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A DFT Study on Reaction Mechanism of Dimerization of Methyl Methacrylate Catalyzed by N-Heterocyclic Carbene

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Supporting Information

Contents

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Table S1 The E(elec), ZPVE, E(elec)+ZPVE (unit: a.u.) of All the Reactants, Intermediates, Transition States, and Products Calculated at M05-2X/6-311++G(2d, 2p)//M05-2X/6-31G(d, p) level of theory

Species	E(elec)	ZPVE	E (E(elec)+ZPVE)
R	-345.853556	0.125875	-345.727681
Cat	-935.557750	0.307451	-935.250299
TS1(A)	-1281.395774	0.434460	-1280.961314
M1(A)	-1281.424375	0.435770	-1280.988605
TS2(A)	-1281.350683	0.431399	-1280.919284
M2(A)	-1281.446038	0.436762	-1281.009276
TS3(A)	-1627.279273	0.564654	-1626.714619
M3(A)	-1627.295090	0.566503	-1626.728587
TS4(A)	-1627.242323	0.560813	-1626.681510
M4(A)	-1627.326516	0.567369	-1626.759147
TS5(A)	-1627.251124	0.563292	-1626.687832
M5(A)	-1627.311271	0.567588	-1626.743683
TS6(A)	-1627.288241	0.565747	-1626.722494
P(E)	-691.744375	0.256825	-691.487550
TS1(B)	-1627.242142	0.560043	-1626.682099
M1(B)	-1627.255525	0.564210	-1626.691315
TS2(B)	-1627.235069	0.559912	-1626.675157
M2(B)+R′	-1627.305920	0.563924	-1626.741996
TS3(B)	-1627.276551	0.564990	-1626.711561
M3(B)	-1627.292639	0.567077	-1626.725562
TS4(B)	-1627.261245	0.561869	-1626.699376
M4(B)	-1627.311263	0.566738	-1626.744525

TS5(B)	-1627.291591	0.565747	-1626.725844
TS4(C)	-1627.241285	0.561801	-1626.679484
M4(C)	-1627.327329	0.567657	-1626.759672
TS5(C)	-1627.236518	0.562465	-1626.674053
M5(C)	-1627.296458	0.566933	-1626.729525
TS6(C)	-1627.283537	0.566135	-1626.717402
P(Z)	-691.743058	0.257242	-691.485816
TS3(D)	-1627.272365	0.565442	-1626.706923
M3(D)	-1627.286102	0.566692	-1626.719410
TS4(D)	-1627.262534	0.561628	-1626.700906
M4(D)	-1627.302512	0.566432	-1626.736080
TS5(D)	-1627.285046	0.565502	-1626.719544

Part S1: channel A

As shown in Figure 2 for channel A, obviously, the distance between the C1 atom and the C2 atom shortens from 1.909 Å in **TS1(A)** to 1.486 Å in **M1(A)**, indicating the formation of C1–C2 bond in the first step. Secondly, the distance between C2 and H4 varies from 1.100 Å in **M1(A)** to 1.233 Å in **TS2(A)**, and finally to 2.162 Å in **M2(A)**, concerted with distance of C3–H4 changing from 2.141 Å in **M1(A)** to 1.366 Å in **TS2(A)** and finally to 1.087 Å in **M2(A)**. Additionally, the dihedral angle of N6–C1–C2–C3 changed from -69.0° in **M1(A)** to -37.1° in **TS2(A)**, and finally to -5.2° in **M2(A)**, implying that these four atoms (N6C1C2C3) are almost in the same plane in **M2(A)**. Thirdly, the distance of C2–C2′ shortens from 1.991 Å in **TS3(A)** to 1.586 Å in **M3(A)**, indicating the formation of C2–C2′ bond in **M3(A)**. Fourthly, the distance between the C2 atom and the H5 proton changes from 1.091 Å in **M3(A)** to 1.417 Å in **TS4(A)**, accompanied with the distance of C3′–H5 changing from 1.470 Å in **TS4(A)** to 1.092 Å in **M4(A)**, which demonstrates that the H5 proton has transferred from the C2 atom to the C3′ atom in the intermediate **M4(A)**. Specifically, the dihedral angle of C1–C2–C3–C2′ changed from 125.7° in **M3(A)** to 152.2° in **TS4(A)**, and finally to 171.7° in **M4(A)**, which indicates that these four atoms (C1C2C3C2′**)** are almost in the same plane in **M4(A)**. Fifthly, the distances of

C3–H4 and C2–H4 are separately 1.367 Å and 1.234 Å in **TS5(A)**, which indicates that the H4 proton is transferring from the C3 atom to the C2 atom. The length between the C2 atom and H4 atom is 1.094 Å in **M5(A)**, demonstrating the formation of C2–H4 bond. Lastly, the distance between the C1 atom and the C2 atom lengthens from 1.503 Å in **M5(A)** to 1.885 Å in **TS6(A)**, however, the bond length of C2–C3 shortens from 1.503 Å in **M5(A)** to 1.410 Å in **TS6(A)** and finally to 1.337 Å in the final product **P(E)**, which indicates the break of the C1–C2 bond and the formation of C2=C3 bond.

Part S2: channel B

As shown in Figure 3 for channel B, the first step is the same with the first step in channel A. Secondly, the distance between the H5 proton and the O7′ atom shortens from 1.344 Å in **TS1(B)** and finally to 0.983 Å in **M1(B)**, as well as the distance of C2–H5 changing from 1.263 Å in **TS1(B)** to 1.951 Å in **M1(B)**. All these changes indicate that H5 proton has transferred from the C2 atom to the O7′ atom in **M1(B)**. Thirdly, in **TS2(B)**, the distances of C3–H5 and H5–O7′ are 1.557 Å and 1.130 Å, respectively. Fourthly, the distance between the C2 atom and the C2′ atom shortens from 1.990 Å in **TS3(B)** to 1.576 Å in **M3(B)**, which indicates the fully formation of C2–C2′ bond in **M3(B)**. Fifthly, the distance between the C3 atom and the H5 proton changes from 1.092 Å in **M3(B)** to 1.401 Å in **TS4(B)** and then to 2.860 Å in **M4(B)**, which is accompanied with the distance of the C3′ atom and the H5 proton shortening from initially 2.770 Å in **M3(B)** to 1.489 Å in **TS4(B)** and finally to 1.091 Å in **M4(B)**, indicating that the H5 proton has transferred from the C3 atom to the C3′ atom in **M4(B)**. Lastly, the distance between the C1 atom and the C2 atom lengthens from 1.499 Å in **M4(B)** to 1.863 Å in **TS5(B)**. Moreover, the bond length of C2–C3 bond shortens from 1.512 Å in **M4(B)** to 1.410 Å in **TS5(B)** and finally to 1.337 Å in **P(E)**. All these changes indicate the break of C1–C2 bond and the formation of C2=C3 bond.

Part S3: channel C

There are seven reaction steps in channel C, and the former four steps of channel C are the same with those of channel B, so we only focus on the later three steps (the fifth step to the seventh step) in channel C as follows: As shown in Figure 4, fifthly**,** the distance between the C2 atom and the H4 proton is elongated from 1.091 Å in **M3(B)** (as shown in Figure 3) to 1.410 Å in **TS4(C)**, while the distance between the C3′ atom and the H4 proton is shortened from 1.463 Å in **TS4(C)** to 1.091 Å in **M4(C)**, indicating that the H4 proton has transferred from the C2 atom to the C3′ atom. Specifically, the dihedral angle of C1–C2–C3–C2′ changed from 146.5° in **TS4**(C) to 170.9° in **M4(C)**, demonstrating the four members (C1C2C3C2′) are almost in the same plane in **M4(C)**. It should be noted that **M4(C)** is the configurational isomer of **M4** (depicted in Scheme 2). Sixthly, the distance of C3–H5 is lengthened from 1.099 Å in **M4(C)** to 1.382 Å in **TS5(C)**, while the distance between the C2 atom and the H5 proton is shortened from 1.221 Å in **TS5(C)** to 1.097 Å in **M5(C)**. All these changes show that the H5 proton has transferred from the C3 atom to the C2 atom. This is to say, the C2–H5 bond forms with the break of the C3–H5 bond. Seventhly, the distance between the C1 atom and the C2 atom lengthens from 1.524 Å in **M5(C)** to 1.847 Å in **TS6(C)**, as well as, the bond length of C2–C3 bond shortens from 1.496 Å in **M5(C)** to 1.416 Å in **TS6(C)** and finally to 1.341 Å in **P(Z)**, indicating the breaking of C1–C2 bond and the formation of C2=C3 bond.

Part S4: channel D

There are six reaction steps in channel D, and the former three steps of channel D are the same with those of channel B, so we only discussed the later three reaction steps (the fourth step to the sixth step) in channel D as follows.

As shown in Figure 5, fourthly, the distance between the C2 atom and the C2′ atom shortens from 1.914 Å in **TS3(D)** to 1.576 Å in **M3(D)**, showing the formation

of the C2–C2′ bond in **M3(D)**. Fifthly, the distance between the C3 atom and the H5 proton varies from 1.097 Å in **M3(D)** to 1.346 Å in **TS4(D)** and finally to 2.656 Å in **M4(D)**, concerted with the distance of the C3′ atom and the H5 proton changing from 2.555 Å in **M3(D)** to 1.501 Å in **TS4(D)** and then to 1.092 Å in **M4(D)**, which demonstrates the H5 proton has transferred from the C3 atom to the C3′ atom in **M4(D)**. Sixthly, the distance between the C1 atom and C2 atom lengthens from 1.507 Å in **M4(D)** to 1.874 Å in **TS5(D)**. Meanwhile, the bond length of C2–C3 bond shortens from 1.498 Å in **M4(D)** to 1.415 Å in **TS5(D)**. Especially, the bond length of C2=C3 is 1.341 Å in **P(Z)** (Figure 4). All these changes show that the product **P(Z)** is formed *via* transition state **TS5(D)**.

List of the Cartesian Coordinates of All Structures

Cat

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.253004	0.642345	-0.022891
2	7	0	-1.698683	-0.127774	-0.002258
3	6	0	-3.120409	-0.070071	-0.001138
4	6	0	-3.844210	-1.260049	0.034064
5	6	0	-3.767135	1.161390	-0.034489
6	6	0	-5.231740	-1.207998	0.035021
7	1	0	-3.306319	-2.196737	0.060727
8	6	0	-5.158120	1.194420	-0.032224
9	1	0	-3.183542	2.069700	-0.063740
10	6	0	-5.895648	0.015987	0.002497
11	1	0	-5.796122	-2.131600	0.062874
12	1	0	-5.664229	2.151216	-0.058886
13	1	0	-6.977615	0.049637	0.003973
14	7	0	0.294697	-0.744585	0.000573
15	6	0	1.449367	-1.577072	0.092660
16	6	0	1.529704	-2.695883	-0.729737
17	6	0	2.455539	-1.288807	1.009992
18	6	0	2.638068	-3.529821	-0.638207

19	1	0	0.715342	-2.901461	-1.411000
20	6	0	3.565385	-2.123319	1.084482
21	1	0	2.365566	-0.424543	1.654991
22	6	0	3.660280	-3.242211	0.262068
23	1	0	2.702693	-4.403727	-1.273787
24	1	0	4.351557	-1.902383	1.794959
25	1	0	4.523990	-3.891423	0.327719
26	7	0	-0.984121	1.037048	-0.020100
27	6	0	1.392640	1.570532	-0.093204
28	6	0	2.512429	1.294609	-0.882446
29	6	0	1.315865	2.777093	0.606368
30	6	0	3.550013	2.216016	-0.956900
31	1	0	2.567554	0.368867	-1.440384
32	6	0	2.356451	3.694518	0.526615
33	1	0	0.436503	2.981637	1.203086
34	6	0	3.476072	3.414101	-0.251484
35	1	0	4.414290	1.999689	-1.571786
36	1	0	2.293472	4.627177	1.072546
37	1	0	4.287489	4.128412	-0.311564
38	6	0	-0.973202	-1.265328	0.006080

R

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.097220	-0.941732	-0.000035
2	1	0	-1.781453	-1.976703	-0.000016
3	1	0	-3.156915	-0.719178	-0.000088
4	6	0	-1.187940	0.031809	0.000005
5	6	0	-1.506909	1.499936	-0.000014
6	1	0	-2.585476	1.651809	-0.000044
7	1	0	-1.078990	1.988152	0.876756
8	1	0	-1.078938	1.988144	-0.876762
9	6	0	0.245883	-0.390486	0.000061
10	8	0	0.642571	-1.532581	0.000229
11	8	0	1.074390	0.669170	-0.000109
12	6	0	2.466961	0.333087	-0.000102
13	1	0	2.998004	1.280168	-0.000692
14	1	0	2.711830	-0.249891	0.886131
15	1	0	2.711603	-0.250893	-0.885735

TS1(A)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.525090	1.254031	-0.457367
2	7	0	1.458493	0.658878	-0.802985
3	6	0	2.870145	0.776060	-0.808071
4	6	0	3.595161	0.164204	-1.824693
5	6	0	3.498693	1.480195	0.213245
6	6	0	4.982745	0.261678	-1.817495
7	1	0	3.067530	-0.369041	-2.605393
8	6	0	4.882869	1.584707	0.196734
9	1	0	2.899331	1.898898	1.008209
10	6	0	5.626597	0.978131	-0.813793
11	1	0	5.556475	-0.211832	-2.603827
12	1	0	5.385283	2.126769	0.987537
13	1	0	6.706112	1.059511	-0.814375
14	7	0	-0.521108	-0.042652	-0.938618
15	6	0	-1.615486	-0.946895	-1.025695
16	6	0	-2.469138	-1.108349	0.060739
17	6	0	-1.779417	-1.686024	-2.191538
18	6	0	-3.520296	-2.011930	-0.038417
19	1	0	-2.289602	-0.553279	0.972518
20	6	0	-2.825987	-2.598690	-2.273656
21	1	0	-1.088226	-1.537868	-3.011320
22	6	0	-3.699288	-2.757428	-1.201145
23	1	0	-4.187693	-2.148176	0.802605
24	1	0	-2.961514	-3.179384	-3.177006
25	1	0	-4.515284	-3.465470	-1.268705
26	7	0	0.692525	1.702251	-0.378152
27	6	0	-1.705672	2.068976	-0.137094
28	6	0	-2.882554	1.983402	-0.885073
29	6	0	-1.612700	2.981104	0.916744
30	6	0	-3.960288	2.802458	-0.570945
31	1	0	-2.951391	1.288800	-1.712170
32	6	0	-2.693712	3.797933	1.223350
33	1	0	-0.690970	3.036856	1.481022
34	6	0	-3.869357	3.707424	0.483149
35	1	0	-4.870140	2.737129	-1.153706
36	1	0	-2.619388	4.502286	2.041927
37	1	0	-4.712133	4.342721	0.724846
38	6	0	0.771002	-0.445873	-1.135794
39	6	0	1.405584	-2.093279	-0.409059

40	1	0	2.402629	-1.682346	-0.288653
41	1	0	1.310153	-2.782205	-1.240840
42	6	0	0.680618	-2.375520	0.752800
43	6	0	-0.329711	-3.490366	0.840635
44	1	0	-0.669029	-3.777186	-0.157678
45	1	0	0.096669	-4.380643	1.315346
46	1	0	-1.205639	-3.207763	1.424061
47	6	0	0.931045	-1.499437	1.859101
48	8	0	1.654347	-0.503646	1.848190
49	8	0	0.239516	-1.843293	2.988323
50	6	0	0.455426	-0.972419	4.092429
51	1	0	-0.143531	-1.370291	4.908483
52	1	0	1.509432	-0.950246	4.368206
53	1	0	0.143510	0.044376	3.850540

M1(A)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.695827	-1.452191	-0.223595
2	7	0	-1.358420	-1.082086	-0.536886
3	6	0	-2.761908	-1.316426	-0.403661
4	6	0	-3.323944	-2.406296	-1.056634
5	6	0	-3.502390	-0.463296	0.406642
6	6	0	-4.685994	-2.637241	-0.909207
7	1	0	-2.698527	-3.053273	-1.657822
8	6	0	-4.867932	-0.703043	0.529065
9	1	0	-2.984263	0.328165	0.938711
10	6	0	-5.457221	-1.781063	-0.125569
11	1	0	-5.145291	-3.480652	-1.408123
12	1	0	-5.468123	-0.052064	1.151433
13	1	0	-6.519374	-1.961717	-0.018659
14	7	0	0.554746	-0.158362	-0.689227
15	6	0	1.557371	0.869516	-0.758056
16	6	0	1.980446	1.455081	0.428520
17	6	0	2.071976	1.238891	-1.993268
18	6	0	2.962474	2.434469	0.367873
19	1	0	1.492909	1.161931	1.350272
20	6	0	3.053002	2.225992	-2.038964
21	1	0	1.713133	0.756864	-2.894492
22	6	0	3.498987	2.816524	-0.860856
23	1	0	3.296835	2.912581	1.279076

24	1	0	3.466111	2.529931	-2.991952
25	1	0	4.261736	3.583876	-0.900252
26	7	0	-0.468366	-2.030424	-0.143328
27	6	0	1.951662	-2.117655	0.149014
28	6	0	3.175129	-1.807244	-0.449322
29	6	0	1.885120	-3.119592	1.122127
30	6	0	4.322249	-2.493454	-0.067398
31	1	0	3.235976	-1.042335	-1.210498
32	6	0	3.035062	-3.801658	1.494675
33	1	0	0.930730	-3.345377	1.578650
34	6	0	4.256088	-3.487814	0.903105
35	1	0	5.268365	-2.250662	-0.533543
36	1	0	2.979118	-4.573019	2.251981
37	1	0	5.153471	-4.016687	1.198388
38	6	0	-0.766617	0.071295	-0.825874
39	6	0	-1.378258	1.322929	-1.342680
40	1	0	-2.418259	1.095748	-1.611925
41	1	0	-0.857343	1.543941	-2.285772
42	6	0	-1.193375	2.469230	-0.385061
43	6	0	-1.177134	3.848147	-0.968030
44	1	0	-0.368059	3.973076	-1.702729
45	1	0	-2.112308	4.102771	-1.484429
46	1	0	-1.025091	4.581441	-0.178645
47	6	0	-0.989917	2.165538	0.936593
48	8	0	-0.948978	0.999840	1.451248
49	8	0	-0.765515	3.251076	1.771023
50	6	0	-0.636856	2.924574	3.142524
51	1	0	-0.538321	3.874191	3.666808
52	1	0	-1.509853	2.382693	3.508670
53	1	0	0.243577	2.306068	3.330996

TS2(A)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.431585	-1.515147	-0.123905
2	7	0	1.590488	-0.967018	0.180501
3	6	0	2.990447	-1.174973	0.160285
4	6	0	3.787893	-0.713997	1.204381
5	6	0	3.546028	-1.874809	-0.909125
6	6	0	5.163203	-0.922753	1.153860
7	1	0	3.333391	-0.231432	2.059209

8	6	0	4.916526	-2.092871	-0.937989
9	1	0	2.897273	-2.233353	-1.696345
10	6	0	5.729273	-1.609089	0.085848
11	1	0	5.787128	-0.561981	1.961404
12	1	0	5.353251	-2.632577	-1.768449
13	1	0	6.798468	-1.774303	0.053242
14	7	0	-0.419663	-0.164442	0.187216
15	6	0	-1.518231	0.534044	0.799631
16	6	0	-2.308473	1.418264	0.074250
17	6	0	-1.768648	0.279630	2.145135
18	6	0	-3.373811	2.044382	0.711532
19	1	0	-2.055496	1.606429	-0.960854
20	6	0	-2.835267	0.913535	2.774138
21	1	0	-1.132905	-0.414081	2.682415
22	6	0	-3.637607	1.794650	2.056039
23	1	0	-3.994534	2.735751	0.156374
24	1	0	-3.040532	0.714328	3.818000
25	1	0	-4.469321	2.286970	2.543941
26	7	0	0.763980	-2.008534	-0.148116
27	6	0	-1.637401	-2.310597	-0.386351
28	6	0	-2.728061	-1.776080	-1.074665
29	6	0	-1.659662	-3.643378	0.032077
30	6	0	-3.839935	-2.570685	-1.327279
31	1	0	-2.694646	-0.754447	-1.426514
32	6	0	-2.772502	-4.432313	-0.227433
33	1	0	-0.801566	-4.043650	0.555947
34	6	0	-3.866253	-3.895681	-0.901959
35	1	0	-4.683335	-2.155532	-1.863937
36	1	0	-2.788622	-5.463937	0.100450
37	1	0	-4.735577	-4.510186	-1.099906
38	6	0	0.900346	0.197934	0.373014
39	6	0	1.426485	1.443576	0.734618
40	1	0	2.463789	1.457235	1.043304
41	1	0	0.504098	2.015115	1.320264
42	6	0	0.852179	2.779631	0.243382
43	6	0	1.423640	4.012039	0.896067
44	1	0	1.575441	3.852648	1.967289
45	1	0	2.394135	4.294279	0.469581
46	1	0	0.749961	4.858883	0.776819
47	6	0	0.261802	2.807312	-1.041229
48	8	0	0.003741	1.836853	-1.762559
49	8	0	-0.054394	4.081211	-1.449947
50	6	0	-0.651187	4.149382	-2.737693
51	1	0	-0.774248	5.208593	-2.952923

52	1	0	-0.017245	3.677712	-3.487916
53	1	0	-1.622510	3.650933	-2.748328

M2(A)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.112076	1.210411	0.202638
2	7	0	0.967357	1.418467	-0.172971
3	6	0	2.167366	2.142144	-0.289512
4	6	0	3.106862	1.823676	-1.271691
5	6	0	2.388171	3.223829	0.566638
6	6	0	4.278229	2.567082	-1.368326
7	1	0	2.906039	1.020155	-1.966349
8	6	0	3.554841	3.966332	0.447264
9	1	0	1.637418	3.468105	1.305065
10	6	0	4.510810	3.637018	-0.510934
11	1	0	5.003787	2.314341	-2.131468
12	1	0	3.721527	4.802899	1.114366
13	1	0	5.423289	4.213458	-0.592425
14	7	0	-0.633018	-0.074799	-0.055666
15	6	0	-1.463597	-1.097317	-0.624169
16	6	0	-1.769333	-2.239613	0.110704
17	6	0	-1.976898	-0.912817	-1.904350
18	6	0	-2.595680	-3.206920	-0.451752
19	1	0	-1.319137	-2.377273	1.085463
20	6	0	-2.809527	-1.881109	-2.456008
21	1	0	-1.725399	-0.012199	-2.451318
22	6	0	-3.118195	-3.027940	-1.730386
23	1	0	-2.828667	-4.101934	0.110639
24	1	0	-3.216084	-1.738858	-3.449097
25	1	0	-3.764675	-3.782112	-2.161188
26	7	0	-0.176296	2.093623	0.169182
27	6	0	-2.511465	1.546845	0.497365
28	6	0	-3.360322	0.661704	1.165710
29	6	0	-2.978473	2.813433	0.133267
30	6	0	-4.665663	1.040485	1.457207
31	1	0	-2.998566	-0.311426	1.466707
32	6	0	-4.281572	3.187112	0.432214
33	1	0	-2.307423	3.489815	-0.379638
34	6	0	-5.129750	2.300018	1.090736
35	1	0	-5.318435	0.351080	1.977374

36	1	0	-4.637538	4.168674	0.146140
37	1	0	-6.147750	2.590224	1.318675
38	6	0	0.753829	0.040684	-0.289350
39	6	0	1.686656	-0.908953	-0.520344
40	1	0	2.708847	-0.569148	-0.595297
41	1	0	0.496064	-2.700513	-0.740344
42	6	0	1.511810	-2.408418	-0.487806
43	6	0	2.492603	-3.088416	-1.445911
44	1	0	2.267788	-2.780798	-2.467385
45	1	0	3.516603	-2.799115	-1.210381
46	1	0	2.420515	-4.175440	-1.381987
47	6	0	1.720925	-2.837315	0.951757
48	8	0	0.839900	-3.052124	1.755653
49	8	0	3.022929	-2.896240	1.278268
50	6	0	3.282048	-3.183276	2.657170
51	1	0	4.363352	-3.195674	2.757303
52	1	0	2.843620	-2.412396	3.289035
53	1	0	2.856303	-4.148054	2.928141

TS3(A)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.924962	1.031435	-0.547913
2	7	0	0.124323	1.467893	-0.268023
3	6	0	1.259942	2.329105	-0.181515
4	6	0	2.447907	1.975193	-0.807355
5	6	0	1.120797	3.520856	0.525173
6	6	0	3.536231	2.836389	-0.686636
7	1	0	2.503071	1.067116	-1.401347
8	6	0	2.213151	4.372776	0.623691
9	1	0	0.166605	3.764333	0.974759
10	6	0	3.423474	4.026308	0.024854
11	1	0	4.470585	2.575646	-1.167026
12	1	0	2.121252	5.304263	1.167466
13	1	0	4.274727	4.690406	0.107053
14	7	0	-1.338176	-0.070738	0.053508
15	6	0	-1.979590	-1.341473	0.250843
16	6	0	-2.427525	-1.699398	1.519251
17	6	0	-2.193060	-2.157417	-0.853921
18	6	0	-3.089653	-2.912810	1.677170
19	1	0	-2.231003	-1.037131	2.354425

20	6	0	-2.859542	-3.366306	-0.683063
21	1	0	-1.839018	-1.843354	-1.827386
22	6	0	-3.306003	-3.743379	0.580185
23	1	0	-3.437740	-3.207184	2.658807
24	1	0	-3.027080	-4.010756	-1.535991
25	1	0	-3.822907	-4.685635	0.710020
26	7	0	-1.049373	1.969556	-0.738165
27	6	0	-3.326363	1.150423	-0.977614
28	6	0	-4.387389	0.601696	-0.253174
29	6	0	-3.582973	1.886397	-2.138671
30	6	0	-5.692115	0.783926	-0.696681
31	1	0	-4.201131	0.049031	0.656682
32	6	0	-4.889449	2.065656	-2.573101
33	1	0	-2.751237	2.308752	-2.686877
34	6	0	-5.945903	1.511717	-1.855270
35	1	0	-6.511657	0.360121	-0.130674
36	1	0	-5.081953	2.632929	-3.474601
37	1	0	-6.964166	1.648337	-2.196727
38	6	0	-0.006679	0.217107	0.240970
39	6	0	1.029099	-0.634849	0.711796
40	1	0	1.986759	-0.128481	0.648678
41	6	0	0.849817	-1.288365	2.086294
42	1	0	-0.017139	-1.948544	2.090160
43	6	0	1.256604	-2.054230	-0.665189
44	1	0	0.705324	-2.821189	-0.124296
45	1	0	0.682507	-1.551313	-1.435338
46	6	0	2.584023	-2.332982	-1.025687
47	6	0	3.117404	-1.517876	-2.063616
48	8	0	2.546976	-0.576005	-2.630614
49	8	0	4.392921	-1.858698	-2.431505
50	6	0	4.931999	-1.067535	-3.481351
51	1	0	5.928389	-1.461183	-3.670463
52	1	0	4.317465	-1.137399	-4.378756
53	1	0	4.988817	-0.017807	-3.188961
54	6	0	2.096532	-2.064894	2.503727
55	1	0	2.012241	-2.395819	3.539867
56	1	0	2.222601	-2.937375	1.868334
57	1	0	2.984866	-1.440222	2.412950
58	6	0	0.529384	-0.150903	3.030962
59	8	0	-0.591195	0.218579	3.322064
60	8	0	1.629235	0.491139	3.446841
61	6	0	1.386949	1.689942	4.193207
62	1	0	0.776007	1.475145	5.067794
63	1	0	2.366690	2.057118	4.482679

64	1	0	0.874903	2.418353	3.565311
65	6	0	3.424945	-3.401642	-0.380411
66	1	0	4.111342	-3.022951	0.386577
67	1	0	2.789417	-4.157627	0.088977
68	1	0	4.038226	-3.903870	-1.129324

M3(A)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.250391	0.010802	-0.455162
2	6	0	-1.748085	-1.338452	-0.413971
3	6	0	-2.461524	-1.741875	0.709545
4	6	0	-1.562344	-2.185026	-1.501059
5	6	0	-2.964016	-3.037125	0.759506
6	1	0	-2.603847	-1.042302	1.522902
7	6	0	-2.065916	-3.480159	-1.437574
8	1	0	-1.039601	-1.829096	-2.378337
9	6	0	-2.758744	-3.907055	-0.307730
10	1	0	-3.512498	-3.365544	1.632752
11	1	0	-1.916462	-4.152281	-2.272087
12	1	0	-3.144949	-4.917042	-0.262470
13	7	0	-0.048616	1.749582	-0.158287
14	6	0	0.977206	2.701141	0.167425
15	6	0	2.231975	2.601694	-0.413869
16	6	0	0.647130	3.715164	1.062526
17	6	0	3.198366	3.536629	-0.051491
18	1	0	2.513212	1.800645	-1.091777
19	6	0	1.615747	4.654365	1.387133
20	1	0	-0.345661	3.753954	1.489269
21	6	0	2.893267	4.563057	0.834574
22	1	0	4.188060	3.433719	-0.475989
23	1	0	1.377051	5.450545	2.080376
24	1	0	3.648632	5.291121	1.102559
25	6	0	0.010329	0.416981	-0.145267
26	6	0	1.218320	-0.420881	0.058400
27	1	0	2.016512	0.261141	0.354704
28	6	0	1.078593	-1.505010	1.148150
29	6	0	0.108247	-1.126399	2.241006
30	8	0	-0.387842	-0.030675	2.411206
31	8	0	-0.126974	-2.157115	3.063601
32	6	0	-0.956253	-1.861562	4.193034

33	1	0	-0.969115	-2.767057	4.791685
34	1	0	-0.542969	-1.027273	4.756549
35	1	0	-1.964121	-1.604577	3.867346
36	6	0	1.680319	-1.026641	-1.332393
37	1	0	0.931502	-1.765731	-1.627425
38	1	0	1.645875	-0.194146	-2.047587
39	6	0	3.025807	-1.657824	-1.307646
40	6	0	3.161191	-3.153613	-1.317414
41	1	0	2.532207	-3.616062	-2.090510
42	1	0	4.194323	-3.429346	-1.525619
43	1	0	2.887082	-3.642567	-0.367364
44	6	0	4.086640	-0.772929	-1.296181
45	8	0	4.013293	0.485415	-1.287526
46	8	0	5.349570	-1.358722	-1.277638
47	6	0	6.417743	-0.432790	-1.325456
48	1	0	7.331687	-1.024827	-1.282828
49	1	0	6.397601	0.153964	-2.245915
50	1	0	6.380655	0.261688	-0.484540
51	7	0	-1.300589	2.208500	-0.403673
52	6	0	-2.032162	1.146294	-0.570664
53	6	0	-3.478724	1.199978	-0.826218
54	6	0	-4.142641	0.259484	-1.617950
55	6	0	-4.186971	2.274782	-0.279731
56	6	0	-5.506849	0.392884	-1.848152
57	1	0	-3.602788	-0.563428	-2.064279
58	6	0	-5.548628	2.401832	-0.517165
59	1	0	-3.658657	3.000329	0.324269
60	6	0	-6.211586	1.459181	-1.298776
61	1	0	-6.016762	-0.335393	-2.465247
62	1	0	-6.091911	3.234947	-0.090359
63	1	0	-7.273929	1.557782	-1.482238
64	6	0	2.442344	-1.743588	1.830863
65	1	0	3.195710	-1.893857	1.059005
66	1	0	2.717936	-0.864300	2.417581
67	1	0	2.389201	-2.608264	2.490759
68	1	0	0.736148	-2.445376	0.706804

TS4(A)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.603600	-0.841071	-0.821673

2	7	0	-0.497320	-0.950938	-0.773044
3	6	0	-1.792918	-1.344272	-1.204299
4	6	0	-2.600933	-0.415182	-1.853977
5	6	0	-2.210175	-2.651263	-0.993286
6	6	0	-3.869198	-0.804889	-2.265903
7	1	0	-2.224885	0.587796	-2.021051
8	6	0	-3.476029	-3.032821	-1.420074
9	1	0	-1.536091	-3.341287	-0.500035
10	6	0	-4.309027	-2.109097	-2.047388
11	1	0	-4.512088	-0.092629	-2.766119
12	1	0	-3.817190	-4.049883	-1.258297
13	1	0	-5.295624	-2.407105	-2.371451
14	7	0	1.151983	0.117163	0.067961
15	6	0	1.952810	0.849618	1.000623
16	6	0	2.305245	0.233191	2.194058
17	6	0	2.351252	2.148457	0.696790
18	6	0	3.099149	0.930354	3.100518
19	1	0	1.939333	-0.766482	2.395047
20	6	0	3.145356	2.832052	1.610134
21	1	0	1.992138	2.597710	-0.222267
22	6	0	3.522947	2.223669	2.806470
23	1	0	3.386463	0.463573	4.032992
24	1	0	3.461546	3.845218	1.393428
25	1	0	4.139867	2.760105	3.514433
26	7	0	0.610122	-1.500652	-1.335864
27	6	0	3.005645	-1.146420	-1.147882
28	6	0	3.313551	-2.474271	-1.468843
29	6	0	4.007773	-0.172752	-1.188828
30	6	0	4.611345	-2.821220	-1.821377
31	1	0	2.528167	-3.216159	-1.438588
32	6	0	5.304325	-0.530951	-1.537308
33	1	0	3.774427	0.857480	-0.962140
34	6	0	5.610025	-1.853173	-1.851134
35	1	0	4.842983	-3.852802	-2.066653
36	1	0	6.076047	0.227897	-1.566612
37	1	0	6.623014	-2.123901	-2.119596
38	6	0	-0.210828	0.023791	0.121567
39	6	0	-1.178677	0.657019	0.952092
40	1	0	-2.078748	1.393280	0.142801
41	6	0	-1.960006	-0.229057	1.935691
42	1	0	-1.739622	0.173785	2.935250
43	6	0	-1.007428	2.130484	1.387830
44	1	0	-1.488436	2.262569	2.359607
45	1	0	0.017981	2.486616	1.475524

46	6	0	-1.846121	2.834245	0.319586
47	6	0	-1.188354	2.961064	-0.939236
48	8	0	-0.156602	2.355753	-1.267110
49	8	0	-1.856681	3.718199	-1.861456
50	6	0	-1.276083	3.715116	-3.159552
51	1	0	-1.889286	4.385225	-3.759698
52	1	0	-0.246829	4.068922	-3.126827
53	1	0	-1.281845	2.713068	-3.588790
54	6	0	-3.478665	-0.157774	1.738502
55	1	0	-4.014305	-0.640784	2.555708
56	1	0	-3.777148	0.888576	1.686403
57	1	0	-3.761867	-0.639082	0.800574
58	6	0	-1.437213	-1.649839	2.068894
59	8	0	-0.283085	-1.998577	1.934197
60	8	0	-2.395991	-2.510377	2.451475
61	6	0	-1.942874	-3.843900	2.708223
62	1	0	-1.172414	-3.837436	3.479881
63	1	0	-2.818833	-4.391062	3.041858
64	1	0	-1.531986	-4.286818	1.803177
65	6	0	-2.927221	3.803298	0.725778
66	1	0	-3.570209	3.367500	1.496053
67	1	0	-2.517815	4.734785	1.136941
68	1	0	-3.549004	4.065894	-0.127765

M4(A)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.877744	-0.961703	-0.467026
2	7	0	-0.132106	-1.444131	0.122001
3	6	0	-1.215775	-2.081340	-0.568999
4	6	0	-1.822959	-1.471031	-1.665588
5	6	0	-1.611045	-3.347299	-0.152103
6	6	0	-2.854880	-2.132523	-2.323023
7	1	0	-1.506767	-0.483633	-1.980689
8	6	0	-2.639063	-4.002644	-0.820776
9	1	0	-1.108946	-3.799247	0.692637
10	6	0	-3.269044	-3.393955	-1.902445
11	1	0	-3.325427	-1.667862	-3.181072
12	1	0	-2.951352	-4.986192	-0.493330
13	1	0	-4.073150	-3.902351	-2.419331
14	7	0	1.238576	0.280121	-0.298228

15	6	0	1.964137	1.359923	0.321550
16	6	0	2.140612	1.350078	1.703757
17	6	0	2.457202	2.402901	-0.453144
18	6	0	2.840761	2.390937	2.304213
19	1	0	1.696997	0.554239	2.292107
20	6	0	3.162000	3.437097	0.155120
21	1	0	2.260707	2.408778	-1.517639
22	6	0	3.357584	3.429314	1.532737
23	1	0	2.981926	2.389778	3.377593
24	1	0	3.549006	4.250179	-0.445736
25	1	0	3.903819	4.235485	2.006208
26	7	0	1.113342	-1.970410	-0.263185
27	6	0	3.289101	-1.109888	-0.854330
28	6	0	4.031773	-2.148478	-0.289319
29	6	0	3.874826	-0.275188	-1.807219
30	6	0	5.354052	-2.342351	-0.668638
31	1	0	3.559082	-2.790537	0.442054
32	6	0	5.198170	-0.472761	-2.182392
33	1	0	3.287866	0.506772	-2.267950
34	6	0	5.940628	-1.502602	-1.611618
35	1	0	5.927915	-3.146338	-0.225416
36	1	0	5.647326	0.173519	-2.925824
37	1	0	6.972598	-1.652101	-1.903389
38	6	0	-0.054660	-0.039236	0.179691
39	6	0	-0.977888	0.775735	0.729549
40	1	0	-3.044491	2.670073	0.806755
41	6	0	-2.011745	0.226431	1.704463
42	1	0	-2.212281	1.065506	2.384082
43	6	0	-0.914311	2.273191	0.565545
44	1	0	-0.625442	2.756069	1.508128
45	1	0	-0.165661	2.538660	-0.178507
46	6	0	-2.239719	2.891616	0.103152
47	6	0	-2.630302	2.320799	-1.240297
48	8	0	-1.860590	2.020280	-2.123054
49	8	0	-3.965646	2.227007	-1.372047
50	6	0	-4.410173	1.699725	-2.628363
51	1	0	-5.494889	1.737987	-2.596230
52	1	0	-4.022016	2.299993	-3.449213
53	1	0	-4.065128	0.672543	-2.738378
54	6	0	-3.365809	-0.246290	1.153605
55	1	0	-4.065793	-0.409043	1.974438
56	1	0	-3.783362	0.507245	0.486356
57	1	0	-3.271920	-1.178097	0.603082
58	6	0	-1.338479	-0.790243	2.624056

59	8	0	-0.306915	-0.588565	3.223148
60	8	0	-2.030325	-1.930988	2.749836
61	6	0	-1.403003	-2.911500	3.583484
62	1	0	-1.304046	-2.535578	4.600443
63	1	0	-2.051788	-3.782109	3.552634
64	1	0	-0.412548	-3.146308	3.195272
65	6	0	-2.113713	4.414761	-0.044272
66	1	0	-1.826143	4.857081	0.910390
67	1	0	-1.345580	4.655296	-0.781498
68	1	0	-3.057518	4.858403	-0.363381

TS5(A)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.468513	-1.278232	0.043802
2	7	0	0.637592	-1.075239	0.215677
3	6	0	1.944138	-1.545327	0.457745
4	6	0	2.908373	-0.686641	0.974444
5	6	0	2.249798	-2.874296	0.153856
6	6	0	4.208694	-1.159167	1.154686
7	1	0	2.628144	0.308160	1.282666
8	6	0	3.542676	-3.329541	0.351449
9	1	0	1.478867	-3.513019	-0.252256
10	6	0	4.531365	-2.470518	0.840554
11	1	0	4.963503	-0.489137	1.546923
12	1	0	3.788069	-4.355562	0.107383
13	1	0	5.542895	-2.830723	0.978211
14	7	0	-1.158839	0.038446	-0.220403
15	6	0	-2.014651	0.991631	-0.849691
16	6	0	-1.837976	1.227091	-2.211377
17	6	0	-3.002486	1.634197	-0.114142
18	6	0	-2.684706	2.125120	-2.850576
19	1	0	-1.046505	0.703811	-2.736418
20	6	0	-3.850238	2.522820	-0.770254
21	1	0	-3.075259	1.445805	0.948311
22	6	0	-3.692038	2.767812	-2.131322
23	1	0	-2.564290	2.317693	-3.908849
24	1	0	-4.629605	3.028209	-0.214644
25	1	0	-4.352389	3.463097	-2.634142
26	7	0	-0.398867	-1.960276	0.309513
27	6	0	-2.815202	-1.874797	0.083883

28	6	0	-3.823784	-1.534970	-0.822091
29	6	0	-3.053602	-2.858757	1.048538
30	6	0	-5.059763	-2.167960	-0.748162
31	1	0	-3.645547	-0.794920	-1.589747
32	6	0	-4.289745	-3.487125	1.114439
33	1	0	-2.260459	-3.119480	1.736664
34	6	0	-5.297411	-3.139325	0.218923
35	1	0	-5.836178	-1.903590	-1.454562
36	1	0	-4.467442	-4.244636	1.867117
37	1	0	-6.262821	-3.626607	0.272455
38	6	0	0.218472	0.178657	-0.124609
39	6	0	0.942450	1.348729	-0.460312
40	1	0	1.871357	2.884536	1.709972
41	6	0	2.361330	1.231300	-1.028321
42	1	0	1.190176	1.566253	-1.649267
43	6	0	0.469507	2.697314	0.060126
44	1	0	0.930727	3.489435	-0.535147
45	1	0	-0.609865	2.811267	-0.057651
46	6	0	0.795171	2.957512	1.545774
47	6	0	0.115423	1.876345	2.355283
48	8	0	-1.085297	1.744339	2.447175
49	8	0	0.986650	1.045105	2.943017
50	6	0	0.399845	-0.083481	3.608428
51	1	0	1.235557	-0.658674	3.994843
52	1	0	-0.253555	0.252904	4.411240
53	1	0	-0.174670	-0.676152	2.896881
54	6	0	3.454614	2.170121	-0.598391
55	1	0	4.319991	2.038594	-1.243633
56	1	0	3.148586	3.217351	-0.658743
57	1	0	3.777160	1.989253	0.434949
58	6	0	2.589760	0.121447	-1.900121
59	8	0	1.722882	-0.652595	-2.319715
60	8	0	3.897862	-0.028535	-2.259843
61	6	0	4.144435	-1.163516	-3.084587
62	1	0	3.594008	-1.090247	-4.022294
63	1	0	5.215940	-1.164234	-3.271017
64	1	0	3.844750	-2.078525	-2.573450
65	6	0	0.266858	4.327030	1.975782
66	1	0	0.699734	5.108676	1.349686
67	1	0	-0.818238	4.349670	1.867602
68	1	0	0.514592	4.542920	3.015793

M5(A)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.470394	-0.411746	-0.976809
2	7	0	0.628173	-0.533927	-0.727299
3	6	0	1.954628	-0.849201	-1.201977
4	6	0	2.535187	-2.067135	-0.884551
5	6	0	2.558614	0.056742	-2.065882
6	6	0	3.781933	-2.373276	-1.429920
7	1	0	2.026997	-2.759320	-0.227004
8	6	0	3.806281	-0.252913	-2.585553
9	1	0	2.051236	0.987661	-2.285470
10	6	0	4.417037	-1.467485	-2.270221
11	1	0	4.251781	-3.318673	-1.191497
12	1	0	4.301973	0.456894	-3.234571
13	1	0	5.389201	-1.705201	-2.683410
14	7	0	-1.098309	0.458984	0.024867
15	6	0	-1.949605	1.328738	0.784468
16	6	0	-1.834218	2.699815	0.572323
17	6	0	-2.872472	0.777508	1.662975
18	6	0	-2.699509	3.541798	1.262698
19	1	0	-1.054044	3.062903	-0.091815
20	6	0	-3.734772	1.637432	2.336596
21	1	0	-2.894775	-0.294611	1.806348
22	6	0	-3.651883	3.012272	2.132335
23	1	0	-2.628525	4.612387	1.120714
24	1	0	-4.467262	1.232733	3.022900
25	1	0	-4.325586	3.675319	2.660442
26	7	0	-0.420734	-1.022014	-1.446624
27	6	0	-2.833672	-0.654629	-1.470886
28	6	0	-3.799297	0.353360	-1.530918
29	6	0	-3.135526	-1.937970	-1.934992
30	6	0	-5.061032	0.066879	-2.039404
31	1	0	-3.567408	1.355710	-1.198239
32	6	0	-4.397214	-2.214541	-2.443595
33	1	0	-2.372383	-2.704150	-1.895316
34	6	0	-5.363870	-1.213701	-2.491485
35	1	0	-5.805955	0.850627	-2.087974
36	1	0	-4.626532	-3.210548	-2.799861
37	1	0	-6.348984	-1.430013	-2.885133
38	6	0	0.236530	0.363260	0.181177
39	6	0	1.032449	1.052929	1.252887
40	1	0	2.291082	-1.345016	1.733284

41	6	0	2.365962	1.505222	0.726959
42	1	0	0.430943	1.940059	1.470645
43	6	0	1.029325	0.221876	2.553047
44	1	0	1.696668	0.742028	3.242091
45	1	0	0.027578	0.242487	2.989053
46	6	0	1.468742	-1.238209	2.445287
47	6	0	0.329509	-2.110611	1.957656
48	8	0	-0.836187	-1.789386	1.877058
49	8	0	0.750610	-3.345651	1.632617
50	6	0	-0.274628	-4.218435	1.134118
51	1	0	0.222138	-5.158747	0.916345
52	1	0	-1.051616	-4.352804	1.883892
53	1	0	-0.712960	-3.792281	0.232264
54	6	0	3.688282	0.989332	1.207309
55	1	0	4.470659	1.679950	0.894239
56	1	0	3.748783	0.906964	2.299258
57	1	0	3.956016	0.002367	0.796321
58	6	0	2.204962	2.376380	-0.326411
59	8	0	1.094557	2.701928	-0.847964
60	8	0	3.371118	2.860786	-0.901140
61	6	0	3.166943	3.815435	-1.927674
62	1	0	2.601865	4.675514	-1.565627
63	1	0	4.160319	4.128725	-2.246361
64	1	0	2.621731	3.389387	-2.772795
65	6	0	1.939739	-1.775451	3.807530
66	1	0	2.814238	-1.211525	4.132671
67	1	0	1.154183	-1.653750	4.556391
68	1	0	2.205756	-2.829850	3.744511

TS6(A)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.660715	-0.660227	-0.922740
2	7	0	-0.439910	-0.739906	-0.974622
3	6	0	-1.694027	-1.372172	-1.209477
4	6	0	-2.726023	-0.682675	-1.830433
5	6	0	-1.839790	-2.692718	-0.797473
6	6	0	-3.941975	-1.332440	-2.028335
7	1	0	-2.573650	0.337202	-2.154758
8	6	0	-3.057548	-3.328327	-0.997743
9	1	0	-1.006920	-3.181047	-0.309746

10	6	0	-4.109092	-2.649173	-1.611395
11	1	0	-4.755118	-0.807841	-2.513716
12	1	0	-3.189390	-4.349520	-0.664837
13	1	0	-5.057551	-3.148181	-1.764698
14	7	0	1.150207	0.388534	-0.179989
15	6	0	1.894636	1.218298	0.716895
16	6	0	2.566564	0.603170	1.770756
17	6	0	1.911194	2.595624	0.536106
18	6	0	3.304061	1.394466	2.643427
19	1	0	2.464990	-0.467187	1.903656
20	6	0	2.647193	3.374290	1.425447
21	1	0	1.342606	3.040782	-0.269220
22	6	0	3.349325	2.776087	2.467853
23	1	0	3.831858	0.932910	3.467902
24	1	0	2.669021	4.449114	1.300010
25	1	0	3.923053	3.387842	3.152622
26	7	0	0.687905	-1.356869	-1.428725
27	6	0	3.080277	-0.961622	-1.153882
28	6	0	4.050252	0.041599	-1.220077
29	6	0	3.444603	-2.296487	-1.348963
30	6	0	5.374823	-0.294763	-1.473061
31	1	0	3.772816	1.077885	-1.080053
32	6	0	4.769533	-2.624146	-1.604187
33	1	0	2.681018	-3.060972	-1.293323
34	6	0	5.737330	-1.624859	-1.663206
35	1	0	6.123501	0.485409	-1.524816
36	1	0	5.047631	-3.659950	-1.751022
37	1	0	6.771055	-1.881930	-1.857564
38	6	0	-0.214025	0.323386	-0.185416
39	6	0	-1.063928	0.568235	1.478939
40	1	0	-3.083370	1.382933	-0.085745
41	6	0	-1.812256	-0.578740	1.815138
42	1	0	-0.083126	0.558710	1.947314
43	6	0	-1.696225	1.948246	1.485964
44	1	0	-2.290376	2.020135	2.401174
45	1	0	-0.917198	2.710873	1.545675
46	6	0	-2.589466	2.280584	0.288187
47	6	0	-1.772481	2.874153	-0.836880
48	8	0	-0.826548	3.617637	-0.708261
49	8	0	-2.278966	2.567618	-2.046913
50	6	0	-1.583820	3.153579	-3.156220
51	1	0	-2.119129	2.828689	-4.043290
52	1	0	-1.589937	4.238679	-3.072536
53	1	0	-0.553233	2.802145	-3.177014

54	6	0	-3.314819	-0.657903	1.812540
55	1	0	-3.650300	-1.345798	2.588536
56	1	0	-3.763781	0.317405	2.020351
57	1	0	-3.730623	-1.016926	0.863485
58	6	0	-1.009673	-1.733696	2.048023
59	8	0	0.213105	-1.819966	1.871068
60	8	0	-1.714892	-2.826324	2.477086
61	6	0	-0.922122	-3.977707	2.732491
62	1	0	-0.164078	-3.769621	3.487326
63	1	0	-1.611232	-4.741696	3.085711
64	1	0	-0.414900	-4.315344	1.827019
65	6	0	-3.653237	3.327458	0.658288
66	1	0	-4.317011	2.922323	1.423112
67	1	0	-3.172767	4.224126	1.054100
68	1	0	-4.252853	3.605706	-0.209530

P(E)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.259452	-0.481244	-0.112725
2	1	0	0.030699	0.547288	-0.378971
3	1	0	-1.997507	-0.607251	-1.648878
4	6	0	1.548981	-0.778965	0.077494
5	6	0	2.089829	-2.127167	0.463454
6	1	0	1.289058	-2.856170	0.571568
7	1	0	2.798899	-2.487651	-0.283418
8	1	0	2.630355	-2.064354	1.409189
9	6	0	2.513618	0.343571	-0.103468
10	8	0	2.229854	1.481722	-0.402550
11	8	0	3.782172	-0.054531	0.108549
12	6	0	4.761569	0.978585	-0.048213
13	1	0	5.719728	0.508738	0.152376
14	1	0	4.728046	1.377276	-1.060821
15	1	0	4.570096	1.787226	0.655316
16	6	0	-0.892065	-1.440296	0.013175
17	1	0	-0.649333	-2.396709	-0.457229
18	1	0	-1.095577	-1.644528	1.070440
19	6	0	-2.187212	-0.899714	-0.614852
20	6	0	-3.302593	-1.941995	-0.535939
21	1	0	-3.518583	-2.167268	0.508726
22	1	0	-4.217785	-1.578677	-1.004476

23	1	0	-2.997704	-2.859228	-1.041676
24	6	0	-2.599554	0.333768	0.160769
25	8	0	-3.002869	0.314603	1.299557
26	8	0	-2.437111	1.462847	-0.545134
27	6	0	-2.755278	2.666701	0.170059
28	1	0	-2.560941	3.478757	-0.523409
29	1	0	-3.800173	2.654662	0.475082
30	1	0	-2.126144	2.751293	1.054278

TS1(B)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.623219	0.939661	0.047069
2	7	0	0.631425	1.620994	-0.183468
3	6	0	-0.444205	2.536676	0.037161
4	6	0	-1.482187	2.158337	0.878956
5	6	0	-0.385745	3.793366	-0.550562
6	6	0	-2.505496	3.069060	1.113236
7	1	0	-1.507322	1.165306	1.315152
8	6	0	-1.410779	4.696792	-0.295597
9	1	0	0.450290	4.048699	-1.188208
10	6	0	-2.471148	4.333661	0.531399
11	1	0	-3.330288	2.781209	1.752601
12	1	0	-1.383081	5.680396	-0.746090
13	1	0	-3.270010	5.038873	0.723409
14	7	0	1.832178	-0.145697	-0.292750
15	6	0	2.225296	-1.515487	-0.425010
16	6	0	3.196053	-1.861333	-1.357627
17	6	0	1.625649	-2.466278	0.397668
18	6	0	3.587902	-3.191549	-1.458400
19	1	0	3.636907	-1.096323	-1.983811
20	6	0	2.017437	-3.795196	0.273635
21	1	0	0.848934	-2.173366	1.097108
22	6	0	2.999375	-4.156451	-0.645469
23	1	0	4.346166	-3.473332	-2.177224
24	1	0	1.550959	-4.546040	0.898018
25	1	0	3.301826	-5.192049	-0.732985
26	7	0	1.905065	2.018159	0.112743
27	6	0	4.069622	0.909978	0.309157
28	6	0	4.838037	1.993580	-0.123053
29	6	0	4.669116	-0.135537	1.016564

30	6	0	6.201697	2.024563	0.139381
31	1	0	4.355377	2.801132	-0.657765
32	6	0	6.034074	-0.096505	1.274595
33	1	0	4.074365	-0.965282	1.374967
34	6	0	6.801694	0.977899	0.833905
35	1	0	6.795030	2.864097	-0.199168
36	1	0	6.496406	-0.904505	1.826676
37	1	0	7.864936	1.001704	1.036464
38	6	0	0.552967	0.307079	-0.456618
39	6	0	-0.579819	-0.514614	-0.772447
40	1	0	-0.990445	-0.941569	0.343198
41	1	0	-0.224008	-1.426626	-1.259508
42	6	0	-1.740029	0.107343	-1.486133
43	6	0	-1.505601	0.613171	-2.884032
44	1	0	-0.719123	1.378025	-2.888151
45	1	0	-1.171864	-0.191997	-3.547485
46	1	0	-2.408259	1.052004	-3.301907
47	6	0	-2.965658	0.108626	-0.925347
48	8	0	-3.308331	-0.220142	0.324221
49	8	0	-4.026091	0.542150	-1.675823
50	6	0	-5.144415	1.051522	-0.955758
51	1	0	-5.867023	1.345782	-1.713898
52	1	0	-5.570317	0.294503	-0.299145
53	1	0	-4.859219	1.922192	-0.361649
54	6	0	-2.178200	-3.526332	-0.233932
55	1	0	-1.198218	-3.430626	0.213990
56	1	0	-2.359118	-4.349751	-0.914720
57	6	0	-3.136310	-2.653449	0.060060
58	6	0	-4.529341	-2.721356	-0.498637
59	1	0	-4.680425	-3.653025	-1.044205
60	1	0	-5.255299	-2.657188	0.312789
61	1	0	-4.713030	-1.885934	-1.177609
62	6	0	-2.839446	-1.532913	1.046047
63	8	0	-1.602749	-1.387145	1.453790
64	8	0	-3.783986	-1.627832	2.060146
65	6	0	-3.544593	-0.753337	3.151386
66	1	0	-4.356853	-0.921510	3.856295
67	1	0	-2.585061	-0.969380	3.619267
68	1	0	-3.558636	0.288278	2.819678

M1(B)

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	2.678049	0.851489	0.041563
2	7	0	0.740905	1.684478	-0.253379
3	6	0	-0.223793	2.693035	-0.011568
4	6	0	-1.366167	2.416357	0.736184
5	6	0	0.028379	3.980520	-0.481180
6	6	0	-2.265369	3.444141	0.999248
7	1	0	-1.547872	1.418131	1.111673
8	6	0	-0.876136	4.997802	-0.204435
9	1	0	0.934258	4.168621	-1.041385
10	6	0	-2.028526	4.733165	0.531209
11	1	0	-3.149311	3.231548	1.588393
12	1	0	-0.680675	5.998641	-0.567983
13	1	0	-2.732360	5.527767	0.743523
14	7	0	1.806996	-0.208943	-0.165053
15	6	0	2.139171	-1.577220	-0.360420
16	6	0	3.042080	-1.935863	-1.357374
17	6	0	1.556247	-2.544876	0.456426
18	6	0	3.376740	-3.275063	-1.525520
19	1	0	3.478505	-1.166746	-1.981697
20	6	0	1.882188	-3.883551	0.266487
21	1	0	0.854511	-2.249109	1.227171
22	6	0	2.795515	-4.249284	-0.718940
23	1	0	4.084681	-3.556980	-2.294208
24	1	0	1.426711	-4.637715	0.895512
25	1	0	3.052248	-5.291436	-0.858949
26	7	0	2.061623	1.984312	0.003570
27	6	0	4.117298	0.733407	0.317707
28	6	0	4.960510	1.755531	-0.126619
29	6	0	4.644905	-0.335739	1.046741
30	6	0	6.320239	1.704555	0.150595
31	1	0	4.534632	2.580422	-0.682409
32	6	0	6.007400	-0.380553	1.318391
33	1	0	3.995062	-1.121265	1.409054
34	6	0	6.846948	0.634723	0.869453
35	1	0	6.969342	2.497909	-0.197358
36	1	0	6.411776	-1.208449	1.886602
37	1	0	7.907872	0.593714	1.081710
38	6	0	0.537381	0.326716	-0.407563
39	6	0	-0.576010	-0.374416	-0.766508
40	1	0	-1.205351	-1.063113	0.947342
41	1	0	-0.423025	-1.438455	-0.911605
42	6	0	-1.770066	0.232527	-1.400517

43	6	0	-1.583023	0.866661	-2.756554
44	1	0	-0.800283	1.628806	-2.697848
45	1	0	-1.258390	0.122824	-3.488881
46	1	0	-2.500724	1.331867	-3.108487
47	6	0	-2.986795	0.152439	-0.845915
48	8	0	-3.260961	-0.227163	0.439058
49	8	0	-4.098948	0.548582	-1.528377
50	6	0	-5.092653	1.216335	-0.751319
51	1	0	-5.848015	1.545459	-1.460716
52	1	0	-5.533262	0.540276	-0.018725
53	1	0	-4.661970	2.080568	-0.241417
54	6	0	-2.289656	-3.482745	-0.401923
55	1	0	-1.341316	-3.457765	0.117063
56	1	0	-2.442081	-4.249202	-1.151993
57	6	0	-3.251506	-2.610199	-0.119266
58	6	0	-4.611919	-2.623909	-0.758171
59	1	0	-4.694973	-3.457866	-1.454288
60	1	0	-5.376271	-2.724759	0.013605
61	1	0	-4.801067	-1.695475	-1.299138
62	6	0	-3.036065	-1.564455	0.959746
63	8	0	-1.784150	-1.583820	1.547187
64	8	0	-4.002690	-1.774656	1.919668
65	6	0	-3.953889	-0.880413	3.030318
66	1	0	-4.764332	-1.184323	3.688500
67	1	0	-2.999408	-0.961265	3.547707
68	1	0	-4.110454	0.148192	2.701329

TS2(B)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.874770	0.722101	0.005908
2	7	0	-0.958823	1.642082	0.184763
3	6	0	-0.091529	2.691362	-0.182959
4	6	0	0.993630	2.457129	-1.027023
5	6	0	-0.360937	3.980152	0.281699
6	6	0	1.827952	3.515360	-1.372101
7	1	0	1.172157	1.461129	-1.410101
8	6	0	0.472974	5.027666	-0.084545
9	1	0	-1.222614	4.140555	0.915155
10	6	0	1.576849	4.800481	-0.903875
11	1	0	2.669549	3.330122	-2.028543

12	1	0	0.262585	6.025934	0.278409
13	1	0	2.229120	5.619327	-1.179074
14	7	0	-1.940269	-0.304136	-0.031289
15	6	0	-2.183545	-1.693503	0.106595
16	6	0	-2.939423	-2.179249	1.170560
17	6	0	-1.645727	-2.568219	-0.836350
18	6	0	-3.169029	-3.546714	1.278667
19	1	0	-3.344323	-1.485123	1.895885
20	6	0	-1.862874	-3.935561	-0.709929
21	1	0	-1.071018	-2.161937	-1.659640
22	6	0	-2.628368	-4.426142	0.344923
23	1	0	-3.762756	-3.925300	2.100751
24	1	0	-1.444197	-4.616019	-1.440840
25	1	0	-2.803030	-5.490225	0.439110
26	7	0	-2.318631	1.879769	0.112990
27	6	0	-4.328989	0.550288	-0.125430
28	6	0	-5.164827	1.471689	0.511535
29	6	0	-4.885609	-0.469742	-0.901591
30	6	0	-6.543004	1.370963	0.375747
31	1	0	-4.717672	2.259594	1.103094
32	6	0	-6.266257	-0.565666	-1.030939
33	1	0	-4.245067	-1.176117	-1.412496
34	6	0	-7.097139	0.349658	-0.391822
35	1	0	-7.185095	2.087255	0.872425
36	1	0	-6.692368	-1.355215	-1.636732
37	1	0	-8.172184	0.269010	-0.493582
38	6	0	-0.672983	0.278054	0.188407
39	6	0	0.477377	-0.376415	0.461194
40	1	0	2.392349	-1.085396	1.245123
41	1	0	0.429133	-1.454928	0.406529
42	6	0	1.665544	0.280738	1.076872
43	6	0	1.441820	1.120987	2.320236
44	1	0	1.135802	2.141110	2.069127
45	1	0	0.659478	0.668689	2.929649
46	1	0	2.355683	1.194440	2.910080
47	6	0	2.815755	0.535018	0.322496
48	8	0	3.186290	-0.175789	-0.676567
49	8	0	3.641518	1.494847	0.790453
50	6	0	4.836693	1.738483	0.050915
51	1	0	5.223835	2.679619	0.432945
52	1	0	5.561183	0.941086	0.211092
53	1	0	4.618882	1.822716	-1.012796
54	6	0	5.511245	-1.627088	1.413088
55	1	0	4.832146	-1.756195	2.244668

56	1	0	6.557335	-1.444316	1.625569
57	6	0	5.075090	-1.701300	0.156422
58	6	0	5.935902	-1.557557	-1.063498
59	1	0	6.955064	-1.291940	-0.783800
60	1	0	5.953361	-2.490040	-1.629134
61	1	0	5.521463	-0.786610	-1.714775
62	6	0	3.621318	-1.927979	-0.076789
63	8	0	2.817465	-2.082014	0.923214
64	8	0	3.389708	-2.593039	-1.207920
65	6	0	2.013654	-2.834561	-1.518652
66	1	0	2.017157	-3.338789	-2.481056
67	1	0	1.556572	-3.463498	-0.755634
68	1	0	1.496929	-1.877589	-1.578672

M2(B)+R´

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.898103	0.645452	0.022477
2	7	0	-1.064342	1.709030	0.280193
3	6	0	-0.281337	2.800664	-0.152558
4	6	0	0.810212	2.602163	-0.995318
5	6	0	-0.633511	4.087551	0.258180
6	6	0	1.572908	3.695649	-1.393301
7	1	0	1.054804	1.604778	-1.333204
8	6	0	0.127699	5.170134	-0.161746
9	1	0	-1.498812	4.218267	0.893507
10	6	0	1.240422	4.981283	-0.979244
11	1	0	2.419766	3.534075	-2.049401
12	1	0	-0.146182	6.167473	0.159042
13	1	0	1.835153	5.828914	-1.294683
14	7	0	-1.888952	-0.307776	0.012869
15	6	0	-2.047255	-1.708307	0.174951
16	6	0	-2.774197	-2.217650	1.247728
17	6	0	-1.460451	-2.566154	-0.753216
18	6	0	-2.925710	-3.593680	1.379816
19	1	0	-3.219249	-1.534738	1.960304
20	6	0	-1.600035	-3.941136	-0.603745
21	1	0	-0.908427	-2.141806	-1.582682
22	6	0	-2.336107	-4.456184	0.460187
23	1	0	-3.497006	-3.991777	2.208578
24	1	0	-1.142652	-4.609162	-1.322813

25	1	0	-2.449722	-5.526875	0.572494
26	7	0	-2.439191	1.841564	0.154579
27	6	0	-4.329864	0.361089	-0.155617
28	6	0	-5.254823	1.209931	0.458204
29	6	0	-4.779633	-0.696501	-0.950464
30	6	0	-6.615973	0.999928	0.281029
31	1	0	-4.889897	2.027533	1.065552
32	6	0	-6.143703	-0.900949	-1.122551
33	1	0	-4.068529	-1.348958	-1.439580
34	6	0	-7.063692	-0.057902	-0.506148
35	1	0	-7.327869	1.659764	0.760550
36	1	0	-6.486981	-1.719234	-1.742597
37	1	0	-8.125250	-0.223673	-0.640221
38	6	0	-0.677900	0.365848	0.297734
39	6	0	0.488465	-0.223806	0.627102
40	1	0	2.143295	-0.424093	1.846140
41	1	0	0.515485	-1.300740	0.547456
42	6	0	1.688178	0.405124	1.289945
43	6	0	1.390213	1.513943	2.310642
44	1	0	1.147957	2.462331	1.835746
45	1	0	0.546245	1.206206	2.928144
46	1	0	2.256996	1.673754	2.949783
47	6	0	2.815055	0.759217	0.331273
48	8	0	2.986945	0.284881	-0.772802
49	8	0	3.690067	1.611688	0.884573
50	6	0	4.829043	1.922641	0.075833
51	1	0	5.399548	2.652945	0.642347
52	1	0	5.417516	1.023433	-0.100406
53	1	0	4.508927	2.338811	-0.877923
54	6	0	5.528498	-1.678296	1.392183
55	1	0	4.834859	-1.862549	2.202038
56	1	0	6.526908	-1.332869	1.630600
57	6	0	5.150262	-1.880033	0.130495
58	6	0	6.014625	-1.643369	-1.073944
59	1	0	6.999896	-1.288158	-0.772074
60	1	0	6.129357	-2.558881	-1.655955
61	1	0	5.543100	-0.905039	-1.725068
62	6	0	3.741648	-2.329563	-0.092891
63	8	0	2.908904	-2.463148	0.778709
64	8	0	3.500523	-2.571297	-1.385348
65	6	0	2.118109	-2.763238	-1.707101
66	1	0	2.094903	-3.022700	-2.761946
67	1	0	1.692255	-3.558917	-1.097471
68	1	0	1.591230	-1.827938	-1.520394

TS3(B)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.305219	-0.700151	-0.503752
2	7	0	-0.448112	-1.709091	-0.606865
3	6	0	0.381092	-2.853790	-0.790874
4	6	0	0.458267	-3.794580	0.230367
5	6	0	1.054402	-3.026288	-1.993835
6	6	0	1.254007	-4.920016	0.047438
7	1	0	-0.075445	-3.613886	1.153543
8	6	0	1.854512	-4.151294	-2.163805
9	1	0	0.947537	-2.285062	-2.775243
10	6	0	1.955893	-5.093577	-1.143943
11	1	0	1.331902	-5.657892	0.835555
12	1	0	2.392845	-4.293483	-3.091712
13	1	0	2.579514	-5.968221	-1.279343
14	7	0	-1.320409	0.193775	-0.120056
15	6	0	-1.545862	1.410785	0.606925
16	6	0	-1.095494	2.618891	0.092406
17	6	0	-2.207354	1.339708	1.830307
18	6	0	-1.307935	3.781828	0.827316
19	1	0	-0.533225	2.662528	-0.830886
20	6	0	-2.439629	2.511536	2.539399
21	1	0	-2.525937	0.377698	2.211571
22	6	0	-1.989443	3.732100	2.038936
23	1	0	-0.921849	4.716387	0.442546
24	1	0	-2.959467	2.469461	3.487809
25	1	0	-2.160402	4.641013	2.601956
26	7	0	-1.793362	-1.853508	-0.799622
27	6	0	-3.742860	-0.411415	-0.600699
28	6	0	-4.222789	0.867028	-0.895829
29	6	0	-4.638220	-1.472170	-0.436058
30	6	0	-5.591307	1.077702	-1.017154
31	1	0	-3.534091	1.689247	-1.036196
32	6	0	-6.003282	-1.253335	-0.560978
33	1	0	-4.249558	-2.457284	-0.214241
34	6	0	-6.482553	0.022360	-0.848310
35	1	0	-5.959812	2.068719	-1.248504
36	1	0	-6.693279	-2.077164	-0.430708
37	1	0	-7.547589	0.193234	-0.942049

38	6	0	-0.107608	-0.471830	-0.161529
39	6	0	1.136582	0.157884	0.044991
40	1	0	2.966669	0.400179	1.005643
41	1	0	0.950982	1.161957	0.412414
42	6	0	2.302827	-0.445488	0.811052
43	6	0	3.185559	-1.534704	0.168642
44	1	0	3.443387	-1.256211	-0.849869
45	1	0	4.107596	-1.616849	0.744598
46	1	0	2.703297	-2.508637	0.154716
47	6	0	1.845995	-0.971596	2.159157
48	8	0	0.738142	-1.383204	2.425397
49	8	0	2.853121	-0.985882	3.046755
50	6	0	2.520624	-1.537307	4.326447
51	1	0	3.430333	-1.480590	4.916491
52	1	0	1.722303	-0.959123	4.788633
53	1	0	2.193017	-2.570096	4.217268
54	6	0	1.804774	0.776490	-1.724826
55	1	0	1.977330	-0.194650	-2.180642
56	1	0	0.864083	1.236103	-2.010154
57	6	0	2.903265	1.637042	-1.603161
58	6	0	4.334155	1.174280	-1.706911
59	1	0	4.393174	0.240241	-2.271798
60	1	0	4.936274	1.916864	-2.231501
61	1	0	4.819468	1.004609	-0.738089
62	6	0	2.597932	3.001294	-1.314622
63	8	0	1.475030	3.491489	-1.152688
64	8	0	3.707674	3.797741	-1.221142
65	6	0	3.428729	5.167829	-0.964377
66	1	0	4.395447	5.663418	-0.908117
67	1	0	2.826715	5.598827	-1.764736
68	1	0	2.885867	5.283976	-0.026040

M3(B)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.201998	0.655411	-0.616631
2	7	0	0.370513	1.701101	-0.710845
3	6	0	-0.428045	2.886318	-0.801231
4	6	0	-0.296666	3.822303	0.218425
5	6	0	-1.258185	3.093711	-1.892399
6	6	0	-1.050142	4.987695	0.155067

7	1	0	0.365028	3.610115	1.048250
8	6	0	-2.017868	4.259263	-1.936830
9	1	0	-1.307550	2.355962	-2.681539
10	6	0	-1.916491	5.199526	-0.915956
11	1	0	-0.969143	5.724390	0.943563
12	1	0	-2.682445	4.432803	-2.772737
13	1	0	-2.509277	6.104253	-0.957597
14	7	0	1.189360	-0.210780	-0.259433
15	6	0	1.373602	-1.516063	0.324751
16	6	0	0.879729	-2.635705	-0.327288
17	6	0	2.058479	-1.592844	1.534110
18	6	0	1.081716	-3.880535	0.264672
19	1	0	0.270594	-2.548742	-1.219905
20	6	0	2.278192	-2.845203	2.091944
21	1	0	2.398768	-0.686370	2.017616
22	6	0	1.790859	-3.987252	1.455892
23	1	0	0.659126	-4.754011	-0.213078
24	1	0	2.815813	-2.929056	3.027460
25	1	0	1.951236	-4.959980	1.903762
26	7	0	1.711602	1.830364	-0.889783
27	6	0	3.634914	0.341276	-0.705153
28	6	0	4.097616	-0.928005	-1.061950
29	6	0	4.542299	1.378563	-0.472329
30	6	0	5.464491	-1.152713	-1.173640
31	1	0	3.400000	-1.730765	-1.258685
32	6	0	5.905779	1.144441	-0.586870
33	1	0	4.166992	2.357769	-0.206010
34	6	0	6.368608	-0.122125	-0.934148
35	1	0	5.821395	-2.135284	-1.453178
36	1	0	6.606239	1.948758	-0.402801
37	1	0	7.432106	-0.305123	-1.021245
38	6	0	0.022710	0.479497	-0.299535
39	6	0	-1.313860	-0.132612	-0.068804
40	1	0	-1.089054	-1.177909	0.148771
41	1	0	-2.799364	-0.437129	1.377872
42	6	0	-2.128756	0.388734	1.131864
43	6	0	-3.020391	1.625754	0.923363
44	1	0	-3.682560	1.461234	0.076527
45	1	0	-3.635453	1.765018	1.812955
46	1	0	-2.447013	2.534517	0.753713
47	6	0	-1.237992	0.635019	2.326315
48	8	0	-0.056916	0.923397	2.281995
49	8	0	-1.911124	0.548878	3.477030
50	6	0	-1.140786	0.818217	4.656359

51	1	0	-1.828210	0.698910	5.487761
52	1	0	-0.314957	0.112928	4.730771
53	1	0	-0.743620	1.831421	4.622877
54	6	0	-2.166332	-0.232976	-1.390621
55	1	0	-2.536492	0.760139	-1.656135
56	1	0	-1.467775	-0.562267	-2.170325
57	6	0	-3.283685	-1.206960	-1.238742
58	6	0	-4.710206	-0.759599	-1.077155
59	1	0	-4.925008	0.123296	-1.694165
60	1	0	-5.385418	-1.552902	-1.397925
61	1	0	-5.004926	-0.498679	-0.048131
62	6	0	-2.898776	-2.531998	-1.275745
63	8	0	-1.723314	-2.973959	-1.406499
64	8	0	-3.935006	-3.453930	-1.146776
65	6	0	-3.525155	-4.802873	-1.244528
66	1	0	-4.426126	-5.401872	-1.112332
67	1	0	-3.075558	-5.016809	-2.216279
68	1	0	-2.792732	-5.054113	-0.474639

TS4(B)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.422813	0.603548	-0.336859
2	7	0	0.711611	1.842820	-0.361705
3	6	0	0.028190	3.097683	-0.466442
4	6	0	0.177640	4.017936	0.563207
5	6	0	-0.703360	3.388769	-1.609184
6	6	0	-0.464613	5.245043	0.463125
7	1	0	0.774123	3.758655	1.428002
8	6	0	-1.352782	4.616696	-1.693091
9	1	0	-0.759035	2.668102	-2.413642
10	6	0	-1.238305	5.538752	-0.657651
11	1	0	-0.369283	5.967120	1.263208
12	1	0	-1.938678	4.852855	-2.571498
13	1	0	-1.745300	6.492452	-0.727249
14	7	0	1.305022	-0.204568	-0.276828
15	6	0	1.302737	-1.639705	-0.153582
16	6	0	0.632679	-2.404938	-1.096895
17	6	0	1.974459	-2.212742	0.919785
18	6	0	0.631359	-3.788962	-0.951778
19	1	0	0.061794	-1.942426	-1.891009

20	6	0	1.995463	-3.594654	1.030843
21	1	0	2.447028	-1.581450	1.659966
22	6	0	1.324077	-4.382107	0.096785
23	1	0	0.066382	-4.386954	-1.653421
24	1	0	2.511241	-4.056104	1.862527
25	1	0	1.323581	-5.459467	0.202986
26	7	0	2.070153	1.856603	-0.383371
27	6	0	3.826622	0.166682	-0.376449
28	6	0	4.223504	-0.987704	-1.057111
29	6	0	4.780260	0.981068	0.239122
30	6	0	5.570530	-1.324023	-1.108056
31	1	0	3.488964	-1.613549	-1.545891
32	6	0	6.124367	0.636247	0.183620
33	1	0	4.457360	1.876848	0.753089
34	6	0	6.520135	-0.518000	-0.486226
35	1	0	5.877592	-2.216771	-1.637101
36	1	0	6.860999	1.266068	0.665296
37	1	0	7.567842	-0.788067	-0.526657
38	6	0	0.209040	0.602918	-0.277852
39	6	0	-1.178460	0.105809	-0.154150
40	1	0	-1.062412	-0.977406	-0.110979
41	1	0	-2.999243	-0.185446	0.497414
42	6	0	-1.916220	0.435849	1.132571
43	6	0	-2.380602	1.853087	1.428522
44	1	0	-2.693308	2.363977	0.515570
45	1	0	-3.237529	1.821591	2.101536
46	1	0	-1.616949	2.469922	1.910866
47	6	0	-1.425098	-0.329940	2.263123
48	8	0	-0.642773	-1.273175	2.223683
49	8	0	-1.957357	0.081410	3.449500
50	6	0	-1.568790	-0.706093	4.570930
51	1	0	-2.069795	-0.267107	5.430396
52	1	0	-1.875536	-1.743125	4.437635
53	1	0	-0.487237	-0.681347	4.704890
54	6	0	-2.166446	0.334716	-1.349934
55	1	0	-2.357967	1.398075	-1.495890
56	1	0	-1.735091	-0.081557	-2.264738
57	6	0	-3.435418	-0.360041	-0.915153
58	6	0	-4.749342	0.383217	-1.059429
59	1	0	-5.053311	0.519500	-2.104811
60	1	0	-5.550412	-0.155010	-0.554532
61	1	0	-4.677925	1.375130	-0.605922
62	6	0	-3.405210	-1.766932	-1.217787
63	8	0	-2.402526	-2.429500	-1.498855

64	8	0	-4.623898	-2.376595	-1.129452
65	6	0	-4.594158	-3.785002	-1.326299
66	1	0	-5.623146	-4.121956	-1.221897
67	1	0	-4.211971	-4.030538	-2.317235
68	1	0	-3.958283	-4.266167	-0.582820

M4(B)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.020578	-0.928583	-0.647825
2	7	0	-0.035625	-1.637782	-0.753911
3	6	0	0.997964	-2.621624	-0.896585
4	6	0	1.243831	-3.476301	0.171107
5	6	0	1.686103	-2.717302	-2.095846
6	6	0	2.222817	-4.448840	0.026279
7	1	0	0.692058	-3.343174	1.092254
8	6	0	2.661600	-3.703845	-2.231499
9	1	0	1.454452	-2.036235	-2.904876
10	6	0	2.926948	-4.564743	-1.173185
11	1	0	2.442992	-5.111482	0.852683
12	1	0	3.206870	-3.796400	-3.161664
13	1	0	3.688194	-5.327435	-1.278072
14	7	0	-1.168967	0.105342	-0.307071
15	6	0	-1.525550	1.374056	0.266581
16	6	0	-1.419051	2.521690	-0.506847
17	6	0	-1.947086	1.402041	1.590945
18	6	0	-1.777678	3.741375	0.059366
19	1	0	-1.035107	2.465863	-1.516582
20	6	0	-2.315468	2.626583	2.136320
21	1	0	-1.919422	0.487348	2.167586
22	6	0	-2.237498	3.790055	1.372583
23	1	0	-1.690842	4.646090	-0.528400
24	1	0	-2.647448	2.674508	3.165198
25	1	0	-2.522500	4.739440	1.808582
26	7	0	-1.333121	-1.995003	-0.941382
27	6	0	-3.489277	-0.884949	-0.681057
28	6	0	-4.203636	0.287925	-0.937205
29	6	0	-4.173810	-2.087646	-0.479691
30	6	0	-5.592719	0.252506	-0.982565
31	1	0	-3.684909	1.220695	-1.107147
32	6	0	-5.560478	-2.114156	-0.530409

33	1	0	-3.607071	-2.987733	-0.282384
34	6	0	-6.273023	-0.943574	-0.778479
35	1	0	-6.142034	1.163463	-1.182121
36	1	0	-6.084944	-3.047127	-0.369434
37	1	0	-7.355010	-0.964130	-0.812933
38	6	0	0.088683	-0.385650	-0.329071
39	6	0	1.339803	0.333245	0.077687
40	1	0	0.955596	1.248680	0.550188
41	1	0	3.464881	1.835060	0.192272
42	6	0	2.096457	-0.516339	1.073717
43	6	0	3.513136	-0.965550	0.860073
44	1	0	4.224150	-0.146870	0.691962
45	1	0	3.841019	-1.492320	1.754995
46	1	0	3.630830	-1.665244	0.018429
47	6	0	1.284099	-0.999141	2.077044
48	8	0	0.037633	-0.800107	2.175124
49	8	0	1.891350	-1.835275	3.006026
50	6	0	1.050456	-2.221195	4.079075
51	1	0	1.649418	-2.878452	4.708072
52	1	0	0.720152	-1.355158	4.655629
53	1	0	0.161804	-2.745354	3.723880
54	6	0	2.164353	0.755454	-1.153018
55	1	0	2.783428	-0.080665	-1.481495
56	1	0	1.515471	1.046336	-1.983362
57	6	0	3.054235	1.950891	-0.811624
58	6	0	4.199803	2.117811	-1.819802
59	1	0	3.799419	2.222723	-2.830146
60	1	0	4.800018	2.998372	-1.588030
61	1	0	4.845254	1.239227	-1.789386
62	6	0	2.237656	3.225617	-0.822885
63	8	0	1.295779	3.451721	-1.550847
64	8	0	2.717225	4.128844	0.043273
65	6	0	2.015920	5.378475	0.060562
66	1	0	2.534229	5.995654	0.788075
67	1	0	2.038562	5.837923	-0.926395
68	1	0	0.980530	5.217318	0.358091

TS5(B)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.040491	0.901950	-0.652678

2	7	0	0.172735	1.810370	-0.969863
3	6	0	-0.766162	2.864506	-1.028502
4	6	0	-0.563214	4.007637	-0.262332
5	6	0	-1.891599	2.719509	-1.831997
6	6	0	-1.523548	5.010972	-0.290096
7	1	0	0.325273	4.085548	0.348223
8	6	0	-2.851498	3.724404	-1.838070
9	1	0	-1.994368	1.832736	-2.443346
10	6	0	-2.671907	4.868599	-1.066232
11	1	0	-1.380408	5.902084	0.307495
12	1	0	-3.733940	3.617918	-2.456084
13	1	0	-3.419551	5.651317	-1.075368
14	7	0	1.084406	-0.083315	-0.823297
15	6	0	1.264875	-1.493538	-0.703859
16	6	0	0.738296	-2.318602	-1.690823
17	6	0	1.924204	-2.013818	0.407141
18	6	0	0.892881	-3.696300	-1.576846
19	1	0	0.209968	-1.878482	-2.527039
20	6	0	2.101069	-3.389521	0.490931
21	1	0	2.249682	-1.344961	1.190643
22	6	0	1.591060	-4.229628	-0.498468
23	1	0	0.460836	-4.346147	-2.325614
24	1	0	2.619440	-3.807846	1.344185
25	1	0	1.721353	-5.301518	-0.417013
26	7	0	1.488797	2.075409	-0.737348
27	6	0	3.480584	0.694767	-0.445694
28	6	0	4.187293	-0.274683	-1.161465
29	6	0	4.149136	1.522098	0.458110
30	6	0	5.555423	-0.415307	-0.965053
31	1	0	3.671183	-0.908929	-1.870780
32	6	0	5.517580	1.375892	0.649435
33	1	0	3.584382	2.266303	1.004042
34	6	0	6.221354	0.406397	-0.059506
35	1	0	6.102239	-1.164956	-1.522417
36	1	0	6.033189	2.015343	1.354409
37	1	0	7.287125	0.291057	0.092926
38	6	0	-0.136303	0.499852	-0.987905
39	6	0	-1.533753	-0.233049	0.001597
40	1	0	-0.910308	-1.087862	0.261392
41	1	0	-3.993206	-1.236599	0.619514
42	6	0	-1.776667	0.602954	1.111244
43	6	0	-2.952752	1.533074	1.267923
44	1	0	-3.715004	1.341652	0.511386
45	1	0	-3.416316	1.391750	2.247123

46	1	0	-2.678563	2.589991	1.196156
47	6	0	-0.724635	0.616012	2.079226
48	8	0	0.349720	0.010239	2.005019
49	8	0	-0.987807	1.418564	3.153512
50	6	0	0.051098	1.461314	4.123185
51	1	0	-0.291694	2.142978	4.898283
52	1	0	0.234253	0.471284	4.540788
53	1	0	0.979530	1.822906	3.679841
54	6	0	-2.646934	-0.607122	-0.954906
55	1	0	-3.216766	0.272500	-1.258437
56	1	0	-2.220511	-1.055983	-1.855152
57	6	0	-3.612343	-1.627547	-0.324272
58	6	0	-4.750158	-1.963505	-1.288557
59	1	0	-4.342970	-2.416784	-2.192854
60	1	0	-5.454940	-2.665467	-0.840880
61	1	0	-5.293860	-1.057102	-1.559129
62	6	0	-2.805955	-2.874620	-0.036338
63	8	0	-2.352164	-3.600738	-0.892867
64	8	0	-2.604032	-3.065238	1.272606
65	6	0	-1.729435	-4.155611	1.593520
66	1	0	-1.684970	-4.183924	2.677994
67	1	0	-2.127026	-5.087190	1.194220
68	1	0	-0.742229	-3.973988	1.170607

TS4(C)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.043741	1.675388	-0.238194
2	7	0	1.034610	1.447644	-0.515851
3	6	0	2.371299	1.934910	-0.606768
4	6	0	3.078793	1.805148	-1.794159
5	6	0	2.914622	2.573807	0.502899
6	6	0	4.377266	2.301227	-1.861351
7	1	0	2.614209	1.325756	-2.644376
8	6	0	4.206074	3.079125	0.417799
9	1	0	2.330854	2.622222	1.412124
10	6	0	4.939313	2.937762	-0.758857
11	1	0	4.942476	2.201103	-2.779073
12	1	0	4.645853	3.571623	1.275410
13	1	0	5.948161	3.326211	-0.816565
14	7	0	-0.787799	0.325050	-0.417309

15	6	0	-1.746180	-0.690058	-0.101078
16	6	0	-1.619880	-1.384701	1.098903
17	6	0	-2.861371	-0.841646	-0.916586
18	6	0	-2.637214	-2.253658	1.480772
19	1	0	-0.756200	-1.202286	1.723899
20	6	0	-3.888640	-1.684784	-0.505304
21	1	0	-2.914299	-0.297090	-1.849133
22	6	0	-3.775533	-2.392456	0.689396
23	1	0	-2.549290	-2.800622	2.410611
24	1	0	-4.771135	-1.794007	-1.122783
25	1	0	-4.574445	-3.052199	1.004036
26	7	0	0.052991	2.362027	-0.290176
27	6	0	-2.360392	2.312328	-0.050258
28	6	0	-3.339129	1.798917	0.806196
29	6	0	-2.588620	3.518829	-0.718353
30	6	0	-4.537529	2.483102	0.972712
31	1	0	-3.164126	0.881316	1.350801
32	6	0	-3.787925	4.197763	-0.544828
33	1	0	-1.816797	3.912967	-1.366094
34	6	0	-4.766900	3.677932	0.296756
35	1	0	-5.290658	2.082741	1.639248
36	1	0	-3.958489	5.129628	-1.068435
37	1	0	-5.703555	4.204414	0.430286
38	6	0	0.578930	0.169652	-0.536821
39	6	0	1.319380	-1.050901	-0.524836
40	1	0	1.830052	-2.909013	-1.375980
41	1	0	1.094417	-1.825324	0.631359
42	6	0	1.309399	-2.011507	-1.718240
43	6	0	2.012130	-1.437379	-2.950965
44	1	0	3.003455	-1.071903	-2.679586
45	1	0	2.122301	-2.192904	-3.731970
46	1	0	1.419573	-0.616614	-3.356966
47	6	0	-0.075588	-2.465055	-2.118916
48	8	0	-0.809404	-1.868788	-2.875117
49	8	0	-0.387227	-3.642670	-1.562992
50	6	0	-1.657337	-4.183147	-1.948120
51	1	0	-1.730077	-5.143072	-1.445345
52	1	0	-2.458109	-3.520397	-1.632192
53	1	0	-1.695295	-4.308528	-3.029626
54	6	0	2.693561	-1.052478	0.211214
55	1	0	3.423849	-1.636543	-0.353938
56	1	0	3.121807	-0.072051	0.398361
57	6	0	2.280099	-1.782523	1.486561
58	6	0	3.008587	-3.023450	1.937403

59	1	0	3.118776	-3.726494	1.107923
60	1	0	4.013572	-2.801132	2.314554
61	1	0	2.460659	-3.521665	2.735569
62	6	0	1.648185	-0.913997	2.430259
63	8	0	1.207128	0.214320	2.169865
64	8	0	1.415400	-1.476006	3.655805
65	6	0	0.671100	-0.656484	4.550595
66	1	0	0.633197	-1.201688	5.490749
67	1	0	1.156179	0.309209	4.686655
68	1	0	-0.339253	-0.481543	4.176362

M4(C)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.131808	0.785511	-0.227582
2	7	0	0.350543	1.954512	-0.161323
3	6	0	-0.199032	3.239514	0.063130
4	6	0	-0.865902	3.552064	1.247838
5	6	0	-0.008397	4.217477	-0.913757
6	6	0	-1.355100	4.839332	1.439481
7	1	0	-0.990700	2.791148	2.006524
8	6	0	-0.492363	5.502060	-0.704019
9	1	0	0.526232	3.956991	-1.816826
10	6	0	-1.173398	5.819298	0.468607
11	1	0	-1.871348	5.077477	2.361176
12	1	0	-0.341274	6.257234	-1.465240
13	1	0	-1.555732	6.819771	0.624807
14	7	0	1.179203	0.016678	0.454396
15	6	0	1.206408	-1.412171	0.388006
16	6	0	0.549652	-2.051423	-0.663808
17	6	0	1.979407	-2.126273	1.294893
18	6	0	0.694623	-3.426647	-0.806981
19	1	0	-0.052487	-1.465354	-1.349054
20	6	0	2.109119	-3.503066	1.147263
21	1	0	2.490008	-1.595119	2.087779
22	6	0	1.471467	-4.152176	0.095704
23	1	0	0.209111	-3.932676	-1.633041
24	1	0	2.709305	-4.065375	1.850395
25	1	0	1.579375	-5.223126	-0.023192
26	7	0	1.668544	1.931349	-0.577808
27	6	0	3.541197	0.409641	-0.463698

28	6	0	3.934566	-0.841846	-0.947865
29	6	0	4.508029	1.393945	-0.233939
30	6	0	5.281493	-1.101908	-1.178224
31	1	0	3.199041	-1.605197	-1.160248
32	6	0	5.850841	1.127255	-0.467464
33	1	0	4.188752	2.362764	0.126599
34	6	0	6.240973	-0.124425	-0.935120
35	1	0	5.578584	-2.072047	-1.555805
36	1	0	6.591386	1.894783	-0.281394
37	1	0	7.287813	-0.335514	-1.114451
38	6	0	-0.022221	0.750245	0.436332
39	6	0	-1.260542	0.368220	0.850365
40	1	0	-2.511408	-0.449616	2.308631
41	1	0	-3.883729	-0.552988	0.393134
42	6	0	-1.481351	-0.635863	1.973401
43	6	0	-0.572268	-0.404875	3.183777
44	1	0	-0.708910	0.614501	3.546092
45	1	0	-0.806004	-1.108670	3.981136
46	1	0	0.475151	-0.535756	2.917754
47	6	0	-1.523201	-2.120840	1.633245
48	8	0	-1.028460	-3.002289	2.292394
49	8	0	-2.302994	-2.372054	0.562030
50	6	0	-2.569834	-3.758653	0.326816
51	1	0	-3.257172	-3.779395	-0.513574
52	1	0	-1.645021	-4.285419	0.099491
53	1	0	-3.023503	-4.206036	1.210191
54	6	0	-2.468320	1.108785	0.325513
55	1	0	-2.961199	1.698178	1.112142
56	1	0	-2.162663	1.814202	-0.446725
57	6	0	-3.536719	0.207398	-0.307342
58	6	0	-4.741170	1.038524	-0.776147
59	1	0	-5.180240	1.565398	0.072162
60	1	0	-4.427369	1.781781	-1.512003
61	1	0	-5.503405	0.401494	-1.224291
62	6	0	-2.969833	-0.527061	-1.499109
63	8	0	-1.972222	-0.227263	-2.113137
64	8	0	-3.760733	-1.555085	-1.870743
65	6	0	-3.300674	-2.264130	-3.024997
66	1	0	-4.046931	-3.029199	-3.220789
67	1	0	-3.205167	-1.589427	-3.874020
68	1	0	-2.328798	-2.716520	-2.824482

TS5(C)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.776877	-1.021277	-0.336277
2	7	0	-0.228397	-1.662992	-0.559833
3	6	0	-1.231579	-2.612611	-0.903582
4	6	0	-1.943249	-2.460835	-2.091355
5	6	0	-1.444019	-3.701890	-0.067214
6	6	0	-2.896835	-3.410863	-2.433557
7	1	0	-1.746891	-1.608811	-2.729257
8	6	0	-2.389921	-4.654699	-0.430029
9	1	0	-0.891598	-3.774431	0.858586
10	6	0	-3.119266	-4.509510	-1.606009
11	1	0	-3.456161	-3.299822	-3.353590
12	1	0	-2.565252	-5.504240	0.217185
13	1	0	-3.861106	-5.249467	-1.878248
14	7	0	0.999002	0.119733	-0.486952
15	6	0	1.440162	1.468691	-0.388524
16	6	0	0.703249	2.372223	0.370266
17	6	0	2.568814	1.873541	-1.104317
18	6	0	1.094674	3.710518	0.387513
19	1	0	-0.145949	2.027768	0.942563
20	6	0	2.963540	3.201063	-1.050298
21	1	0	3.108802	1.158160	-1.710513
22	6	0	2.216778	4.125099	-0.316099
23	1	0	0.504059	4.425615	0.945259
24	1	0	3.833784	3.522860	-1.607441
25	1	0	2.509081	5.167291	-0.303350
26	7	0	1.052190	-2.094595	-0.387257
27	6	0	3.224683	-1.076942	-0.068394
28	6	0	3.838740	-0.213791	0.844397
29	6	0	3.969967	-2.084983	-0.683478
30	6	0	5.192339	-0.355846	1.124126
31	1	0	3.262245	0.563566	1.328907
32	6	0	5.323413	-2.220844	-0.398338
33	1	0	3.476970	-2.755105	-1.375597
34	6	0	5.936821	-1.354801	0.501975
35	1	0	5.664855	0.313511	1.831513
36	1	0	5.897898	-3.001221	-0.880742
37	1	0	6.991878	-1.459175	0.721189
38	6	0	-0.318894	-0.294548	-0.580561
39	6	0	-1.506330	0.464779	-0.673260
40	1	0	-2.073320	0.662622	-1.736386

41	1	0	-2.097851	1.232019	1.908297
42	6	0	-1.449843	1.837375	-1.360888
43	6	0	-0.639286	2.006680	-2.626150
44	1	0	-0.376296	1.030437	-3.048885
45	1	0	-1.208565	2.569100	-3.368148
46	1	0	0.290002	2.554949	-2.454562
47	6	0	-2.029000	3.039709	-0.846909
48	8	0	-2.042461	4.120717	-1.421149
49	8	0	-2.598211	2.909709	0.402918
50	6	0	-3.214664	4.100483	0.883992
51	1	0	-3.623405	3.849453	1.860916
52	1	0	-2.486001	4.906585	0.968830
53	1	0	-4.006304	4.425481	0.209512
54	6	0	-2.687362	0.051925	0.203243
55	1	0	-3.533925	0.674205	-0.092254
56	1	0	-2.971227	-0.990784	0.028613
57	6	0	-2.486587	0.233575	1.722805
58	6	0	-3.821032	0.035455	2.443881
59	1	0	-4.539023	0.776694	2.089739
60	1	0	-4.209134	-0.963641	2.243638
61	1	0	-3.711161	0.146655	3.523566
62	6	0	-1.494388	-0.781337	2.241353
63	8	0	-1.740316	-1.948188	2.447615
64	8	0	-0.275175	-0.250770	2.460195
65	6	0	0.695190	-1.171357	2.983266
66	1	0	1.603231	-0.591723	3.124170
67	1	0	0.346314	-1.581327	3.929544
68	1	0	0.865852	-1.983899	2.279158

M5(C)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.264815	1.979800	0.115878
2	7	0	1.652083	1.140722	-0.126349
3	6	0	3.072923	1.157140	-0.274044
4	6	0	3.620366	1.991499	-1.242065
5	6	0	3.859801	0.355015	0.542942
6	6	0	5.000219	2.015071	-1.399233
7	1	0	2.966712	2.597537	-1.855313
8	6	0	5.239872	0.382423	0.364306
9	1	0	3.385984	-0.251172	1.304299

10	6	0	5.808236	1.208073	-0.600700
11	1	0	5.443302	2.655409	-2.150696
12	1	0	5.870268	-0.236832	0.989146
13	1	0	6.882665	1.225396	-0.731497
14	7	0	-0.408302	0.609884	-0.022823
15	6	0	-1.668185	-0.067722	-0.208818
16	6	0	-2.302211	-0.659903	0.876231
17	6	0	-2.238184	-0.054870	-1.474370
18	6	0	-3.545868	-1.256066	0.682529
19	1	0	-1.836632	-0.653461	1.853326
20	6	0	-3.468478	-0.671950	-1.660611
21	1	0	-1.705118	0.386155	-2.305320
22	6	0	-4.124899	-1.261450	-0.582232
23	1	0	-4.052695	-1.719257	1.519213
24	1	0	-3.894376	-0.710242	-2.653215
25	1	0	-5.085090	-1.738809	-0.732688
26	7	0	0.993281	2.311869	0.062752
27	6	0	-1.332519	2.986184	0.244034
28	6	0	-2.565241	2.735249	0.851638
29	6	0	-1.052559	4.265086	-0.250886
30	6	0	-3.505847	3.754408	0.950789
31	1	0	-2.795494	1.757801	1.247282
32	6	0	-1.996086	5.276818	-0.145288
33	1	0	-0.093891	4.449333	-0.716518
34	6	0	-3.227312	5.022728	0.453220
35	1	0	-4.459295	3.552466	1.421472
36	1	0	-1.772447	6.261221	-0.535619
37	1	0	-3.966300	5.810202	0.530866
38	6	0	0.836935	0.081440	-0.201492
39	6	0	1.252743	-1.261307	-0.791133
40	1	0	2.276652	-1.033946	-1.112331
41	1	0	-0.590029	-2.454572	0.951100
42	6	0	0.459133	-1.419431	-2.049497
43	6	0	0.815489	-0.457283	-3.148758
44	1	0	1.893823	-0.447107	-3.358841
45	1	0	0.289314	-0.751172	-4.055840
46	1	0	0.539162	0.595869	-2.943799
47	6	0	-0.616317	-2.283578	-2.266900
48	8	0	-1.316770	-2.376058	-3.284755
49	8	0	-0.920764	-3.114621	-1.177388
50	6	0	-1.947692	-4.057906	-1.442358
51	1	0	-2.129208	-4.575822	-0.499900
52	1	0	-2.856513	-3.563576	-1.781601
53	1	0	-1.638264	-4.770680	-2.208689

54	6	0	1.425730	-2.435167	0.200276
55	1	0	1.402654	-3.331035	-0.417544
56	1	0	2.419301	-2.359940	0.650015
57	6	0	0.419183	-2.608698	1.331448
58	6	0	0.487415	-4.036797	1.895875
59	1	0	0.215131	-4.732671	1.102388
60	1	0	1.499866	-4.273563	2.231564
61	1	0	-0.198555	-4.165314	2.731985
62	6	0	0.662532	-1.615487	2.441015
63	8	0	1.581926	-0.827221	2.516072
64	8	0	-0.283934	-1.682217	3.396637
65	6	0	-0.099028	-0.776450	4.493991
66	1	0	-0.922838	-0.969004	5.174522
67	1	0	0.857113	-0.963993	4.978644
68	1	0	-0.120304	0.253165	4.139273

TS6(C)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.146151	1.738477	0.303194
2	7	0	0.934413	1.756913	-0.007139
3	6	0	2.195005	2.356983	-0.271593
4	6	0	2.229531	3.560880	-0.972168
5	6	0	3.361532	1.730355	0.154623
6	6	0	3.459888	4.140931	-1.251061
7	1	0	1.303166	4.021536	-1.284273
8	6	0	4.585628	2.319333	-0.147399
9	1	0	3.313083	0.815217	0.730370
10	6	0	4.639758	3.521203	-0.845430
11	1	0	3.496176	5.076458	-1.794247
12	1	0	5.497046	1.836976	0.181295
13	1	0	5.595785	3.976344	-1.070114
14	7	0	-0.689380	0.433474	0.270346
15	6	0	-1.534783	-0.723549	0.275866
16	6	0	-1.526751	-1.573387	1.375618
17	6	0	-2.380919	-0.938081	-0.805172
18	6	0	-2.384203	-2.669233	1.385378
19	1	0	-0.851318	-1.378615	2.197536
20	6	0	-3.231444	-2.037303	-0.785576
21	1	0	-2.354878	-0.271922	-1.656991
22	6	0	-3.235968	-2.898658	0.308149

23	1	0	-2.385744	-3.339643	2.235242
24	1	0	-3.869913	-2.227095	-1.637769
25	1	0	-3.899521	-3.754384	0.317801
26	7	0	-0.155891	2.563797	0.139421
27	6	0	-2.536675	2.183480	0.487343
28	6	0	-3.443644	1.499951	1.301467
29	6	0	-2.930287	3.360136	-0.156476
30	6	0	-4.734574	1.990651	1.458627
31	1	0	-3.145904	0.594793	1.812343
32	6	0	-4.221617	3.843894	0.006135
33	1	0	-2.216609	3.881518	-0.780448
34	6	0	-5.126952	3.158293	0.811440
35	1	0	-5.433704	1.458504	2.090712
36	1	0	-4.521949	4.752802	-0.499099
37	1	0	-6.135100	3.533283	0.934441
38	6	0	0.662865	0.434043	0.044404
39	6	0	1.482149	-0.641828	-1.213697
40	1	0	2.138747	0.173844	-1.516669
41	1	0	0.720543	-2.431449	0.735397
42	6	0	0.509417	-0.881876	-2.214959
43	6	0	0.112454	0.276600	-3.091589
44	1	0	0.976818	0.899284	-3.341865
45	1	0	-0.337360	-0.090860	-4.012558
46	1	0	-0.626266	0.943183	-2.616596
47	6	0	-0.218256	-2.099226	-2.410917
48	8	0	-1.042051	-2.309071	-3.295361
49	8	0	0.079260	-3.096312	-1.506602
50	6	0	-0.556776	-4.341018	-1.780294
51	1	0	-0.293809	-4.996487	-0.951687
52	1	0	-1.636223	-4.218512	-1.840541
53	1	0	-0.200399	-4.757708	-2.722949
54	6	0	2.315410	-1.739893	-0.549195
55	1	0	2.407765	-2.542744	-1.278407
56	1	0	3.316878	-1.347887	-0.358619
57	6	0	1.802853	-2.339459	0.758715
58	6	0	2.411053	-3.733744	0.984713
59	1	0	2.085830	-4.394385	0.180866
60	1	0	3.501472	-3.677614	0.975053
61	1	0	2.090777	-4.155388	1.938809
62	6	0	2.207067	-1.492994	1.941087
63	8	0	3.247852	-0.882642	2.051939
64	8	0	1.312426	-1.552543	2.947322
65	6	0	1.690714	-0.831227	4.128655
66	1	0	0.881217	-0.981688	4.836857

67	1	0	2.627786	-1.220152	4.522248
68	1	0	1.813770	0.225647	3.897747

P(Z)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.509990	-1.077085	0.944884
2	1	0	0.015100	-1.990700	1.204087
3	1	0	0.535734	0.907547	-0.579854
4	6	0	-1.639662	-1.226254	0.237302
5	6	0	-2.180388	-2.584159	-0.127134
6	1	0	-1.519207	-3.368861	0.237246
7	1	0	-3.174427	-2.723278	0.299813
8	1	0	-2.287509	-2.680911	-1.208983
9	6	0	-2.505532	-0.115490	-0.244766
10	8	0	-3.609730	-0.291622	-0.708619
11	8	0	-1.956214	1.113573	-0.156129
12	6	0	-2.795896	2.171585	-0.636368
13	1	0	-2.219929	3.083367	-0.506036
14	1	0	-3.038314	2.011340	-1.685363
15	1	0	-3.719894	2.210381	-0.062216
16	6	0	0.161388	0.184835	1.415035
17	1	0	-0.574104	0.940493	1.681808
18	1	0	0.759327	-0.051056	2.297386
19	6	0	1.091739	0.781237	0.351402
20	6	0	1.640024	2.145997	0.787961
21	1	0	0.811067	2.836708	0.948508
22	1	0	2.194021	2.054113	1.724622
23	1	0	2.302255	2.560811	0.029501
24	6	0	2.239582	-0.162780	0.067928
25	8	0	2.506550	-1.160680	0.696026
26	8	0	2.968338	0.253418	-0.981685
27	6	0	4.090348	-0.580347	-1.300136
28	1	0	4.567138	-0.116509	-2.158204
29	1	0	4.774668	-0.629218	-0.454766
30	1	0	3.752840	-1.586966	-1.540942

TS3(D)

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	1.887411	-1.434493	-0.277568
2	7	0	-0.219667	-1.693846	-0.290513
3	6	0	-1.383319	-2.429098	-0.662462
4	6	0	-2.292258	-1.904636	-1.572505
5	6	0	-1.499707	-3.738909	-0.199709
6	6	0	-3.349936	-2.700259	-2.005706
7	1	0	-2.156169	-0.906127	-1.959581
8	6	0	-2.542094	-4.530846	-0.660328
9	1	0	-0.762497	-4.122449	0.492460
10	6	0	-3.470759	-4.012815	-1.563011
11	1	0	-4.064009	-2.292688	-2.708952
12	1	0	-2.631192	-5.552388	-0.313530
13	1	0	-4.282810	-4.632788	-1.920625
14	7	0	1.315969	-0.238716	0.103475
15	6	0	2.017524	0.892650	0.636111
16	6	0	2.775184	0.732710	1.792962
17	6	0	1.925655	2.113700	-0.017952
18	6	0	3.469390	1.827114	2.295037
19	1	0	2.822644	-0.233871	2.279000
20	6	0	2.607115	3.206126	0.510417
21	1	0	1.301465	2.242272	-0.896314
22	6	0	3.384333	3.062940	1.655592
23	1	0	4.068252	1.716808	3.189878
24	1	0	2.511006	4.162477	0.013136
25	1	0	3.918243	3.914318	2.058461
26	7	0	0.974218	-2.323301	-0.515511
27	6	0	3.324976	-1.704594	-0.426205
28	6	0	3.773716	-3.005658	-0.183614
29	6	0	4.224609	-0.721822	-0.847432
30	6	0	5.115491	-3.319484	-0.353594
31	1	0	3.062515	-3.757410	0.132541
32	6	0	5.566053	-1.044857	-1.014327
33	1	0	3.880431	0.282777	-1.053187
34	6	0	6.014115	-2.338737	-0.765092
35	1	0	5.459886	-4.327656	-0.162392
36	1	0	6.260241	-0.283106	-1.344726
37	1	0	7.060833	-2.582980	-0.894677
38	6	0	-0.057200	-0.405785	0.123096
39	6	0	-0.970295	0.641467	0.444130
40	1	0	-2.500146	1.439775	1.608568
41	1	0	-0.371045	1.502796	0.717288
42	6	0	-2.006475	0.465536	1.560745

43	6	0	-1.324478	0.172149	2.900103
44	1	0	-0.822207	-0.795631	2.873435
45	1	0	-0.581394	0.945526	3.101400
46	1	0	-2.044140	0.155345	3.719815
47	6	0	-3.140499	-0.494348	1.257509
48	8	0	-4.058052	-0.258614	0.504921
49	8	0	-3.049518	-1.641040	1.948897
50	6	0	-4.148911	-2.542437	1.755578
51	1	0	-3.883778	-3.448037	2.293207
52	1	0	-5.059136	-2.102848	2.161600
53	1	0	-4.285179	-2.744383	0.696797
54	6	0	-1.825768	1.482609	-1.046626
55	1	0	-1.064140	1.316479	-1.803959
56	1	0	-2.686880	0.825688	-1.108959
57	6	0	-2.120921	2.837769	-0.785563
58	6	0	-3.413580	3.268726	-0.137591
59	1	0	-3.945916	3.995014	-0.757861
60	1	0	-4.062677	2.402467	0.005782
61	1	0	-3.267306	3.750286	0.835840
62	6	0	-1.151497	3.801068	-1.173469
63	8	0	-0.042634	3.598570	-1.690115
64	8	0	-1.559347	5.089820	-0.936360
65	6	0	-0.633887	6.085899	-1.343449
66	1	0	-1.106430	7.041007	-1.123993
67	1	0	0.304720	5.995658	-0.793792
68	1	0	-0.414343	6.004719	-2.408038

M3(D)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.080192	-1.104769	-0.451169
2	7	0	0.026457	-1.587647	-0.579402
3	6	0	-1.071740	-2.478267	-0.838015
4	6	0	-1.882925	-2.285299	-1.946542
5	6	0	-1.210946	-3.579118	-0.002747
6	6	0	-2.901430	-3.200003	-2.190122
7	1	0	-1.721575	-1.436130	-2.595123
8	6	0	-2.216586	-4.498980	-0.273248
9	1	0	-0.540515	-3.701760	0.838063
10	6	0	-3.068188	-4.301640	-1.357329
11	1	0	-3.556870	-3.053571	-3.038104

12	1	0	-2.337548	-5.365288	0.364695
13	1	0	-3.858219	-5.013690	-1.558293
14	7	0	1.351082	0.002199	-0.069680
15	6	0	1.900246	1.218344	0.480294
16	6	0	2.654913	1.122911	1.646244
17	6	0	1.673199	2.424489	-0.165320
18	6	0	3.207461	2.280639	2.176967
19	1	0	2.804826	0.160340	2.119305
20	6	0	2.212452	3.579021	0.398352
21	1	0	1.018285	2.493290	-1.027862
22	6	0	2.983630	3.508108	1.553154
23	1	0	3.800143	2.226888	3.080747
24	1	0	2.001610	4.529202	-0.073644
25	1	0	3.402807	4.410592	1.979648
26	7	0	1.277853	-2.084398	-0.758047
27	6	0	3.544559	-1.206164	-0.522996
28	6	0	4.129071	-2.442180	-0.235993
29	6	0	4.339969	-0.126725	-0.916951
30	6	0	5.506071	-2.593960	-0.330365
31	1	0	3.497543	-3.271047	0.055861
32	6	0	5.716631	-0.288901	-1.009959
33	1	0	3.888984	0.827148	-1.155893
34	6	0	6.300916	-1.517112	-0.713627
35	1	0	5.958058	-3.550841	-0.103842
36	1	0	6.332125	0.545858	-1.318766
37	1	0	7.374633	-1.636114	-0.785472
38	6	0	0.032210	-0.320259	-0.150287
39	6	0	-1.091189	0.619914	0.117795
40	1	0	-2.540567	1.205722	1.456189
41	1	0	-0.610691	1.594149	0.217121
42	6	0	-1.810188	0.386624	1.463920
43	6	0	-0.861388	0.550130	2.650822
44	1	0	-0.111379	-0.244183	2.675683
45	1	0	-0.348835	1.510134	2.575691
46	1	0	-1.403833	0.514639	3.594526
47	6	0	-2.654265	-0.872817	1.529471
48	8	0	-3.578545	-1.129837	0.795571
49	8	0	-2.308804	-1.679407	2.555013
50	6	0	-3.218217	-2.763110	2.787216
51	1	0	-2.797562	-3.327719	3.614701
52	1	0	-4.199921	-2.369964	3.048541
53	1	0	-3.311402	-3.377761	1.895401
54	6	0	-2.067930	0.852961	-1.097368
55	1	0	-1.434243	0.872854	-1.994922

56	1	0	-2.764785	0.019258	-1.161851
57	6	0	-2.797514	2.139365	-0.908264
58	6	0	-4.286378	2.145256	-0.686268
59	1	0	-4.866521	2.034860	-1.614035
60	1	0	-4.593067	1.322533	-0.031177
61	1	0	-4.600304	3.082589	-0.226259
62	6	0	-2.031743	3.275913	-1.061851
63	8	0	-0.784968	3.325342	-1.276719
64	8	0	-2.722215	4.479193	-0.949467
65	6	0	-1.908974	5.628464	-1.063339
66	1	0	-2.579197	6.482819	-0.969892
67	1	0	-1.151179	5.664383	-0.276330
68	1	0	-1.393812	5.660412	-2.024837

TS4(D)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.375137	-0.923491	-0.080743
2	7	0	-0.412469	-1.696187	-0.233901
3	6	0	0.511918	-2.768998	-0.491224
4	6	0	0.826211	-3.643603	0.540173
5	6	0	0.932341	-2.983767	-1.795536
6	6	0	1.624743	-4.743494	0.253057
7	1	0	0.484039	-3.429505	1.542211
8	6	0	1.742504	-4.081020	-2.066315
9	1	0	0.629821	-2.300554	-2.578481
10	6	0	2.087731	-4.957914	-1.043065
11	1	0	1.890692	-5.431595	1.045071
12	1	0	2.093714	-4.252192	-3.075305
13	1	0	2.715210	-5.813777	-1.256489
14	7	0	-1.491089	0.136611	-0.107573
15	6	0	-1.849396	1.527312	-0.041358
16	6	0	-1.506346	2.371784	-1.088484
17	6	0	-2.520015	1.987066	1.086559
18	6	0	-1.818685	3.722753	-0.984647
19	1	0	-0.961835	1.997813	-1.944497
20	6	0	-2.848830	3.333608	1.165069
21	1	0	-2.760256	1.300594	1.888097
22	6	0	-2.492172	4.201183	0.134374
23	1	0	-1.512963	4.397397	-1.772324
24	1	0	-3.365263	3.708283	2.038903

25	1	0	-2.729401	5.254336	0.211210
26	7	0	-1.723992	-2.046355	-0.154435
27	6	0	-3.841163	-0.848141	0.010602
28	6	0	-4.495153	-1.839355	0.746799
29	6	0	-4.580072	0.133695	-0.655077
30	6	0	-5.881655	-1.840497	0.826697
31	1	0	-3.908608	-2.598827	1.246848
32	6	0	-5.966940	0.123998	-0.569970
33	1	0	-4.079124	0.893708	-1.239775
34	6	0	-6.618307	-0.857493	0.172044
35	1	0	-6.385600	-2.606914	1.401107
36	1	0	-6.538626	0.882750	-1.088293
37	1	0	-7.699008	-0.857709	0.236945
38	6	0	-0.228820	-0.373601	-0.187715
39	6	0	1.003651	0.455690	-0.222856
40	1	0	2.882337	0.896501	0.223791
41	1	0	0.928878	1.088552	-1.113082
42	6	0	2.354065	-0.231460	-0.287043
43	6	0	3.051828	-0.376899	-1.625001
44	1	0	2.671602	-1.193823	-2.245824
45	1	0	2.952441	0.557334	-2.182855
46	1	0	4.113843	-0.561689	-1.466467
47	6	0	2.602968	-1.173777	0.778054
48	8	0	1.948791	-1.268016	1.816418
49	8	0	3.716396	-1.930393	0.583680
50	6	0	4.134077	-2.670127	1.727422
51	1	0	5.027925	-3.208547	1.421398
52	1	0	4.358137	-1.997525	2.555873
53	1	0	3.359130	-3.366436	2.044796
54	6	0	1.060264	1.518188	0.969634
55	1	0	0.255510	2.240649	0.859916
56	1	0	0.956915	0.978196	1.910434
57	6	0	2.413335	2.167120	0.871110
58	6	0	3.242613	2.320180	2.125858
59	1	0	2.828920	3.052951	2.829801
60	1	0	3.301677	1.361204	2.648232
61	1	0	4.255894	2.638038	1.881472
62	6	0	2.487765	3.123845	-0.185403
63	8	0	1.702393	3.209974	-1.142100
64	8	0	3.578482	3.949978	-0.125875
65	6	0	3.732438	4.802541	-1.251561
66	1	0	4.632409	5.384774	-1.064350
67	1	0	3.840639	4.222230	-2.168887
68	1	0	2.870748	5.460995	-1.363806

M4(D)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.239567	-1.311065	-0.065982
2	7	0	0.177506	-1.792708	-0.112894
3	6	0	-0.952001	-2.683210	-0.187072
4	6	0	-1.809504	-2.624288	-1.273383
5	6	0	-1.075118	-3.649174	0.806493
6	6	0	-2.858131	-3.534410	-1.337783
7	1	0	-1.692621	-1.859842	-2.026959
8	6	0	-2.122893	-4.554269	0.724688
9	1	0	-0.368662	-3.670186	1.625617
10	6	0	-3.015390	-4.494517	-0.344911
11	1	0	-3.560589	-3.471612	-2.157740
12	1	0	-2.247041	-5.302055	1.496964
13	1	0	-3.837600	-5.196655	-0.399558
14	7	0	1.513395	-0.146484	0.095659
15	6	0	2.012739	1.194489	0.235054
16	6	0	1.972893	1.799556	1.485796
17	6	0	2.524586	1.843769	-0.879185
18	6	0	2.459157	3.094200	1.617203
19	1	0	1.558057	1.261523	2.329728
20	6	0	3.013093	3.137281	-0.732969
21	1	0	2.535836	1.340164	-1.837393
22	6	0	2.979382	3.759506	0.510376
23	1	0	2.425687	3.583700	2.581466
24	1	0	3.411847	3.659118	-1.592733
25	1	0	3.353254	4.769517	0.616715
26	7	0	1.425399	-2.321185	-0.192544
27	6	0	3.702431	-1.442286	-0.128530
28	6	0	4.218967	-2.505634	-0.876191
29	6	0	4.569579	-0.581699	0.549910
30	6	0	5.591007	-2.700871	-0.949445
31	1	0	3.535130	-3.168134	-1.390150
32	6	0	5.942653	-0.783716	0.467827
33	1	0	4.183663	0.231034	1.148622
34	6	0	6.455618	-1.837710	-0.281140
35	1	0	5.985125	-3.524187	-1.530999
36	1	0	6.611120	-0.117154	0.997223
37	1	0	7.525966	-1.988682	-0.341546

38	6	0	0.196277	-0.473579	0.061919
39	6	0	-0.959204	0.474800	0.250003
40	1	0	-3.029065	1.969955	-0.205124
41	1	0	-0.522792	1.278761	0.858903
42	6	0	-2.063741	-0.178087	1.022303
43	6	0	-1.743320	-0.456840	2.462172
44	1	0	-0.994194	-1.258555	2.602502
45	1	0	-1.337726	0.432102	2.968213
46	1	0	-2.636044	-0.768257	2.999345
47	6	0	-3.246883	-0.575392	0.412345
48	8	0	-3.603564	-0.433984	-0.781716
49	8	0	-4.125385	-1.218764	1.282027
50	6	0	-5.374576	-1.549207	0.705772
51	1	0	-5.971637	-1.975525	1.511699
52	1	0	-5.870716	-0.668105	0.296218
53	1	0	-5.262807	-2.277834	-0.099064
54	6	0	-1.289986	1.121551	-1.113624
55	1	0	-0.370559	1.506105	-1.566688
56	1	0	-1.750038	0.380429	-1.759751
57	6	0	-2.280104	2.269405	-0.941598
58	6	0	-3.004749	2.577721	-2.256631
59	1	0	-2.290765	2.810250	-3.051158
60	1	0	-3.573310	1.690518	-2.532818
61	1	0	-3.686467	3.419305	-2.142635
62	6	0	-1.583502	3.494135	-0.396960
63	8	0	-0.398926	3.602189	-0.161309
64	8	0	-2.447267	4.503929	-0.183077
65	6	0	-1.859481	5.693307	0.350011
66	1	0	-2.676310	6.399366	0.467614
67	1	0	-1.388770	5.484183	1.309632
68	1	0	-1.107139	6.083844	-0.333914

TS5(D)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.488929	1.024694	-0.126982
2	7	0	0.574783	1.851349	0.173589
3	6	0	-0.375342	2.897088	0.311784
4	6	0	-1.483436	2.682996	1.117843
5	6	0	-0.179328	4.099355	-0.364578
6	6	0	-2.436233	3.691798	1.228484

7	1	0	-1.601586	1.751461	1.654158
8	6	0	-1.130205	5.100843	-0.228862
9	1	0	0.698165	4.230067	-0.981851
10	6	0	-2.262417	4.897284	0.560512
11	1	0	-3.309310	3.516205	1.843098
12	1	0	-0.992413	6.039777	-0.749379
13	1	0	-3.004171	5.680451	0.652891
14	7	0	1.609241	0.009631	0.200999
15	6	0	1.979698	-1.335318	0.544625
16	6	0	1.603819	-2.397382	-0.267130
17	6	0	2.717696	-1.537665	1.707151
18	6	0	1.957597	-3.689853	0.108507
19	1	0	1.016540	-2.234048	-1.158598
20	6	0	3.087426	-2.829758	2.059344
21	1	0	2.993487	-0.687452	2.318279
22	6	0	2.703419	-3.906139	1.262362
23	1	0	1.634865	-4.520972	-0.504129
24	1	0	3.663977	-2.996257	2.959977
25	1	0	2.980526	-4.913295	1.546588
26	7	0	1.860545	2.162880	-0.151920
27	6	0	3.929574	0.892670	-0.387056
28	6	0	4.755571	1.972617	-0.060317
29	6	0	4.477838	-0.249598	-0.976208
30	6	0	6.118663	1.906282	-0.315296
31	1	0	4.315632	2.852494	0.390090
32	6	0	5.843750	-0.308488	-1.226616
33	1	0	3.843672	-1.083056	-1.245486
34	6	0	6.665558	0.764579	-0.895601
35	1	0	6.754251	2.743791	-0.057823
36	1	0	6.264425	-1.193727	-1.685629
37	1	0	7.729135	0.712276	-1.091182
38	6	0	0.360553	0.544680	0.397686
39	6	0	-1.181794	-0.379245	-0.131781
40	1	0	-3.531577	-1.747677	0.548429
41	1	0	-0.598876	-0.899592	-0.888924
42	6	0	-2.162626	0.443978	-0.733901
43	6	0	-1.892489	1.017872	-2.101985
44	1	0	-1.625068	2.080775	-2.063113
45	1	0	-1.062242	0.487158	-2.576798
46	1	0	-2.764435	0.935382	-2.752113
47	6	0	-3.354094	0.818487	-0.039487
48	8	0	-3.696271	0.527635	1.111434
49	8	0	-4.185882	1.579970	-0.818466
50	6	0	-5.431426	1.900752	-0.214397

51	1	0	-5.983479	2.471676	-0.957801
52	1	0	-5.977645	0.996588	0.054727
53	1	0	-5.288013	2.494544	0.688267
54	6	0	-1.490676	-1.294947	1.041542
55	1	0	-0.584467	-1.842507	1.312369
56	1	0	-1.815359	-0.707534	1.897757
57	6	0	-2.605875	-2.292823	0.726517
58	6	0	-2.823026	-3.254594	1.905063
59	1	0	-1.910977	-3.818973	2.112945
60	1	0	-3.085235	-2.680622	2.794251
61	1	0	-3.630123	-3.955515	1.692470
62	6	0	-2.305428	-3.111414	-0.504279
63	8	0	-1.214038	-3.295781	-1.002259
64	8	0	-3.416822	-3.688494	-0.991121
65	6	0	-3.212454	-4.518235	-2.138548
66	1	0	-4.194099	-4.897363	-2.406629
67	1	0	-2.788276	-3.934366	-2.953910
68	1	0	-2.534663	-5.336425	-1.898698