754418	1.534439	-1.835138
106	8	0	1.228862	3.394447	2.186293
107	8	0	-0.584248	3.829710	1.094520

TS3(RR)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.722519	-1.508461	0.428117
2	8	0	3.907260	-0.077026	0.075396
3	7	0	-0.862190	2.178386	-1.462137
4	7	0	0.065793	2.464310	-2.443518
5	7	0	0.580398	0.676285	-1.255743
6	6	0	-2.176315	3.422696	0.141950
7	1	0	-1.635103	2.909815	0.933514
8	6	0	-3.174233	4.352650	0.420312
9	1	0	-3.408934	4.591351	1.452676
10	6	0	-3.865136	4.973638	-0.618325
11	1	0	-4.641034	5.698991	-0.397263
12	6	0	-3.557917	4.667137	-1.943201
13	1	0	-4.094163	5.152268	-2.751854
14	6	0	-2.566247	3.737199	-2.238206
15	1	0	-2.308475	3.486273	-3.261223

16	6	0	-1.894290	3.120598	-1.188727
17	6	0	-0.605134	1.077641	-0.734295
18	6	0	0.933464	1.516604	-2.285838
19	6	0	2.199984	1.080977	-2.939296
20	1	0	3.000076	1.796047	-2.737693
21	1	0	2.085930	0.986959	-4.020542
22	6	0	2.434525	-0.283732	-2.242967
23	1	0	3.489177	-0.509624	-2.117208
24	1	0	1.978122	-1.077847	-2.842416
25	6	0	1.683736	-0.229418	-0.884978
26	1	0	1.277022	-1.205164	-0.621878
27	6	0	2.572047	0.340019	0.311393
28	6	0	3.828117	-2.978668	-0.331122
29	6	0	4.982285	-1.784707	2.263096
30	1	0	4.060509	-2.093114	2.764016
31	1	0	5.339844	-0.873695	2.750977
32	1	0	5.732894	-2.568275	2.414722
33	6	0	6.395524	-1.222230	-0.419796
34	6	0	7.215579	-2.520262	-0.402902
35	1	0	8.200391	-2.351202	-0.857544
36	1	0	6.723100	-3.318186	-0.969695
37	1	0	7.385176	-2.884764	0.616477
38	6	0	7.160078	-0.125897	0.335900
39	1	0	8.110796	0.091423	-0.168664
40	1	0	7.392379	-0.430129	1.362044
41	1	0	6.582605	0.804218	0.382009
42	6	0	6.196005	-0.777484	-1.874192
43	1	0	7.168170	-0.638881	-2.365425
44	1	0	5.655347	0.173973	-1.929526
45	1	0	5.639105	-1.522499	-2.455697
46	6	0	2.559876	1.872448	0.265041
47	6	0	1.475326	2.585010	0.794190
48	6	0	3.607292	2.572988	-0.330366
49	6	0	1.422407	3.969499	0.674433
50	1	0	0.675936	2.048305	1.306041
51	6	0	3.556310	3.962770	-0.439960
52	1	0	4.463020	2.022046	-0.707730
53	6	0	2.459209	4.662564	0.049686
54	1	0	4.377973	4.495011	-0.909107
55	6	0	2.164886	-0.160101	1.707235
56	6	0	1.483946	-1.353537	1.939245
57	6	0	2.666527	0.540296	2.813449
58	6	0	1.288628	-1.824205	3.238145
59	1	0	1.059746	-1.928636	1.128640

60	6	0	2.479463	0.071629	4.106528
61	1	0	3.219045	1.461183	2.654388
62	6	0	1.784724	-1.116810	4.325474
63	1	0	2.878300	0.634000	4.944875
64	6	0	-3.008807	-0.359911	0.303587
65	6	0	-1.574673	0.121605	0.791943
66	8	0	-1.280181	0.754732	1.790147
67	6	0	-4.035565	-0.272290	1.414171
68	6	0	-4.943969	-1.308773	1.640651
69	6	0	-4.162293	0.902786	2.162552
70	6	0	-5.950115	-1.181323	2.596019
71	1	0	-4.875517	-2.232052	1.073636
72	6	0	-5.164422	1.029895	3.118310
73	1	0	-3.456526	1.708906	2.000466
74	6	0	-6.063110	-0.011243	3.339614
75	1	0	-6.643094	-2.001035	2.756757
76	1	0	-5.241579	1.947025	3.694442
77	1	0	-6.843456	0.088960	4.087368
78	6	0	-3.618582	0.118875	-1.034207
79	6	0	-4.672274	1.223921	-0.962131
80	1	0	-5.567946	0.870609	-0.445109
81	1	0	-4.319058	2.115889	-0.442640
82	1	0	-4.956327	1.517325	-1.976803
83	1	0	0.739076	-2.747389	3.390913
84	1	0	1.630208	-1.484095	5.334982
85	1	0	0.571384	4.510345	1.077491
86	1	0	2.414920	5.743091	-0.041622
87	1	0	3.758328	-2.903454	-1.421129
88	1	0	4.361983	-3.904067	-0.091885
89	1	0	2.815751	-3.075579	0.071819
90	6	0	-2.260929	-2.473067	-1.124238
91	6	0	-3.119843	-3.516257	-1.488571
92	6	0	-3.134743	-4.087110	-2.757482
93	6	0	-2.235247	-3.639997	-3.713729
94	6	0	-1.358827	-2.608254	-3.388420
95	6	0	-1.385256	-2.035351	-2.122549
96	1	0	-3.844576	-4.878061	-2.968212
97	1	0	-2.225075	-4.088145	-4.700775
98	1	0	-0.657446	-2.236455	-4.128553
99	1	0	-0.731933	-1.202935	-1.892955
100	7	0	-4.082786	-4.096214	-0.538937
101	6	0	-2.279113	-1.749286	0.205573
102	8	0	-1.009436	-1.166216	0.511625
103	1	0	-2.577963	-2.421656	1.008816

104	8	0	-5.184543	-4.385540	-0.968072
105	8	0	-3.723944	-4.273775	0.612891
106	1	0	-2.814123	0.401751	-1.721968
107	1	0	-4.098393	-0.758339	-1.487129

TS(SR)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-4.262533	1.451815	0.680807
2	8	0	-3.750954	0.166495	-0.283418
3	7	0	1.484862	-2.066381	-0.537176
4	7	0	1.049060	-2.211392	-1.836317
5	7	0	-0.194107	-0.821222	-0.669163
6	6	0	2.950831	-2.856254	1.234887
7	1	0	2.263274	-2.451236	1.971868
8	6	0	4.138962	-3.466598	1.622685
9	1	0	4.370942	-3.547550	2.679833
10	6	0	5.017510	-3.979980	0.670208
11	1	0	5.939953	-4.458791	0.982169
12	6	0	4.702639	-3.883467	-0.682300
13	1	0	5.381974	-4.280425	-1.429644
14	6	0	3.526679	-3.263169	-1.091473
15	1	0	3.282179	-3.150347	-2.140192
16	6	0	2.669150	-2.746311	-0.126075
17	6	0	0.791224	-1.170416	0.192885
18	6	0	0.026785	-1.417127	-1.884977
19	6	0	-0.908293	-0.896595	-2.926265
20	1	0	-1.632238	-1.657440	-3.228503
21	1	0	-0.359307	-0.569557	-3.811237
22	6	0	-1.565711	0.290713	-2.164697
23	1	0	-2.609299	0.447741	-2.437629
24	1	0	-1.008237	1.208867	-2.377282
25	6	0	-1.425919	-0.025288	-0.653706
26	1	0	-1.267942	0.866640	-0.050156
27	6	0	-2.702838	-0.772308	-0.107495
28	6	0	-2.869071	2.679680	0.980582
29	6	0	-4.993684	0.896775	2.314522
30	1	0	-4.220405	0.551607	3.007411
31	1	0	-5.705011	0.078294	2.172713
32	1	0	-5.525094	1.732686	2.782906
33	6	0	-5.594947	2.230683	-0.418285

34	6	0	-6.004023	3.600335	0.141286
35	1	0	-6.816697	4.027708	-0.460514
36	1	0	-5.170294	4.310785	0.121129
37	1	0	-6.364048	3.531508	1.174377
38	6	0	-6.821169	1.307349	-0.455235
39	1	0	-7.579075	1.707163	-1.141606
40	1	0	-7.284808	1.213659	0.532600
41	1	0	-6.554174	0.301327	-0.798433
42	6	0	-5.059385	2.408322	-1.845343
43	1	0	-5.809763	2.905643	-2.474068
44	1	0	-4.824305	1.441158	-2.301210
45	1	0	-4.150596	3.022216	-1.868872
46	6	0	-3.007991	-1.979050	-0.993933
47	6	0	-2.235892	-3.140860	-0.887486
48	6	0	-4.014868	-1.919101	-1.957473
49	6	0	-2.434539	-4.202129	-1.764702
50	1	0	-1.472606	-3.213326	-0.115777
51	6	0	-4.221911	-2.987485	-2.828241
52	1	0	-4.629255	-1.027733	-2.021267
53	6	0	-3.423956	-4.125125	-2.743821
54	1	0	-5.007359	-2.927285	-3.575156
55	6	0	-2.633971	-1.196448	1.357520
56	6	0	-1.735707	-0.636566	2.258728
57	6	0	-3.595928	-2.099194	1.832890
58	6	0	-1.775169	-0.982692	3.610397
59	1	0	-0.990989	0.078275	1.938193
60	6	0	-3.652890	-2.426632	3.180342
61	1	0	-4.307493	-2.536772	1.138560
62	6	0	-2.736576	-1.870326	4.075671
63	1	0	-4.407734	-3.121445	3.534946
64	6	0	2.837112	0.646751	1.292502
65	6	0	1.456518	-0.038791	1.716141
66	8	0	1.264026	-0.626079	2.767223
67	6	0	3.541961	0.257057	-0.000050
68	6	0	4.856892	-0.227406	-0.001315
69	6	0	2.908748	0.384633	-1.245949
70	6	0	5.515689	-0.536692	-1.187746
71	1	0	5.382476	-0.387245	0.931199
72	6	0	3.558025	0.065551	-2.433342
73	1	0	1.881381	0.733752	-1.296858
74	6	0	4.874551	-0.385051	-2.411907
75	1	0	6.534637	-0.908428	-1.146819
76	1	0	3.030636	0.175775	-3.376011
77	1	0	5.389328	-0.623915	-3.337084

78	6	0	3.776028	0.591311	2.514232
79	6	0	3.325881	1.341292	3.767085
80	1	0	3.448716	2.421513	3.644170
81	1	0	2.287452	1.120759	4.021431
82	1	0	3.950273	1.041164	4.612725
83	1	0	-1.032196	-0.560325	4.277629
84	1	0	-2.771177	-2.138302	5.127020
85	1	0	-1.816999	-5.090564	-1.681735
86	1	0	-3.579337	-4.952991	-3.428075
87	1	0	-2.489725	3.083914	0.034782
88	1	0	-3.243494	3.521661	1.572477
89	1	0	-2.031383	2.241169	1.534465
90	6	0	1.863204	2.814267	-0.010118
91	6	0	2.962830	3.408171	-0.634693
92	6	0	2.861014	4.173567	-1.789557
93	6	0	1.607067	4.407998	-2.337114
94	6	0	0.482916	3.862778	-1.721325
95	6	0	0.616423	3.072982	-0.583476
96	1	0	3.764703	4.571974	-2.234564
97	1	0	1.511434	5.014217	-3.230800
98	1	0	-0.506267	4.046925	-2.130350
99	1	0	-0.256696	2.639362	-0.112325
100	7	0	4.307782	3.228754	-0.083343
101	6	0	1.931581	1.925272	1.209543
102	8	0	0.721108	1.171386	1.390795
103	1	0	2.098576	2.565672	2.079136
104	8	0	4.400567	3.089688	1.126372
105	8	0	5.250338	3.254793	-0.850745
106	1	0	3.899587	-0.472477	2.751569
107	1	0	4.753378	0.982488	2.227683

TS3(RS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.815310	-0.868920	-0.348722
2	8	0	3.550142	0.238260	-0.276837
3	7	0	-1.019019	3.260548	-0.590954
4	7	0	0.046880	3.893222	-1.199682
5	7	0	0.371176	1.732989	-0.932444
6	6	0	-2.917574	3.706740	0.867289
7	1	0	-2.640600	2.845155	1.465113

8	6	0	-4.039360	4.471713	1.174570
9	1	0	-4.641606	4.204537	2.036792
10	6	0	-4.379220	5.576553	0.398167
11	1	0	-5.251203	6.171446	0.648715
12	6	0	-3.592319	5.918279	-0.699651
13	1	0	-3.849463	6.779293	-1.307621
14	6	0	-2.476904	5.156253	-1.031318
15	1	0	-1.857195	5.405345	-1.884497
16	6	0	-2.154843	4.052593	-0.244501
17	6	0	-0.869969	1.927787	-0.422465
18	6	0	0.877525	2.920685	-1.394029
19	6	0	2.198769	2.717469	-2.056031
20	1	0	3.009976	2.969355	-1.366095
21	1	0	2.308106	3.312491	-2.962853
22	6	0	2.133435	1.195038	-2.318424
23	1	0	3.113959	0.735096	-2.405867
24	1	0	1.571067	1.016481	-3.240000
25	6	0	1.309839	0.616947	-1.140758
26	1	0	0.732757	-0.251977	-1.445167
27	6	0	2.197566	0.240712	0.147180
28	6	0	4.699909	-1.930528	-1.897111
29	6	0	4.956301	-1.963353	1.166396
30	1	0	4.234581	-2.785017	1.142526
31	1	0	4.791616	-1.392218	2.084905
32	1	0	5.963717	-2.392978	1.210161
33	6	0	6.334417	0.262671	-0.474292
34	6	0	7.547760	-0.540613	-0.964732
35	1	0	8.446367	0.089726	-0.953163
36	1	0	7.409669	-0.899713	-1.989842
37	1	0	7.750835	-1.409254	-0.326955
38	6	0	6.655538	0.848198	0.908617
39	1	0	7.479915	1.569704	0.833365
40	1	0	6.964082	0.066967	1.611916
41	1	0	5.796200	1.366865	1.347136
42	6	0	6.061135	1.403071	-1.464329
43	1	0	6.945107	2.047734	-1.557274
44	1	0	5.220705	2.024906	-1.138977
45	1	0	5.825525	1.021179	-2.465569
46	6	0	2.046822	1.337103	1.210104
47	6	0	0.897575	1.428977	2.004999
48	6	0	3.019214	2.331371	1.331133
49	6	0	0.723725	2.493309	2.882552
50	1	0	0.124716	0.672335	1.940361
51	6	0	2.849684	3.393375	2.219333

52	1	0	3.913213	2.273508	0.720684
53	6	0	1.698822	3.482501	2.994366
54	1	0	3.621052	4.153165	2.298460
55	6	0	1.837206	-1.169201	0.644696
56	6	0	1.657869	-2.198531	-0.288341
57	6	0	1.797209	-1.498093	1.999645
58	6	0	1.414281	-3.507742	0.115639
59	1	0	1.715742	-1.988681	-1.353442
60	6	0	1.542200	-2.805668	2.409310
61	1	0	1.963222	-0.732025	2.748205
62	6	0	1.342614	-3.814887	1.472834
63	1	0	1.500547	-3.032331	3.470085
64	6	0	-2.727685	-0.372171	-0.650330
65	6	0	-1.953826	0.387947	0.485204
66	8	0	-2.350726	0.803767	1.562091
67	6	0	-4.144623	-0.768068	-0.302894
68	6	0	-4.687318	-1.936077	-0.849400
69	6	0	-4.965899	0.062903	0.464066
70	6	0	-6.013837	-2.281779	-0.613006
71	1	0	-4.063799	-2.572431	-1.472441
72	6	0	-6.295332	-0.283621	0.696845
73	1	0	-4.556807	0.976180	0.880617
74	6	0	-6.822758	-1.456696	0.165610
75	1	0	-6.416939	-3.194633	-1.040449
76	1	0	-6.921134	0.370116	1.296656
77	1	0	-7.858257	-1.723959	0.351828
78	6	0	-2.668771	0.210758	-2.068253
79	6	0	-3.591398	1.407378	-2.276604
80	1	0	-4.639753	1.100769	-2.245272
81	1	0	-3.445964	2.162397	-1.497895
82	1	0	-3.401650	1.877530	-3.245050
83	1	0	1.260211	-4.282809	-0.630445
84	1	0	1.126305	-4.829488	1.792524
85	1	0	-0.183766	2.542814	3.476333
86	1	0	1.561983	4.312733	3.679789
87	1	0	4.591399	-1.326000	-2.803657
88	1	0	5.617512	-2.519333	-2.000478
89	1	0	3.865357	-2.633543	-1.849420
90	6	0	-1.882445	-2.709125	0.289363
91	6	0	-1.833543	-3.983750	-0.278525
92	6	0	-1.991880	-5.153862	0.458811
93	6	0	-2.254114	-5.057556	1.816559
94	6	0	-2.331251	-3.799223	2.413338
95	6	0	-2.133958	-2.646712	1.663884

96	1	0	-1.915676	-6.110175	-0.044302
97	1	0	-2.399733	-5.957504	2.403690
98	1	0	-2.537305	-3.715640	3.475291
99	1	0	-2.160086	-1.670449	2.138253
100	7	0	-1.580462	-4.148857	-1.709964
101	6	0	-1.581759	-1.423896	-0.444568
102	8	0	-0.874567	-0.536915	0.431198
103	1	0	-1.008715	-1.609918	-1.355760
104	8	0	-1.991717	-3.285388	-2.473327
105	8	0	-0.981359	-5.146845	-2.071705
106	1	0	-1.630996	0.482415	-2.295639
107	1	0	-2.936356	-0.598705	-2.758904

M01'(Re)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	3.906982	-1.374496	-0.074684
2	8	0	3.204380	0.154893	-0.146623
3	7	0	-2.385228	1.268677	-0.224270
4	7	0	-2.021017	2.022641	-1.328186
5	7	0	-0.428978	0.694454	-0.600820
6	6	0	-3.995925	0.908589	1.554816
7	1	0	-3.177662	0.576403	2.184422
8	6	0	-5.309885	0.912758	2.007980
9	1	0	-5.525299	0.576856	3.017219
10	6	0	-6.341372	1.351434	1.178835
11	1	0	-7.364968	1.357949	1.538633
12	6	0	-6.048925	1.792650	-0.109016
13	1	0	-6.845666	2.140687	-0.758914
14	6	0	-4.739340	1.783919	-0.581247
15	1	0	-4.497800	2.109093	-1.586145
16	6	0	-3.720572	1.333325	0.254030
17	6	0	-1.443384	0.419165	0.261921
18	6	0	-0.799572	1.639404	-1.522863
19	6	0	0.315413	1.944775	-2.464409
20	1	0	0.783638	2.894269	-2.182192
21	1	0	-0.019727	2.014784	-3.499846
22	6	0	1.261163	0.740852	-2.215738
23	1	0	2.314462	1.014811	-2.282250
24	1	0	1.060221	-0.039083	-2.953525
25	6	0	0.922132	0.177544	-0.809796

26	1	0	0.884868	-0.913321	-0.841165
27	6	0	1.937516	0.619641	0.286862
28	6	0	2.805932	-2.690415	-0.842907
29	1	0	1.897426	-2.863425	-0.257343
30	1	0	3.351956	-3.639126	-0.883882
31	1	0	2.503370	-2.433023	-1.863575
32	6	0	4.358161	-1.863606	1.679226
33	1	0	3.473081	-2.134769	2.262709
34	1	0	4.861988	-1.042545	2.197218
35	1	0	5.035726	-2.724584	1.665797
36	6	0	5.470311	-1.115831	-1.113180
37	6	0	6.163711	-2.460996	-1.370757
38	1	0	7.102140	-2.303223	-1.918434
39	1	0	5.539441	-3.129536	-1.973466
40	1	0	6.413186	-2.979843	-0.437838
41	6	0	6.430390	-0.185384	-0.358452
42	1	0	7.314125	0.030223	-0.973693
43	1	0	6.780142	-0.638051	0.575727
44	1	0	5.951944	0.769422	-0.112401
45	6	0	5.102311	-0.472013	-2.456362
46	1	0	5.998937	-0.354689	-3.079581
47	1	0	4.659343	0.518338	-2.309788
48	1	0	4.386300	-1.082350	-3.019632
49	6	0	1.986010	2.146781	0.316907
50	6	0	0.950704	2.873566	0.916510
51	6	0	3.014957	2.838327	-0.323747
52	6	0	0.928962	4.262323	0.843873
53	1	0	0.158781	2.345013	1.440640
54	6	0	2.996048	4.230824	-0.389628
55	1	0	3.828802	2.277089	-0.769940
56	6	0	1.949137	4.946029	0.183847
57	1	0	3.802900	4.755257	-0.892088
58	6	0	1.631617	0.034965	1.668526
59	6	0	0.830392	-1.093376	1.850859
60	6	0	2.293567	0.574306	2.776599
61	6	0	0.690156	-1.667104	3.114533
62	1	0	0.294287	-1.534926	1.018374
63	6	0	2.158575	0.002050	4.036221
64	1	0	2.926923	1.447004	2.642174
65	6	0	1.353807	-1.122950	4.209277
66	1	0	2.682048	0.433956	4.883306
67	1	0	0.114793	4.810613	1.306782
68	1	0	1.931472	6.029705	0.127149
69	1	0	1.243331	-1.569929	5.192137

70	1	0	0.054808	-2.539340	3.236882
71	6	0	-3.661609	-2.034697	-0.066482
72	6	0	-3.039555	-1.791861	-1.295028
73	6	0	-3.742589	-1.392002	-2.424202
74	6	0	-5.121699	-1.243103	-2.336568
75	6	0	-5.775227	-1.502496	-1.134196
76	6	0	-5.048815	-1.893660	-0.014944
77	1	0	-3.207084	-1.215712	-3.348382
78	1	0	-5.682859	-0.929987	-3.210031
79	1	0	-6.851113	-1.383518	-1.062894
80	1	0	-5.537431	-2.064246	0.938346
81	7	0	-1.596857	-1.999976	-1.450435
82	6	0	-2.967491	-2.305742	1.242919
83	8	0	-3.524762	-2.928660	2.117730
84	1	0	-1.986111	-1.832670	1.382072
85	8	0	-1.050201	-1.523626	-2.430317
86	8	0	-1.016664	-2.652502	-0.596583

M01'(Si)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-3.616463	0.906005	-0.032539
2	8	0	-2.834887	-0.582111	0.044072
3	7	0	2.615196	-1.887910	-0.731048
4	7	0	2.033792	-2.914451	-1.459340
5	7	0	0.650672	-1.271463	-0.994481
6	6	0	4.499602	-1.175400	0.632561
7	1	0	3.843113	-0.482483	1.147375
8	6	0	5.848807	-1.261208	0.957870
9	1	0	6.244517	-0.619457	1.738162
10	6	0	6.681202	-2.164220	0.300134
11	1	0	7.731653	-2.230029	0.563285
12	6	0	6.155315	-2.984509	-0.694491
13	1	0	6.794784	-3.693370	-1.210567
14	6	0	4.810469	-2.901918	-1.043107
15	1	0	4.389299	-3.531864	-1.816862
16	6	0	3.991238	-1.992013	-0.378603
17	6	0	1.808950	-0.841198	-0.416370
18	6	0	0.818102	-2.494150	-1.594535
19	6	0	-0.451569	-2.985053	-2.203360

20	1	0	-0.868476	-3.789630	-1.589116
21	1	0	-0.310004	-3.360076	-3.217847
22	6	0	-1.328744	-1.705589	-2.150558
23	1	0	-2.378214	-1.922586	-1.950795
24	1	0	-1.266993	-1.181125	-3.108114
25	6	0	-0.730828	-0.795297	-1.044512
26	1	0	-0.754166	0.254750	-1.346762
27	6	0	-1.488009	-0.932311	0.317706
28	6	0	-2.760196	2.062039	-1.242742
29	1	0	-1.778696	2.364185	-0.865099
30	1	0	-3.354108	2.973726	-1.369561
31	1	0	-2.624227	1.606498	-2.230005
32	6	0	-3.748345	1.745250	1.637416
33	1	0	-2.785831	2.158331	1.954560
34	1	0	-4.083215	1.045525	2.408506
35	1	0	-4.471886	2.566746	1.585349
36	6	0	-5.327701	0.408528	-0.674854
37	6	0	-6.116445	1.658339	-1.089724
38	1	0	-7.131236	1.378737	-1.401426
39	1	0	-5.643082	2.173304	-1.932831
40	1	0	-6.212732	2.375399	-0.266263
41	6	0	-6.090763	-0.332434	0.432387
42	1	0	-7.057753	-0.689540	0.054332
43	1	0	-6.290324	0.318323	1.290488
44	1	0	-5.529081	-1.202270	0.791604
45	6	0	-5.179521	-0.519363	-1.887899
46	1	0	-6.166803	-0.768121	-2.299455
47	1	0	-4.683413	-1.455080	-1.611106
48	1	0	-4.595421	-0.052529	-2.690310
49	6	0	-1.469134	-2.401450	0.741239
50	6	0	-0.303339	-2.967467	1.270268
51	6	0	-2.582039	-3.216623	0.530781
52	6	0	-0.240365	-4.330167	1.540873
53	1	0	0.560225	-2.336329	1.466075
54	6	0	-2.521059	-4.580703	0.811913
55	1	0	-3.493366	-2.775212	0.142455
56	6	0	-1.347717	-5.143477	1.305652
57	1	0	-3.393916	-5.203404	0.641517
58	6	0	-0.934612	-0.022875	1.416797
59	6	0	-0.160974	1.108117	1.149242
60	6	0	-1.331458	-0.267735	2.735818
61	6	0	0.203875	1.979412	2.174521
62	1	0	0.182220	1.319108	0.142145
63	6	0	-0.970099	0.598714	3.760400

64	1	0	-1.937111	-1.142656	2.954554
65	6	0	-0.201878	1.727839	3.481222
66	1	0	-1.289479	0.393875	4.777354
67	1	0	0.675786	-4.755302	1.937620
68	1	0	-1.298260	-6.206814	1.517022
69	1	0	0.084874	2.405185	4.279096
70	1	0	0.810921	2.850898	1.951180
71	6	0	2.286196	2.553483	-0.977752
72	6	0	1.790358	3.789870	-0.565349
73	6	0	0.704742	4.399026	-1.173376
74	6	0	0.116017	3.772449	-2.269318
75	6	0	0.615369	2.556994	-2.732584
76	6	0	1.691287	1.952347	-2.086671
77	1	0	0.347558	5.352258	-0.801308
78	1	0	-0.732943	4.236747	-2.759098
79	1	0	0.156500	2.073254	-3.588783
80	1	0	2.058076	0.982588	-2.409972
81	7	0	2.461001	4.552497	0.501670
82	6	0	3.300555	1.786084	-0.192162
83	8	0	3.482844	1.970277	0.986753
84	1	0	3.850392	1.015415	-0.759846
85	8	0	1.749526	5.051225	1.357142
86	8	0	3.662885	4.687893	0.417955

TS1'(Re)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.301313	-0.811454	-0.407163
2	8	0	3.136496	0.346747	-0.041789
3	7	0	-2.359475	1.377100	-0.587437
4	7	0	-1.767435	2.364591	-1.344581
5	7	0	-0.422088	0.666359	-0.947562
6	6	0	-4.090503	1.158391	1.109297
7	1	0	-3.370161	0.662161	1.756655
8	6	0	-5.408121	1.366552	1.508534
9	1	0	-5.721965	1.037980	2.494161
10	6	0	-6.313736	1.998363	0.660920
11	1	0	-7.336356	2.163995	0.983948
12	6	0	-5.905173	2.421451	-0.603076
13	1	0	-6.607494	2.913861	-1.267413
14	6	0	-4.597452	2.210040	-1.023302

15	1	0	-4.256951	2.530475	-2.001021
16	6	0	-3.707125	1.575943	-0.160864
17	6	0	-1.571147	0.317614	-0.321708
18	6	0	-0.577315	1.894583	-1.538274
19	6	0	0.664410	2.348437	-2.219758
20	1	0	1.124257	3.159440	-1.649219
21	1	0	0.469641	2.702534	-3.232956
22	6	0	1.513038	1.054219	-2.190739
23	1	0	2.572546	1.252313	-2.044511
24	1	0	1.389379	0.522971	-3.137567
25	6	0	0.952263	0.150179	-1.056066
26	1	0	0.912222	-0.883904	-1.397042
27	6	0	1.763043	0.253941	0.297993
28	6	0	3.742876	-1.870484	-1.857360
29	1	0	2.891889	-2.503522	-1.591971
30	1	0	4.554747	-2.533629	-2.173624
31	1	0	3.456748	-1.257318	-2.718322
32	6	0	4.753584	-1.880747	1.065785
33	1	0	3.977637	-2.616510	1.295223
34	1	0	4.907436	-1.265772	1.957360
35	1	0	5.685294	-2.419552	0.860842
36	6	0	5.784804	0.263118	-0.899914
37	6	0	6.891696	-0.621024	-1.490946
38	1	0	7.775123	-0.013603	-1.726804
39	1	0	6.568500	-1.105917	-2.418484
40	1	0	7.210293	-1.403643	-0.792820
41	6	0	6.318497	0.989800	0.342672
42	1	0	7.141398	1.661743	0.065236
43	1	0	6.702970	0.285365	1.087751
44	1	0	5.536891	1.592965	0.818557
45	6	0	5.367119	1.306422	-1.943907
46	1	0	6.238635	1.892785	-2.264094
47	1	0	4.629875	2.004623	-1.533358
48	1	0	4.936582	0.842225	-2.839496
49	6	0	1.372369	1.558178	0.998077
50	6	0	0.202757	1.628902	1.767506
51	6	0	2.137814	2.709149	0.816874
52	6	0	-0.209305	2.844282	2.302902
53	1	0	-0.384533	0.729394	1.953726
54	6	0	1.727202	3.924276	1.366138
55	1	0	3.057068	2.647866	0.243246
56	6	0	0.547569	3.997440	2.099462
57	1	0	2.332497	4.813189	1.217081
58	6	0	1.583954	-0.964485	1.217950

59	6	0	1.264564	-2.241095	0.748093
60	6	0	1.932476	-0.827117	2.567283
61	6	0	1.265923	-3.341127	1.606243
62	1	0	0.985964	-2.410548	-0.286497
63	6	0	1.940287	-1.921283	3.422935
64	1	0	2.206603	0.151861	2.947539
65	6	0	1.602246	-3.185804	2.945545
66	1	0	2.210519	-1.785479	4.465122
67	1	0	-1.123928	2.885925	2.886163
68	1	0	0.222828	4.944315	2.519012
69	1	0	1.600819	-4.041736	3.612501
70	1	0	0.997630	-4.318565	1.218443
71	6	0	-3.172484	-1.816172	0.238039
72	6	0	-3.337988	-2.056931	-1.128073
73	6	0	-4.545845	-2.442214	-1.692647
74	6	0	-5.636336	-2.654121	-0.856199
75	6	0	-5.501722	-2.448443	0.514191
76	6	0	-4.287224	-2.023886	1.046260
77	1	0	-4.614031	-2.575550	-2.766058
78	1	0	-6.583532	-2.973546	-1.276392
79	1	0	-6.350941	-2.607223	1.171023
80	1	0	-4.168008	-1.821840	2.105804
81	7	0	-2.217516	-1.868460	-2.057988
82	6	0	-1.897031	-1.314141	0.915583
83	8	0	-1.954062	-0.952592	2.105367
84	1	0	-0.989157	-1.771649	0.517016
85	8	0	-2.450061	-1.327204	-3.122541
86	8	0	-1.115074	-2.276762	-1.722060

TS1'(Si)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	3.983327	0.323613	0.153777
2	8	0	2.744490	-0.781876	-0.131956
3	7	0	-2.600114	-1.700416	0.920725
4	7	0	-1.959673	-2.806102	1.443117
5	7	0	-0.641651	-1.048978	1.274900
6	6	0	-4.326879	-1.266773	-0.745144
7	1	0	-3.623792	-0.656941	-1.310383
8	6	0	-5.633271	-1.451161	-1.189971
9	1	0	-5.948177	-0.981381	-2.115687

10	6	0	-6.524007	-2.239212	-0.465604
11	1	0	-7.537185	-2.383422	-0.825771
12	6	0	-6.111598	-2.846518	0.718642
13	1	0	-6.800473	-3.464803	1.284410
14	6	0	-4.815711	-2.659889	1.186802
15	1	0	-4.472634	-3.124270	2.104383
16	6	0	-3.940396	-1.864714	0.452893
17	6	0	-1.834320	-0.597862	0.815467
18	6	0	-0.759337	-2.366712	1.642910
19	6	0	0.524382	-2.918509	2.157534
20	1	0	0.896230	-3.695632	1.487042
21	1	0	0.406643	-3.350221	3.152884
22	6	0	1.422263	-1.653783	2.162690
23	1	0	2.441688	-1.865243	1.847790
24	1	0	1.456971	-1.238889	3.173309
25	6	0	0.758231	-0.603198	1.229338
26	1	0	0.844558	0.395438	1.659766
27	6	0	1.340835	-0.608562	-0.243013
28	6	0	3.662183	1.272750	1.746829
29	1	0	2.801091	1.941160	1.651535
30	1	0	4.530202	1.894275	1.989820
31	1	0	3.486919	0.599797	2.593104
32	6	0	4.259085	1.504798	-1.273972
33	1	0	3.475986	2.265811	-1.334690
34	1	0	4.273279	0.964257	-2.224538
35	1	0	5.223522	2.011109	-1.156245
36	6	0	5.486820	-0.815725	0.344808
37	6	0	6.690107	-0.009735	0.853881
38	1	0	7.580016	-0.650581	0.903033
39	1	0	6.515236	0.388289	1.859559
40	1	0	6.930318	0.831963	0.194355
41	6	0	5.825486	-1.432659	-1.020035
42	1	0	6.651083	-2.149532	-0.918610
43	1	0	6.137509	-0.670676	-1.742482
44	1	0	4.965842	-1.966490	-1.441104
45	6	0	5.185777	-1.944223	1.339305
46	1	0	6.078156	-2.566284	1.489502
47	1	0	4.385134	-2.594602	0.970937
48	1	0	4.887125	-1.556141	2.320947
49	6	0	0.779131	-1.826810	-0.980994
50	6	0	-0.480692	-1.764209	-1.592385
51	6	0	1.484061	-3.029318	-0.993686
52	6	0	-1.042964	-2.905499	-2.153372
53	1	0	-1.011114	-0.812191	-1.636676

54	6	0	0.923023	-4.169059	-1.570319
55	1	0	2.474349	-3.065644	-0.549898
56	6	0	-0.346102	-4.113639	-2.136769
57	1	0	1.481688	-5.099860	-1.574428
58	6	0	1.076463	0.681628	-1.029556
59	6	0	0.847887	1.923257	-0.439071
60	6	0	1.252171	0.631373	-2.419471
61	6	0	0.780116	3.079846	-1.217596
62	1	0	0.705772	2.027666	0.631672
63	6	0	1.172624	1.777889	-3.196802
64	1	0	1.456151	-0.323395	-2.893656
65	6	0	0.930600	3.011731	-2.595893
66	1	0	1.300774	1.708593	-4.272281
67	1	0	-2.025868	-2.847315	-2.610909
68	1	0	-0.786368	-5.002790	-2.576532
69	1	0	0.856358	3.912713	-3.196037
70	1	0	0.584417	4.034179	-0.741534
71	6	0	-1.999887	2.217080	0.964234
72	6	0	-1.902094	3.541108	0.534625
73	6	0	-1.306414	4.546330	1.285750
74	6	0	-0.823274	4.244566	2.552721
75	6	0	-0.966507	2.949712	3.044968
76	6	0	-1.547601	1.957106	2.259641
77	1	0	-1.240698	5.546766	0.872933
78	1	0	-0.357671	5.017366	3.154050
79	1	0	-0.616014	2.706267	4.042778
80	1	0	-1.629422	0.950451	2.652911
81	7	0	-2.495397	3.972064	-0.742323
82	6	0	-2.570853	1.163644	0.009221
83	8	0	-2.262379	1.197874	-1.190478
84	1	0	-3.579640	0.845131	0.335467
85	8	0	-1.841484	4.735604	-1.433185
86	8	0	-3.628470	3.609425	-0.983154

M1'(Re)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.282738	-1.083214	-0.456894
2	8	0	3.195065	0.171122	-0.187382
3	7	0	-2.384884	1.399468	-0.522934
4	7	0	-1.795583	2.450693	-1.184821

5	7	0	-0.387816	0.782334	-0.865756
6	6	0	-4.091503	1.175376	1.197286
7	1	0	-3.321693	0.766227	1.851480
8	6	0	-5.421754	1.314981	1.583755
9	1	0	-5.714669	1.034277	2.590086
10	6	0	-6.369326	1.812627	0.692672
11	1	0	-7.402462	1.922066	1.005947
12	6	0	-5.995291	2.171348	-0.601908
13	1	0	-6.732709	2.558280	-1.296842
14	6	0	-4.674995	2.027508	-1.011300
15	1	0	-4.357892	2.295700	-2.013029
16	6	0	-3.747616	1.527646	-0.102705
17	6	0	-1.550946	0.368012	-0.336215
18	6	0	-0.582081	2.039039	-1.373580
19	6	0	0.654870	2.571530	-2.005499
20	1	0	1.112129	3.314293	-1.345473
21	1	0	0.452811	3.034315	-2.971888
22	6	0	1.511952	1.286845	-2.117383
23	1	0	2.573319	1.476154	-1.967251
24	1	0	1.378184	0.846415	-3.108153
25	6	0	0.983457	0.276763	-1.057994
26	1	0	0.931859	-0.726376	-1.483736
27	6	0	1.852434	0.262731	0.254433
28	6	0	3.692021	-2.183561	-1.862616
29	1	0	2.843511	-2.807228	-1.570489
30	1	0	4.497564	-2.856138	-2.174978
31	1	0	3.397605	-1.588165	-2.733591
32	6	0	4.648739	-2.085134	1.084410
33	1	0	3.821419	-2.746714	1.354540
34	1	0	4.845139	-1.426312	1.935353
35	1	0	5.540736	-2.700577	0.920837
36	6	0	5.835346	-0.127667	-0.982896
37	6	0	6.878529	-1.096106	-1.557869
38	1	0	7.807618	-0.557602	-1.785702
39	1	0	6.530443	-1.559023	-2.487452
40	1	0	7.129037	-1.897558	-0.853286
41	6	0	6.426742	0.588376	0.239812
42	1	0	7.283643	1.206406	-0.059139
43	1	0	6.779405	-0.124483	0.992580
44	1	0	5.689467	1.244694	0.716464
45	6	0	5.482173	0.916407	-2.050434
46	1	0	6.392111	1.415379	-2.409618
47	1	0	4.817476	1.686999	-1.646676
48	1	0	4.988599	0.464463	-2.919285

49	6	0	1.681824	1.615126	0.950458
50	6	0	0.525339	1.887844	1.694303
51	6	0	2.644283	2.612585	0.787773
52	6	0	0.331459	3.158137	2.229521
53	1	0	-0.215189	1.100132	1.860567
54	6	0	2.446440	3.880408	1.334120
55	1	0	3.547930	2.390271	0.230744
56	6	0	1.284838	4.159458	2.047018
57	1	0	3.203180	4.647258	1.200739
58	6	0	1.555495	-0.924426	1.179140
59	6	0	1.196299	-2.178272	0.678745
60	6	0	1.834734	-0.813901	2.544366
61	6	0	1.076727	-3.280568	1.522318
62	1	0	0.995159	-2.324964	-0.376936
63	6	0	1.727234	-1.913168	3.387595
64	1	0	2.143178	0.143362	2.951061
65	6	0	1.340197	-3.151259	2.881398
66	1	0	1.944972	-1.800552	4.444782
67	1	0	-0.570628	3.364093	2.797411
68	1	0	1.127003	5.147195	2.468699
69	1	0	1.248548	-4.008349	3.540729
70	1	0	0.778106	-4.239396	1.110680
71	6	0	-3.121941	-1.576441	0.175556
72	6	0	-3.706717	-1.838613	-1.068657
73	6	0	-4.955322	-2.444470	-1.208799
74	6	0	-5.639066	-2.850211	-0.073958
75	6	0	-5.068505	-2.635475	1.181004
76	6	0	-3.838325	-2.000753	1.294848
77	1	0	-5.359642	-2.594836	-2.201925
78	1	0	-6.605193	-3.333208	-0.169675
79	1	0	-5.594112	-2.955873	2.075361
80	1	0	-3.378422	-1.784137	2.253972
81	7	0	-3.019107	-1.497518	-2.317116
82	6	0	-1.757653	-0.898333	0.493468
83	8	0	-1.578914	-0.568214	1.769826
84	1	0	-1.010603	-1.601743	0.068334
85	8	0	-3.677668	-1.403003	-3.337146
86	8	0	-1.803995	-1.341271	-2.282481

M1'(Si)

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

1	14	0	-3.962197	0.284509	-0.216468
2	8	0	-2.697931	-0.797433	0.047073
3	7	0	2.822044	-1.458947	-0.918946
4	7	0	2.208163	-2.592900	-1.386471
5	7	0	0.785124	-0.910793	-1.179557
6	6	0	4.564389	-0.913665	0.695440
7	1	0	3.826337	-0.345602	1.265524
8	6	0	5.890334	-1.029281	1.102761
9	1	0	6.205704	-0.544048	2.020165
10	6	0	6.802362	-1.766632	0.351146
11	1	0	7.831360	-1.855115	0.683609
12	6	0	6.396205	-2.394443	-0.824919
13	1	0	7.104308	-2.972075	-1.409270
14	6	0	5.080440	-2.279889	-1.259207
15	1	0	4.738479	-2.761000	-2.168714
16	6	0	4.189033	-1.535235	-0.494131
17	6	0	1.987322	-0.413936	-0.821447
18	6	0	0.977030	-2.222944	-1.539521
19	6	0	-0.275371	-2.849546	-2.042689
20	1	0	-0.634017	-3.597433	-1.332955
21	1	0	-0.117651	-3.330489	-3.009218
22	6	0	-1.208179	-1.617251	-2.132921
23	1	0	-2.241930	-1.855087	-1.894695
24	1	0	-1.170683	-1.209742	-3.146990
25	6	0	-0.650357	-0.543120	-1.159675
26	1	0	-0.780993	0.456409	-1.573087
27	6	0	-1.309401	-0.620655	0.276912
28	6	0	-3.618322	1.322867	-1.748680
29	1	0	-2.786316	2.016469	-1.594298
30	1	0	-4.498549	1.923519	-1.999461
31	1	0	-3.386264	0.694127	-2.615458
32	6	0	-4.340266	1.362455	1.268109
33	1	0	-3.593071	2.146658	1.414367
34	1	0	-4.372895	0.758560	2.179569
35	1	0	-5.319607	1.837320	1.141383
36	6	0	-5.416480	-0.893659	-0.528523
37	6	0	-6.622579	-0.103451	-1.055849
38	1	0	-7.489074	-0.768497	-1.166494
39	1	0	-6.421152	0.339041	-2.037613
40	1	0	-6.915856	0.703531	-0.374423
41	6	0	-5.799379	-1.583498	0.788715
42	1	0	-6.601699	-2.313171	0.616941
43	1	0	-6.160502	-0.863120	1.530132

44	1	0	-4.947374	-2.117621	1.224658
45	6	0	-5.031129	-1.963625	-1.557502
46	1	0	-5.897679	-2.595639	-1.793050
47	1	0	-4.239360	-2.615448	-1.172945
48	1	0	-4.682649	-1.520656	-2.498618
49	6	0	-0.792887	-1.871711	0.990529
50	6	0	0.479275	-1.864382	1.578324
51	6	0	-1.560305	-3.035744	1.023743
52	6	0	0.984947	-3.029200	2.147028
53	1	0	1.062386	-0.938724	1.589439
54	6	0	-1.050962	-4.196974	1.605086
55	1	0	-2.554534	-3.027404	0.588918
56	6	0	0.226171	-4.199761	2.156633
57	1	0	-1.655901	-5.098248	1.625102
58	6	0	-1.125697	0.635704	1.134848
59	6	0	-0.963445	1.912402	0.597867
60	6	0	-1.322092	0.516744	2.514580
61	6	0	-0.974652	3.037733	1.420112
62	1	0	-0.810059	2.067041	-0.464952
63	6	0	-1.331533	1.636681	3.336874
64	1	0	-1.471955	-0.466084	2.949592
65	6	0	-1.154825	2.905509	2.791610
66	1	0	-1.476740	1.516029	4.405714
67	1	0	1.976291	-3.018971	2.590065
68	1	0	0.625474	-5.105425	2.602248
69	1	0	-1.149135	3.783319	3.429308
70	1	0	-0.823126	4.019078	0.983713
71	6	0	1.771416	2.094187	-1.055507
72	6	0	1.709910	3.361729	-0.477515
73	6	0	1.058138	4.435722	-1.064378
74	6	0	0.465166	4.266100	-2.312659
75	6	0	0.565855	3.035293	-2.952979
76	6	0	1.215894	1.969313	-2.329708
77	1	0	1.028514	5.386421	-0.543375
78	1	0	-0.050044	5.094518	-2.785660
79	1	0	0.129917	2.897546	-3.937312
80	1	0	1.268316	1.013562	-2.844784
81	7	0	2.409180	3.639857	0.786775
82	6	0	2.375927	0.939353	-0.234672
83	8	0	2.028726	0.910129	1.053784
84	1	0	3.470772	1.012287	-0.441782
85	8	0	1.829762	4.324700	1.611187
86	8	0	3.555495	3.251525	0.882411

M02'(SS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	5.262452	-0.814379	-0.006004
2	8	0	3.798956	-0.273212	-0.670726
3	7	0	-1.125011	2.287169	-0.480583
4	7	0	-0.275654	3.061889	-1.226060
5	7	0	0.404141	0.962405	-1.101794
6	6	0	-2.555108	2.595509	1.458164
7	1	0	-1.931795	1.886065	2.003296
8	6	0	-3.671509	3.192920	2.038841
9	1	0	-3.908085	2.974606	3.074584
10	6	0	-4.482541	4.047269	1.294429
11	1	0	-5.348466	4.510263	1.756063
12	6	0	-4.190307	4.302389	-0.045288
13	1	0	-4.827904	4.958352	-0.628351
14	6	0	-3.082460	3.711942	-0.643995
15	1	0	-2.836122	3.885716	-1.685422
16	6	0	-2.281075	2.872420	0.121546
17	6	0	-0.755780	1.004124	-0.425561
18	6	0	0.644218	2.224690	-1.589124
19	6	0	1.878496	2.259030	-2.423901
20	1	0	2.674868	2.792484	-1.900205
21	1	0	1.701969	2.748995	-3.382270
22	6	0	2.173287	0.745292	-2.568672
23	1	0	3.233626	0.521058	-2.645087
24	1	0	1.665830	0.367334	-3.460020
25	6	0	1.540043	0.052442	-1.333772
26	1	0	1.161530	-0.942319	-1.573167
27	6	0	2.528412	-0.053146	-0.077605
28	6	0	5.501503	-2.620063	-0.466019
29	1	0	4.795032	-3.255937	0.071328
30	1	0	6.513551	-2.947216	-0.209723
31	1	0	5.359398	-2.781852	-1.539975
32	6	0	5.320148	-0.623525	1.857826
33	1	0	4.620848	-1.309128	2.344110
34	1	0	5.082263	0.395695	2.176133
35	1	0	6.329748	-0.861863	2.211552
36	6	0	6.631885	0.227854	-0.850547
37	6	0	7.851886	-0.670356	-1.121201
38	1	0	8.662487	-0.072238	-1.557193

39	1	0	7.620837	-1.477757	-1.822914
40	1	0	8.238911	-1.123479	-0.200772
41	6	0	7.110859	1.388159	0.038493
42	1	0	7.892417	1.955836	-0.483346
43	1	0	7.541639	1.020946	0.975874
44	1	0	6.314267	2.090788	0.299798
45	6	0	6.133652	0.779051	-2.194786
46	1	0	6.949827	1.297560	-2.714559
47	1	0	5.312352	1.492663	-2.068569
48	1	0	5.776824	-0.022259	-2.853042
49	6	0	2.521788	1.273948	0.691044
50	6	0	1.451106	1.651311	1.514923
51	6	0	3.554945	2.188252	0.481501
52	6	0	1.434631	2.911517	2.107250
53	1	0	0.611541	0.970151	1.680394
54	6	0	3.542066	3.444008	1.084757
55	1	0	4.365806	1.918566	-0.183626
56	6	0	2.477417	3.811723	1.900875
57	1	0	4.360408	4.134843	0.904730
58	6	0	2.178212	-1.304367	0.750414
59	6	0	2.276993	-2.535141	0.089033
60	6	0	1.879381	-1.311740	2.113000
61	6	0	2.078941	-3.736293	0.759658
62	1	0	2.547779	-2.553714	-0.963945
63	6	0	1.660793	-2.513881	2.785548
64	1	0	1.824690	-0.388419	2.672714
65	6	0	1.757297	-3.729143	2.115333
66	1	0	1.418020	-2.492317	3.842853
67	1	0	0.592020	3.189088	2.733595
68	1	0	2.456178	4.791949	2.366304
69	1	0	1.592429	-4.662255	2.644797
70	1	0	2.174431	-4.675182	0.222331
71	6	0	-1.574879	-1.384508	-0.516449
72	6	0	-2.292397	-1.622959	-1.699867
73	6	0	-2.411820	-2.890030	-2.267045
74	6	0	-1.781911	-3.968738	-1.663024
75	6	0	-1.038297	-3.761895	-0.503340
76	6	0	-0.950269	-2.491851	0.057768
77	1	0	-2.995266	-3.006291	-3.171369
78	1	0	-1.871459	-4.958216	-2.098190
79	1	0	-0.535428	-4.593806	-0.019380
80	1	0	-0.424330	-2.310041	0.990091
81	7	0	-2.953168	-0.534016	-2.435591
82	6	0	-1.519855	-0.080304	0.332714

83	8	0	-1.003795	-0.232607	1.553109
84	1	0	-2.564513	0.296286	0.295631
85	8	0	-3.659574	-0.819815	-3.384636
86	8	0	-2.735849	0.616557	-2.082011
87	6	0	-4.266072	-1.384688	1.577591
88	6	0	-3.937431	-0.464229	2.470965
89	8	0	-3.686216	0.336613	3.280241
90	6	0	-5.016138	-0.990316	0.372285
91	6	0	-5.509982	-1.974087	-0.496725
92	6	0	-5.230145	0.357387	0.038298
93	6	0	-6.193640	-1.619368	-1.656059
94	1	0	-5.354582	-3.023615	-0.268282
95	6	0	-5.909445	0.705180	-1.121481
96	1	0	-4.840177	1.143604	0.682629
97	6	0	-6.397962	-0.280852	-1.977247
98	1	0	-6.558671	-2.398285	-2.318573
99	1	0	-6.042705	1.755729	-1.361153
100	1	0	-6.916269	-0.008474	-2.890317
101	6	0	-3.794282	-2.807752	1.812302
102	6	0	-2.737592	-2.907980	2.910883
103	1	0	-3.374779	-3.173339	0.867898
104	1	0	-4.656602	-3.446267	2.045894
105	1	0	-2.329811	-3.920861	2.963238
106	1	0	-1.926210	-2.200563	2.704891
107	1	0	-3.165380	-2.669238	3.890751

M02'(RR)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.685809	-1.245688	-0.186133
2	8	0	3.805293	0.188465	-0.068116
3	7	0	-1.300359	2.372170	-0.779863
4	7	0	-0.451299	2.990840	-1.657484
5	7	0	0.350161	1.053036	-0.955485
6	6	0	-2.954587	3.059307	0.873093
7	1	0	-2.364346	2.551346	1.636505
8	6	0	-4.142630	3.728202	1.160165
9	1	0	-4.476786	3.798907	2.189756
10	6	0	-4.894308	4.310007	0.142176
11	1	0	-5.816197	4.830573	0.379571
12	6	0	-4.464004	4.228622	-1.181391

13	1	0	-5.050445	4.678087	-1.975516
14	6	0	-3.277409	3.573634	-1.489856
15	1	0	-2.913244	3.501340	-2.508546
16	6	0	-2.543413	3.001048	-0.455608
17	6	0	-0.853230	1.181818	-0.367216
18	6	0	0.539377	2.162581	-1.746020
19	6	0	1.807404	2.080994	-2.519876
20	1	0	2.542586	2.783960	-2.123053
21	1	0	1.642886	2.301531	-3.575239
22	6	0	2.198028	0.605466	-2.272973
23	1	0	3.273059	0.453498	-2.261383
24	1	0	1.755501	-0.017289	-3.055252
25	6	0	1.550290	0.185426	-0.926684
26	1	0	1.246815	-0.860648	-0.970517
27	6	0	2.473247	0.449745	0.337174
28	6	0	3.787501	-2.476314	-1.290460
29	1	0	2.872562	-2.852566	-0.822599
30	1	0	4.431704	-3.341349	-1.480032
31	1	0	3.521782	-2.041870	-2.259817
32	6	0	5.084176	-2.014842	1.475455
33	1	0	4.214800	-2.492295	1.934710
34	1	0	5.461801	-1.262490	2.173736
35	1	0	5.861868	-2.775725	1.345684
36	6	0	6.290819	-0.646453	-1.000991
37	6	0	7.159036	-1.849204	-1.397470
38	1	0	8.111571	-1.502188	-1.818639
39	1	0	6.670922	-2.469739	-2.156977
40	1	0	7.395636	-2.487139	-0.538490
41	6	0	7.061360	0.228906	-0.002070
42	1	0	7.971399	0.627841	-0.469373
43	1	0	7.366725	-0.341386	0.881625
44	1	0	6.456941	1.078058	0.336325
45	6	0	5.984036	0.180792	-2.255988
46	1	0	6.917330	0.493788	-2.742372
47	1	0	5.418648	1.085754	-2.007831
48	1	0	5.408235	-0.393671	-2.992271
49	6	0	2.387648	1.928760	0.728550
50	6	0	1.283102	2.396027	1.453948
51	6	0	3.385988	2.822089	0.344723
52	6	0	1.168058	3.752172	1.741518
53	1	0	0.507792	1.700046	1.787259
54	6	0	3.269363	4.179358	0.645894
55	1	0	4.253116	2.449135	-0.191116
56	6	0	2.156163	4.648699	1.334617

57	1	0	4.052101	4.866747	0.340264
58	6	0	2.166195	-0.450197	1.542816
59	6	0	1.569448	-1.704619	1.442848
60	6	0	2.694932	-0.064142	2.783152
61	6	0	1.499308	-2.550544	2.551449
62	1	0	1.142271	-2.061903	0.511681
63	6	0	2.622617	-0.901179	3.886776
64	1	0	3.176562	0.903900	2.876570
65	6	0	2.024070	-2.155758	3.774231
66	1	0	3.037479	-0.576317	4.835527
67	1	0	0.302981	4.107297	2.293438
68	1	0	2.061774	5.705574	1.563206
69	1	0	1.967204	-2.815367	4.634073
70	1	0	1.024753	-3.520793	2.445955
71	6	0	-1.474083	-1.221311	0.168780
72	6	0	-1.318314	-1.784041	-1.101430
73	6	0	-1.126281	-3.149073	-1.313527
74	6	0	-1.187707	-4.010448	-0.228388
75	6	0	-1.407635	-3.488798	1.047194
76	6	0	-1.509239	-2.115873	1.238403
77	1	0	-0.972585	-3.510540	-2.323325
78	1	0	-1.079713	-5.078980	-0.380464
79	1	0	-1.475885	-4.154414	1.902899
80	1	0	-1.596331	-1.672154	2.225491
81	7	0	-1.307388	-0.950117	-2.307928
82	6	0	-1.653370	0.268669	0.565068
83	8	0	-1.372478	0.550848	1.836828
84	1	0	-2.706244	0.477518	0.243704
85	8	0	-0.553469	-1.272856	-3.214826
86	8	0	-2.041104	0.023385	-2.349603
87	6	0	-4.781155	-1.223238	1.117238
88	6	0	-4.408797	-1.992354	2.128367
89	8	0	-4.080368	-2.670721	3.020207
90	6	0	-4.727297	-1.803061	-0.240284
91	6	0	-4.817036	-0.986422	-1.373495
92	6	0	-4.551261	-3.184351	-0.432372
93	6	0	-4.713200	-1.531239	-2.652119
94	1	0	-4.940939	0.086192	-1.265770
95	6	0	-4.443919	-3.721500	-1.705828
96	1	0	-4.492142	-3.844069	0.430405
97	6	0	-4.520240	-2.896692	-2.828873
98	1	0	-4.767088	-0.872365	-3.513202
99	1	0	-4.297202	-4.791140	-1.823451
100	1	0	-4.435832	-3.316189	-3.825982

101	6	0	-5.199016	0.203736	1.432460
102	6	0	-4.650392	0.684671	2.774847
103	1	0	-6.292857	0.281670	1.400260
104	1	0	-4.813382	0.861759	0.645915
105	1	0	-4.985121	1.702995	2.982934
106	1	0	-5.003043	0.053476	3.598578
107	1	0	-3.553429	0.662287	2.752252

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-4.743929	-2.136535	-0.025251
2	8	0	-3.787639	-0.897999	0.628827
3	7	0	0.324825	3.113940	0.578237
4	7	0	-0.707291	3.758859	1.217378
5	7	0	-1.108445	1.603567	0.974192
6	6	0	1.894353	3.839562	-1.145423
7	1	0	1.411913	3.135078	-1.820408
8	6	0	2.970665	4.642401	-1.515206
9	1	0	3.339778	4.600058	-2.534755
10	6	0	3.566889	5.496771	-0.591749
11	1	0	4.402355	6.121265	-0.890915
12	6	0	3.092458	5.554377	0.718161
13	1	0	3.553396	6.222095	1.438075
14	6	0	2.026929	4.752172	1.108886
15	1	0	1.635930	4.781885	2.120044
16	6	0	1.450868	3.902300	0.169490
17	6	0	0.104109	1.799250	0.422555
18	6	0	-1.561661	2.811065	1.435052
19	6	0	-2.904946	2.689864	2.062423
20	1	0	-3.667026	3.038825	1.358600
21	1	0	-2.983265	3.269963	2.982099
22	6	0	-2.986977	1.163765	2.295150
23	1	0	-3.993686	0.768040	2.172677
24	1	0	-2.650752	0.932100	3.308160
25	6	0	-2.015409	0.484174	1.291158
26	1	0	-1.429954	-0.296904	1.776190
27	6	0	-2.742797	-0.136367	0.039141
28	6	0	-4.133057	-3.778981	0.653681

29	1	0	-3.146573	-4.022584	0.253553
30	1	0	-4.816602	-4.586586	0.375777
31	1	0	-4.064205	-3.758045	1.746543
32	6	0	-4.691815	-2.157078	-1.899249
33	1	0	-3.739759	-2.552517	-2.262819
34	1	0	-4.831550	-1.156168	-2.319569
35	1	0	-5.494326	-2.799168	-2.279337
36	6	0	-6.528236	-1.837961	0.604570
37	6	0	-7.195322	-3.201774	0.858632
38	1	0	-8.241563	-3.051773	1.155012
39	1	0	-6.698851	-3.757864	1.659667
40	1	0	-7.196870	-3.831342	-0.039311
41	6	0	-7.394439	-1.092635	-0.424297
42	1	0	-8.401512	-0.936675	-0.015525
43	1	0	-7.501333	-1.668597	-1.349371
44	1	0	-6.994811	-0.111634	-0.696574
45	6	0	-6.510725	-1.057895	1.927026
46	1	0	-7.526697	-0.991224	2.338065
47	1	0	-6.139963	-0.036018	1.796543
48	1	0	-5.878501	-1.544983	2.678509
49	6	0	-3.314915	1.013201	-0.794709
50	6	0	-2.501810	1.841247	-1.583924
51	6	0	-4.663677	1.344862	-0.649047
52	6	0	-3.049114	2.954484	-2.218579
53	1	0	-1.436716	1.631684	-1.708677
54	6	0	-5.208226	2.455106	-1.290590
55	1	0	-5.286364	0.734996	-0.007198
56	6	0	-4.399544	3.266630	-2.079870
57	1	0	-6.261543	2.685967	-1.162012
58	6	0	-1.784693	-1.103569	-0.672452
59	6	0	-1.305833	-2.177217	0.093914
60	6	0	-1.405811	-1.022621	-2.010715
61	6	0	-0.467662	-3.137717	-0.455140
62	1	0	-1.622734	-2.279919	1.128169
63	6	0	-0.543290	-1.973587	-2.558048
64	1	0	-1.773520	-0.224838	-2.641492
65	6	0	-0.070864	-3.028897	-1.788268
66	1	0	-0.234712	-1.875871	-3.593289
67	1	0	-2.405411	3.583691	-2.825408
68	1	0	-4.815772	4.136698	-2.577630
69	1	0	0.601580	-3.763281	-2.222063
70	1	0	-0.126386	-3.968321	0.156160
71	6	0	2.392298	0.792394	-0.105070
72	6	0	2.994604	0.482147	1.122718

73	6	0	4.379004	0.428828	1.295869
74	6	0	5.207717	0.675618	0.214654
75	6	0	4.641884	0.968354	-1.025414
76	6	0	3.261732	1.025536	-1.172223
77	1	0	4.780376	0.167285	2.266726
78	1	0	6.283865	0.603726	0.332254
79	1	0	5.282947	1.143854	-1.884268
80	1	0	2.786499	1.225848	-2.126640
81	7	0	2.194685	0.115230	2.294085
82	6	0	0.878220	0.817275	-0.474669
83	8	0	0.613488	1.161895	-1.732547
84	1	0	0.497358	-0.181425	-0.166574
85	8	0	2.767624	-0.121487	3.343859
86	8	0	0.978649	0.033472	2.167190
87	6	0	3.738343	-2.484497	-0.325305
88	6	0	3.199976	-2.102495	-1.472970
89	8	0	2.735584	-1.764948	-2.486808
90	6	0	5.207019	-2.582784	-0.225721
91	6	0	5.816291	-2.855735	1.005176
92	6	0	6.035803	-2.356339	-1.337153
93	6	0	7.204382	-2.883277	1.122377
94	1	0	5.208927	-3.039179	1.885582
95	6	0	7.417404	-2.382314	-1.215884
96	1	0	5.589421	-2.144872	-2.306486
97	6	0	8.014497	-2.643908	0.017956
98	1	0	7.651153	-3.092780	2.089546
99	1	0	8.033075	-2.197169	-2.090835
100	1	0	9.094944	-2.664620	0.112584
101	6	0	2.811456	-2.782327	0.839261
102	6	0	2.639337	-4.281753	1.085703
103	1	0	1.834031	-2.319879	0.659312
104	1	0	3.216599	-2.294128	1.734844
105	1	0	1.994985	-4.465669	1.950394
106	1	0	2.191970	-4.760603	0.209579
107	1	0	3.604326	-4.763527	1.267331

M02'(RS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-4.901400	-1.336460	0.241311
2	8	0	-3.716664	-0.191501	0.622189

3	7	0	1.065228	2.802170	0.350104
4	7	0	0.121898	3.722234	0.738431
5	7	0	-0.583016	1.647467	0.992334
6	6	0	2.551138	2.983064	-1.561771
7	1	0	1.852422	2.361751	-2.112996
8	6	0	3.749420	3.429287	-2.111577
9	1	0	3.971435	3.219258	-3.152547
10	6	0	4.664719	4.127261	-1.327360
11	1	0	5.599578	4.468068	-1.760691
12	6	0	4.387598	4.391849	0.013288
13	1	0	5.102708	4.934711	0.621808
14	6	0	3.191250	3.959879	0.575033
15	1	0	2.949698	4.152487	1.614983
16	6	0	2.298290	3.255468	-0.222736
17	6	0	0.663833	1.537019	0.514870
18	6	0	-0.869910	2.979961	1.122753
19	6	0	-2.231887	3.189391	1.686700
20	1	0	-2.907358	3.543838	0.903967
21	1	0	-2.226428	3.917379	2.498848
22	6	0	-2.581693	1.757645	2.164950
23	1	0	-3.636518	1.517463	2.050489
24	1	0	-2.317919	1.657743	3.220337
25	6	0	-1.699466	0.764245	1.355867
26	1	0	-1.317298	-0.035314	1.991729
27	6	0	-2.435873	0.134413	0.103315
28	6	0	-4.877532	-2.671080	1.563447
29	1	0	-4.993626	-2.242370	2.564468
30	1	0	-3.946927	-3.241088	1.540584
31	1	0	-5.700565	-3.374135	1.403432
32	6	0	-4.684738	-2.089551	-1.460158
33	1	0	-3.862602	-2.810304	-1.478758
34	1	0	-4.486319	-1.322483	-2.215771
35	1	0	-5.605961	-2.611354	-1.743370
36	6	0	-6.580474	-0.432349	0.340967
37	6	0	-7.665711	-1.457751	0.714825
38	1	0	-8.653523	-0.980122	0.680624
39	1	0	-7.524125	-1.854361	1.724833
40	1	0	-7.689390	-2.305764	0.019226
41	6	0	-6.976115	0.185872	-1.009358
42	1	0	-7.930515	0.719790	-0.909864
43	1	0	-7.109695	-0.586191	-1.774182
44	1	0	-6.236977	0.896046	-1.390378
45	6	0	-6.549793	0.651716	1.426943
46	1	0	-7.548142	1.091368	1.552437

47	1	0	-5.859570	1.464989	1.180434
48	1	0	-6.243912	0.242174	2.397204
49	6	0	-2.558536	1.209501	-0.979882
50	6	0	-1.466279	1.574774	-1.782629
51	6	0	-3.745385	1.933796	-1.091307
52	6	0	-1.583874	2.635388	-2.676933
53	1	0	-0.516753	1.035253	-1.713097
54	6	0	-3.861155	2.989744	-1.994516
55	1	0	-4.576882	1.678872	-0.446499
56	6	0	-2.778195	3.344916	-2.791174
57	1	0	-4.797679	3.534740	-2.065371
58	6	0	-1.766972	-1.178139	-0.349688
59	6	0	-1.674658	-2.205117	0.601646
60	6	0	-1.440787	-1.480456	-1.672363
61	6	0	-1.335206	-3.502607	0.236013
62	1	0	-1.933478	-2.004362	1.638320
63	6	0	-1.083845	-2.778548	-2.040674
64	1	0	-1.504607	-0.723809	-2.442970
65	6	0	-1.048593	-3.797601	-1.096645
66	1	0	-0.841435	-2.984626	-3.077725
67	1	0	-0.730390	2.906695	-3.290946
68	1	0	-2.861058	4.168657	-3.492952
69	1	0	-0.783856	-4.808911	-1.387886
70	1	0	-1.294246	-4.282342	0.990754
71	6	0	2.834616	0.308357	0.659811
72	6	0	3.238045	0.179823	1.992669
73	6	0	4.574491	0.241688	2.392041
74	6	0	5.554559	0.459371	1.439291
75	6	0	5.190508	0.563575	0.095157
76	6	0	3.858608	0.463753	-0.278440
77	1	0	4.815200	0.118076	3.440297
78	1	0	6.594175	0.530913	1.740328
79	1	0	5.952210	0.717846	-0.663767
80	1	0	3.541321	0.494598	-1.314395
81	7	0	2.262980	-0.052539	3.058820
82	6	0	1.387623	0.257838	0.074941
83	8	0	1.335535	0.158643	-1.251892
84	1	0	0.852176	-0.534017	0.639298
85	8	0	2.662103	-0.453723	4.137588
86	8	0	1.081374	0.172041	2.823705
87	6	0	3.432328	-2.386620	-1.835310
88	6	0	2.420732	-2.011839	-2.608668
89	8	0	1.607460	-1.745655	-3.397485
90	6	0	3.261015	-2.674379	-0.403732

91	6	0	4.378616	-2.870872	0.420990
92	6	0	1.989684	-2.736846	0.185602
93	6	0	4.228283	-3.116452	1.782773
94	1	0	5.379410	-2.808287	0.005509
95	6	0	1.845166	-2.974755	1.546901
96	1	0	1.111411	-2.539293	-0.424456
97	6	0	2.962257	-3.173261	2.357950
98	1	0	5.112523	-3.251747	2.398920
99	1	0	0.847317	-2.991459	1.976962
100	1	0	2.846330	-3.348712	3.422299
101	6	0	4.785858	-2.483227	-2.522404
102	6	0	5.287864	-3.922600	-2.658019
103	1	0	5.503976	-1.877282	-1.953796
104	1	0	4.727174	-2.023478	-3.513876
105	1	0	6.290611	-3.948494	-3.094312
106	1	0	5.323757	-4.420985	-1.685906
107	1	0	4.616892	-4.498035	-3.300995

TS2'(SS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	5.040066	-0.697115	0.007845
2	8	0	3.632383	0.107831	-0.450763
3	7	0	-1.429423	2.028865	-1.300269
4	7	0	-0.502493	2.803143	-1.952242
5	7	0	0.256819	0.770546	-1.570045
6	6	0	-3.098360	2.503810	0.427548
7	1	0	-2.578240	1.856402	1.131812
8	6	0	-4.250971	3.188231	0.807987
9	1	0	-4.623033	3.063608	1.817707
10	6	0	-4.906136	4.027169	-0.087584
11	1	0	-5.801247	4.556201	0.222358
12	6	0	-4.412382	4.194068	-1.380150
13	1	0	-4.920461	4.847989	-2.080662
14	6	0	-3.267044	3.519010	-1.778100
15	1	0	-2.861221	3.628558	-2.777056
16	6	0	-2.632212	2.678859	-0.869760
17	6	0	-1.000613	0.776580	-1.090717
18	6	0	0.505768	2.003109	-2.106920
19	6	0	1.857408	2.059947	-2.735619
20	1	0	2.527023	2.683594	-2.139246

21	1	0	1.813862	2.463555	-3.747990
22	6	0	2.249829	0.563339	-2.695376
23	1	0	3.321685	0.407281	-2.613232
24	1	0	1.886044	0.075134	-3.603615
25	6	0	1.485232	-0.046974	-1.493074
26	1	0	1.229244	-1.088118	-1.665538
27	6	0	2.260422	0.099610	-0.094408
28	6	0	5.279613	-2.236369	-1.042924
29	1	0	4.536870	-3.003783	-0.815559
30	1	0	6.267415	-2.666877	-0.850054
31	1	0	5.220576	-2.002830	-2.111371
32	6	0	5.117244	-1.126961	1.828634
33	1	0	4.504168	-2.000548	2.067562
34	1	0	4.777913	-0.292028	2.448986
35	1	0	6.155306	-1.350042	2.100942
36	6	0	6.406309	0.556550	-0.419631
37	6	0	7.746212	-0.178486	-0.581725
38	1	0	8.555077	0.547000	-0.738445
39	1	0	7.737197	-0.854143	-1.443047
40	1	0	8.003883	-0.767001	0.307024
41	6	0	6.555050	1.590240	0.707271
42	1	0	7.301013	2.346748	0.429427
43	1	0	6.892097	1.120504	1.637426
44	1	0	5.616995	2.111660	0.923730
45	6	0	6.077531	1.273734	-1.736474
46	1	0	6.882955	1.971305	-2.001814
47	1	0	5.145259	1.844082	-1.665796
48	1	0	5.970977	0.563680	-2.566104
49	6	0	1.920617	1.450069	0.553535
50	6	0	0.690380	1.664398	1.192854
51	6	0	2.812925	2.517378	0.450695
52	6	0	0.360678	2.923929	1.684267
53	1	0	-0.005749	0.831943	1.291960
54	6	0	2.485665	3.776610	0.953372
55	1	0	3.765345	2.360545	-0.041363
56	6	0	1.254734	3.987046	1.564228
57	1	0	3.196585	4.591608	0.858815
58	6	0	2.008081	-1.109266	0.818445
59	6	0	2.132449	-2.394039	0.280201
60	6	0	1.829059	-0.989199	2.195984
61	6	0	2.064656	-3.524996	1.084750
62	1	0	2.307972	-2.524852	-0.784768
63	6	0	1.744129	-2.121140	3.004885
64	1	0	1.761562	-0.009534	2.655215

65	6	0	1.861685	-3.393111	2.455902
66	1	0	1.593750	-2.000570	4.073363
67	1	0	-0.603345	3.069196	2.164724
68	1	0	0.993115	4.968494	1.946501
69	1	0	1.793852	-4.273014	3.086983
70	1	0	2.157360	-4.509680	0.637468
71	6	0	-2.010113	-1.492798	-1.564448
72	6	0	-3.204948	-1.617610	-2.281467
73	6	0	-3.483272	-2.683801	-3.132535
74	6	0	-2.522978	-3.667171	-3.316896
75	6	0	-1.322665	-3.584051	-2.614425
76	6	0	-1.086559	-2.527473	-1.741958
77	1	0	-4.443946	-2.721799	-3.631344
78	1	0	-2.719105	-4.497121	-3.986571
79	1	0	-0.575860	-4.363911	-2.724469
80	1	0	-0.213036	-2.518725	-1.098948
81	7	0	-4.262365	-0.615380	-2.154562
82	6	0	-1.664662	-0.445467	-0.456979
83	8	0	-0.776276	-0.950303	0.424056
84	1	0	-2.620794	-0.103501	-0.023817
85	8	0	-5.415874	-0.970452	-2.319418
86	8	0	-3.926444	0.530855	-1.903647
87	6	0	-2.947129	-2.045363	1.708642
88	6	0	-1.785752	-2.586966	1.284565
89	8	0	-1.052807	-3.470951	1.036170
90	6	0	-3.007716	-0.778135	2.428617
91	6	0	-4.239465	-0.147018	2.677005
92	6	0	-1.853322	-0.180425	2.980369
93	6	0	-4.312193	1.023086	3.430721
94	1	0	-5.155810	-0.578874	2.288147
95	6	0	-1.929279	0.999470	3.706361
96	1	0	-0.893359	-0.664989	2.833128
97	6	0	-3.161720	1.617321	3.940066
98	1	0	-5.284085	1.473491	3.615160
99	1	0	-1.018024	1.429025	4.115183
100	1	0	-3.221042	2.529423	4.525361
101	6	0	-4.214667	-2.828825	1.402455
102	6	0	-3.993708	-4.132325	0.637965
103	1	0	-4.876187	-2.189731	0.797948
104	1	0	-4.758374	-3.032621	2.335566
105	1	0	-4.951558	-4.615575	0.431901
106	1	0	-3.492743	-3.943426	-0.318514
107	1	0	-3.371291	-4.827744	1.206803

TS2'(RR)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-3.773988	-2.441960	-0.060695
2	8	0	-3.814718	-0.758596	-0.205775
3	7	0	0.593725	2.872987	0.263421
4	7	0	-0.473888	3.588843	0.728019
5	7	0	-0.918441	1.431002	0.604587
6	6	0	2.600972	3.106045	-1.089673
7	1	0	2.312429	2.213137	-1.640585
8	6	0	3.774910	3.798607	-1.374351
9	1	0	4.403185	3.465134	-2.193233
10	6	0	4.138016	4.912646	-0.620938
11	1	0	5.050923	5.449797	-0.855865
12	6	0	3.333367	5.338440	0.434999
13	1	0	3.620043	6.201106	1.026412
14	6	0	2.161993	4.656885	0.741448
15	1	0	1.521473	4.961066	1.560810
16	6	0	1.815828	3.551409	-0.030344
17	6	0	0.382452	1.550722	0.253479
18	6	0	-1.369776	2.678322	0.957145
19	6	0	-2.696899	2.610938	1.634405
20	1	0	-3.481696	3.075885	1.033556
21	1	0	-2.642959	3.117251	2.600090
22	6	0	-2.875682	1.074110	1.792510
23	1	0	-3.911447	0.755924	1.680743
24	1	0	-2.514500	0.765418	2.776227
25	6	0	-1.986594	0.411802	0.709940
26	1	0	-1.554681	-0.533349	1.040663
27	6	0	-2.819494	0.161688	-0.612620
28	6	0	-2.341889	-2.986143	1.025526
29	1	0	-1.381077	-2.756992	0.552180
30	1	0	-2.376435	-4.071527	1.168894
31	1	0	-2.354508	-2.517425	2.015921
32	6	0	-3.658848	-3.314625	-1.714550
33	1	0	-2.655719	-3.228493	-2.143400
34	1	0	-4.369704	-2.903497	-2.436610
35	1	0	-3.883896	-4.379100	-1.583017
36	6	0	-5.437687	-2.792628	0.774031

37	6	0	-5.468735	-4.245182	1.269890
38	1	0	-6.451001	-4.476281	1.702066
39	1	0	-4.716483	-4.422402	2.046030
40	1	0	-5.292065	-4.960311	0.457932
41	6	0	-6.574370	-2.573343	-0.233940
42	1	0	-7.547900	-2.715658	0.253205
43	1	0	-6.514631	-3.280344	-1.068266
44	1	0	-6.552360	-1.559190	-0.649056
45	6	0	-5.632100	-1.846872	1.966210
46	1	0	-6.560219	-2.091591	2.499400
47	1	0	-5.698492	-0.804897	1.636685
48	1	0	-4.808309	-1.921438	2.686410
49	6	0	-3.524149	1.451978	-1.034182
50	6	0	-2.801495	2.463762	-1.674974
51	6	0	-4.874067	1.656684	-0.748275
52	6	0	-3.404283	3.681921	-1.970901
53	1	0	-1.762291	2.294195	-1.949057
54	6	0	-5.481641	2.872247	-1.057922
55	1	0	-5.439183	0.859110	-0.278278
56	6	0	-4.745349	3.892480	-1.654545
57	1	0	-6.532151	3.022265	-0.829763
58	6	0	-2.041250	-0.402920	-1.795098
59	6	0	-0.760580	-0.924046	-1.681196
60	6	0	-2.694645	-0.470468	-3.034595
61	6	0	-0.124294	-1.505054	-2.780118
62	1	0	-0.212997	-0.879400	-0.750396
63	6	0	-2.076314	-1.065321	-4.124159
64	1	0	-3.695829	-0.060209	-3.132760
65	6	0	-0.785911	-1.587515	-3.997792
66	1	0	-2.596077	-1.119592	-5.075620
67	1	0	-2.828141	4.464157	-2.454125
68	1	0	-5.216939	4.842047	-1.885928
69	1	0	-0.297625	-2.042896	-4.853599
70	1	0	0.890270	-1.867828	-2.660608
71	6	0	1.171989	-0.560884	1.368408
72	6	0	0.690180	-0.348339	2.670388
73	6	0	0.378196	-1.383737	3.547412
74	6	0	0.588731	-2.695875	3.146179
75	6	0	1.073050	-2.945105	1.865584
76	6	0	1.341631	-1.893547	0.992184
77	1	0	-0.005340	-1.143601	4.531766
78	1	0	0.371459	-3.511188	3.826998
79	1	0	1.231874	-3.966290	1.534224
80	1	0	1.677930	-2.078442	-0.022327

81	7	0	0.476105	1.005801	3.200888
82	6	0	1.561258	0.517788	0.306934
83	8	0	1.947605	0.033396	-0.873090
84	1	0	2.323926	1.137498	0.823444
85	8	0	-0.417417	1.167368	4.016964
86	8	0	1.204532	1.903317	2.808863
87	6	0	4.690874	-0.891690	-0.588516
88	6	0	3.618646	-1.335641	-1.256772
89	8	0	3.003558	-2.091793	-1.917027
90	6	0	5.782481	-1.888694	-0.464293
91	6	0	6.778593	-1.714091	0.512118
92	6	0	5.872408	-3.029442	-1.281494
93	6	0	7.810592	-2.635362	0.663498
94	1	0	6.742471	-0.849549	1.167391
95	6	0	6.901155	-3.948997	-1.123673
96	1	0	5.128413	-3.194367	-2.053741
97	6	0	7.881776	-3.761091	-0.151313
98	1	0	8.562764	-2.469815	1.429292
99	1	0	6.939816	-4.818173	-1.773739
100	1	0	8.686500	-4.479138	-0.032940
101	6	0	4.849941	0.506576	-0.052934
102	6	0	6.020027	1.259355	-0.694591
103	1	0	4.970705	0.496508	1.039189
104	1	0	3.930509	1.044732	-0.273172
105	1	0	6.085862	2.276641	-0.296292
106	1	0	6.976350	0.759818	-0.519125
107	1	0	5.874483	1.322036	-1.777354

TS2'(SR)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-4.601530	1.031087	-1.153709
2	8	0	-3.786076	0.274406	0.111776
3	7	0	0.903407	-2.831235	0.922545
4	7	0	-0.089304	-3.605853	1.461583
5	7	0	-0.894380	-2.017564	0.153919
6	6	0	2.927683	-2.155454	2.091693
7	1	0	2.416006	-1.245055	2.383125
8	6	0	4.258378	-2.398919	2.419675
9	1	0	4.794854	-1.687942	3.038650
10	6	0	4.901624	-3.539774	1.945161

11	1	0	5.941392	-3.718514	2.199486
12	6	0	4.219510	-4.454520	1.143907
13	1	0	4.723738	-5.340884	0.774353
14	6	0	2.888654	-4.228543	0.811198
15	1	0	2.333992	-4.918363	0.183376
16	6	0	2.271168	-3.077349	1.285556
17	6	0	0.437794	-1.872793	0.113265
18	6	0	-1.170622	-3.080499	0.975282
19	6	0	-2.632250	-3.341793	1.066961
20	1	0	-3.001801	-3.024410	2.045313
21	1	0	-2.862668	-4.398766	0.928974
22	6	0	-3.170223	-2.453159	-0.080714
23	1	0	-4.133049	-2.002495	0.153270
24	1	0	-3.282538	-3.056229	-0.984988
25	6	0	-2.106850	-1.353411	-0.360326
26	1	0	-1.996487	-1.197986	-1.433693
27	6	0	-2.419725	0.006491	0.366111
28	6	0	-4.266586	0.144877	-2.778149
29	1	0	-3.238941	0.290167	-3.121914
30	1	0	-4.925346	0.539319	-3.558754
31	1	0	-4.454123	-0.931263	-2.696858
32	6	0	-4.201115	2.857033	-1.282395
33	1	0	-3.220539	3.033263	-1.733113
34	1	0	-4.202412	3.320548	-0.291558
35	1	0	-4.956002	3.363019	-1.894271
36	6	0	-6.410837	0.800177	-0.636848
37	6	0	-7.338348	1.195483	-1.794727
38	1	0	-8.386563	1.142699	-1.473081
39	1	0	-7.223707	0.524447	-2.652785
40	1	0	-7.154106	2.219705	-2.139237
41	6	0	-6.705856	1.691354	0.578490
42	1	0	-7.732737	1.526543	0.930545
43	1	0	-6.607045	2.754010	0.332718
44	1	0	-6.025977	1.472855	1.409954
45	6	0	-6.676450	-0.662663	-0.258812
46	1	0	-7.739438	-0.809061	-0.025911
47	1	0	-6.099219	-0.952901	0.625241
48	1	0	-6.420918	-1.350183	-1.074235
49	6	0	-2.257853	-0.199454	1.874101
50	6	0	-0.984342	-0.180788	2.458909
51	6	0	-3.373850	-0.457454	2.670324
52	6	0	-0.839415	-0.457025	3.814956
53	1	0	-0.104612	0.070893	1.862990
54	6	0	-3.221917	-0.730244	4.029502

55	1	0	-4.361070	-0.441373	2.220628
56	6	0	-1.954297	-0.740325	4.602831
57	1	0	-4.097882	-0.931257	4.638505
58	6	0	-1.584176	1.184854	-0.146739
59	6	0	-1.102290	1.256389	-1.456766
60	6	0	-1.464537	2.317379	0.665357
61	6	0	-0.494070	2.416204	-1.932388
62	1	0	-1.187243	0.414711	-2.136518
63	6	0	-0.864557	3.477742	0.192676
64	1	0	-1.844244	2.288575	1.681154
65	6	0	-0.369754	3.530004	-1.107250
66	1	0	-0.774078	4.339163	0.846450
67	1	0	0.151441	-0.435796	4.258070
68	1	0	-1.835131	-0.953046	5.660485
69	1	0	0.112587	4.432534	-1.469826
70	1	0	-0.116481	2.440078	-2.949980
71	6	0	2.465222	-1.509982	-1.289917
72	6	0	2.375571	-2.452277	-2.323948
73	6	0	3.497073	-3.065873	-2.883578
74	6	0	4.756723	-2.731321	-2.414466
75	6	0	4.880410	-1.783142	-1.398835
76	6	0	3.750447	-1.187632	-0.853706
77	1	0	3.360320	-3.790396	-3.675669
78	1	0	5.634430	-3.202191	-2.843038
79	1	0	5.862873	-1.511768	-1.025254
80	1	0	3.811689	-0.457551	-0.052713
81	7	0	1.080477	-2.857011	-2.883775
82	6	0	1.298859	-0.798251	-0.545148
83	8	0	1.686942	0.027780	0.445348
84	1	0	0.666700	-0.341174	-1.320909
85	8	0	1.053265	-3.779003	-3.677575
86	8	0	0.076621	-2.246713	-2.532887
87	6	0	2.816331	2.555443	-0.129868
88	6	0	2.043360	2.047988	0.847733
89	8	0	1.516508	2.072162	1.899300
90	6	0	3.534245	3.789112	0.263056
91	6	0	4.784299	4.080128	-0.311278
92	6	0	3.031635	4.698177	1.210517
93	6	0	5.491800	5.225912	0.036219
94	1	0	5.212665	3.387304	-1.029728
95	6	0	3.746023	5.837191	1.563724
96	1	0	2.068657	4.503256	1.673174
97	6	0	4.979099	6.115380	0.977014
98	1	0	6.455730	5.417929	-0.426362

99	1	0	3.329338	6.520100	2.298545
100	1	0	5.531134	7.008838	1.249747
101	6	0	3.014214	1.952578	-1.498104
102	6	0	2.879541	2.960843	-2.645333
103	1	0	2.265013	1.171435	-1.627548
104	1	0	3.991779	1.454958	-1.580431
105	1	0	2.924228	2.446146	-3.610099
106	1	0	1.927777	3.492493	-2.581662
107	1	0	3.671498	3.712434	-2.629824

TS2'(RS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-4.859842	1.076486	-0.473111
2	8	0	-3.614280	-0.040634	-0.727179
3	7	0	1.305253	-2.760853	-0.167110
4	7	0	0.396764	-3.752645	-0.437874
5	7	0	-0.391004	-1.748988	-0.922813
6	6	0	2.771855	-2.674751	1.764475
7	1	0	2.033800	-2.043754	2.249562
8	6	0	3.983659	-3.000447	2.366580
9	1	0	4.180907	-2.675096	3.382425
10	6	0	4.942836	-3.726532	1.664225
11	1	0	5.888134	-3.970941	2.137937
12	6	0	4.697576	-4.140173	0.355463
13	1	0	5.448311	-4.702588	-0.188914
14	6	0	3.488813	-3.829062	-0.257540
15	1	0	3.270973	-4.134514	-1.275484
16	6	0	2.552250	-3.094293	0.458149
17	6	0	0.852933	-1.541200	-0.473309
18	6	0	-0.625544	-3.098099	-0.896435
19	6	0	-1.981318	-3.423574	-1.418231
20	1	0	-2.638004	-3.700819	-0.589688
21	1	0	-1.953995	-4.245924	-2.133962
22	6	0	-2.382601	-2.074210	-2.064601
23	1	0	-3.447281	-1.865254	-1.986629
24	1	0	-2.108432	-2.087593	-3.122072
25	6	0	-1.550215	-0.959615	-1.369304
26	1	0	-1.205579	-0.212914	-2.085956
27	6	0	-2.317974	-0.238812	-0.184465
28	6	0	-4.905985	2.248007	-1.942606

29	1	0	-4.978185	1.697876	-2.886812
30	1	0	-4.014402	2.876906	-1.978964
31	1	0	-5.775429	2.908596	-1.873142
32	6	0	-4.679822	2.035411	1.125270
33	1	0	-3.902491	2.800957	1.046274
34	1	0	-4.429656	1.378740	1.964613
35	1	0	-5.628380	2.533174	1.357347
36	6	0	-6.484040	0.070201	-0.460886
37	6	0	-7.622745	0.972035	-0.968913
38	1	0	-8.581586	0.445078	-0.880339
39	1	0	-7.489269	1.244115	-2.020388
40	1	0	-7.704451	1.898552	-0.387550
41	6	0	-6.855698	-0.388653	0.958305
42	1	0	-7.771491	-0.993630	0.928212
43	1	0	-7.049102	0.468721	1.611520
44	1	0	-6.075908	-0.990295	1.433890
45	6	0	-6.379923	-1.142919	-1.396608
46	1	0	-7.351145	-1.650639	-1.466160
47	1	0	-5.647842	-1.876717	-1.044617
48	1	0	-6.088462	-0.846829	-2.411482
49	6	0	-2.383362	-1.191415	1.013145
50	6	0	-1.274986	-1.417511	1.843910
51	6	0	-3.539882	-1.942622	1.220925
52	6	0	-1.343669	-2.374529	2.852825
53	1	0	-0.352305	-0.847070	1.713453
54	6	0	-3.607806	-2.894186	2.237420
55	1	0	-4.385873	-1.790154	0.563525
56	6	0	-2.506234	-3.115761	3.056312
57	1	0	-4.522372	-3.461933	2.380161
58	6	0	-1.721664	1.150034	0.119545
59	6	0	-1.698168	2.074287	-0.935887
60	6	0	-1.399993	1.606542	1.398621
61	6	0	-1.431517	3.420710	-0.713390
62	1	0	-1.955776	1.748378	-1.940169
63	6	0	-1.105396	2.953168	1.620534
64	1	0	-1.392289	0.935711	2.247385
65	6	0	-1.144271	3.869115	0.575978
66	1	0	-0.853154	3.274674	2.626177
67	1	0	-0.478444	-2.535177	3.488916
68	1	0	-2.551774	-3.857970	3.846932
69	1	0	-0.928018	4.917242	0.755890
70	1	0	-1.443680	4.116754	-1.546483
71	6	0	2.982702	-0.264544	-0.776293
72	6	0	3.371855	-0.235969	-2.118996

73	6	0	4.702973	-0.295034	-2.528536
74	6	0	5.695475	-0.411325	-1.569135
75	6	0	5.346185	-0.401543	-0.218440
76	6	0	4.015124	-0.300310	0.162232
77	1	0	4.931492	-0.248374	-3.586029
78	1	0	6.734087	-0.484501	-1.872702
79	1	0	6.118050	-0.461092	0.542845
80	1	0	3.720367	-0.234286	1.203436
81	7	0	2.376725	-0.085270	-3.179775
82	6	0	1.536724	-0.203169	-0.220437
83	8	0	1.458259	0.042328	1.101793
84	1	0	0.971668	0.499766	-0.859572
85	8	0	2.732712	0.387971	-4.243211
86	8	0	1.226572	-0.443057	-2.950822
87	6	0	2.609615	2.505550	2.002331
88	6	0	1.758307	1.612059	2.521566
89	8	0	1.117621	1.106145	3.370202
90	6	0	2.892073	2.722526	0.573986
91	6	0	4.188381	3.024116	0.130852
92	6	0	1.870112	2.689528	-0.380843
93	6	0	4.454058	3.231111	-1.219628
94	1	0	5.004338	3.060437	0.848109
95	6	0	2.131304	2.892881	-1.732038
96	1	0	0.868666	2.458091	-0.042994
97	6	0	3.428802	3.161992	-2.162415
98	1	0	5.471476	3.436642	-1.539644
99	1	0	1.314051	2.834832	-2.448182
100	1	0	3.639685	3.308406	-3.217204
101	6	0	3.176263	3.486099	3.024025
102	6	0	2.681197	4.915702	2.797332
103	1	0	4.273501	3.468686	2.980804
104	1	0	2.908784	3.156074	4.032541
105	1	0	3.112292	5.608970	3.525839
106	1	0	2.950289	5.260791	1.794802
107	1	0	1.590902	4.956481	2.882410

M2'(SS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-5.133159	-0.139797	0.289088
2	8	0	-3.581017	-0.359363	-0.360016

3	7	0	1.188919	-2.360481	-0.370437
4	7	0	0.243134	-3.094123	-1.028482
5	7	0	-0.296447	-0.959752	-0.927996
6	6	0	2.756237	-2.811029	1.433312
7	1	0	2.172032	-2.156419	2.072682
8	6	0	3.894365	-3.469637	1.891732
9	1	0	4.211448	-3.334441	2.920127
10	6	0	4.613578	-4.303624	1.039417
11	1	0	5.494844	-4.819533	1.406468
12	6	0	4.212215	-4.475286	-0.285779
13	1	0	4.781461	-5.117185	-0.949089
14	6	0	3.086536	-3.816693	-0.764338
15	1	0	2.753660	-3.923155	-1.790702
16	6	0	2.376994	-2.999252	0.109761
17	6	0	0.899966	-1.057260	-0.328370
18	6	0	-0.645998	-2.207398	-1.363372
19	6	0	-1.915818	-2.152239	-2.148301
20	1	0	-2.759798	-2.480100	-1.534931
21	1	0	-1.866033	-2.764175	-3.048868
22	6	0	-2.000874	-0.631843	-2.430868
23	1	0	-3.021524	-0.289854	-2.585467
24	1	0	-1.394148	-0.389110	-3.308272
25	6	0	-1.349737	0.036354	-1.197897
26	1	0	-0.876428	0.984926	-1.439374
27	6	0	-2.355042	0.236649	0.038567
28	6	0	-5.851722	1.530452	-0.177391
29	1	0	-5.357586	2.345304	0.360078
30	1	0	-6.916130	1.556354	0.078793
31	1	0	-5.755493	1.728852	-1.249124
32	6	0	-5.149257	-0.322030	2.155752
33	1	0	-4.534661	0.447376	2.631746
34	1	0	-4.779001	-1.294450	2.488878
35	1	0	-6.173694	-0.196669	2.522945
36	6	0	-6.115132	-1.529663	-0.551053
37	6	0	-7.602745	-1.390073	-0.194475
38	1	0	-8.174662	-2.211552	-0.644914
39	1	0	-8.025152	-0.452276	-0.569648
40	1	0	-7.769186	-1.429854	0.888074
41	6	0	-5.621952	-2.904623	-0.081713
42	1	0	-6.206926	-3.700918	-0.560260
43	1	0	-5.721067	-3.028041	1.002404
44	1	0	-4.571532	-3.069657	-0.346229
45	6	0	-5.951162	-1.433931	-2.073940
46	1	0	-6.543705	-2.213367	-2.570784

47	1	0	-4.905339	-1.571115	-2.370198
48	1	0	-6.288312	-0.465562	-2.460460
49	6	0	-1.811331	-0.490302	1.272770
50	6	0	-0.825735	0.059683	2.090752
51	6	0	-2.207720	-1.813217	1.510733
52	6	0	-0.268015	-0.673142	3.138388
53	1	0	-0.446285	1.061931	1.934672
54	6	0	-1.653255	-2.548296	2.552343
55	1	0	-2.963408	-2.264724	0.877340
56	6	0	-0.682585	-1.977592	3.376355
57	1	0	-1.978610	-3.570662	2.717737
58	6	0	-2.582216	1.745693	0.216253
59	6	0	-2.791243	2.525916	-0.928525
60	6	0	-2.716992	2.355256	1.464650
61	6	0	-3.099705	3.876814	-0.832425
62	1	0	-2.728967	2.073711	-1.915472
63	6	0	-3.022668	3.712875	1.565212
64	1	0	-2.580472	1.778703	2.371914
65	6	0	-3.211296	4.478828	0.420120
66	1	0	-3.112413	4.166679	2.546623
67	1	0	0.514741	-0.197699	3.721021
68	1	0	-0.248407	-2.552842	4.188221
69	1	0	-3.448418	5.534665	0.500531
70	1	0	-3.257237	4.458582	-1.735105
71	6	0	1.552965	1.291141	-0.765130
72	6	0	1.831879	1.446112	-2.129418
73	6	0	1.458837	2.580215	-2.850408
74	6	0	0.765848	3.593270	-2.207038
75	6	0	0.500458	3.482658	-0.841913
76	6	0	0.901216	2.356404	-0.132606
77	1	0	1.714813	2.640221	-3.901015
78	1	0	0.451007	4.469515	-2.762929
79	1	0	-0.024907	4.275735	-0.319642
80	1	0	0.741224	2.318383	0.939814
81	7	0	2.531342	0.409239	-2.897596
82	6	0	1.908378	0.027320	0.015539
83	8	0	1.963267	0.168220	1.401063
84	1	0	2.853137	-0.366512	-0.376895
85	8	0	3.196473	0.761548	-3.850924
86	8	0	2.383334	-0.760263	-2.562994
87	6	0	3.701935	1.880494	1.399442
88	6	0	2.556950	1.368312	1.979815
89	8	0	1.840758	1.843649	2.878946
90	6	0	4.531756	1.133899	0.453371

91	6	0	4.928617	1.684635	-0.782268
92	6	0	4.906535	-0.201376	0.703169
93	6	0	5.605272	0.926761	-1.732946
94	1	0	4.653558	2.711990	-1.011270
95	6	0	5.562868	-0.967782	-0.254347
96	1	0	4.638904	-0.636908	1.661419
97	6	0	5.909384	-0.412179	-1.485324
98	1	0	5.867183	1.374582	-2.687341
99	1	0	5.806087	-2.003761	-0.034095
100	1	0	6.417285	-1.007627	-2.237031
101	6	0	4.057314	3.295721	1.794207
102	6	0	4.693692	3.382843	3.185916
103	1	0	3.152208	3.919415	1.786547
104	1	0	4.745744	3.720142	1.053372
105	1	0	4.930506	4.415785	3.464738
106	1	0	3.996160	2.972687	3.920072
107	1	0	5.616986	2.796254	3.222293

M2'(RR)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-5.172430	-0.542749	-0.695820
2	8	0	-3.791544	0.067845	0.080078
3	7	0	0.720177	2.765800	0.456513
4	7	0	-0.405534	3.458203	0.806031
5	7	0	-0.697654	1.273733	0.946328
6	6	0	2.379119	3.391324	-1.206102
7	1	0	1.797335	2.853778	-1.947786
8	6	0	3.581419	4.016548	-1.520992
9	1	0	3.951840	3.985235	-2.539598
10	6	0	4.312505	4.667136	-0.528612
11	1	0	5.254010	5.144216	-0.780288
12	6	0	3.849916	4.702414	0.785901
13	1	0	4.426069	5.204525	1.555102
14	6	0	2.648938	4.083904	1.117818
15	1	0	2.268714	4.078209	2.134012
16	6	0	1.938163	3.440841	0.111239
17	6	0	0.574978	1.446695	0.573332
18	6	0	-1.249867	2.517672	1.107891
19	6	0	-2.626717	2.403162	1.676514
20	1	0	-3.377556	2.488368	0.886025

21	1	0	-2.816612	3.157712	2.439422
22	6	0	-2.572695	0.956844	2.226603
23	1	0	-3.555062	0.499851	2.315063
24	1	0	-2.077557	0.959721	3.202518
25	6	0	-1.666061	0.197296	1.231486
26	1	0	-1.133128	-0.629341	1.696320
27	6	0	-2.438608	-0.331783	-0.075803
28	6	0	-5.661228	-2.224895	-0.020394
29	1	0	-5.000271	-3.012735	-0.394254
30	1	0	-6.681520	-2.465696	-0.336991
31	1	0	-5.629597	-2.250703	1.072689
32	6	0	-4.950901	-0.675437	-2.553625
33	1	0	-4.120667	-1.339503	-2.809670
34	1	0	-4.764359	0.289151	-3.031765
35	1	0	-5.860076	-1.105872	-2.987744
36	6	0	-6.490668	0.745850	-0.253132
37	6	0	-7.834993	0.327245	-0.868076
38	1	0	-8.604614	1.072157	-0.628118
39	1	0	-8.181982	-0.636662	-0.481415
40	1	0	-7.778423	0.254722	-1.959926
41	6	0	-6.110268	2.128254	-0.798763
42	1	0	-6.903743	2.854094	-0.578067
43	1	0	-5.966116	2.117844	-1.885105
44	1	0	-5.189830	2.501976	-0.337535
45	6	0	-6.636453	0.836515	1.271985
46	1	0	-7.413872	1.564914	1.537625
47	1	0	-5.701059	1.163784	1.740371
48	1	0	-6.920464	-0.125643	1.712691
49	6	0	-1.853026	0.320510	-1.330554
50	6	0	-0.648486	-0.117506	-1.879055
51	6	0	-2.455416	1.460207	-1.876686
52	6	0	-0.065342	0.535622	-2.962204
53	1	0	-0.127909	-0.971420	-1.465890
54	6	0	-1.878709	2.116026	-2.960501
55	1	0	-3.384348	1.831353	-1.457341
56	6	0	-0.684519	1.652501	-3.512404
57	1	0	-2.364951	2.994382	-3.373411
58	6	0	-2.375418	-1.868677	-0.052752
59	6	0	-2.643222	-2.518013	1.159457
60	6	0	-2.184677	-2.650695	-1.192916
61	6	0	-2.689866	-3.903633	1.240655
62	1	0	-2.841319	-1.935860	2.056617
63	6	0	-2.229183	-4.043335	-1.115250
64	1	0	-1.995597	-2.181918	-2.151643

65	6	0	-2.476306	-4.674787	0.099263
66	1	0	-2.067548	-4.630616	-2.013249
67	1	0	0.883485	0.157342	-3.329895
68	1	0	-0.238782	2.165859	-4.358702
69	1	0	-2.508839	-5.757942	0.156154
70	1	0	-2.898323	-4.381263	2.192788
71	6	0	1.407201	-0.813633	1.234865
72	6	0	1.321337	-0.907722	2.635318
73	6	0	0.953588	-2.081237	3.288784
74	6	0	0.640928	-3.206364	2.540169
75	6	0	0.750861	-3.154165	1.154234
76	6	0	1.143659	-1.981843	0.514481
77	1	0	0.911837	-2.086882	4.370632
78	1	0	0.326547	-4.117046	3.037747
79	1	0	0.522484	-4.030225	0.555827
80	1	0	1.291319	-1.980080	-0.561444
81	7	0	1.586750	0.240556	3.512876
82	6	0	1.742962	0.481116	0.492398
83	8	0	2.032545	0.366681	-0.862540
84	1	0	2.547136	0.987692	1.041928
85	8	0	1.903113	0.017634	4.663619
86	8	0	1.453618	1.369429	3.052194
87	6	0	4.299562	-0.495673	-0.767251
88	6	0	3.033926	-0.602597	-1.318526
89	8	0	2.535329	-1.392216	-2.139879
90	6	0	5.251989	-1.602267	-0.917662
91	6	0	6.389427	-1.676934	-0.081189
92	6	0	5.096593	-2.654875	-1.848724
93	6	0	7.301421	-2.722538	-0.163865
94	1	0	6.557941	-0.904738	0.663357
95	6	0	6.011830	-3.698024	-1.925636
96	1	0	4.242282	-2.634834	-2.511130
97	6	0	7.125401	-3.748235	-1.089230
98	1	0	8.157957	-2.734351	0.505244
99	1	0	5.854313	-4.482370	-2.661907
100	1	0	7.839507	-4.562695	-1.159649
101	6	0	4.776797	0.774730	-0.092607
102	6	0	5.959077	1.433112	-0.819913
103	1	0	5.050372	0.615655	0.963331
104	1	0	3.976534	1.517834	-0.094699
105	1	0	6.283765	2.340060	-0.298236
106	1	0	6.814317	0.758523	-0.904223
107	1	0	5.655929	1.710948	-1.834160

M2'(SR)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-4.923037	-1.348593	0.476259
2	8	0	-4.057983	-0.062559	-0.194105
3	7	0	0.884710	2.693724	0.621836
4	7	0	-0.083131	3.611112	0.900196
5	7	0	-0.896844	1.556367	0.859512
6	6	0	2.789132	3.126243	-0.840875
7	1	0	2.252761	2.681589	-1.669425
8	6	0	4.099847	3.574237	-0.993031
9	1	0	4.566821	3.508943	-1.968952
10	6	0	4.805933	4.065797	0.100111
11	1	0	5.827505	4.408676	-0.027119
12	6	0	4.212163	4.115621	1.362824
13	1	0	4.765288	4.498596	2.213464
14	6	0	2.911211	3.661837	1.534351
15	1	0	2.427511	3.675123	2.505464
16	6	0	2.230885	3.164095	0.426835
17	6	0	0.418944	1.440390	0.600518
18	6	0	-1.154095	2.891591	1.033157
19	6	0	-2.581963	3.159528	1.340197
20	1	0	-3.074396	3.573145	0.456289
21	1	0	-2.692964	3.862108	2.166478
22	6	0	-3.079099	1.738653	1.680505
23	1	0	-4.107749	1.570097	1.371061
24	1	0	-3.012508	1.580634	2.759746
25	6	0	-2.126998	0.726287	0.985660
26	1	0	-1.914501	-0.099615	1.658502
27	6	0	-2.678525	0.184991	-0.387252
28	6	0	-4.350884	-1.671964	2.237084
29	1	0	-3.331813	-2.066352	2.276380
30	1	0	-5.001258	-2.418060	2.705279
31	1	0	-4.392233	-0.765268	2.850165
32	6	0	-4.832641	-2.901869	-0.567035
33	1	0	-3.861317	-3.397526	-0.493827
34	1	0	-5.013843	-2.670347	-1.620606
35	1	0	-5.601385	-3.610703	-0.239978
36	6	0	-6.694711	-0.675172	0.467592

37	6	0	-7.610025	-1.622069	1.257797
38	1	0	-8.649763	-1.275042	1.200402
39	1	0	-7.334819	-1.661886	2.317343
40	1	0	-7.584777	-2.643734	0.862299
41	6	0	-7.194401	-0.576445	-0.981353
42	1	0	-8.196930	-0.129584	-1.006650
43	1	0	-7.260460	-1.562465	-1.453025
44	1	0	-6.532852	0.047487	-1.592976
45	6	0	-6.746415	0.717705	1.107943
46	1	0	-7.783922	1.073207	1.159138
47	1	0	-6.176153	1.445805	0.520997
48	1	0	-6.349587	0.714648	2.130384
49	6	0	-2.555479	1.289606	-1.439779
50	6	0	-1.335810	1.531476	-2.082256
51	6	0	-3.646869	2.111469	-1.724903
52	6	0	-1.204621	2.597952	-2.965778
53	1	0	-0.481770	0.879993	-1.910634
54	6	0	-3.514378	3.176169	-2.615702
55	1	0	-4.600700	1.908464	-1.249555
56	6	0	-2.292229	3.428182	-3.231115
57	1	0	-4.372482	3.805015	-2.831430
58	6	0	-2.023411	-1.133683	-0.824541
59	6	0	-1.501886	-2.062341	0.083878
60	6	0	-2.155335	-1.518931	-2.163698
61	6	0	-1.131392	-3.339916	-0.335412
62	1	0	-1.368500	-1.821676	1.133416
63	6	0	-1.784382	-2.791322	-2.582818
64	1	0	-2.570271	-0.817555	-2.880631
65	6	0	-1.279561	-3.711784	-1.667111
66	1	0	-1.897814	-3.066522	-3.626217
67	1	0	-0.250934	2.769010	-3.454866
68	1	0	-2.189908	4.257253	-3.923707
69	1	0	-0.991175	-4.705623	-1.993056
70	1	0	-0.716676	-4.036695	0.386779
71	6	0	2.402082	-0.013488	1.236510
72	6	0	2.271539	-0.799231	2.387973
73	6	0	3.340049	-1.152198	3.209321
74	6	0	4.603287	-0.681030	2.894321
75	6	0	4.772992	0.114238	1.762382
76	6	0	3.693010	0.438209	0.947819
77	1	0	3.155909	-1.779570	4.073162
78	1	0	5.450508	-0.942165	3.518211
79	1	0	5.760587	0.465088	1.483046
80	1	0	3.875778	1.000279	0.038804

81	7	0	0.963090	-1.292985	2.802011
82	6	0	1.229473	0.198447	0.260576
83	8	0	1.567461	0.368055	-1.091595
84	1	0	0.541059	-0.643405	0.380086
85	8	0	0.883228	-2.391177	3.312511
86	8	0	0.001194	-0.546285	2.632601
87	6	0	3.127469	-1.491541	-1.302239
88	6	0	2.818979	-0.182756	-1.651766
89	8	0	3.430070	0.676411	-2.290791
90	6	0	4.534646	-1.869186	-1.210055
91	6	0	4.926376	-2.900511	-0.323480
92	6	0	5.581458	-1.191866	-1.878165
93	6	0	6.259915	-3.233306	-0.120847
94	1	0	4.165796	-3.432172	0.241175
95	6	0	6.913749	-1.529513	-1.668082
96	1	0	5.326178	-0.395984	-2.564596
97	6	0	7.273517	-2.552760	-0.792904
98	1	0	6.508362	-4.030204	0.575667
99	1	0	7.685599	-0.985820	-2.207488
100	1	0	8.315817	-2.814277	-0.639781
101	6	0	2.061285	-2.455064	-0.846249
102	6	0	2.102323	-3.788451	-1.606381
103	1	0	1.082187	-2.007893	-1.040454
104	1	0	2.094889	-2.663638	0.242198
105	1	0	1.394643	-4.509599	-1.185419
106	1	0	1.843422	-3.625256	-2.656768
107	1	0	3.097896	-4.237271	-1.577413

M2'(RS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.796662	-1.244788	-0.240835
2	8	0	3.878715	0.135995	0.084008
3	7	0	-1.113656	2.454528	-0.838616
4	7	0	-0.180668	3.244152	-1.442773
5	7	0	0.576483	1.199099	-1.108477
6	6	0	-2.751933	3.046200	0.863077
7	1	0	-2.153241	2.555354	1.622580
8	6	0	-3.989704	3.596461	1.188920
9	1	0	-4.319921	3.563429	2.220975
10	6	0	-4.795883	4.150368	0.198603

11	1	0	-5.759371	4.575364	0.460734
12	6	0	-4.375228	4.159257	-1.132641
13	1	0	-5.005545	4.591526	-1.902093
14	6	0	-3.151346	3.600883	-1.477925
15	1	0	-2.805153	3.578608	-2.505613
16	6	0	-2.369646	3.044613	-0.470625
17	6	0	-0.685776	1.198579	-0.652533
18	6	0	0.835252	2.451318	-1.597692
19	6	0	2.188319	2.543482	-2.209205
20	1	0	2.838519	3.172767	-1.599169
21	1	0	2.139449	2.963143	-3.214918
22	6	0	2.611998	1.055513	-2.202459
23	1	0	3.678890	0.927911	-2.042838
24	1	0	2.342011	0.598219	-3.157932
25	6	0	1.788097	0.346988	-1.094530
26	1	0	1.523657	-0.659572	-1.408462
27	6	0	2.498416	0.329512	0.322261
28	6	0	4.095612	-2.159107	-1.726157
29	1	0	3.107399	-2.578328	-1.512854
30	1	0	4.749497	-2.998452	-1.984632
31	1	0	4.013638	-1.518125	-2.609909
32	6	0	4.932530	-2.398684	1.229154
33	1	0	4.005071	-2.950755	1.405386
34	1	0	5.172591	-1.846782	2.142114
35	1	0	5.732132	-3.125941	1.051198
36	6	0	6.493490	-0.496819	-0.630957
37	6	0	7.439912	-1.594653	-1.138688
38	1	0	8.437743	-1.175276	-1.321163
39	1	0	7.088874	-2.030311	-2.080618
40	1	0	7.555474	-2.406171	-0.411513
41	6	0	7.073492	0.123533	0.648674
42	1	0	8.034790	0.608594	0.434197
43	1	0	7.250919	-0.634520	1.418949
44	1	0	6.400181	0.879856	1.067508
45	6	0	6.371484	0.592680	-1.703514
46	1	0	7.363510	0.989170	-1.956451
47	1	0	5.760241	1.430961	-1.351217
48	1	0	5.927798	0.207196	-2.629706
49	6	0	2.337574	1.699950	0.992531
50	6	0	1.160080	2.029588	1.676865
51	6	0	3.353469	2.650008	0.893885
52	6	0	0.991609	3.304338	2.208422
53	1	0	0.374010	1.287849	1.813170
54	6	0	3.183750	3.925502	1.432093

55	1	0	4.278520	2.382289	0.393811
56	6	0	1.999608	4.259129	2.080630
57	1	0	3.982644	4.655237	1.345804
58	6	0	2.019831	-0.800954	1.245563
59	6	0	1.425199	-1.982182	0.798797
60	6	0	2.393683	-0.713001	2.594580
61	6	0	1.224077	-3.050381	1.677962
62	1	0	1.105034	-2.109143	-0.232533
63	6	0	2.178717	-1.766907	3.470156
64	1	0	2.871715	0.193298	2.952899
65	6	0	1.594889	-2.946777	3.011525
66	1	0	2.473151	-1.670969	4.510060
67	1	0	0.075069	3.545668	2.737255
68	1	0	1.866103	5.251513	2.498698
69	1	0	1.426461	-3.775923	3.690457
70	1	0	0.756474	-3.960698	1.317455
71	6	0	-2.719446	-0.187931	-1.044198
72	6	0	-2.733493	-1.002113	-2.188230
73	6	0	-3.891856	-1.263510	-2.914492
74	6	0	-5.086595	-0.685312	-2.515640
75	6	0	-5.103785	0.146489	-1.400431
76	6	0	-3.941110	0.382921	-0.674137
77	1	0	-3.832347	-1.912580	-3.778390
78	1	0	-5.994476	-0.880627	-3.075423
79	1	0	-6.029084	0.612611	-1.078000
80	1	0	-3.991511	1.004481	0.209544
81	7	0	-1.513177	-1.611006	-2.724745
82	6	0	-1.486551	0.004655	-0.148724
83	8	0	-1.695140	0.218394	1.218119
84	1	0	-0.834138	-0.858350	-0.289572
85	8	0	-1.615013	-2.560451	-3.471761
86	8	0	-0.436099	-1.100614	-2.426278
87	6	0	-3.630432	-1.228348	1.815276
88	6	0	-2.879389	-0.077963	2.036691
89	8	0	-3.073911	0.843208	2.837241
90	6	0	-3.285276	-2.308315	0.910152
91	6	0	-4.277875	-2.990379	0.168450
92	6	0	-1.954807	-2.729649	0.702865
93	6	0	-3.949932	-3.952935	-0.776889
94	1	0	-5.321474	-2.726733	0.312638
95	6	0	-1.626536	-3.674860	-0.263652
96	1	0	-1.181849	-2.283449	1.320720
97	6	0	-2.619384	-4.290409	-1.024883
98	1	0	-4.743018	-4.433558	-1.344009

99	1	0	-0.584592	-3.945933	-0.425070
100	1	0	-2.362918	-5.022747	-1.783007
101	6	0	-5.002715	-1.229739	2.454332
102	6	0	-5.293210	-2.465241	3.310915
103	1	0	-5.787752	-1.138882	1.682655
104	1	0	-5.082600	-0.332568	3.071721
105	1	0	-6.300740	-2.430052	3.738665
106	1	0	-5.208416	-3.384525	2.722640
107	1	0	-4.573049	-2.531497	4.131536

TS3'(SS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-5.110341	-0.725869	0.123782
2	8	0	-3.479971	-0.518506	-0.266874
3	7	0	0.975688	-2.069791	-0.451580
4	7	0	0.208151	-2.547591	-1.492714
5	7	0	-0.413934	-0.551105	-0.808125
6	6	0	2.373169	-2.785966	1.393997
7	1	0	1.805324	-2.124153	2.040934
8	6	0	3.407567	-3.581190	1.878837
9	1	0	3.662032	-3.541425	2.933132
10	6	0	4.098703	-4.435730	1.023477
11	1	0	4.894935	-5.063727	1.410528
12	6	0	3.773813	-4.479823	-0.331608
13	1	0	4.322495	-5.132728	-1.002158
14	6	0	2.750545	-3.685030	-0.834508
15	1	0	2.479284	-3.699971	-1.883666
16	6	0	2.053691	-2.855082	0.040060
17	6	0	0.650381	-0.838303	-0.013391
18	6	0	-0.631910	-1.579014	-1.683296
19	6	0	-1.740755	-1.257087	-2.626723
20	1	0	-2.632689	-1.834432	-2.378662
21	1	0	-1.463314	-1.461418	-3.661665
22	6	0	-1.952701	0.252422	-2.343212
23	1	0	-3.001139	0.532186	-2.441589
24	1	0	-1.357132	0.847535	-3.043286
25	6	0	-1.417469	0.510291	-0.907144
26	1	0	-0.928292	1.478692	-0.813698
27	6	0	-2.522227	0.413463	0.209569
28	6	0	-6.135692	0.720715	-0.493832

29	1	0	-6.029200	1.603945	0.142007
30	1	0	-7.195994	0.445836	-0.522091
31	1	0	-5.834412	0.999581	-1.508580
32	6	0	-5.383110	-1.018403	1.958268
33	1	0	-5.056870	-0.180093	2.576354
34	1	0	-4.856193	-1.913447	2.302555
35	1	0	-6.453471	-1.162789	2.140106
36	6	0	-5.565674	-2.295476	-0.838758
37	6	0	-6.941890	-2.801547	-0.380776
38	1	0	-7.240799	-3.672195	-0.978725
39	1	0	-7.720875	-2.039515	-0.500794
40	1	0	-6.930811	-3.111783	0.669341
41	6	0	-4.523476	-3.392343	-0.580152
42	1	0	-4.780471	-4.302596	-1.137231
43	1	0	-4.479582	-3.660416	0.482350
44	1	0	-3.518507	-3.081973	-0.884030
45	6	0	-5.630285	-1.978776	-2.339779
46	1	0	-5.809783	-2.894837	-2.917498
47	1	0	-4.700294	-1.529958	-2.706769
48	1	0	-6.443895	-1.280551	-2.564252
49	6	0	-1.871396	-0.117727	1.486380
50	6	0	-1.098212	0.720090	2.292616
51	6	0	-1.905603	-1.484124	1.768710
52	6	0	-0.361516	0.205165	3.354640
53	1	0	-1.069897	1.784399	2.081155
54	6	0	-1.181398	-2.000059	2.840663
55	1	0	-2.482595	-2.145116	1.129724
56	6	0	-0.403604	-1.158585	3.632696
57	1	0	-1.214179	-3.065318	3.047447
58	6	0	-3.161150	1.798782	0.409314
59	6	0	-3.246312	2.726112	-0.634738
60	6	0	-3.749996	2.134411	1.633765
61	6	0	-3.919553	3.933853	-0.468688
62	1	0	-2.782508	2.528092	-1.594954
63	6	0	-4.425533	3.339529	1.803126
64	1	0	-3.662854	1.452389	2.472543
65	6	0	-4.519700	4.242874	0.747925
66	1	0	-4.872450	3.572377	2.764308
67	1	0	0.261066	0.865444	3.950165
68	1	0	0.171187	-1.563973	4.459598
69	1	0	-5.044172	5.184080	0.876447
70	1	0	-3.971684	4.634645	-1.295855
71	6	0	1.613589	1.643040	-0.332206
72	6	0	1.522639	1.921876	-1.710801

73	6	0	0.889645	3.067342	-2.201088
74	6	0	0.292368	3.959072	-1.328437
75	6	0	0.368397	3.712604	0.047670
76	6	0	1.014773	2.588402	0.529492
77	1	0	0.865894	3.221408	-3.272733
78	1	0	-0.222057	4.834046	-1.708371
79	1	0	-0.093725	4.400406	0.749025
80	1	0	1.068790	2.410870	1.597683
81	7	0	2.037457	1.003382	-2.727951
82	6	0	2.214240	0.436254	0.251286
83	8	0	2.330730	0.357807	1.641511
84	1	0	2.779949	-0.262216	-0.343539
85	8	0	2.261950	1.455542	-3.838219
86	8	0	2.187320	-0.175121	-2.436970
87	6	0	4.042802	1.544703	0.656597
88	6	0	3.321064	1.292352	1.909832
89	8	0	3.339348	1.870670	2.967299
90	6	0	4.967694	0.541441	0.121867
91	6	0	5.651400	0.775956	-1.087056
92	6	0	5.169367	-0.703806	0.749224
93	6	0	6.485934	-0.186819	-1.640706
94	1	0	5.522212	1.721952	-1.603552
95	6	0	6.004117	-1.663211	0.189780
96	1	0	4.672661	-0.917552	1.692002
97	6	0	6.669598	-1.414632	-1.008779
98	1	0	6.995697	0.025226	-2.575758
99	1	0	6.139431	-2.610593	0.701549
100	1	0	7.325452	-2.163460	-1.440394
101	6	0	4.313931	3.007338	0.386042
102	6	0	5.635485	3.496697	0.989399
103	1	0	3.489535	3.598503	0.799997
104	1	0	4.300861	3.189880	-0.696591
105	1	0	5.789654	4.561007	0.789384
106	1	0	5.625216	3.344223	2.071732
107	1	0	6.481887	2.941983	0.574740

TS3'(RR)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	5.172783	0.121309	0.041887
2	8	0	3.517274	0.155281	-0.294815

3	7	0	-0.533101	2.462539	-0.612670
4	7	0	0.260298	2.672556	-1.720087
5	7	0	0.538729	0.680752	-0.821672
6	6	0	-1.794231	3.600540	1.110828
7	1	0	-1.219289	3.051023	1.850278
8	6	0	-2.812241	4.477288	1.473343
9	1	0	-3.036603	4.631223	2.523524
10	6	0	-3.535983	5.157629	0.495472
11	1	0	-4.327822	5.840624	0.784749
12	6	0	-3.245421	4.960295	-0.853622
13	1	0	-3.812613	5.483968	-1.615727
14	6	0	-2.237899	4.079822	-1.233693
15	1	0	-2.006089	3.889433	-2.275605
16	6	0	-1.522023	3.412682	-0.242527
17	6	0	-0.420671	1.244798	-0.044880
18	6	0	0.904250	1.550600	-1.812692
19	6	0	1.900730	0.928802	-2.729671
20	1	0	2.891261	1.351036	-2.555124
21	1	0	1.633438	1.073757	-3.777230
22	6	0	1.838388	-0.556492	-2.289308
23	1	0	2.815150	-1.033096	-2.366797
24	1	0	1.126628	-1.099409	-2.918976
25	6	0	1.305243	-0.566377	-0.828266
26	1	0	0.630813	-1.401997	-0.632464
27	6	0	2.437712	-0.577599	0.262518
28	6	0	5.927577	-1.519304	-0.473451
29	1	0	5.740524	-2.315117	0.252357
30	1	0	7.011615	-1.412186	-0.591992
31	1	0	5.515712	-1.839300	-1.436048
32	6	0	5.555430	0.522867	1.836203
33	1	0	5.097789	-0.175871	2.538615
34	1	0	5.220650	1.530634	2.100082
35	1	0	6.639512	0.476321	1.985561
36	6	0	5.845673	1.503702	-1.067843
37	6	0	7.292730	1.828700	-0.666514
38	1	0	7.716353	2.571784	-1.354364
39	1	0	7.939245	0.943927	-0.702773
40	1	0	7.347337	2.246103	0.344409
41	6	0	4.993852	2.770706	-0.908728
42	1	0	5.377228	3.572290	-1.553407
43	1	0	5.018546	3.141063	0.123369
44	1	0	3.945192	2.597207	-1.171053
45	6	0	5.832063	1.040508	-2.532022
46	1	0	6.119423	1.864940	-3.197413

47	1	0	4.843120	0.687520	-2.845426
48	1	0	6.539475	0.220432	-2.695399
49	6	0	1.906897	0.134191	1.506220
50	6	0	1.005521	-0.511497	2.355864
51	6	0	2.182704	1.485622	1.712844
52	6	0	0.373093	0.182995	3.381375
53	1	0	0.791542	-1.565182	2.203186
54	6	0	1.565316	2.178475	2.752754
55	1	0	2.859200	1.999842	1.037447
56	6	0	0.654031	1.532241	3.583528
57	1	0	1.786871	3.230797	2.902506
58	6	0	2.853087	-2.027264	0.563060
59	6	0	2.741880	-3.044979	-0.389885
60	6	0	3.432960	-2.344044	1.797101
61	6	0	3.225860	-4.325205	-0.131012
62	1	0	2.269358	-2.861294	-1.348495
63	6	0	3.918801	-3.621206	2.058961
64	1	0	3.489372	-1.585619	2.570565
65	6	0	3.825893	-4.616865	1.089733
66	1	0	4.365168	-3.836899	3.024395
67	1	0	-0.354759	-0.322622	4.008376
68	1	0	0.160298	2.076297	4.382539
69	1	0	4.204764	-5.613939	1.289265
70	1	0	3.128044	-5.096047	-0.888614
71	6	0	-1.920919	-0.969735	-0.157821
72	6	0	-2.033611	-1.394720	-1.495093
73	6	0	-1.780286	-2.708186	-1.887611
74	6	0	-1.371019	-3.642707	-0.950735
75	6	0	-1.261255	-3.256057	0.386832
76	6	0	-1.538651	-1.953360	0.772598
77	1	0	-1.903552	-2.966918	-2.932037
78	1	0	-1.153141	-4.659822	-1.254748
79	1	0	-0.953935	-3.977479	1.137651
80	1	0	-1.470196	-1.667785	1.815839
81	7	0	-2.403893	-0.471228	-2.566593
82	6	0	-2.178863	0.395448	0.323444
83	8	0	-2.268155	0.586010	1.706846
84	1	0	-2.573281	1.150159	-0.333479
85	8	0	-2.885771	-0.937816	-3.582789
86	8	0	-2.186421	0.724965	-2.410034
87	6	0	-4.250527	-0.065631	0.759411
88	6	0	-3.466982	-0.066314	1.999128
89	8	0	-3.608169	-0.600749	3.071406
90	6	0	-4.870743	-1.293150	0.281231

91	6	0	-5.504225	-1.315969	-0.980215
92	6	0	-4.721837	-2.528108	0.948824
93	6	0	-5.945506	-2.504529	-1.548012
94	1	0	-5.637210	-0.390079	-1.532417
95	6	0	-5.168505	-3.711627	0.376019
96	1	0	-4.261064	-2.546546	1.929809
97	6	0	-5.777637	-3.714374	-0.877389
98	1	0	-6.418916	-2.483644	-2.525140
99	1	0	-5.039123	-4.644781	0.916951
100	1	0	-6.124468	-4.642485	-1.320050
101	6	0	-4.796913	1.284410	0.320218
102	6	0	-6.236784	1.523811	0.782678
103	1	0	-4.738039	1.384907	-0.772563
104	1	0	-4.157778	2.077411	0.727559
105	1	0	-6.587826	2.510093	0.464433
106	1	0	-6.911895	0.768461	0.371298
107	1	0	-6.301042	1.469662	1.873213

TS3'(SR)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.863129	-1.386745	0.322265
2	8	0	3.598009	-0.605058	-0.491150
3	7	0	-1.071820	2.412001	0.083501
4	7	0	-0.488541	3.160015	-0.917205
5	7	0	0.402600	1.158989	-0.716815
6	6	0	-2.369319	2.493083	2.123508
7	1	0	-1.684086	1.770784	2.555266
8	6	0	-3.481130	2.951583	2.821593
9	1	0	-3.660413	2.596290	3.830747
10	6	0	-4.355264	3.862522	2.231708
11	1	0	-5.221322	4.216676	2.781033
12	6	0	-4.112389	4.325528	0.939340
13	1	0	-4.790435	5.037692	0.480829
14	6	0	-3.011569	3.869927	0.223087
15	1	0	-2.817132	4.195619	-0.792165
16	6	0	-2.160804	2.946445	0.823220
17	6	0	-0.571223	1.164295	0.229468
18	6	0	0.417784	2.355957	-1.381892
19	6	0	1.497253	2.388124	-2.411620
20	1	0	2.293453	3.068008	-2.091932

21	1	0	1.119723	2.714934	-3.381352
22	6	0	1.953757	0.903422	-2.422310
23	1	0	3.027081	0.787750	-2.577610
24	1	0	1.420216	0.371796	-3.214095
25	6	0	1.517913	0.285330	-1.072236
26	1	0	1.166662	-0.736212	-1.218817
27	6	0	2.623131	0.272935	0.042209
28	6	0	4.272880	-2.850601	1.339718
29	1	0	3.824472	-2.529468	2.284490
30	1	0	5.128778	-3.493707	1.573234
31	1	0	3.534678	-3.452802	0.802950
32	6	0	5.800106	-0.216486	1.454438
33	1	0	5.117980	0.335560	2.108233
34	1	0	6.401006	0.515458	0.907637
35	1	0	6.470120	-0.802775	2.092447
36	6	0	5.953540	-1.991371	-1.103771
37	6	0	7.261460	-2.564378	-0.538551
38	1	0	7.890388	-2.942775	-1.354842
39	1	0	7.082560	-3.398546	0.148900
40	1	0	7.838509	-1.801986	-0.003227
41	6	0	6.287367	-0.836039	-2.056557
42	1	0	6.945291	-1.187853	-2.861942
43	1	0	6.810078	-0.020986	-1.541251
44	1	0	5.382098	-0.427250	-2.518099
45	6	0	5.209528	-3.083365	-1.886247
46	1	0	5.814030	-3.416813	-2.739983
47	1	0	4.254887	-2.713666	-2.276235
48	1	0	5.005610	-3.960866	-1.263134
49	6	0	3.178303	1.694080	0.176601
50	6	0	2.449859	2.711070	0.809138
51	6	0	4.365204	2.038037	-0.475131
52	6	0	2.896774	4.028995	0.786264
53	1	0	1.518641	2.478499	1.319201
54	6	0	4.817995	3.354974	-0.492435
55	1	0	4.928104	1.268016	-0.989359
56	6	0	4.082751	4.357045	0.134071
57	1	0	5.742513	3.596823	-1.007123
58	6	0	2.047503	-0.320405	1.337064
59	6	0	1.376148	-1.546988	1.255511
60	6	0	2.239316	0.239488	2.602399
61	6	0	0.858566	-2.165647	2.386925
62	1	0	1.293953	-2.049436	0.295817
63	6	0	1.727160	-0.381837	3.741394
64	1	0	2.793140	1.165039	2.712194

65	6	0	1.020187	-1.574501	3.638009
66	1	0	1.882221	0.076238	4.712941
67	1	0	2.310250	4.799932	1.275165
68	1	0	4.429408	5.385100	0.114815
69	1	0	0.607672	-2.047215	4.522966
70	1	0	0.336552	-3.114598	2.293002
71	6	0	-2.773874	0.075686	-0.556757
72	6	0	-2.698876	0.289298	-1.947923
73	6	0	-3.723225	0.898718	-2.677307
74	6	0	-4.883796	1.283780	-2.035302
75	6	0	-4.991262	1.084930	-0.652840
76	6	0	-3.955333	0.523228	0.067922
77	1	0	-3.585775	1.037217	-3.743152
78	1	0	-5.695246	1.732597	-2.595938
79	1	0	-5.891708	1.388162	-0.128290
80	1	0	-4.047051	0.412078	1.142973
81	7	0	-1.524501	-0.104341	-2.701934
82	6	0	-1.646597	-0.413506	0.251971
83	8	0	-1.822131	-0.574778	1.638243
84	1	0	-0.863083	-0.989633	-0.212732
85	8	0	-1.197378	0.574677	-3.666619
86	8	0	-0.911448	-1.109590	-2.349134
87	6	0	-2.705322	-2.325266	0.428374
88	6	0	-2.555644	-1.728506	1.783494
89	8	0	-2.965857	-2.051119	2.867992
90	6	0	-4.056930	-2.535701	-0.085245
91	6	0	-4.238589	-2.830258	-1.453385
92	6	0	-5.212631	-2.331141	0.692033
93	6	0	-5.506556	-2.919461	-2.007969
94	1	0	-3.367121	-2.942786	-2.092614
95	6	0	-6.482646	-2.429568	0.131206
96	1	0	-5.107751	-2.116870	1.750604
97	6	0	-6.641510	-2.721794	-1.219811
98	1	0	-5.612644	-3.134669	-3.067253
99	1	0	-7.354973	-2.276397	0.760166
100	1	0	-7.632589	-2.795440	-1.655603
101	6	0	-1.639753	-3.344006	0.070210
102	6	0	-1.775136	-4.633932	0.888355
103	1	0	-0.641064	-2.925109	0.232563
104	1	0	-1.698998	-3.569653	-0.998186
105	1	0	-0.983626	-5.347416	0.638677
106	1	0	-1.721114	-4.415341	1.959733
107	1	0	-2.742124	-5.107617	0.697505

TS3'(RS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	3.892068	-1.266153	-0.260597
2	8	0	3.483096	0.373057	-0.283986
3	7	0	-1.847597	2.379857	-0.220977
4	7	0	-1.292788	3.107042	-1.253034
5	7	0	-0.070129	1.372524	-0.671237
6	6	0	-3.282978	2.507758	1.724148
7	1	0	-2.541240	1.937939	2.273980
8	6	0	-4.486841	2.891189	2.305554
9	1	0	-4.685053	2.633668	3.340350
10	6	0	-5.428589	3.605929	1.567723
11	1	0	-6.364237	3.905792	2.027803
12	6	0	-5.164445	3.942795	0.241132
13	1	0	-5.894114	4.503530	-0.333556
14	6	0	-3.972178	3.554585	-0.359813
15	1	0	-3.753825	3.789043	-1.395094
16	6	0	-3.050152	2.829212	0.388691
17	6	0	-1.156809	1.273530	0.132513
18	6	0	-0.206865	2.445817	-1.510399
19	6	0	0.894726	2.492478	-2.515186
20	1	0	1.575271	3.322389	-2.307362
21	1	0	0.500921	2.610592	-3.525810
22	6	0	1.558048	1.102369	-2.294333
23	1	0	2.638163	1.120915	-2.441114
24	1	0	1.121424	0.376630	-2.984704
25	6	0	1.198574	0.664005	-0.849436
26	1	0	1.027265	-0.410851	-0.785618
27	6	0	2.330485	1.059428	0.164259
28	6	0	2.696250	-2.272540	-1.301681
29	1	0	1.727883	-2.410585	-0.809898
30	1	0	3.106292	-3.276161	-1.462875
31	1	0	2.520756	-1.819500	-2.283144
32	6	0	3.969663	-1.962431	1.476914
33	1	0	2.974936	-1.988117	1.931386
34	1	0	4.619537	-1.366564	2.123495
35	1	0	4.352295	-2.988821	1.446488
36	6	0	5.608802	-1.216962	-1.057029

37	6	0	6.180080	-2.636242	-1.179410
38	1	0	7.179970	-2.602343	-1.631676
39	1	0	5.554824	-3.273606	-1.814400
40	1	0	6.278352	-3.122384	-0.202367
41	6	0	6.542688	-0.364067	-0.186642
42	1	0	7.531042	-0.278824	-0.657326
43	1	0	6.685920	-0.808388	0.804523
44	1	0	6.144156	0.647037	-0.048831
45	6	0	5.510420	-0.591210	-2.455209
46	1	0	6.501231	-0.556896	-2.927341
47	1	0	5.127317	0.434025	-2.408367
48	1	0	4.851283	-1.169995	-3.112435
49	6	0	2.611753	2.559520	0.050791
50	6	0	1.723855	3.479447	0.618817
51	6	0	3.714548	3.030902	-0.661367
52	6	0	1.907588	4.845254	0.432140
53	1	0	0.882384	3.123037	1.209325
54	6	0	3.905709	4.400682	-0.836891
55	1	0	4.416224	2.316952	-1.078366
56	6	0	2.996259	5.310222	-0.303643
57	1	0	4.767136	4.755311	-1.394240
58	6	0	2.077041	0.707355	1.632025
59	6	0	0.984682	-0.012187	2.104304
60	6	0	3.070373	1.100786	2.540323
61	6	0	0.875314	-0.315340	3.464643
62	1	0	0.207912	-0.361435	1.436380
63	6	0	2.973838	0.782096	3.886018
64	1	0	3.929595	1.654874	2.170771
65	6	0	1.865071	0.075376	4.355629
66	1	0	3.756853	1.089293	4.571961
67	1	0	1.201178	5.546536	0.864177
68	1	0	3.141069	6.375963	-0.448432
69	1	0	1.775879	-0.164403	5.410301
70	1	0	0.003107	-0.853783	3.820567
71	6	0	-3.043946	-0.414847	-0.787714
72	6	0	-2.949732	-0.846255	-2.124845
73	6	0	-3.999554	-0.737773	-3.030316
74	6	0	-5.191161	-0.151219	-2.632533
75	6	0	-5.326671	0.269877	-1.309939
76	6	0	-4.282217	0.133659	-0.406258
77	1	0	-3.860623	-1.119873	-4.034487
78	1	0	-6.005348	-0.041244	-3.339004
79	1	0	-6.257878	0.711978	-0.970682
80	1	0	-4.418475	0.434712	0.625641

81	7	0	-1.755154	-1.531070	-2.612176
82	6	0	-1.983801	-0.570713	0.235713
83	8	0	-2.370367	-0.561369	1.574491
84	1	0	-1.031174	-1.003938	-0.024229
85	8	0	-1.900593	-2.403230	-3.449222
86	8	0	-0.665704	-1.190190	-2.169093
87	6	0	-2.701160	-2.643759	0.613052
88	6	0	-3.184899	-1.710948	1.619731
89	8	0	-4.208198	-1.692383	2.256349
90	6	0	-1.381550	-3.263138	0.758886
91	6	0	-0.848258	-4.095621	-0.246512
92	6	0	-0.590928	-3.048577	1.902761
93	6	0	0.401008	-4.686567	-0.100336
94	1	0	-1.414317	-4.276038	-1.156131
95	6	0	0.668090	-3.622377	2.035159
96	1	0	-0.990554	-2.447142	2.713323
97	6	0	1.172751	-4.453768	1.038044
98	1	0	0.782243	-5.323702	-0.892919
99	1	0	1.247685	-3.428230	2.933836
100	1	0	2.151766	-4.910266	1.144254
101	6	0	-3.774101	-3.367808	-0.163546
102	6	0	-4.188670	-4.700435	0.470066
103	1	0	-3.428684	-3.534772	-1.193797
104	1	0	-4.649730	-2.712661	-0.240318
105	1	0	-4.967016	-5.192852	-0.119767
106	1	0	-3.332645	-5.377278	0.544069
107	1	0	-4.574763	-4.525862	1.477694

P(SS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.727857	-0.831976	0.168174
2	6	0	0.431796	-2.230587	-0.504500
3	8	0	-0.101284	-3.181917	0.016384
4	6	0	2.080623	-0.163414	-0.032705
5	6	0	2.807146	0.379560	1.030801
6	6	0	2.604700	0.003149	-1.322946
7	6	0	4.031212	1.011036	0.821111
8	1	0	2.421990	0.326318	2.040691
9	6	0	3.831734	0.617821	-1.535769

10	1	0	2.039720	-0.366251	-2.175077
11	6	0	4.559449	1.120357	-0.459150
12	1	0	4.569616	1.420440	1.670234
13	1	0	4.214558	0.718897	-2.547382
14	1	0	5.515760	1.607258	-0.621279
15	6	0	0.203726	-0.803890	1.606032
16	6	0	0.915124	-1.767691	2.559478
17	1	0	-0.853890	-1.081507	1.587343
18	1	0	0.252675	0.228548	1.967955
19	1	0	0.585547	-1.589200	3.587349
20	1	0	0.668750	-2.795046	2.289289
21	1	0	2.003327	-1.672285	2.530210
22	6	0	-1.701870	-0.123929	-0.558225
23	6	0	-2.197150	1.089140	-0.064550
24	6	0	-3.533348	1.278714	0.272018
25	6	0	-4.421018	0.221172	0.139485
26	6	0	-3.959027	-1.002153	-0.338892
27	6	0	-2.623626	-1.167187	-0.688968
28	1	0	-3.846977	2.250477	0.631920
29	1	0	-5.463342	0.352380	0.407961
30	1	0	-4.643710	-1.837109	-0.446609
31	1	0	-2.265275	-2.118600	-1.064875
32	7	0	-1.304631	2.240926	0.129092
33	6	0	-0.262612	-0.358226	-0.960904
34	8	0	-0.129205	-1.594037	-1.678919
35	1	0	0.119004	0.479929	-1.544680
36	8	0	-0.104612	2.025484	0.202413
37	8	0	-1.809102	3.345208	0.210168

P(RR)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.727857	-0.831976	0.168174
2	6	0	-0.431796	-2.230587	-0.504500
3	8	0	0.101284	-3.181917	0.016384
4	6	0	-2.080623	-0.163414	-0.032705
5	6	0	-2.807146	0.379560	1.030801
6	6	0	-2.604700	0.003149	-1.322946
7	6	0	-4.031212	1.011036	0.821111
8	1	0	-2.421990	0.326318	2.040691
9	6	0	-3.831734	0.617821	-1.535769

10	1	0	-2.039720	-0.366251	-2.175077
11	6	0	-4.559449	1.120357	-0.459150
12	1	0	-4.569616	1.420440	1.670234
13	1	0	-4.214558	0.718897	-2.547382
14	1	0	-5.515760	1.607258	-0.621279
15	6	0	-0.203726	-0.803890	1.606032
16	6	0	-0.915124	-1.767691	2.559478
17	1	0	0.853890	-1.081507	1.587343
18	1	0	-0.252675	0.228548	1.967955
19	1	0	-0.585547	-1.589200	3.587349
20	1	0	-0.668750	-2.795046	2.289289
21	1	0	-2.003327	-1.672285	2.530210
22	6	0	1.701870	-0.123929	-0.558225
23	6	0	2.197150	1.089140	-0.064550
24	6	0	3.533348	1.278714	0.272018
25	6	0	4.421018	0.221172	0.139485
26	6	0	3.959027	-1.002153	-0.338892
27	6	0	2.623626	-1.167187	-0.688968
28	1	0	3.846977	2.250477	0.631920
29	1	0	5.463342	0.352380	0.407961
30	1	0	4.643710	-1.837109	-0.446609
31	1	0	2.265275	-2.118600	-1.064875
32	7	0	1.304631	2.240926	0.129092
33	6	0	0.262612	-0.358226	-0.960904
34	8	0	0.129205	-1.594037	-1.678919
35	1	0	-0.119004	0.479929	-1.544680
36	8	0	0.104612	2.025484	0.202413
37	8	0	1.809102	3.345208	0.210168

P(SR)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.563839	0.097644	0.089557
2	6	0	2.275016	-0.731375	-0.980770
3	8	0	3.065206	-0.546177	-1.851236
4	6	0	0.658950	1.192363	-0.433632
5	6	0	0.109897	2.142268	0.433975
6	6	0	0.296283	1.229558	-1.783949
7	6	0	-0.797117	3.088981	-0.033183
8	1	0	0.366103	2.131562	1.488835
9	6	0	-0.602772	2.182442	-2.251874

10	1	0	0.728515	0.517889	-2.481340
11	6	0	-1.157668	3.111731	-1.376924
12	1	0	-1.223046	3.806472	0.660513
13	1	0	-0.868713	2.196987	-3.303965
14	1	0	-1.864082	3.850607	-1.741121
15	6	0	2.553300	0.565828	1.170135
16	6	0	3.637963	-0.452713	1.519374
17	1	0	3.217469	-1.394343	1.884697
18	1	0	4.266066	-0.676104	0.652186
19	1	0	4.282733	-0.056059	2.306468
20	6	0	-0.580512	-1.426426	0.050672
21	6	0	-1.621642	-0.801644	0.751421
22	6	0	-2.953604	-0.903300	0.371295
23	6	0	-3.285654	-1.665197	-0.740218
24	6	0	-2.277424	-2.301842	-1.456053
25	6	0	-0.946383	-2.175918	-1.068868
26	1	0	-3.702435	-0.380350	0.952669
27	1	0	-4.322652	-1.757150	-1.042706
28	1	0	-2.523997	-2.898512	-2.328088
29	1	0	-0.163426	-2.662144	-1.637896
30	7	0	-1.344755	0.009915	1.942039
31	6	0	0.881926	-1.284233	0.395492
32	8	0	1.717656	-1.922292	-0.609619
33	1	0	1.110292	-1.686393	1.381241
34	8	0	-0.250457	-0.117909	2.473111
35	8	0	-2.209596	0.764073	2.338407
36	1	0	3.019073	1.486245	0.803152
37	1	0	1.982509	0.821329	2.067080

P(RS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.563948	0.097678	0.089509
2	6	0	-2.275216	-0.731082	-0.981015
3	8	0	-3.065579	-0.545767	-1.851289
4	6	0	-0.658950	1.192315	-0.433688
5	6	0	-0.109375	2.141733	0.434074
6	6	0	-0.296563	1.229807	-1.784095
7	6	0	0.797883	3.088284	-0.032992
8	1	0	-0.365230	2.130732	1.489021
9	6	0	0.602701	2.182522	-2.251914

10	1	0	-0.729155	0.518464	-2.481603
11	6	0	1.158118	3.111366	-1.376807
12	1	0	1.224250	3.805324	0.660899
13	1	0	0.868380	2.197351	-3.304071
14	1	0	1.864678	3.850105	-1.740987
15	6	0	-2.553128	0.565873	1.170302
16	6	0	-3.637697	-0.452727	1.519773
17	1	0	-3.217063	-1.394393	1.884849
18	1	0	-4.266009	-0.676049	0.652716
19	1	0	-4.282274	-0.056225	2.307091
20	6	0	0.580517	-1.426356	0.050499
21	6	0	1.621455	-0.801534	0.751430
22	6	0	2.953526	-0.903182	0.371733
23	6	0	3.285897	-1.665282	-0.739554
24	6	0	2.277855	-2.301984	-1.455613
25	6	0	0.946697	-2.175994	-1.068847
26	1	0	3.702168	-0.380156	0.953286
27	1	0	4.322987	-1.757342	-1.041684
28	1	0	2.524681	-2.898728	-2.327526
29	1	0	0.163869	-2.662258	-1.638024
30	7	0	1.344158	0.010081	1.941934
31	6	0	-0.881973	-1.284253	0.395043
32	8	0	-1.717399	-1.922045	-0.610459
33	1	0	-1.110511	-1.686719	1.380647
34	8	0	0.249944	-0.118455	2.473009
35	8	0	2.208589	0.764836	2.338022
36	1	0	-3.018995	1.486288	0.803449
37	1	0	-1.982130	0.821396	2.067103

M02X(SS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	5.129688	-0.991228	-0.513890
2	8	0	3.662268	-0.197843	-0.268029
3	7	0	-0.124725	3.104854	-0.434926
4	7	0	0.989947	3.373958	-1.186015
5	7	0	0.783139	1.223171	-0.770114
6	6	0	-1.735494	4.110622	1.108062
7	1	0	-1.669131	3.232646	1.743822
8	6	0	-2.570180	5.178564	1.426995
9	1	0	-3.165095	5.130958	2.332594

10	6	0	-2.637403	6.299722	0.604879
11	1	0	-3.287185	7.127734	0.867633
12	6	0	-1.867081	6.359936	-0.554794
13	1	0	-1.913856	7.231709	-1.198386
14	6	0	-1.037088	5.300483	-0.899167
15	1	0	-0.433649	5.324479	-1.798667
16	6	0	-0.988114	4.187057	-0.062831
17	6	0	-0.300770	1.790633	-0.217448
18	6	0	1.505783	2.201091	-1.393174
19	6	0	2.552485	1.602527	-2.274355
20	1	0	3.536002	1.648358	-1.806591
21	1	0	2.583624	2.102421	-3.243062
22	6	0	2.040728	0.138358	-2.353587
23	1	0	2.848428	-0.564250	-2.543447
24	1	0	1.297486	0.052740	-3.152393
25	6	0	1.340294	-0.123366	-0.995448
26	1	0	0.511844	-0.832812	-1.040519
27	6	0	2.355396	-0.577000	0.145298
28	6	0	5.239013	-1.560021	-2.304856
29	6	0	5.453572	-2.456786	0.606809
30	1	0	4.880954	-3.338538	0.306447
31	1	0	5.215930	-2.235686	1.650761
32	1	0	6.519813	-2.705549	0.548827
33	6	0	6.446172	0.338488	-0.182716
34	6	0	7.779965	-0.111371	-0.799438
35	1	0	8.570697	0.606338	-0.545243
36	1	0	7.723309	-0.167047	-1.891677
37	1	0	8.098681	-1.092071	-0.427484
38	6	0	6.632765	0.516829	1.331738
39	1	0	7.355335	1.319135	1.530841
40	1	0	7.016554	-0.396009	1.799546
41	1	0	5.694873	0.780284	1.833401
42	6	0	6.050908	1.683374	-0.804176
43	1	0	6.850028	2.420909	-0.653083
44	1	0	5.139740	2.087438	-0.350338
45	1	0	5.885614	1.599286	-1.885660
46	6	0	2.039173	0.170767	1.439669
47	6	0	0.924544	-0.165339	2.207465
48	6	0	2.822495	1.264497	1.820851
49	6	0	0.626626	0.552510	3.363232
50	1	0	0.279812	-0.981572	1.893613
51	6	0	2.519990	1.982919	2.973250
52	1	0	3.672059	1.545441	1.210035
53	6	0	1.424898	1.620849	3.754961

54	1	0	3.140713	2.826627	3.258524
55	6	0	2.277899	-2.102748	0.291515
56	6	0	2.153462	-2.909185	-0.844981
57	6	0	2.429450	-2.726251	1.530983
58	6	0	2.184902	-4.296371	-0.748261
59	1	0	2.018499	-2.462077	-1.825799
60	6	0	2.448602	-4.114567	1.633579
61	1	0	2.540015	-2.125317	2.426466
62	6	0	2.330386	-4.905712	0.495605
63	1	0	2.563522	-4.576303	2.608924
64	6	0	-2.528765	0.869175	-0.656653
65	6	0	-1.591365	1.153577	0.329125
66	8	0	-1.653982	1.048186	1.584234
67	6	0	-3.910229	0.498448	-0.301014
68	6	0	-4.858708	0.208966	-1.307586
69	6	0	-4.367658	0.396670	1.034470
70	6	0	-6.163558	-0.161904	-1.006362
71	1	0	-4.578613	0.264403	-2.353528
72	6	0	-5.676401	0.025170	1.326785
73	1	0	-3.677297	0.614488	1.837522
74	6	0	-6.587979	-0.265701	0.315620
75	1	0	-6.850998	-0.383449	-1.818541
76	1	0	-5.979536	-0.054726	2.367255
77	1	0	-7.602367	-0.569503	0.553346
78	6	0	-2.211341	1.033771	-2.131299
79	6	0	-2.764556	2.325352	-2.749833
80	1	0	-3.840820	2.409828	-2.579010
81	1	0	-2.296495	3.201300	-2.290443
82	1	0	-2.582215	2.364629	-3.828555
83	1	0	2.084529	-4.899936	-1.644707
84	1	0	2.346685	-5.987753	0.575819
85	1	0	-0.254587	0.286465	3.935985
86	1	0	1.186943	2.179287	4.654636
87	1	0	5.165488	-0.727933	-3.013470
88	1	0	6.200217	-2.056172	-2.474389
89	1	0	4.452739	-2.284668	-2.538970
90	6	0	-3.058638	-2.521333	-0.389383
91	6	0	-4.317212	-2.904799	0.077767
92	6	0	-5.321227	-3.353943	-0.767949
93	6	0	-5.068639	-3.428197	-2.132781
94	6	0	-3.818841	-3.065320	-2.628068
95	6	0	-2.826213	-2.620281	-1.760900
96	1	0	-6.276373	-3.639503	-0.345746
97	1	0	-5.845717	-3.775732	-2.804501

98	1	0	-3.617125	-3.128975	-3.692358
99	1	0	-1.849488	-2.325455	-2.131288
100	7	0	-4.594937	-2.918851	1.519012
101	6	0	-1.950169	-1.928969	0.434714
102	8	0	-0.794497	-2.185714	0.161520
103	8	0	-3.646580	-2.799354	2.277589
104	8	0	-5.746272	-3.072829	1.879501
105	1	0	-1.130798	1.000069	-2.309324
106	1	0	-2.602190	0.168576	-2.683033
107	1	0	-2.214991	-1.225955	1.236577

M02X(RR)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.189670	-1.596693	-0.362446
2	8	0	3.748431	0.030745	-0.282689
3	7	0	-1.354585	2.679087	-0.599469
4	7	0	-0.646627	3.243666	-1.625629
5	7	0	0.360693	1.446445	-0.816715
6	6	0	-2.914696	3.350274	1.137731
7	1	0	-2.166132	3.081936	1.878249
8	6	0	-4.174033	3.818795	1.497891
9	1	0	-4.418934	3.931358	2.548723
10	6	0	-5.112040	4.138900	0.518939
11	1	0	-6.091784	4.503827	0.809035
12	6	0	-4.799421	3.987679	-0.830581
13	1	0	-5.533400	4.228605	-1.591876
14	6	0	-3.549005	3.511471	-1.208683
15	1	0	-3.286245	3.360520	-2.249719
16	6	0	-2.629066	3.201888	-0.214425
17	6	0	-0.779484	1.571713	-0.120688
18	6	0	0.394618	2.474708	-1.725384
19	6	0	1.605751	2.401356	-2.585458
20	1	0	2.340979	3.136907	-2.246535
21	1	0	1.373851	2.591909	-3.633613
22	6	0	2.070491	0.950269	-2.317238
23	1	0	3.153184	0.847762	-2.343077
24	1	0	1.644663	0.286436	-3.074974
25	6	0	1.513882	0.522304	-0.930247
26	1	0	1.136489	-0.498053	-0.969590
27	6	0	2.574579	0.653583	0.218519

28	6	0	2.873204	-2.619005	-1.229137
29	6	0	4.586948	-2.324125	1.316790
30	1	0	3.680131	-2.519841	1.895923
31	1	0	5.218079	-1.645997	1.898215
32	1	0	5.126063	-3.270209	1.193832
33	6	0	5.768752	-1.514658	-1.414546
34	6	0	6.181693	-2.930434	-1.840595
35	1	0	7.136554	-2.899893	-2.381779
36	1	0	5.439793	-3.385402	-2.505754
37	1	0	6.315143	-3.595209	-0.979242
38	6	0	6.897007	-0.882452	-0.587315
39	1	0	7.799684	-0.763292	-1.201542
40	1	0	7.163133	-1.503507	0.274637
41	1	0	6.611353	0.107749	-0.213991
42	6	0	5.532491	-0.661021	-2.666031
43	1	0	6.421001	-0.674563	-3.311434
44	1	0	5.331102	0.381349	-2.397283
45	1	0	4.686780	-1.028725	-3.260430
46	6	0	2.883075	2.135292	0.426166
47	6	0	1.987959	2.940150	1.142469
48	6	0	4.016696	2.711915	-0.146827
49	6	0	2.212853	4.309454	1.244214
50	1	0	1.123862	2.483429	1.626949
51	6	0	4.241498	4.083816	-0.034171
52	1	0	4.720454	2.078647	-0.676888
53	6	0	3.335381	4.886738	0.651439
54	1	0	5.128291	4.522233	-0.481426
55	6	0	2.182998	-0.046624	1.522852
56	6	0	1.257339	-1.089140	1.587867
57	6	0	2.929296	0.264428	2.665106
58	6	0	1.089587	-1.810026	2.770264
59	1	0	0.629922	-1.353943	0.741686
60	6	0	2.756126	-0.446423	3.845458
61	1	0	3.661476	1.065653	2.619229
62	6	0	1.837186	-1.492740	3.898858
63	1	0	3.343692	-0.188058	4.720941
64	6	0	-2.394252	-0.036003	0.909829
65	6	0	-1.287212	0.783240	1.059908
66	8	0	-0.665994	1.093796	2.116278
67	6	0	-3.222233	-0.094953	-0.293684
68	6	0	-4.607518	-0.355608	-0.173233
69	6	0	-2.754304	0.101213	-1.617013
70	6	0	-5.457251	-0.369803	-1.270578
71	1	0	-5.029142	-0.529954	0.810814

72	6	0	-3.610590	0.101345	-2.714013
73	1	0	-1.692784	0.215190	-1.808773
74	6	0	-4.973929	-0.131840	-2.557033
75	1	0	-6.515113	-0.565381	-1.116323
76	1	0	-3.195660	0.263795	-3.705828
77	1	0	-5.639990	-0.136896	-3.413583
78	6	0	-2.907782	-0.597190	2.218431
79	6	0	-3.660552	0.440752	3.060091
80	1	0	-2.044989	-0.947419	2.795396
81	1	0	-3.539060	-1.474841	2.038283
82	1	0	-4.026264	0.008035	3.996904
83	1	0	-2.981467	1.262050	3.304748
84	1	0	-4.514430	0.859321	2.516557
85	1	0	0.368516	-2.620301	2.796091
86	1	0	1.701846	-2.053853	4.818287
87	1	0	1.512370	4.927008	1.797702
88	1	0	3.507960	5.955012	0.736182
89	1	0	2.617504	-2.213357	-2.214633
90	1	0	3.245591	-3.638804	-1.375120
91	1	0	1.952042	-2.690511	-0.642580
92	6	0	-2.541381	-3.156037	-1.142333
93	6	0	-2.676629	-3.565287	0.191305
94	6	0	-3.887058	-4.003296	0.703790
95	6	0	-5.000936	-4.067004	-0.131369
96	6	0	-4.890212	-3.697261	-1.465514
97	6	0	-3.669934	-3.242491	-1.956885
98	1	0	-3.940027	-4.303206	1.743286
99	1	0	-5.947441	-4.415564	0.266695
100	1	0	-5.753360	-3.740256	-2.120593
101	1	0	-3.596014	-2.897680	-2.984213
102	7	0	-1.526793	-3.648208	1.103747
103	6	0	-1.366402	-2.481315	-1.761374
104	8	0	-0.439966	-1.967871	-1.179678
105	8	0	-0.439161	-3.920153	0.633975
106	8	0	-1.753971	-3.507463	2.294232
107	1	0	-1.439144	-2.428943	-2.865168

M02X(SR)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.679464	1.033305	0.392687

2	8	0	3.748781	-0.251114	-0.173178
3	7	0	-1.380836	-2.487524	1.206710
4	7	0	-0.563239	-3.587886	1.205563
5	7	0	0.592671	-1.711146	1.110516
6	6	0	-3.684542	-1.741438	0.850428
7	1	0	-3.320834	-0.931934	0.227158
8	6	0	-5.043038	-1.914140	1.098103
9	1	0	-5.747169	-1.203678	0.676366
10	6	0	-5.496388	-2.984146	1.864851
11	1	0	-6.558040	-3.110859	2.048939
12	6	0	-4.584457	-3.896112	2.392350
13	1	0	-4.930326	-4.734366	2.987531
14	6	0	-3.221766	-3.734292	2.168674
15	1	0	-2.496878	-4.429330	2.575344
16	6	0	-2.790579	-2.654692	1.402638
17	6	0	-0.695818	-1.337528	1.160905
18	6	0	0.628220	-3.080122	1.141284
19	6	0	2.027014	-3.587576	1.130472
20	1	0	2.279607	-3.952652	0.130468
21	1	0	2.172076	-4.394889	1.848739
22	6	0	2.812149	-2.302891	1.496320
23	1	0	3.781117	-2.248029	1.002767
24	1	0	2.977120	-2.273481	2.576304
25	6	0	1.930129	-1.084081	1.096667
26	1	0	1.962092	-0.311522	1.867518
27	6	0	2.352855	-0.466019	-0.284116
28	6	0	4.300004	1.381687	2.202038
29	6	0	4.492914	2.584883	-0.638678
30	1	0	3.542198	3.091347	-0.450598
31	1	0	4.539552	2.346486	-1.705248
32	1	0	5.306599	3.282589	-0.410704
33	6	0	6.435934	0.340789	0.208468
34	6	0	7.432388	1.239696	0.953857
35	1	0	8.457364	0.881537	0.791527
36	1	0	7.250220	1.237903	2.033886
37	1	0	7.390169	2.278183	0.605212
38	6	0	6.807076	0.297910	-1.280832
39	1	0	7.796924	-0.158255	-1.414253
40	1	0	6.844622	1.302542	-1.715562
41	1	0	6.085091	-0.291647	-1.857454
42	6	0	6.511849	-1.078895	0.784849
43	1	0	7.544909	-1.449478	0.749375
44	1	0	5.888395	-1.771913	0.210407
45	1	0	6.183907	-1.114782	1.830952

46	6	0	2.126425	-1.527202	-1.358945
47	6	0	0.830780	-1.788416	-1.816381
48	6	0	3.189971	-2.293411	-1.838177
49	6	0	0.601292	-2.823531	-2.717086
50	1	0	0.000531	-1.165645	-1.484423
51	6	0	2.956848	-3.330438	-2.740330
52	1	0	4.197049	-2.071362	-1.502039
53	6	0	1.662050	-3.604015	-3.173416
54	1	0	3.791039	-3.920871	-3.106908
55	6	0	1.668726	0.864461	-0.615841
56	6	0	1.233871	1.755478	0.366773
57	6	0	1.645927	1.282932	-1.952235
58	6	0	0.765455	3.024186	0.024533
59	1	0	1.215132	1.477489	1.414838
60	6	0	1.195730	2.552733	-2.294403
61	1	0	1.987928	0.605894	-2.728907
62	6	0	0.751047	3.429062	-1.305406
63	1	0	1.176458	2.854420	-3.336957
64	6	0	-1.366821	0.832125	2.115778
65	6	0	-1.251705	0.058153	0.987439
66	8	0	-1.500192	0.273312	-0.246024
67	6	0	-1.750479	2.247852	2.010307
68	6	0	-1.423664	3.167311	3.025496
69	6	0	-2.399507	2.760293	0.869958
70	6	0	-1.678267	4.527994	2.881971
71	1	0	-0.946030	2.821732	3.937254
72	6	0	-2.647591	4.119363	0.725879
73	1	0	-2.686573	2.066153	0.093159
74	6	0	-2.279760	5.018790	1.724966
75	1	0	-1.398595	5.209439	3.680396
76	1	0	-3.120692	4.477453	-0.185257
77	1	0	-2.466167	6.081705	1.609094
78	6	0	-1.038548	0.270549	3.481528
79	6	0	-2.266725	0.184719	4.396120
80	1	0	-2.725862	1.168963	4.523659
81	1	0	-3.016787	-0.475853	3.949829
82	1	0	-2.005239	-0.202695	5.385426
83	1	0	0.398306	3.687418	0.802723
84	1	0	0.368311	4.407572	-1.574900
85	1	0	-0.413192	-2.998019	-3.058863
86	1	0	1.482448	-4.411517	-3.876326
87	1	0	4.363346	0.474577	2.812620
88	1	0	5.021295	2.102472	2.600603
89	1	0	3.305167	1.817016	2.329806

90	6	0	-3.462846	1.478514	-2.341272
91	6	0	-3.597115	0.089158	-2.301000
92	6	0	-4.819667	-0.541211	-2.121955
93	6	0	-5.963393	0.242000	-1.993068
94	6	0	-5.866315	1.630372	-2.044587
95	6	0	-4.625169	2.237539	-2.211372
96	1	0	-4.859638	-1.623823	-2.091394
97	1	0	-6.928263	-0.236107	-1.861419
98	1	0	-6.757932	2.240641	-1.947959
99	1	0	-4.523532	3.317827	-2.234225
100	7	0	-2.431085	-0.770986	-2.526595
101	6	0	-2.151441	2.218596	-2.391611
102	8	0	-2.120722	3.379201	-2.738884
103	1	0	-1.263428	1.682096	-2.036691
104	8	0	-1.529861	-0.321433	-3.209838
105	8	0	-2.451688	-1.896123	-2.058057
106	1	0	-0.609965	-0.734916	3.390102
107	1	0	-0.257763	0.868017	3.973323

M02X(RS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	3.518186	-0.889681	1.202030
2	8	0	2.628289	-1.895594	0.177818
3	7	0	-3.175931	-1.329255	-0.437993
4	7	0	-2.969290	-2.645929	-0.138871
5	7	0	-1.095544	-1.468009	-0.029801
6	6	0	-4.673984	0.017988	-1.807186
7	1	0	-3.810293	0.397636	-2.346439
8	6	0	-5.966038	0.437951	-2.104498
9	1	0	-6.123212	1.143199	-2.913472
10	6	0	-7.048244	-0.036738	-1.366245
11	1	0	-8.053529	0.292559	-1.607661
12	6	0	-6.844073	-0.928612	-0.314849
13	1	0	-7.686060	-1.289439	0.266084
14	6	0	-5.558365	-1.352960	0.002754
15	1	0	-5.366352	-2.031028	0.827017
16	6	0	-4.495681	-0.872210	-0.753665
17	6	0	-2.078041	-0.576755	-0.299990
18	6	0	-1.702239	-2.692368	0.131197
19	6	0	-0.806111	-3.672221	0.801551

20	1	0	-0.381650	-4.387804	0.094161
21	1	0	-1.352934	-4.216985	1.572275
22	6	0	0.253516	-2.707837	1.393750
23	1	0	1.232576	-3.171922	1.502084
24	1	0	-0.085798	-2.366927	2.376450
25	6	0	0.315810	-1.476466	0.443824
26	1	0	0.498582	-0.532668	0.963675
27	6	0	1.474992	-1.688926	-0.613526
28	6	0	2.607347	-0.615968	2.823950
29	6	0	3.942701	0.778104	0.460438
30	1	0	3.050857	1.289824	0.086347
31	1	0	4.646848	0.695246	-0.371705
32	1	0	4.392885	1.408622	1.235842
33	6	0	5.074273	-1.929155	1.481062
34	6	0	6.117638	-1.108297	2.251696
35	1	0	7.010126	-1.716668	2.448145
36	1	0	5.736396	-0.765556	3.220720
37	1	0	6.437341	-0.227663	1.683715
38	6	0	5.659212	-2.351532	0.126225
39	1	0	6.571940	-2.943440	0.275521
40	1	0	5.925758	-1.484599	-0.489640
41	1	0	4.947500	-2.960734	-0.440779
42	6	0	4.714865	-3.185889	2.286414
43	1	0	5.598264	-3.826042	2.409924
44	1	0	3.942758	-3.777099	1.779802
45	1	0	4.345674	-2.934082	3.286744
46	6	0	1.221530	-2.964712	-1.416062
47	6	0	0.213132	-2.979305	-2.384743
48	6	0	1.943027	-4.131121	-1.162794
49	6	0	-0.101887	-4.157523	-3.053203
50	1	0	-0.323969	-2.062860	-2.618167
51	6	0	1.634466	-5.308370	-1.843133
52	1	0	2.737124	-4.109781	-0.424207
53	6	0	0.603188	-5.328483	-2.777861
54	1	0	2.199759	-6.211886	-1.637036
55	6	0	1.747456	-0.539090	-1.576825
56	6	0	0.862715	0.507405	-1.769697
57	6	0	2.947800	-0.554304	-2.299201
58	6	0	1.166832	1.557110	-2.638304
59	1	0	-0.092983	0.551292	-1.274545
60	6	0	3.263405	0.494763	-3.153438
61	1	0	3.640210	-1.382241	-2.166633
62	6	0	2.378003	1.564212	-3.318047
63	1	0	4.204149	0.481187	-3.695299

64	6	0	-2.792361	1.496607	0.771161
65	6	0	-2.182537	0.953018	-0.332529
66	8	0	-1.841211	1.528197	-1.416826
67	6	0	-3.175966	0.696984	1.946804
68	6	0	-4.485944	0.753176	2.456525
69	6	0	-2.266253	-0.153592	2.598884
70	6	0	-4.878332	-0.040049	3.528761
71	1	0	-5.207487	1.412621	1.980565
72	6	0	-2.664047	-0.966567	3.657550
73	1	0	-1.223480	-0.124273	2.293367
74	6	0	-3.974635	-0.919345	4.125629
75	1	0	-5.899566	0.018256	3.894163
76	1	0	-1.938053	-1.614868	4.141692
77	1	0	-4.283853	-1.543432	4.957897
78	6	0	-3.208585	2.949426	0.674125
79	6	0	-4.338160	3.181881	-0.334647
80	1	0	-2.346658	3.553668	0.362114
81	1	0	-3.505011	3.308888	1.666010
82	1	0	-4.608657	4.240933	-0.394583
83	1	0	-4.008249	2.848843	-1.321907
84	1	0	-5.233391	2.610567	-0.067050
85	1	0	0.425899	2.339620	-2.780259
86	1	0	2.626951	2.386550	-3.981295
87	1	0	-0.894879	-4.159919	-3.794074
88	1	0	0.357569	-6.247088	-3.300703
89	1	0	2.199075	-1.544521	3.233997
90	1	0	3.308150	-0.211184	3.563297
91	1	0	1.796282	0.110179	2.712075
92	6	0	1.524443	3.608767	0.624497
93	6	0	1.780067	4.523868	-0.401774
94	6	0	2.853501	5.402591	-0.368927
95	6	0	3.684221	5.407656	0.746025
96	6	0	3.450070	4.518476	1.792856
97	6	0	2.393481	3.619681	1.718448
98	1	0	3.018300	6.070482	-1.205627
99	1	0	4.514226	6.103942	0.792433
100	1	0	4.099630	4.518416	2.661479
101	1	0	2.220473	2.889343	2.502318
102	7	0	0.914120	4.600331	-1.587245
103	6	0	0.471456	2.537141	0.591444
104	8	0	0.509061	1.638740	1.410911
105	1	0	-0.299246	2.567695	-0.191959
106	8	0	-0.281371	4.434939	-1.430125
107	8	0	1.450976	4.837500	-2.654837

TS2X(SS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-4.759911	-0.745256	-0.301673
2	8	0	-3.077428	-0.866915	-0.317872
3	7	0	1.595657	-2.259446	-0.841975
4	7	0	0.681079	-2.712910	-1.751018
5	7	0	0.141875	-0.726089	-0.955188
6	6	0	3.170591	-2.999671	0.854780
7	1	0	2.705705	-2.322476	1.565321
8	6	0	4.254653	-3.795610	1.212384
9	1	0	4.646332	-3.734992	2.223099
10	6	0	4.825812	-4.670451	0.289125
11	1	0	5.669206	-5.289340	0.579143
12	6	0	4.308738	-4.759646	-1.001100
13	1	0	4.747213	-5.444652	-1.719497
14	6	0	3.234976	-3.961732	-1.385174
15	1	0	2.824089	-4.005133	-2.386315
16	6	0	2.691028	-3.087140	-0.451879
17	6	0	1.335335	-1.015790	-0.397758
18	6	0	-0.187712	-1.745273	-1.804156
19	6	0	-1.393174	-1.394251	-2.613699
20	1	0	-2.258238	-1.975244	-2.297350
21	1	0	-1.211305	-1.563957	-3.677370
22	6	0	-1.556949	0.105896	-2.248591
23	1	0	-2.595721	0.423478	-2.297609
24	1	0	-0.957676	0.726652	-2.922270
25	6	0	-0.965466	0.239859	-0.823856
26	1	0	-0.572196	1.232699	-0.613847
27	6	0	-2.002449	-0.193975	0.321230
28	6	0	-5.294561	0.324035	-1.753942
29	6	0	-5.495333	-0.077708	1.288437
30	1	0	-5.371382	1.005122	1.374305
31	1	0	-5.048841	-0.545060	2.169229
32	1	0	-6.568004	-0.302108	1.294223
33	6	0	-5.391415	-2.519547	-0.566570
34	6	0	-6.845398	-2.453959	-1.064762
35	1	0	-7.264359	-3.466508	-1.128265
36	1	0	-6.912541	-2.003797	-2.060330

37	1	0	-7.487801	-1.877230	-0.388830
38	6	0	-5.362264	-3.297704	0.759731
39	1	0	-5.681851	-4.335224	0.594203
40	1	0	-6.040184	-2.858544	1.496560
41	1	0	-4.360567	-3.324606	1.202258
42	6	0	-4.552749	-3.267175	-1.611020
43	1	0	-4.999070	-4.247392	-1.822312
44	1	0	-3.529480	-3.439673	-1.262861
45	1	0	-4.502982	-2.717926	-2.559550
46	6	0	-1.326763	-1.180637	1.272850
47	6	0	-0.339247	-0.749062	2.157739
48	6	0	-1.592143	-2.548104	1.164968
49	6	0	0.339289	-1.671598	2.951871
50	1	0	-0.050580	0.295832	2.197023
51	6	0	-0.910343	-3.468818	1.955912
52	1	0	-2.330328	-2.888842	0.447437
53	6	0	0.052629	-3.030230	2.860227
54	1	0	-1.128978	-4.527122	1.856359
55	6	0	-2.527972	1.074297	1.003842
56	6	0	-2.942239	2.144045	0.198505
57	6	0	-2.731445	1.163628	2.379534
58	6	0	-3.567242	3.256798	0.752498
59	1	0	-2.779335	2.117577	-0.876650
60	6	0	-3.336981	2.285125	2.938280
61	1	0	-2.430338	0.346884	3.025859
62	6	0	-3.766839	3.330607	2.128726
63	1	0	-3.475882	2.338592	4.013277
64	6	0	3.453761	0.337150	-0.583784
65	6	0	2.349612	-0.116716	0.285786
66	8	0	2.282130	0.121319	1.514554
67	6	0	4.560659	1.027811	0.153540
68	6	0	5.169166	2.169742	-0.378290
69	6	0	5.100180	0.453322	1.312375
70	6	0	6.291048	2.725530	0.230870
71	1	0	4.737619	2.619500	-1.264175
72	6	0	6.227588	1.005142	1.911752
73	1	0	4.629423	-0.428104	1.736741
74	6	0	6.824699	2.142845	1.374984
75	1	0	6.745414	3.616335	-0.192952
76	1	0	6.636405	0.545315	2.807079
77	1	0	7.699000	2.575507	1.851525
78	6	0	3.913586	-0.412284	-1.829206
79	6	0	5.189527	-1.235085	-1.612916
80	1	0	6.043170	-0.571407	-1.446562

81	1	0	5.110689	-1.898467	-0.746400
82	1	0	5.393124	-1.846934	-2.494671
83	1	0	-3.887457	4.068686	0.106001
84	1	0	-4.242393	4.203037	2.565913
85	1	0	1.117655	-1.314056	3.617655
86	1	0	0.590456	-3.745864	3.476288
87	1	0	-4.968009	-0.096271	-2.710243
88	1	0	-6.385728	0.404457	-1.778846
89	1	0	-4.892467	1.337605	-1.667487
90	6	0	0.863571	3.226759	-1.093873
91	6	0	-0.072415	3.873914	-0.230317
92	6	0	-0.959753	4.846712	-0.706433
93	6	0	-0.978062	5.186457	-2.043499
94	6	0	-0.077056	4.558382	-2.927890
95	6	0	0.803976	3.608160	-2.470352
96	1	0	-1.634486	5.303052	0.008806
97	1	0	-1.683234	5.924754	-2.407236
98	1	0	-0.082658	4.821282	-3.981618
99	1	0	1.492061	3.116148	-3.147124
100	7	0	-0.188440	3.535625	1.156277
101	6	0	1.827257	2.249744	-0.713627
102	8	0	2.625605	1.714419	-1.594440
103	8	0	0.240499	2.435692	1.529756
104	8	0	-0.729680	4.334389	1.920117
105	1	0	3.110579	-1.041051	-2.219949
106	1	0	4.099447	0.330150	-2.610178
107	1	0	1.964786	2.018642	0.338516

TS2X(RR)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-4.930836	0.087377	-0.148457
2	8	0	-3.595340	-0.939465	-0.021715
3	7	0	1.833966	-1.497314	-0.882128
4	7	0	1.120489	-2.429569	-1.604432
5	7	0	-0.109729	-0.678306	-1.086250
6	6	0	3.254621	-1.751953	1.058350
7	1	0	2.517620	-1.193775	1.633152
8	6	0	4.403212	-2.278057	1.645972
9	1	0	4.571360	-2.137580	2.708167
10	6	0	5.329980	-2.970388	0.873686

11	1	0	6.222797	-3.377547	1.336871
12	6	0	5.120183	-3.137543	-0.496292
13	1	0	5.846382	-3.673267	-1.097913
14	6	0	3.979037	-2.620868	-1.096132
15	1	0	3.787239	-2.739380	-2.156424
16	6	0	3.066084	-1.930148	-0.306018
17	6	0	1.128399	-0.384865	-0.627189
18	6	0	-0.049444	-1.882809	-1.726295
19	6	0	-1.325080	-2.177483	-2.441429
20	1	0	-1.848893	-3.015221	-1.978197
21	1	0	-1.140986	-2.416838	-3.490145
22	6	0	-2.075194	-0.832220	-2.259523
23	1	0	-3.149142	-0.966504	-2.205211
24	1	0	-1.851364	-0.175138	-3.103970
25	6	0	-1.497060	-0.181050	-0.971241
26	1	0	-1.505692	0.909275	-1.023357
27	6	0	-2.245375	-0.693178	0.352961
28	6	0	-4.538032	1.523583	-1.303379
29	6	0	-5.555332	0.722870	1.500490
30	1	0	-4.907153	1.500790	1.911745
31	1	0	-5.613317	-0.086828	2.233036
32	1	0	-6.559675	1.142499	1.374678
33	6	0	-6.236495	-1.063826	-0.910063
34	6	0	-7.463086	-0.243371	-1.334462
35	1	0	-8.239986	-0.906171	-1.737425
36	1	0	-7.212575	0.483713	-2.115070
37	1	0	-7.903538	0.301783	-0.492076
38	6	0	-6.654155	-2.104885	0.138647
39	1	0	-7.374227	-2.812505	-0.293081
40	1	0	-7.130226	-1.635304	1.005843
41	1	0	-5.791659	-2.678633	0.496488
42	6	0	-5.673804	-1.792695	-2.136549
43	1	0	-6.441405	-2.442310	-2.577708
44	1	0	-4.818077	-2.421351	-1.865947
45	1	0	-5.352921	-1.091128	-2.916580
46	6	0	-1.645154	-2.031771	0.797887
47	6	0	-0.417130	-2.048397	1.472186
48	6	0	-2.298102	-3.234380	0.535657
49	6	0	0.164579	-3.260758	1.826887
50	1	0	0.066650	-1.096615	1.700778
51	6	0	-1.713767	-4.448042	0.900050
52	1	0	-3.264837	-3.214273	0.043234
53	6	0	-0.477386	-4.464879	1.535566
54	1	0	-2.230162	-5.378708	0.686654

55	6	0	-2.283497	0.287147	1.536976
56	6	0	-2.162529	1.670862	1.419978
57	6	0	-2.658263	-0.243863	2.777895
58	6	0	-2.421813	2.497815	2.512681
59	1	0	-1.848880	2.136189	0.492405
60	6	0	-2.900705	0.577637	3.871954
61	1	0	-2.773249	-1.318033	2.883641
62	6	0	-2.789112	1.959042	3.740705
63	1	0	-3.187600	0.137568	4.821810
64	6	0	1.152621	2.046474	-1.014139
65	6	0	1.394239	0.962775	0.022833
66	8	0	0.706277	0.950188	1.149975
67	6	0	0.316290	3.182207	-0.621044
68	6	0	-0.633064	3.664460	-1.541950
69	6	0	0.350008	3.740745	0.667241
70	6	0	-1.524832	4.669936	-1.183861
71	1	0	-0.698474	3.226193	-2.533451
72	6	0	-0.489416	4.797886	0.990433
73	1	0	1.036937	3.346610	1.401360
74	6	0	-1.440683	5.254314	0.077756
75	1	0	-2.267690	5.011038	-1.897313
76	1	0	-0.422380	5.249156	1.975307
77	1	0	-2.114921	6.060016	0.350451
78	6	0	1.585473	1.977145	-2.448354
79	6	0	1.178354	0.816265	-3.363151
80	1	0	2.679283	1.987404	-2.350297
81	1	0	1.324267	2.923476	-2.926795
82	1	0	1.531515	1.052441	-4.369723
83	1	0	1.647110	-0.128753	-3.079615
84	1	0	0.094132	0.682039	-3.417286
85	1	0	-2.326509	3.571176	2.394880
86	1	0	-2.985537	2.609430	4.587239
87	1	0	1.122564	-3.268747	2.338293
88	1	0	-0.018833	-5.408371	1.813811
89	1	0	-4.301682	1.185330	-2.317663
90	1	0	-5.403465	2.191515	-1.368368
91	1	0	-3.696826	2.120390	-0.934944
92	6	0	4.269926	1.052120	0.764950
93	6	0	5.257946	0.612117	-0.121786
94	6	0	6.513570	0.185083	0.292257
95	6	0	6.811981	0.180214	1.649461
96	6	0	5.852738	0.606585	2.565570
97	6	0	4.606090	1.036253	2.122574
98	1	0	7.231641	-0.143956	-0.449499

99	1	0	7.787030	-0.154363	1.986010
100	1	0	6.081420	0.616262	3.626572
101	1	0	3.868551	1.395510	2.834514
102	7	0	4.997345	0.532325	-1.560445
103	6	0	3.009453	1.774035	0.339988
104	8	0	3.223533	2.678968	-0.595754
105	8	0	3.871667	0.232208	-1.929715
106	8	0	5.934475	0.716003	-2.319235
107	1	0	2.520052	2.104201	1.271438

TS2X(SR)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-4.837625	-1.372766	0.069257
2	8	0	-3.536373	-0.450355	0.639067
3	7	0	1.269369	2.608741	0.660434
4	7	0	0.233543	3.353999	1.158656
5	7	0	-0.268708	1.199530	1.113102
6	6	0	2.788946	3.219859	-1.155270
7	1	0	2.262487	2.536445	-1.814152
8	6	0	3.852975	3.988378	-1.607554
9	1	0	4.162894	3.904023	-2.643665
10	6	0	4.520849	4.853835	-0.739923
11	1	0	5.352027	5.449568	-1.103243
12	6	0	4.122432	4.959873	0.588812
13	1	0	4.635666	5.637159	1.263033
14	6	0	3.057689	4.194032	1.058526
15	1	0	2.718699	4.266797	2.086667
16	6	0	2.419732	3.328665	0.181750
17	6	0	1.023736	1.283129	0.699704
18	6	0	-0.668604	2.470888	1.445639
19	6	0	-1.976467	2.470320	2.160570
20	1	0	-2.773734	2.865439	1.528868
21	1	0	-1.919918	3.072985	3.068445
22	6	0	-2.132934	0.956825	2.450834
23	1	0	-3.168131	0.633981	2.516252
24	1	0	-1.632583	0.721788	3.395778
25	6	0	-1.383281	0.223422	1.310950
26	1	0	-0.953712	-0.740511	1.599103
27	6	0	-2.335424	0.004424	0.037319
28	6	0	-4.653000	-3.129956	0.706062

29	6	0	-4.959772	-1.373574	-1.801685
30	1	0	-4.169868	-1.982455	-2.249102
31	1	0	-4.885605	-0.361084	-2.211599
32	1	0	-5.927103	-1.790325	-2.103880
33	6	0	-6.404727	-0.584082	0.850972
34	6	0	-7.384041	-1.703963	1.243801
35	1	0	-8.299317	-1.266889	1.663345
36	1	0	-6.959397	-2.374850	1.996557
37	1	0	-7.679147	-2.311010	0.379496
38	6	0	-7.140296	0.339583	-0.134302
39	1	0	-8.058790	0.720689	0.331228
40	1	0	-7.430051	-0.191846	-1.046351
41	1	0	-6.545988	1.207286	-0.436059
42	6	0	-6.043498	0.206109	2.117189
43	1	0	-6.951209	0.627084	2.569354
44	1	0	-5.360725	1.034960	1.903057
45	1	0	-5.563963	-0.433143	2.868095
46	6	0	-2.570173	1.329489	-0.692137
47	6	0	-1.540055	1.964018	-1.399850
48	6	0	-3.813076	1.956874	-0.628177
49	6	0	-1.751614	3.197507	-2.007594
50	1	0	-0.566625	1.488742	-1.487052
51	6	0	-4.031032	3.188462	-1.243053
52	1	0	-4.608701	1.486732	-0.065440
53	6	0	-2.997575	3.816531	-1.930392
54	1	0	-5.008377	3.656512	-1.174118
55	6	0	-1.810210	-1.108015	-0.881738
56	6	0	-1.587886	-2.365269	-0.308658
57	6	0	-1.619757	-0.958634	-2.258442
58	6	0	-1.132078	-3.428807	-1.078543
59	1	0	-1.745669	-2.513127	0.753625
60	6	0	-1.163287	-2.023939	-3.030233
61	1	0	-1.819516	-0.011526	-2.743625
62	6	0	-0.906193	-3.258313	-2.441689
63	1	0	-1.004973	-1.881187	-4.094226
64	6	0	2.330635	-0.610848	1.706382
65	6	0	2.129605	0.264257	0.535868
66	8	0	3.117343	0.674111	-0.186884
67	6	0	3.545039	-1.444795	1.757800
68	6	0	3.471677	-2.686053	2.416804
69	6	0	4.761098	-1.042323	1.187418
70	6	0	4.583859	-3.507808	2.497180
71	1	0	2.510617	-3.024757	2.789201
72	6	0	5.878025	-1.868937	1.288348

73	1	0	4.799110	-0.095497	0.666342
74	6	0	5.793516	-3.098149	1.932379
75	1	0	4.507735	-4.473877	2.985646
76	1	0	6.816859	-1.548993	0.847975
77	1	0	6.665334	-3.742825	1.990717
78	6	0	1.623805	-0.430323	3.013530
79	6	0	2.383390	0.659037	3.794936
80	1	0	3.412708	0.352649	3.995620
81	1	0	2.416394	1.600414	3.236058
82	1	0	1.883156	0.843598	4.748009
83	1	0	-0.935713	-4.385072	-0.604518
84	1	0	-0.533574	-4.083153	-3.040789
85	1	0	-0.935625	3.673144	-2.542162
86	1	0	-3.159417	4.779291	-2.404041
87	1	0	-4.460942	-3.142472	1.784207
88	1	0	-5.566446	-3.702805	0.521112
89	1	0	-3.827924	-3.641563	0.206572
90	6	0	2.229455	-1.905478	-0.942240
91	6	0	2.860536	-1.254562	-2.016939
92	6	0	3.901478	-1.844907	-2.729679
93	6	0	4.324011	-3.122830	-2.393340
94	6	0	3.698014	-3.806211	-1.349526
95	6	0	2.674604	-3.198146	-0.638479
96	1	0	4.362659	-1.290697	-3.537210
97	1	0	5.131882	-3.585879	-2.949892
98	1	0	4.015280	-4.811089	-1.088179
99	1	0	2.175567	-3.691655	0.187819
100	7	0	2.421769	0.056500	-2.497202
101	6	0	1.212207	-1.311562	-0.031719
102	8	0	0.838358	-2.012085	1.046078
103	1	0	0.422004	-0.831702	-0.616306
104	8	0	1.270021	0.416986	-2.267461
105	8	0	3.189817	0.707171	-3.185868
106	1	0	0.589742	-0.130485	2.877139
107	1	0	1.619542	-1.366309	3.572637

TS2X(RS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-4.512566	-0.153363	0.135525
2	8	0	-3.235182	-1.240336	-0.087003

3	7	0	2.273170	-1.262385	-0.899481
4	7	0	1.708470	-1.942310	-1.940058
5	7	0	0.276442	-0.514831	-1.017040
6	6	0	3.497706	-1.928520	1.101930
7	1	0	2.682711	-1.534400	1.716193
8	6	0	4.607857	-2.541097	1.676764
9	1	0	4.669733	-2.637936	2.745500
10	6	0	5.639148	-3.033691	0.870659
11	1	0	6.490222	-3.513749	1.320835
12	6	0	5.559966	-2.901720	-0.513909
13	1	0	6.367402	-3.277457	-1.151256
14	6	0	4.466512	-2.281150	-1.107481
15	1	0	4.386188	-2.161501	-2.182184
16	6	0	3.451194	-1.805852	-0.288954
17	6	0	1.451371	-0.330890	-0.370157
18	6	0	0.505920	-1.467050	-1.989055
19	6	0	-0.700266	-1.704330	-2.837877
20	1	0	-1.059191	-2.723405	-2.707392
21	1	0	-0.474983	-1.541881	-3.894457
22	6	0	-1.678766	-0.646854	-2.275823
23	1	0	-2.702524	-1.006705	-2.233204
24	1	0	-1.646730	0.250097	-2.898073
25	6	0	-1.174928	-0.251045	-0.855348
26	1	0	-1.353813	0.808937	-0.656490
27	6	0	-1.868626	-1.129014	0.285913
28	6	0	-4.046647	1.548161	-0.527955
29	6	0	-5.074097	0.001408	1.911730
30	1	0	-4.373674	0.604347	2.501536
31	1	0	-5.158408	-0.977265	2.381240
32	1	0	-6.060754	0.483371	1.941075
33	6	0	-5.892505	-0.934118	-0.907426
34	6	0	-7.048764	0.064179	-1.077783
35	1	0	-7.882440	-0.408263	-1.601120
36	1	0	-6.729735	0.942468	-1.673714
37	1	0	-7.420602	0.426259	-0.109691
38	6	0	-6.416609	-2.189754	-0.181846
39	1	0	-7.180402	-2.692298	-0.797621
40	1	0	-6.876095	-1.938174	0.779840
41	1	0	-5.615179	-2.906226	0.003573
42	6	0	-5.382937	-1.340047	-2.293912
43	1	0	-6.196182	-1.752692	-2.896158
44	1	0	-4.610045	-2.120064	-2.216037
45	1	0	-4.950903	-0.496473	-2.835998
46	6	0	-1.264124	-2.534762	0.273839

47	6	0	-0.031455	-2.745231	0.905193
48	6	0	-1.887952	-3.584387	-0.389604
49	6	0	0.585391	-3.988236	0.815758
50	1	0	0.417456	-1.930373	1.459613
51	6	0	-1.275786	-4.835741	-0.463258
52	1	0	-2.861144	-3.416835	-0.851059
53	6	0	-0.028902	-5.032020	0.121216
54	1	0	-1.771997	-5.650242	-0.978261
55	6	0	-1.824642	-0.533522	1.698979
56	6	0	-1.528475	0.795509	1.970247
57	6	0	-2.235987	-1.365554	2.745173
58	6	0	-1.634713	1.290187	3.268116
59	1	0	-1.168811	1.462620	1.204218
60	6	0	-2.347449	-0.874596	4.039182
61	1	0	-2.469964	-2.398694	2.528533
62	6	0	-2.055987	0.455866	4.299462
63	1	0	-2.678471	-1.534972	4.830572
64	6	0	3.052103	1.314499	0.845940
65	6	0	1.728889	0.624829	0.749932
66	8	0	1.128534	0.264217	1.848057
67	6	0	4.215667	1.087459	-0.057060
68	6	0	5.422279	0.632430	0.511276
69	6	0	4.147988	1.218618	-1.447886
70	6	0	6.511122	0.330627	-0.291335
71	1	0	5.497975	0.510821	1.590755
72	6	0	5.243055	0.918198	-2.253517
73	1	0	3.245491	1.624817	-1.885083
74	6	0	6.439439	0.468598	-1.680598
75	1	0	7.437842	-0.017872	0.169592
76	1	0	5.174324	1.045621	-3.328556
77	1	0	7.291277	0.231880	-2.305003
78	6	0	3.301528	1.877144	2.206699
79	6	0	4.244680	3.077517	2.280058
80	1	0	3.670646	1.015601	2.803236
81	1	0	2.333124	2.089722	2.653943
82	1	0	4.363604	3.387376	3.326457
83	1	0	5.231121	2.870867	1.856718
84	1	0	3.790924	3.897385	1.707360
85	1	0	-1.367776	2.322732	3.463946
86	1	0	-2.138239	0.841032	5.312650
87	1	0	1.554182	-4.148652	1.296356
88	1	0	0.452576	-6.000681	0.060394
89	1	0	-3.668917	1.518237	-1.553802
90	1	0	-4.918352	2.212652	-0.501731

91	1	0	-3.276422	1.995902	0.106869
92	6	0	0.208897	2.787988	-0.847803
93	6	0	-0.929820	3.601715	-0.726953
94	6	0	-1.803248	3.855473	-1.784338
95	6	0	-1.553631	3.301625	-3.030063
96	6	0	-0.399140	2.536483	-3.212169
97	6	0	0.457088	2.298099	-2.140563
98	1	0	-2.653703	4.505558	-1.610137
99	1	0	-2.228522	3.488953	-3.849402
100	1	0	-0.160039	2.126171	-4.191897
101	1	0	1.360905	1.713045	-2.291668
102	7	0	-1.261299	4.325287	0.521525
103	6	0	1.298408	2.528310	0.177804
104	8	0	2.482337	3.004889	-0.208569
105	1	0	0.967537	2.637051	1.235586
106	8	0	-0.967246	3.800371	1.594201
107	8	0	-1.813108	5.404060	0.407345

M2X(SS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.940275	-0.486192	0.047701
2	8	0	3.281978	-0.676217	0.292081
3	7	0	-1.557249	-1.970221	0.926760
4	7	0	-0.607015	-2.572068	1.713229
5	7	0	-0.035735	-0.514354	1.164088
6	6	0	-3.075546	-2.672711	-0.850960
7	1	0	-2.681736	-1.867822	-1.468323
8	6	0	-4.058020	-3.553685	-1.301686
9	1	0	-4.429327	-3.457568	-2.316950
10	6	0	-4.557725	-4.547814	-0.465897
11	1	0	-5.319014	-5.230723	-0.828113
12	6	0	-4.080330	-4.666278	0.839469
13	1	0	-4.469233	-5.437244	1.495866
14	6	0	-3.105242	-3.795996	1.309395
15	1	0	-2.713512	-3.877416	2.316780
16	6	0	-2.621626	-2.806700	0.455892
17	6	0	-1.269961	-0.686350	0.628596
18	6	0	0.294563	-1.655476	1.848792

19	6	0	1.593654	-1.502881	2.568730
20	1	0	2.373493	-2.092135	2.082296
21	1	0	1.512273	-1.804517	3.613835
22	6	0	1.845174	0.011755	2.373178
23	1	0	2.902539	0.267418	2.382469
24	1	0	1.324521	0.582687	3.147769
25	6	0	1.179993	0.327443	1.018355
26	1	0	0.893190	1.365413	0.921621
27	6	0	2.103055	-0.089276	-0.237867
28	6	0	5.614343	0.658396	1.380006
29	6	0	5.412548	0.150833	-1.649602
30	1	0	5.244769	1.226699	-1.749512
31	1	0	4.852429	-0.356305	-2.440524
32	1	0	6.478503	-0.046108	-1.812983
33	6	0	5.686059	-2.218878	0.288636
34	6	0	7.180037	-2.068036	0.620859
35	1	0	7.655008	-3.056938	0.658010
36	1	0	7.334394	-1.590053	1.593663
37	1	0	7.713285	-1.478064	-0.134272
38	6	0	5.553585	-3.042296	-1.001624
39	1	0	5.940465	-4.057506	-0.842447
40	1	0	6.126640	-2.595828	-1.821196
41	1	0	4.513665	-3.129709	-1.334286
42	6	0	5.001781	-2.963587	1.441977
43	1	0	5.533742	-3.899507	1.657754
44	1	0	3.968192	-3.226122	1.195478
45	1	0	4.988843	-2.370889	2.365175
46	6	0	1.403384	-1.133277	-1.105296
47	6	0	0.337213	-0.776532	-1.932411
48	6	0	1.767719	-2.479345	-1.014587
49	6	0	-0.318453	-1.743868	-2.689637
50	1	0	-0.026649	0.245359	-1.969211
51	6	0	1.105445	-3.446751	-1.765707
52	1	0	2.573264	-2.766138	-0.349584
53	6	0	0.066129	-3.079317	-2.616245
54	1	0	1.402793	-4.487321	-1.681249
55	6	0	2.475037	1.198342	-0.989495
56	6	0	2.946490	2.281787	-0.238202
57	6	0	2.472296	1.310672	-2.380086
58	6	0	3.405331	3.441492	-0.854138
59	1	0	2.962083	2.222038	0.848181
60	6	0	2.907856	2.480385	-2.999173
61	1	0	2.136549	0.482882	-2.992499
62	6	0	3.379627	3.547431	-2.242601

63	1	0	2.882132	2.550554	-4.081485
64	6	0	-3.667606	0.459622	0.777436
65	6	0	-2.245338	0.331330	-0.098695
66	8	0	-2.271268	0.176456	-1.368377
67	6	0	-4.762297	0.945744	-0.152814
68	6	0	-5.429456	2.140151	0.123567
69	6	0	-5.161671	0.189682	-1.258379
70	6	0	-6.483805	2.568187	-0.681354
71	1	0	-5.109066	2.732159	0.975290
72	6	0	-6.214565	0.615371	-2.060818
73	1	0	-4.634572	-0.727083	-1.490731
74	6	0	-6.881132	1.805630	-1.775411
75	1	0	-6.994179	3.498892	-0.452116
76	1	0	-6.511889	0.019355	-2.918447
77	1	0	-7.701309	2.137004	-2.404850
78	6	0	-4.226540	-0.498385	1.846129
79	6	0	-5.405016	-1.392216	1.465616
80	1	0	-6.290361	-0.789134	1.250094
81	1	0	-5.203379	-2.006509	0.586219
82	1	0	-5.640889	-2.063940	2.296108
83	1	0	3.772393	4.264678	-0.248357
84	1	0	3.717642	4.457002	-2.727869
85	1	0	-1.153405	-1.435733	-3.309722
86	1	0	-0.453453	-3.832066	-3.201042
87	1	0	5.435898	0.259718	2.384508
88	1	0	6.695767	0.776471	1.258118
89	1	0	5.166455	1.653600	1.319358
90	6	0	-1.006309	2.603336	1.197961
91	6	0	-0.125045	3.479157	0.548955
92	6	0	0.791165	4.278913	1.223388
93	6	0	0.888096	4.182198	2.603698
94	6	0	0.049352	3.298571	3.283755
95	6	0	-0.888450	2.538603	2.594544
96	1	0	1.423107	4.941104	0.644313
97	1	0	1.608049	4.788147	3.142142
98	1	0	0.114745	3.214122	4.364124
99	1	0	-1.573047	1.890200	3.128197
100	7	0	-0.078006	3.519239	-0.912086
101	6	0	-2.116761	1.848118	0.529457
102	8	0	-3.111907	1.566775	1.500212
103	8	0	-0.437911	2.513626	-1.502737
104	8	0	0.336970	4.531575	-1.449558
105	1	0	-3.414224	-1.086887	2.286932
106	1	0	-4.559821	0.180563	2.642108

107	1	0	-2.522686	2.443013	-0.299614

M2X(RR)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-4.890781	0.065339	-0.147679
2	8	0	-3.554437	-0.954866	-0.013977
3	7	0	1.885236	-1.501148	-0.930216
4	7	0	1.161147	-2.383700	-1.698774
5	7	0	-0.061445	-0.669254	-1.048163
6	6	0	3.372598	-1.932717	0.933254
7	1	0	2.621398	-1.511032	1.595695
8	6	0	4.570751	-2.446009	1.424590
9	1	0	4.764927	-2.422803	2.491459
10	6	0	5.509440	-2.984281	0.550579
11	1	0	6.441471	-3.383505	0.937095
12	6	0	5.257890	-3.009422	-0.822335
13	1	0	5.990887	-3.427090	-1.504008
14	6	0	4.068244	-2.498440	-1.324850
15	1	0	3.847710	-2.501468	-2.386372
16	6	0	3.145045	-1.956774	-0.435738
17	6	0	1.179284	-0.413986	-0.580900
18	6	0	-0.009717	-1.829080	-1.764282
19	6	0	-1.297767	-2.090091	-2.468096
20	1	0	-1.823503	-2.932114	-2.013118
21	1	0	-1.135781	-2.307509	-3.524874
22	6	0	-2.025204	-0.742913	-2.234624
23	1	0	-3.101108	-0.861420	-2.198824
24	1	0	-1.781895	-0.056118	-3.050238
25	6	0	-1.447026	-0.153531	-0.917542
26	1	0	-1.427991	0.934872	-0.921831
27	6	0	-2.212940	-0.693486	0.384599
28	6	0	-4.488262	1.536045	-1.251651
29	6	0	-5.560611	0.662453	1.497188
30	1	0	-4.929298	1.441236	1.933339
31	1	0	-5.624698	-0.157846	2.217143
32	1	0	-6.566567	1.073347	1.355878
33	6	0	-6.172790	-1.072789	-0.966049
34	6	0	-7.390295	-0.246204	-1.404004
35	1	0	-8.156453	-0.901545	-1.838787
36	1	0	-7.122265	0.496777	-2.163682

37	1	0	-7.852233	0.281994	-0.562345
38	6	0	-6.615811	-2.137260	0.048196
39	1	0	-7.319925	-2.838957	-0.418306
40	1	0	-7.118980	-1.687876	0.910981
41	1	0	-5.761508	-2.714907	0.419405
42	6	0	-5.578998	-1.773921	-2.193800
43	1	0	-6.330536	-2.424084	-2.661136
44	1	0	-4.720459	-2.396752	-1.918628
45	1	0	-5.251988	-1.054652	-2.954994
46	6	0	-1.604578	-2.031940	0.819844
47	6	0	-0.391076	-2.049593	1.520430
48	6	0	-2.237829	-3.237339	0.523853
49	6	0	0.189756	-3.262348	1.875275
50	1	0	0.075696	-1.095869	1.771533
51	6	0	-1.652395	-4.451507	0.884245
52	1	0	-3.193811	-3.219111	0.010857
53	6	0	-0.433567	-4.467752	1.551764
54	1	0	-2.155757	-5.382923	0.644252
55	6	0	-2.292080	0.269510	1.583389
56	6	0	-2.155859	1.655389	1.496296
57	6	0	-2.708847	-0.281853	2.800805
58	6	0	-2.430456	2.462492	2.598757
59	1	0	-1.790017	2.129623	0.594362
60	6	0	-2.972885	0.521388	3.904743
61	1	0	-2.838308	-1.357125	2.881569
62	6	0	-2.838120	1.903114	3.805891
63	1	0	-3.292582	0.066156	4.837114
64	6	0	1.536834	2.212374	-0.987888
65	6	0	1.396203	0.924690	0.120867
66	8	0	0.437236	0.995293	1.000037
67	6	0	0.440258	3.198057	-0.658501
68	6	0	-0.676976	3.332229	-1.491445
69	6	0	0.490865	3.968913	0.505243
70	6	0	-1.717338	4.202210	-1.170278
71	1	0	-0.741093	2.758689	-2.412849
72	6	0	-0.537375	4.851348	0.821517
73	1	0	1.358808	3.891445	1.150672
74	6	0	-1.651401	4.966531	-0.008799
75	1	0	-2.572266	4.287545	-1.834520
76	1	0	-0.472622	5.449188	1.726021
77	1	0	-2.455350	5.650980	0.243301
78	6	0	1.774883	2.146923	-2.518524
79	6	0	1.209704	0.983365	-3.331946
80	1	0	2.854228	2.170805	-2.662570

81	1	0	1.393614	3.078638	-2.949896
82	1	0	1.401707	1.161780	-4.393502
83	1	0	1.682727	0.031571	-3.074940
84	1	0	0.127921	0.876423	-3.209816
85	1	0	-2.306760	3.536400	2.504205
86	1	0	-3.045534	2.537377	4.662336
87	1	0	1.130824	-3.272728	2.417227
88	1	0	0.025072	-5.411045	1.830743
89	1	0	-4.250311	1.238453	-2.278119
90	1	0	-5.348029	2.213428	-1.291331
91	1	0	-3.642809	2.108724	-0.855232
92	6	0	4.135020	1.001856	0.939794
93	6	0	5.139687	0.716672	0.010228
94	6	0	6.427436	0.335895	0.368150
95	6	0	6.744973	0.198573	1.712129
96	6	0	5.773053	0.469063	2.672210
97	6	0	4.502276	0.878494	2.285327
98	1	0	7.153810	0.143801	-0.412595
99	1	0	7.742860	-0.108861	2.004245
100	1	0	6.010266	0.381665	3.727590
101	1	0	3.764956	1.128916	3.042472
102	7	0	4.868099	0.757412	-1.424387
103	6	0	2.767400	1.566703	0.645142
104	8	0	2.788357	2.567759	-0.359739
105	8	0	3.776415	0.368060	-1.801441
106	8	0	5.757430	1.127585	-2.169128
107	1	0	2.412841	1.982650	1.596961

M2X(SR)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	4.893245	-1.307441	-0.146942
2	8	0	3.572259	-0.393887	-0.693452
3	7	0	-1.342565	2.553276	-0.544317
4	7	0	-0.365231	3.368877	-1.052581
5	7	0	0.278263	1.254982	-1.009326
6	6	0	-2.909312	3.082549	1.260236
7	1	0	-2.348862	2.430873	1.920857
8	6	0	-4.022642	3.783016	1.702693
9	1	0	-4.337060	3.679758	2.735705
10	6	0	-4.735828	4.602427	0.826492

11	1	0	-5.606951	5.144617	1.180092
12	6	0	-4.332372	4.729851	-0.498587
13	1	0	-4.881554	5.371516	-1.179273
14	6	0	-3.217594	4.031117	-0.957406
15	1	0	-2.875014	4.122479	-1.982865
16	6	0	-2.537659	3.206871	-0.073141
17	6	0	-1.004115	1.253767	-0.557743
18	6	0	0.594747	2.550119	-1.338926
19	6	0	1.902152	2.646306	-2.043087
20	1	0	2.670417	3.055621	-1.383940
21	1	0	1.824805	3.280018	-2.927455
22	6	0	2.140413	1.156849	-2.387505
23	1	0	3.191952	0.888720	-2.446220
24	1	0	1.669372	0.934144	-3.349686
25	6	0	1.413733	0.334138	-1.291943
26	1	0	1.011737	-0.608723	-1.664371
27	6	0	2.379561	0.028157	-0.054484
28	6	0	4.710558	-3.060199	-0.795401
29	6	0	5.033805	-1.319006	1.723149
30	1	0	4.262875	-1.946978	2.176802
31	1	0	4.948464	-0.311165	2.142057
32	1	0	6.012527	-1.720223	2.009462
33	6	0	6.444097	-0.502996	-0.936341
34	6	0	7.429994	-1.614922	-1.335308
35	1	0	8.347459	-1.169604	-1.740685
36	1	0	7.013361	-2.275914	-2.101370
37	1	0	7.719302	-2.233710	-0.477433
38	6	0	7.175995	0.427149	0.045025
39	1	0	8.055564	0.864801	-0.445060
40	1	0	7.527961	-0.117786	0.926965
41	1	0	6.554894	1.254972	0.399815
42	6	0	6.063145	0.282604	-2.199680
43	1	0	6.968190	0.651283	-2.700028
44	1	0	5.435734	1.149878	-1.968018
45	1	0	5.516220	-0.340775	-2.916995
46	6	0	2.614853	1.314011	0.740640
47	6	0	1.598541	1.901993	1.507136
48	6	0	3.837795	1.975977	0.642278
49	6	0	1.809717	3.119350	2.147793
50	1	0	0.633461	1.412899	1.615273
51	6	0	4.055309	3.189582	1.291548
52	1	0	4.614340	1.548551	0.021214
53	6	0	3.038348	3.768342	2.043708
54	1	0	5.017686	3.683237	1.196755

55	6	0	1.851281	-1.142404	0.783572
56	6	0	1.607584	-2.351643	0.118022
57	6	0	1.631457	-1.085412	2.160472
58	6	0	1.102832	-3.453052	0.795921
59	1	0	1.798141	-2.428199	-0.948489
60	6	0	1.116744	-2.188506	2.841558
61	1	0	1.846005	-0.180602	2.715504
62	6	0	0.839338	-3.368816	2.162737
63	1	0	0.928040	-2.114234	3.907456
64	6	0	-2.110771	-0.775222	-1.705664
65	6	0	-2.069084	0.123207	-0.353412
66	8	0	-3.145478	0.563045	0.202119
67	6	0	-3.444655	-1.471368	-1.911324
68	6	0	-3.427899	-2.784674	-2.391821
69	6	0	-4.671369	-0.828344	-1.730609
70	6	0	-4.613097	-3.455871	-2.671134
71	1	0	-2.469930	-3.278848	-2.532827
72	6	0	-5.858463	-1.504244	-2.010501
73	1	0	-4.675760	0.179779	-1.334820
74	6	0	-5.835720	-2.814927	-2.477548
75	1	0	-4.584035	-4.476870	-3.039940
76	1	0	-6.808410	-1.001543	-1.855796
77	1	0	-6.764396	-3.335489	-2.690870
78	6	0	-1.625052	-0.217790	-3.041804
79	6	0	-2.511882	0.920415	-3.547694
80	1	0	-3.506291	0.554118	-3.812418
81	1	0	-2.644973	1.689005	-2.777330
82	1	0	-2.073659	1.391954	-4.430652
83	1	0	0.899155	-4.371385	0.254475
84	1	0	0.417368	-4.218055	2.690496
85	1	0	1.004837	3.559666	2.727457
86	1	0	3.198325	4.718150	2.543211
87	1	0	4.516632	-3.066433	-1.873276
88	1	0	5.625829	-3.631985	-0.616256
89	1	0	3.888250	-3.578204	-0.297657
90	6	0	-2.215814	-1.953462	1.091665
91	6	0	-2.797885	-1.385523	2.230061
92	6	0	-3.700452	-2.071177	3.034937
93	6	0	-4.025649	-3.382145	2.715144
94	6	0	-3.454828	-3.978912	1.591740
95	6	0	-2.572527	-3.266793	0.787822
96	1	0	-4.129575	-1.569216	3.893406
97	1	0	-4.721515	-3.933229	3.338012
98	1	0	-3.708961	-5.002196	1.334189

99	1	0	-2.151044	-3.709745	-0.107510
100	7	0	-2.431329	-0.035091	2.658242
101	6	0	-1.322137	-1.159805	0.195163
102	8	0	-1.144666	-1.695356	-1.124488
103	1	0	-0.373769	-0.980234	0.684760
104	8	0	-1.300867	0.366848	2.397474
105	8	0	-3.229412	0.598198	3.321668
106	1	0	-0.592602	0.129060	-2.946665
107	1	0	-1.609795	-1.038174	-3.770239

M2X(RS)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-4.532635	-0.034806	0.133625
2	8	0	-3.314142	-1.178490	-0.126278
3	7	0	2.218286	-1.200708	-0.884083
4	7	0	1.655041	-1.897032	-1.926836
5	7	0	0.215690	-0.493988	-1.008819
6	6	0	3.473538	-1.904135	1.078349
7	1	0	2.687734	-1.481885	1.705287
8	6	0	4.577626	-2.559404	1.615971
9	1	0	4.652321	-2.676946	2.692200
10	6	0	5.572735	-3.068791	0.784659
11	1	0	6.425698	-3.584782	1.213436
12	6	0	5.474255	-2.918138	-0.597332
13	1	0	6.251708	-3.307571	-1.246078
14	6	0	4.384508	-2.260069	-1.155547
15	1	0	4.284875	-2.131435	-2.227149
16	6	0	3.405451	-1.761251	-0.305913
17	6	0	1.384996	-0.284089	-0.360344
18	6	0	0.449059	-1.433185	-1.981199
19	6	0	-0.740589	-1.647765	-2.848860
20	1	0	-1.116463	-2.665642	-2.736987
21	1	0	-0.492600	-1.481985	-3.898966
22	6	0	-1.713413	-0.578658	-2.293742
23	1	0	-2.745104	-0.919066	-2.287192
24	1	0	-1.645998	0.327512	-2.901430
25	6	0	-1.237120	-0.227051	-0.858570
26	1	0	-1.407465	0.825584	-0.641768
27	6	0	-1.943138	-1.131610	0.243308
28	6	0	-3.974373	1.666759	-0.452312

29	6	0	-5.085684	0.071886	1.919879
30	1	0	-4.360143	0.611289	2.535619
31	1	0	-5.218021	-0.923785	2.351937
32	1	0	-6.044758	0.598731	1.977817
33	6	0	-5.948821	-0.705623	-0.935042
34	6	0	-7.054867	0.353233	-1.052052
35	1	0	-7.913906	-0.058625	-1.597577
36	1	0	-6.711820	1.238444	-1.598614
37	1	0	-7.417636	0.681402	-0.071479
38	6	0	-6.522039	-1.967989	-0.273376
39	1	0	-7.305634	-2.404867	-0.906407
40	1	0	-6.969539	-1.745992	0.701220
41	1	0	-5.747615	-2.728938	-0.124243
42	6	0	-5.452475	-1.065212	-2.340537
43	1	0	-6.292498	-1.392536	-2.967387
44	1	0	-4.725082	-1.883452	-2.305063
45	1	0	-4.983188	-0.209183	-2.840836
46	6	0	-1.374573	-2.548109	0.174795
47	6	0	-0.138319	-2.813648	0.778547
48	6	0	-2.045663	-3.568018	-0.495925
49	6	0	0.443093	-4.070094	0.653452
50	1	0	0.356834	-2.022432	1.345112
51	6	0	-1.466522	-4.833352	-0.603655
52	1	0	-3.018707	-3.365215	-0.932669
53	6	0	-0.217373	-5.082186	-0.043768
54	1	0	-1.994808	-5.624073	-1.127353
55	6	0	-1.865256	-0.611121	1.679750
56	6	0	-1.527403	0.693337	2.009889
57	6	0	-2.294896	-1.473443	2.696646
58	6	0	-1.624040	1.145347	3.325199
59	1	0	-1.169821	1.383905	1.258869
60	6	0	-2.386847	-1.032592	4.009199
61	1	0	-2.567734	-2.495293	2.448310
62	6	0	-2.054091	0.284798	4.327244
63	1	0	-2.723821	-1.713707	4.784296
64	6	0	3.084538	1.484800	0.780868
65	6	0	1.633807	0.698528	0.790086
66	8	0	1.226476	0.117672	1.880513
67	6	0	4.300087	1.101889	-0.041588
68	6	0	5.433168	0.504618	0.527256
69	6	0	4.333779	1.391841	-1.409407
70	6	0	6.542444	0.186119	-0.246683
71	1	0	5.451554	0.276743	1.587401
72	6	0	5.437689	1.058735	-2.191813

73	1	0	3.505790	1.931338	-1.852202
74	6	0	6.547546	0.451180	-1.614723
75	1	0	7.403396	-0.280913	0.221955
76	1	0	5.435503	1.296003	-3.251508
77	1	0	7.412589	0.197194	-2.219294
78	6	0	3.415289	1.775924	2.244627
79	6	0	4.383543	2.942384	2.418939
80	1	0	3.787977	0.855469	2.708355
81	1	0	2.474718	1.981595	2.760982
82	1	0	4.509650	3.185392	3.477221
83	1	0	5.370064	2.726926	2.000277
84	1	0	3.990452	3.826484	1.909451
85	1	0	-1.349387	2.169416	3.553728
86	1	0	-2.125508	0.633458	5.352720
87	1	0	1.412339	-4.258544	1.105633
88	1	0	0.235742	-6.063823	-0.138758
89	1	0	-3.578781	1.658391	-1.474351
90	1	0	-4.816735	2.365726	-0.422560
91	1	0	-3.202615	2.063995	0.216713
92	6	0	0.279945	2.669911	-0.739145
93	6	0	-0.813566	3.551542	-0.716615
94	6	0	-1.519959	3.918845	-1.863174
95	6	0	-1.143152	3.413033	-3.095061
96	6	0	-0.019047	2.589804	-3.172824
97	6	0	0.672880	2.247443	-2.021231
98	1	0	-2.351160	4.605973	-1.763884
99	1	0	-1.699343	3.681960	-3.985881
100	1	0	0.322095	2.218820	-4.134129
101	1	0	1.556830	1.624736	-2.100481
102	7	0	-1.267316	4.227016	0.511035
103	6	0	1.136844	2.235183	0.430473
104	8	0	2.476283	2.635464	0.167117
105	1	0	0.766851	2.635506	1.376569
106	8	0	-1.182320	3.639177	1.576440
107	8	0	-1.720725	5.349845	0.388096
