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SUPPORTING INFORMATION FOR

Computational study on NHC-catalyzed enantioselective and chemoselective fluorination of aliphatic aldehydes

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Part 1: Single-point energies

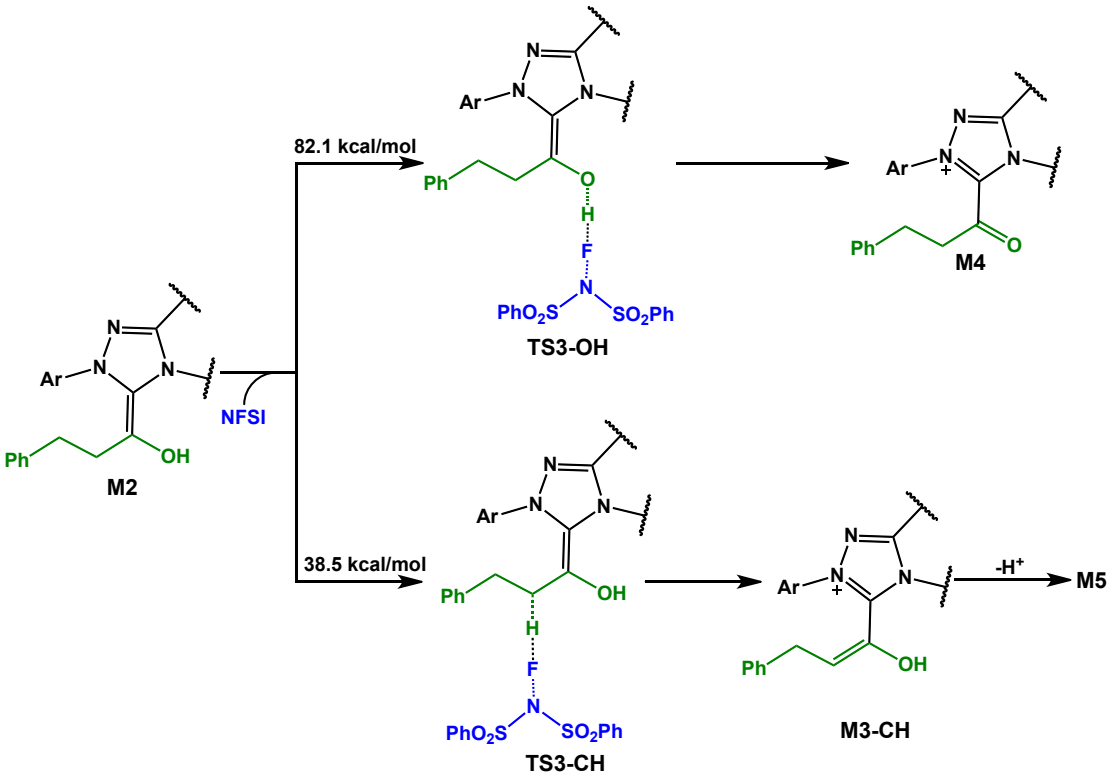
Table S1 Single-point energies of all the stationary points involved in the reaction calculated at M06-2X-GD3/6-311++G(2df,2pd)/IEF-PCM$_{1,4\text{-dioxane}}$ level

R1	-424.15014750	TS4^{D}	-9178.80520680
Cat	-8655.00484630	TS4^{A}	-9407.95607065
NFSI	-1714.97661269	M4	-9078.42050262
CyOH	-311.06037381	M05^{c}	-9469.26078381
AcO^{-}	-228.56943606	M05^{d}	-9776.92106625
AcOH	-229.08207053	M05^{a}	-10693.85421520
NSIA	-1615.35209436	M05^{b}	-9307.07756039
NHSI	-1615.82427372	TS5^{c}	-9469.24780774
HF	-100.44947719	TS5^{d}	-9776.91357141
Re-TS1	-9079.15377897	TS5^{a}	-10693.82691290
Si-TS1	-9079.15546456	TS5^{b}	-9307.06426657
Re-M1	-9079.16291513	M06^{a}	-10693.83549020
Si-M1	-9079.16894060	M06^{b}	-9307.07547705
M02^{A}	-9308.29707272	M5	-9077.97931622
M02^{C}	-9390.26363380	TS6*R*	-10792.93919890
TS2	-9079.09832912	TS6*S*	-10792.94073410
TS2^{A}	-9308.27105282	M6*R*	-9177.65915562
TS2^{C}	-9390.22245108	M6*S*	-9177.65617702
M2	-9079.18666114	M07*R*	-11104.16943490
TS3	-10794.15047070	M07*S*	-11104.15825440
TS3-OH	-10794.13809150	TS7*R*	-11104.14364190
TS3-CH	-10794.12339110	TS7*S*	-11104.13941520
M3	-10794.31646700	M7*R*	-9488.30309843
M3-CH	-10794.30308770	M7*S*	-9488.29905634

Continued

TS8*R*	-9488.29987023	P*R*	-833.28332022
TS8*S*	-9488.28977449	P*S*	-833.28332022
M06*R*[b]	-9717.38096933	TS6[S1]	-9389.00483350
M06*S*[b]	-9717.38184040	M6[S1]	-9389.05059130
TS7*R*[b]	-9717.37738942	M06S[S2-a]	-10793.08430030
TS7*S*[b]	-9717.38065081	TS6S[S2-a]	-10793.04984330
M07*R*[b]	-9717.39563201	M06S[S2-b]	-9406.31479159
M07*S*[b]	-9717.39596982	TS6S[S2-b]	-9406.28725822
NaOAc	-390.82288147	M6S[S2]	-9177.21874897
NaOAc(Dioxane)	-698.47790009		

Part 2: The other possible NFSI participated deprotonation processes



Scheme S1 The other possible NFSI participated deprotonation processes

Part 3: Energy profiles of the direct proton transfer processes

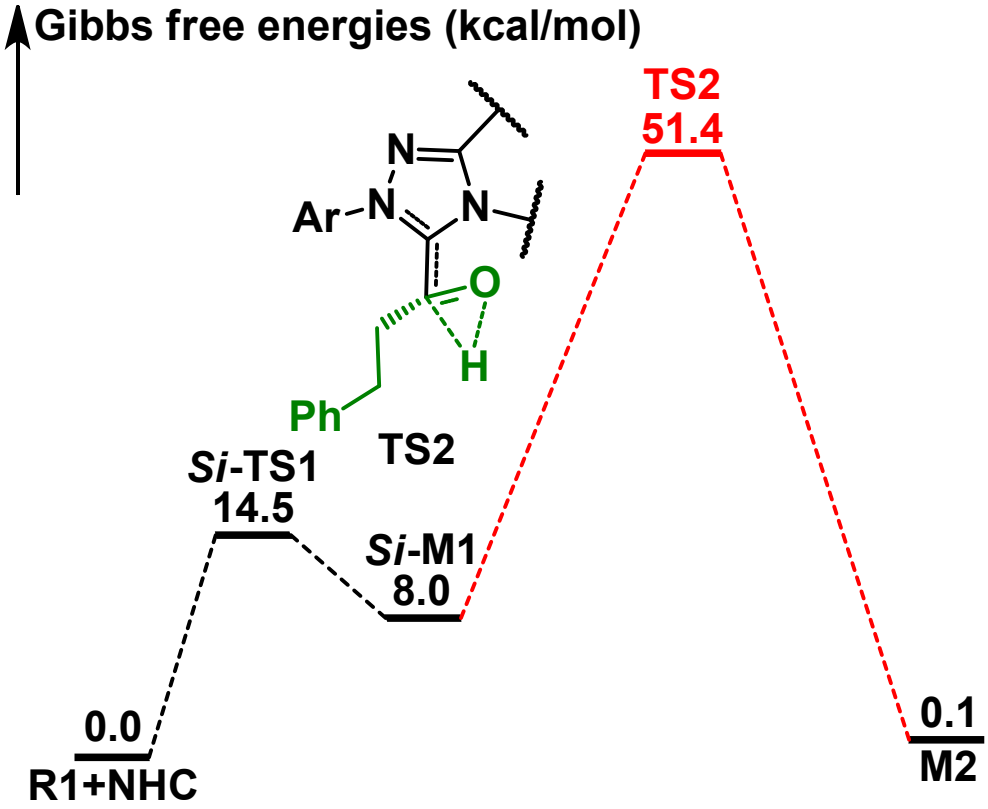


Fig. S1 The Energy profiles of the direct and CyOH-assisted proton transfer processes

Part 4: Relative energies of *E*/*Z*-configured enolate intermediate

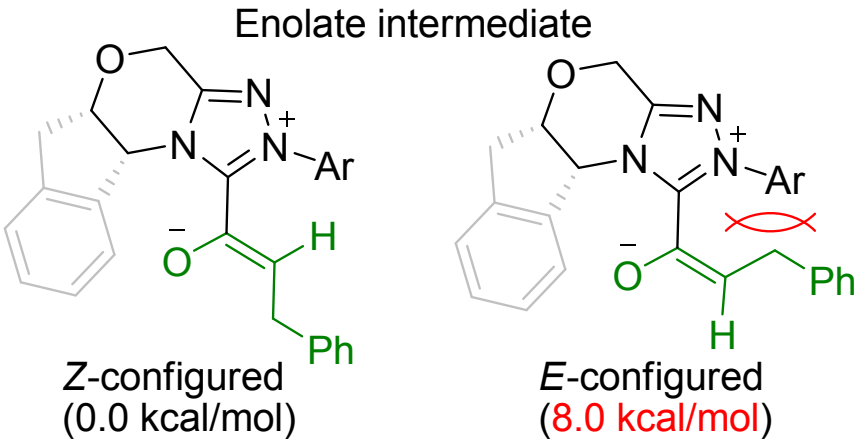


Fig. S2 Relative energies of *E*/*Z*-configured enolate intermediate

Part 5: Energy profile of NSIA-assisted esterification process

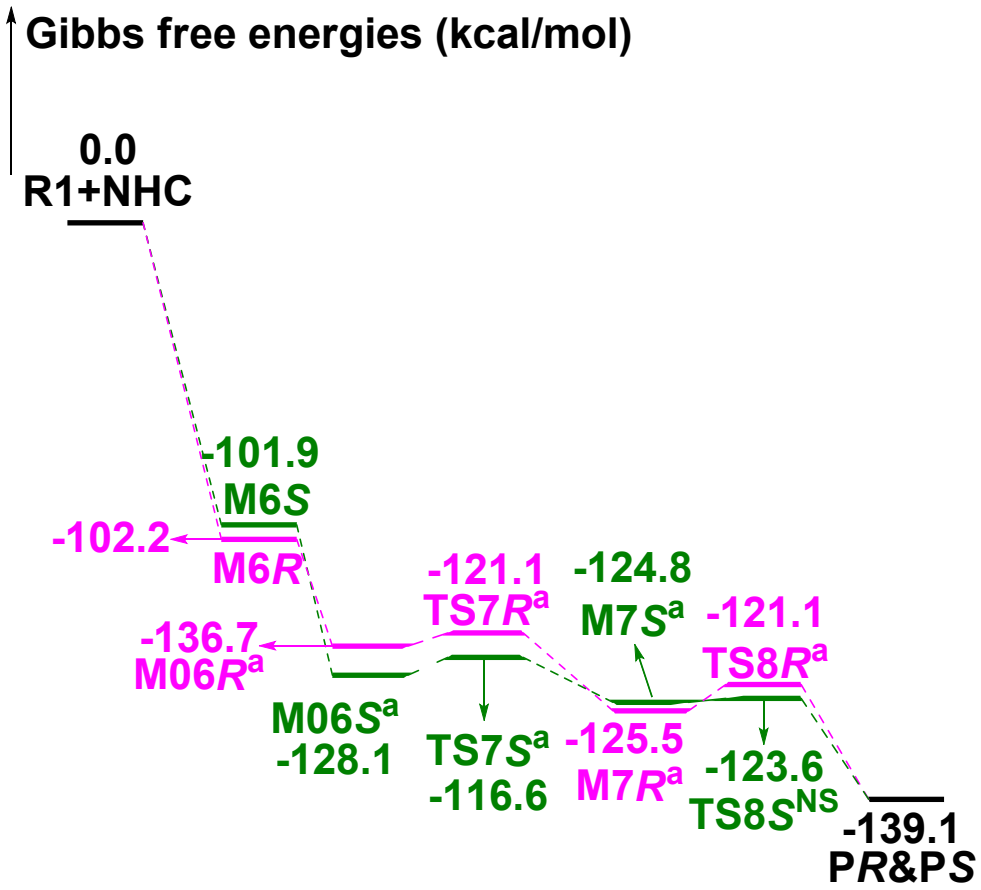


Fig. S3 The energy profile of NSIA-assisted esterification process

Part 6: Energy profile of direct deprotonation

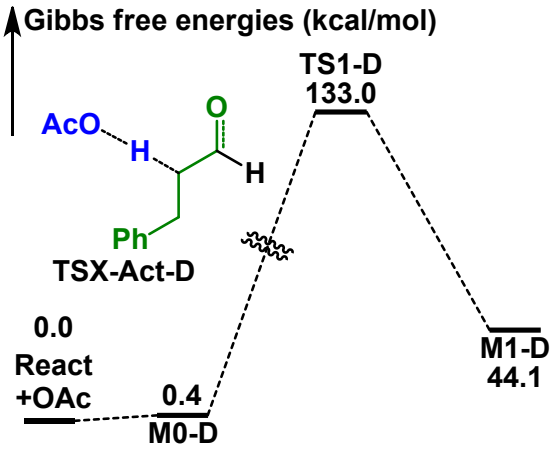


Fig. S4 The energy profile of direct deprotonation process

Part 7: Cartesian coordinates of the stationary points involved in the main text

NHC

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.995434	-0.018103	1.172889
2	6	0	-4.834190	-0.843440	0.420789
3	6	0	-5.404039	-1.972123	0.999355
4	6	0	-5.114606	-2.262922	2.331886
5	6	0	-4.265242	-1.440964	3.074971
6	6	0	-3.695873	-0.307494	2.497994
7	6	0	-3.507472	1.138384	0.336496
8	6	0	-4.515267	1.140191	-0.840820
9	6	0	-4.962023	-0.331045	-0.992505
10	1	0	-6.062614	-2.616424	0.424420
11	1	0	-5.554274	-3.139411	2.797377
12	1	0	-4.048168	-1.686347	4.109461
13	1	0	-3.023649	0.331502	3.061313
14	1	0	-5.378632	1.731228	-0.525414
15	1	0	-4.287589	-0.887729	-1.654786
16	1	0	-3.496290	2.090612	0.872260
17	1	0	-5.969841	-0.412902	-1.405772
18	6	0	-1.842055	0.953502	-1.524846
19	6	0	-1.050693	0.645767	0.573092
20	7	0	-0.578116	0.735298	-1.706857
21	7	0	-2.158787	0.901793	-0.188890
22	7	0	-0.130193	0.553234	-0.412284
23	6	0	-2.883780	1.198166	-2.572381
24	1	0	-3.123934	0.256181	-3.083217
25	1	0	-2.504588	1.898569	-3.318057
26	8	0	-4.034981	1.784678	-2.001065
27	6	0	1.231788	0.232761	-0.213617
28	6	0	1.704141	-1.045862	-0.514979
29	6	0	2.134148	1.176701	0.277788
30	6	0	3.037219	-1.388747	-0.332651
31	6	0	3.471327	0.857134	0.479485

32	6	0	3.903336	-0.425422	0.168794
33	1	0	3.387529	-2.385305	-0.569141
34	1	0	4.159837	1.597052	0.867167
35	35	0	0.503336	-2.338048	-1.165116
36	35	0	5.716024	-0.869430	0.444770
37	35	0	1.545897	2.915317	0.678595

React

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.290008	-0.294657	-0.083078
2	8	0	4.179865	0.473997	-0.355039
3	1	0	3.504051	-1.226323	0.485199
4	6	0	1.843377	-0.093910	-0.450302
5	6	0	0.934670	-0.191467	0.788045
6	1	0	1.559579	-0.884220	-1.158116
7	1	0	1.733356	0.871507	-0.951072
8	1	0	1.115552	-1.146353	1.295209
9	1	0	1.200317	0.602948	1.493610
10	6	0	-0.522947	-0.079485	0.413260
11	6	0	-1.275822	-1.219750	0.125242
12	6	0	-1.130996	1.172894	0.301258
13	6	0	-2.608650	-1.112475	-0.262890
14	1	0	-0.813346	-2.200171	0.212181
15	6	0	-2.463011	1.284833	-0.086643
16	1	0	-0.553839	2.066836	0.525281
17	6	0	-3.205872	0.140946	-0.369406
18	1	0	-3.181677	-2.008642	-0.479300
19	1	0	-2.922128	2.265217	-0.166106
20	1	0	-4.245328	0.225649	-0.669481

CyOH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.136073	1.272608	0.213052
2	6	0	0.340199	1.245089	-0.191531
3	6	0	1.031104	-0.016424	0.319901
4	6	0	0.314223	-1.262601	-0.179293

5	6	0	-1.163245	-1.249032	0.220969
6	6	0	-1.860442	0.017955	-0.280494
7	1	0	0.431722	1.256735	-1.285710
8	1	0	0.861023	2.134090	0.186488
9	1	0	-1.210532	1.323287	1.307956
10	1	0	-1.617476	2.174587	-0.177593
11	1	0	0.407104	-1.286289	-1.273156
12	1	0	0.822994	-2.150292	0.209328
13	1	0	-1.664824	-2.141691	-0.165698
14	1	0	-1.241862	-1.292223	1.315869
15	1	0	-1.865546	0.015179	-1.378767
16	1	0	-2.906418	0.030813	0.042851
17	1	0	0.995642	-0.014255	1.423889
18	8	0	2.374131	-0.097463	-0.127358
19	1	0	2.840527	0.684187	0.197780

NFSI

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.736101	-0.915476	0.412746
2	16	0	0.690656	-1.736742	-0.733543
3	8	0	1.011206	-1.112835	-1.999704
4	8	0	0.928938	-3.134838	-0.458241
5	16	0	2.070547	0.811528	0.329819
6	8	0	2.591660	1.092465	1.648307
7	8	0	2.852637	0.953171	-0.874770
8	6	0	0.510857	1.612638	0.133526
9	6	0	-0.367201	1.635077	1.217044
10	6	0	0.207693	2.189167	-1.095371
11	6	0	-1.595365	2.262448	1.051756
12	1	0	-0.086466	1.179937	2.161218
13	6	0	-1.020323	2.831519	-1.234065
14	1	0	0.922992	2.131964	-1.908964
15	6	0	-1.914082	2.864350	-0.166560
16	1	0	-2.300731	2.289906	1.875046
17	1	0	-1.276270	3.304010	-2.176156
18	1	0	-2.871452	3.362125	-0.283275
19	6	0	-0.971385	-1.344578	-0.266550
20	6	0	-1.717701	-0.541737	-1.123870
21	6	0	-1.502876	-1.891866	0.901111
22	6	0	-3.037125	-0.261149	-0.784077

23	1	0	-1.269755	-0.157313	-2.033507
24	6	0	-2.818331	-1.587785	1.230346
25	1	0	-0.902742	-2.542269	1.526786
26	6	0	-3.580223	-0.774918	0.391106
27	1	0	-3.638091	0.361629	-1.438019
28	1	0	-3.252501	-1.996417	2.136062
29	1	0	-4.609237	-0.549118	0.651381
30	9	0	1.190348	-1.168377	1.667630

AcOH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.091919	0.122594	0.000054
2	8	0	-0.638325	1.197791	-0.000044
3	8	0	-0.778071	-1.036207	-0.000036
4	1	0	-1.720153	-0.805488	-0.000105
5	6	0	1.391992	-0.112822	0.000047
6	1	0	1.670199	-0.694488	0.881398
7	1	0	1.670181	-0.694587	-0.881245
8	1	0	1.910504	0.843259	-0.000010

HF

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	9	0	0.000000	0.000000	0.092255
2	1	0	0.000000	0.000000	-0.830295

NHSI

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.445736	-1.100385	0.654697
2	16	0	0.520700	-1.812814	-0.576433
3	8	0	0.881027	-1.239449	-1.859004
4	8	0	0.644503	-3.235013	-0.308677
5	16	0	2.196292	0.422892	0.514604

6	8	0	2.697955	0.660632	1.857165
7	8	0	3.095932	0.472258	-0.620376
8	6	0	0.787237	1.435589	0.173032
9	6	0	-0.153390	1.635745	1.182145
10	6	0	0.655008	1.985737	-1.096448
11	6	0	-1.267307	2.415188	0.899728
12	1	0	-0.010897	1.183330	2.158578
13	6	0	-0.464031	2.772570	-1.359898
14	1	0	1.410394	1.788494	-1.849167
15	6	0	-1.417455	2.982670	-0.367207
16	1	0	-2.019228	2.578703	1.663913
17	1	0	-0.589662	3.217745	-2.340866
18	1	0	-2.289593	3.592149	-0.581671
19	6	0	-1.116632	-1.263505	-0.166999
20	6	0	-1.804218	-0.470733	-1.076163
21	6	0	-1.659595	-1.636274	1.060571
22	6	0	-3.083126	-0.033423	-0.738087
23	1	0	-1.337196	-0.200129	-2.016841
24	6	0	-2.933874	-1.188977	1.384338
25	1	0	-1.091122	-2.257809	1.745269
26	6	0	-3.642176	-0.389463	0.485520
27	1	0	-3.637153	0.591111	-1.430847
28	1	0	-3.376998	-1.465253	2.334990
29	1	0	-4.637561	-0.043417	0.744542
30	1	0	2.029002	-1.781628	1.142425

OAc^-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.014441	0.209370	0.000000
2	8	0	-0.000377	0.750698	1.129529
3	8	0	-0.000377	0.750698	-1.129529
4	6	0	-0.000377	-1.346817	0.000000
5	1	0	-1.040892	-1.693253	0.000000
6	1	0	0.481276	-1.746612	-0.896437
7	1	0	0.481276	-1.746612	0.896437

NSIA

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	7	0	1.531324	-1.120530	0.668463
2	16	0	0.673050	-1.755035	-0.535946
3	8	0	0.951427	-1.180587	-1.858525
4	8	0	0.731134	-3.211489	-0.397247
5	16	0	2.127321	0.376584	0.561954
6	8	0	2.566541	0.739174	1.912553
7	8	0	3.088921	0.562943	-0.527424
8	6	0	0.736011	1.440727	0.180876
9	6	0	-0.220496	1.674398	1.166632
10	6	0	0.597314	1.958818	-1.100891
11	6	0	-1.336810	2.443455	0.858931
12	1	0	-0.082211	1.247884	2.155617
13	6	0	-0.520364	2.737737	-1.397758
14	1	0	1.356512	1.734071	-1.842207
15	6	0	-1.484462	2.976330	-0.422258
16	1	0	-2.095631	2.621877	1.614395
17	1	0	-0.640184	3.152249	-2.394040
18	1	0	-2.358574	3.575039	-0.661112
19	6	0	-1.021911	-1.296409	-0.156717
20	6	0	-1.750650	-0.531131	-1.056926
21	6	0	-1.569672	-1.694821	1.061136
22	6	0	-3.051415	-0.150803	-0.729342
23	1	0	-1.284045	-0.228525	-1.988068
24	6	0	-2.868664	-1.315793	1.378480
25	1	0	-0.971642	-2.283937	1.749487
26	6	0	-3.609442	-0.541981	0.483593
27	1	0	-3.623612	0.460270	-1.420999
28	1	0	-3.304496	-1.620537	2.324999
29	1	0	-4.622127	-0.242967	0.737181

CyOH-NSIA

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.701013	0.852244	-2.045278
2	6	0	2.968674	-0.358521	-1.462978
3	6	0	3.692670	-0.898892	-0.226809
4	6	0	3.840051	0.201771	0.826466
5	6	0	4.551676	1.433216	0.260057
6	6	0	3.853588	1.958676	-0.997889

7	1	0	1.949549	-0.077993	-1.162050
8	1	0	2.859129	-1.161215	-2.198789
9	1	0	4.701129	0.544861	-2.384016
10	1	0	3.174087	1.232214	-2.927798
11	1	0	2.835035	0.464167	1.186952
12	1	0	4.381040	-0.200703	1.689782
13	1	0	4.618136	2.221129	1.018550
14	1	0	5.584547	1.161056	-0.001500
15	1	0	2.856046	2.333526	-0.727925
16	1	0	4.406230	2.809455	-1.413657
17	1	0	4.703706	-1.213661	-0.534672
18	8	0	3.071934	-2.044627	0.302960
19	1	0	2.144070	-1.802782	0.491260
20	7	0	0.312761	-1.169717	0.550389
21	16	0	-0.326654	-0.427742	1.834086
22	8	0	-1.518487	-1.082045	2.383452
23	8	0	0.780611	-0.125552	2.742587
24	16	0	-0.596378	-2.065609	-0.453507
25	8	0	0.230876	-2.281673	-1.641808
26	8	0	-1.198586	-3.236960	0.183484
27	6	0	-1.957027	-1.017706	-0.955633
28	6	0	-1.700686	0.046075	-1.817829
29	6	0	-3.226246	-1.246122	-0.439233
30	6	0	-2.740619	0.899732	-2.164990
31	1	0	-0.694936	0.192154	-2.201034
32	6	0	-4.265714	-0.391252	-0.802782
33	1	0	-3.375797	-2.077878	0.240556
34	6	0	-4.022412	0.678184	-1.659865
35	1	0	-2.553043	1.739511	-2.826638
36	1	0	-5.263850	-0.558290	-0.410011
37	1	0	-4.833212	1.346621	-1.934053
38	6	0	-0.883621	1.149568	1.183249
39	6	0	-2.213173	1.525429	1.311483
40	6	0	0.036908	1.959383	0.522269
41	6	0	-2.630297	2.736265	0.760067
42	1	0	-2.902663	0.859437	1.819242
43	6	0	-0.385242	3.165455	-0.022921
44	1	0	1.066390	1.625947	0.426849
45	6	0	-1.720879	3.553640	0.096013
46	1	0	-3.671624	3.033225	0.840398
47	1	0	0.324511	3.801531	-0.543363
48	1	0	-2.052068	4.493332	-0.335841

CyOH-OAc$^-$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.092918	-0.379019	-0.894070
2	6	0	-2.121541	-1.326276	-0.186493
3	6	0	-0.765208	-0.668435	0.061769
4	6	0	-0.938347	0.639090	0.839875
5	6	0	-1.902685	1.593221	0.132148
6	6	0	-3.259565	0.928221	-0.114078
7	1	0	-2.533207	-1.621246	0.789673
8	1	0	-1.976042	-2.246670	-0.763109
9	1	0	-2.701702	-0.146437	-1.894696
10	1	0	-4.065675	-0.863058	-1.042202
11	1	0	-1.329413	0.384534	1.836368
12	1	0	0.053444	1.085753	0.957509
13	1	0	-2.029421	2.516164	0.710048
14	1	0	-1.469203	1.887686	-0.834049
15	1	0	-3.730128	0.706907	0.854595
16	1	0	-3.935100	1.607484	-0.648280
17	1	0	-0.325941	-0.410033	-0.921325
18	8	0	0.058926	-1.570815	0.744068
19	1	0	1.006179	-1.309271	0.528989
20	6	0	2.874722	0.197117	-0.087188
21	8	0	2.216636	1.229947	0.131428
22	8	0	2.486809	-1.006230	-0.003976
23	6	0	4.343767	0.358283	-0.524871
24	1	0	4.990624	-0.218565	0.142412
25	1	0	4.470688	-0.056214	-1.529829
26	1	0	4.646587	1.406539	-0.520817

NaOAc

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.529609	0.009965	0.000081
2	8	0	-0.069655	1.121670	-0.000104
3	8	0	-0.056358	-1.110551	-0.000089
4	6	0	2.052180	0.001801	0.000131
5	1	0	2.408196	-0.545207	0.876584
6	1	0	2.407980	-0.535524	-0.882427

7	1	0	2.453675	1.014316	0.005419
8	11	0	-1.977498	-0.008467	0.000063

NaOAc-Dioxane

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.367367	0.077524	-0.094515
2	8	0	2.487683	0.957045	0.119181
3	8	0	3.126162	-1.158732	-0.206297
4	6	0	4.820586	0.516760	-0.224030
5	1	0	5.410728	0.035789	0.560277
6	1	0	5.217434	0.173464	-1.182460
7	1	0	4.915657	1.599267	-0.146168
8	11	0	0.981497	-0.688992	0.133832
9	6	0	-1.685321	1.002169	0.697129
10	6	0	-2.710968	1.399506	-0.349332
11	6	0	-3.329132	-0.827750	-0.620707
12	6	0	-2.312327	-1.250530	0.425162
13	1	0	-2.135972	1.034921	1.698233
14	1	0	-2.232811	1.425977	-1.340850
15	1	0	-4.198959	-1.488407	-0.603879
16	1	0	-1.896214	-2.236302	0.202851
17	8	0	-1.223795	-0.327150	0.438891
18	8	0	-3.789426	0.482126	-0.352237
19	1	0	-2.780930	-1.269879	1.418468
20	1	0	-2.866945	-0.870315	-1.619548
21	1	0	-3.124305	2.386273	-0.128720
22	1	0	-0.810369	1.655745	0.671104

***Re*-TS1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.958156	-0.914428	-0.364316
2	6	0	4.571102	-2.171478	-0.367294
3	6	0	5.256966	-2.611127	-1.492639
4	6	0	5.322870	-1.776576	-2.608405
5	6	0	4.729670	-0.514377	-2.593398
6	6	0	4.047331	-0.068358	-1.462550

7	6	0	3.305381	-0.663186	0.972558
8	6	0	4.075933	-1.651790	1.882961
9	6	0	4.392470	-2.854464	0.966141
10	1	0	5.743571	-3.581726	-1.500668
11	1	0	5.856209	-2.106604	-3.494126
12	1	0	4.806481	0.128533	-3.463708
13	1	0	3.605146	0.923297	-1.441104
14	1	0	5.015765	-1.165420	2.155611
15	1	0	3.554499	-3.561098	0.924675
16	1	0	3.376683	0.370486	1.319533
17	1	0	5.274225	-3.405123	1.300481
18	6	0	1.339147	-1.885268	1.949875
19	6	0	0.883702	-0.592733	0.199032
20	7	0	0.057405	-1.997259	1.793730
21	7	0	1.878796	-1.047170	0.999863
22	7	0	-0.193745	-1.199225	0.705938
23	6	0	2.182901	-2.569514	2.980400
24	1	0	2.301276	-3.628927	2.718686
25	1	0	1.690414	-2.512513	3.952378
26	8	0	3.430525	-1.923140	3.104978
27	6	0	-1.554382	-0.979836	0.354516
28	6	0	-2.298035	-0.044030	1.064235
29	6	0	-2.163274	-1.702560	-0.665900
30	6	0	-3.639884	0.170041	0.782050
31	6	0	-3.501475	-1.508154	-0.971973
32	6	0	-4.221780	-0.574039	-0.235452
33	1	0	-4.211669	0.902287	1.337186
34	1	0	-3.968644	-2.061976	-1.776333
35	35	0	-1.451937	0.968507	2.406149
36	35	0	-6.044214	-0.293406	-0.636353
37	35	0	-1.129364	-2.888199	-1.680858
38	6	0	0.608090	0.570529	-1.291935
39	8	0	-0.558915	0.403685	-1.722287
40	1	0	1.466743	0.184523	-1.885715
41	6	0	0.941775	1.904833	-0.608450
42	6	0	0.811547	3.040861	-1.629733
43	1	0	1.951003	1.899431	-0.172379
44	1	0	0.228426	2.061854	0.208563
45	1	0	1.507077	2.867692	-2.460917
46	1	0	-0.200412	2.993444	-2.044375
47	6	0	1.072557	4.392277	-1.014674
48	6	0	2.246808	5.098613	-1.279540
49	6	0	0.146067	4.949981	-0.126358
50	6	0	2.491935	6.332382	-0.679368

51	1	0	2.974477	4.678309	-1.969683
52	6	0	0.385421	6.180736	0.475121
53	1	0	-0.773226	4.409702	0.089342
54	6	0	1.561530	6.877442	0.200156
55	1	0	3.409180	6.868709	-0.902840
56	1	0	-0.347505	6.600521	1.157389
57	1	0	1.748019	7.839593	0.666564

_Si_-TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.200108	0.604687	-0.651371
2	6	0	5.515450	0.583049	-0.199627
3	6	0	6.459091	-0.211931	-0.846975
4	6	0	6.057988	-0.973545	-1.941629
5	6	0	4.737396	-0.930517	-2.399074
6	6	0	3.792510	-0.133015	-1.759455
7	6	0	3.327394	1.477842	0.222067
8	6	0	4.277180	1.949414	1.385670
9	6	0	5.704406	1.505025	0.977725
10	1	0	7.488930	-0.240264	-0.503121
11	1	0	6.781496	-1.602246	-2.451251
12	1	0	4.450801	-1.516095	-3.266945
13	1	0	2.769734	-0.049651	-2.118925
14	1	0	4.212378	3.031641	1.499119
15	1	0	6.206387	1.031241	1.827783
16	1	0	2.883248	2.304721	-0.336567
17	1	0	6.307210	2.374806	0.697874
18	6	0	2.362986	-0.115567	1.867351
19	6	0	1.034198	0.435263	0.174417
20	7	0	1.319825	-0.865424	2.045663
21	7	0	2.217528	0.688439	0.762486
22	7	0	0.514255	-0.494806	0.987225
23	6	0	3.601282	0.065962	2.681575
24	1	0	4.423951	-0.536470	2.269655
25	1	0	3.430887	-0.227443	3.717489
26	8	0	3.902194	1.448144	2.661309
27	6	0	-0.636356	-1.253317	0.664224
28	6	0	-1.880169	-0.972479	1.224533
29	6	0	-0.529942	-2.291841	-0.264057
30	6	0	-3.001749	-1.722264	0.891888

31	6	0	-1.635084	-3.053950	-0.616151
32	6	0	-2.857468	-2.759519	-0.021725
33	1	0	-3.964646	-1.497365	1.332948
34	1	0	-1.545616	-3.854110	-1.339749
35	35	0	-2.042314	0.466480	2.416308
36	35	0	-4.367400	-3.786937	-0.484651
37	35	0	1.135669	-2.612559	-1.075307
38	6	0	0.359979	1.323853	-1.550531
39	8	0	1.325175	1.829129	-2.147189
40	1	0	-0.064931	0.353387	-1.898344
41	6	0	-0.689755	2.210395	-0.883870
42	6	0	-1.673254	2.718551	-1.942982
43	1	0	-0.178971	3.054333	-0.407272
44	1	0	-1.221269	1.654778	-0.104618
45	1	0	-1.111468	3.235566	-2.727390
46	1	0	-2.150999	1.852016	-2.421529
47	6	0	-2.741542	3.638664	-1.395937
48	6	0	-3.026873	4.843896	-2.041192
49	6	0	-3.478198	3.308325	-0.252309
50	6	0	-4.022183	5.695984	-1.569452
51	1	0	-2.458372	5.116088	-2.926561
52	6	0	-4.472369	4.158402	0.223305
53	1	0	-3.269836	2.386655	0.286313
54	6	0	-4.750755	5.354886	-0.434004
55	1	0	-4.224913	6.627995	-2.088041
56	1	0	-5.032740	3.885877	1.112576
57	1	0	-5.525531	6.016927	-0.060758

***Re*-M1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.784157	-1.396076	-0.300227
2	6	0	4.153696	-2.745797	-0.303089
3	6	0	4.795303	-3.293848	-1.406547
4	6	0	5.070420	-2.473084	-2.499508
5	6	0	4.730740	-1.120185	-2.480902
6	6	0	4.089196	-0.566932	-1.374203
7	6	0	3.140769	-1.046908	1.021540
8	6	0	3.702418	-2.165311	1.935922
9	6	0	3.807979	-3.397566	1.012094
10	1	0	5.089972	-4.338750	-1.412503

11	1	0	5.571203	-2.887366	-3.368584
12	1	0	4.973663	-0.491918	-3.330971
13	1	0	3.841978	0.490239	-1.354471
14	1	0	4.709955	-1.857330	2.225304
15	1	0	2.851027	-3.929069	0.938458
16	1	0	3.371923	-0.046203	1.391807
17	1	0	4.557993	-4.109990	1.361601
18	6	0	0.970074	-1.940026	1.941868
19	6	0	0.746798	-0.590815	0.222958
20	7	0	-0.310446	-1.851284	1.756028
21	7	0	1.662243	-1.189623	1.017757
22	7	0	-0.426309	-1.015835	0.683759
23	6	0	1.665197	-2.754660	2.988578
24	1	0	1.612150	-3.818393	2.723796
25	1	0	1.163246	-2.616412	3.947326
26	8	0	2.996892	-2.321080	3.144040
27	6	0	-1.739258	-0.645537	0.264582
28	6	0	-2.417782	0.351389	0.954777
29	6	0	-2.409972	-1.384760	-0.704701
30	6	0	-3.746217	0.637883	0.673291
31	6	0	-3.735210	-1.119105	-1.006842
32	6	0	-4.386447	-0.106919	-0.307951
33	1	0	-4.265058	1.425331	1.204688
34	1	0	-4.247720	-1.681714	-1.776744
35	35	0	-1.494978	1.340087	2.262029
36	35	0	-6.196010	0.262246	-0.702080
37	35	0	-1.467126	-2.705833	-1.642301
38	6	0	0.808210	0.413475	-0.953932
39	8	0	-0.403576	0.581696	-1.439582
40	1	0	1.568499	-0.038928	-1.643584
41	6	0	1.443810	1.709210	-0.366996
42	6	0	1.496781	2.763130	-1.471677
43	1	0	2.444355	1.549053	0.061200
44	1	0	0.786568	2.057075	0.439331
45	1	0	2.145402	2.407288	-2.283174
46	1	0	0.483343	2.829409	-1.879168
47	6	0	1.982997	4.100813	-0.977694
48	6	0	3.244957	4.585474	-1.325350
49	6	0	1.183632	4.876113	-0.129609
50	6	0	3.699812	5.813185	-0.847921
51	1	0	3.875632	3.994121	-1.985097
52	6	0	1.632823	6.102049	0.350423
53	1	0	0.196932	4.511258	0.147992
54	6	0	2.894321	6.575726	-0.007652

55	1	0	4.682415	6.174362	-1.136136
56	1	0	0.996339	6.693426	1.001759
57	1	0	3.244041	7.533759	0.363669

***Si*-M1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.145882	-0.492258	-0.530814
2	6	0	5.401418	-0.720589	0.023801
3	6	0	6.229167	-1.703457	-0.513235
4	6	0	5.774058	-2.439717	-1.604420
5	6	0	4.518743	-2.186798	-2.166443
6	6	0	3.688932	-1.200454	-1.639048
7	6	0	3.403224	0.587778	0.222933
8	6	0	4.319105	0.910046	1.460531
9	6	0	5.674882	0.224089	1.166286
10	1	0	7.211075	-1.892785	-0.089243
11	1	0	6.406442	-3.212689	-2.030185
12	1	0	4.195680	-2.758490	-3.030904
13	1	0	2.726368	-0.929756	-2.070438
14	1	0	4.426392	1.988982	1.573625
15	1	0	6.045951	-0.270781	2.069800
16	1	0	3.176371	1.442178	-0.415302
17	1	0	6.423279	0.970537	0.880690
18	6	0	2.004927	-0.725828	1.801179
19	6	0	0.907219	0.089182	0.090802
20	7	0	0.806941	-1.203794	1.945646
21	7	0	2.104305	0.069834	0.687913
22	7	0	0.137970	-0.682161	0.866411
23	6	0	3.208472	-0.809622	2.680385
24	1	0	3.916694	-1.558298	2.298705
25	1	0	2.919722	-1.075008	3.697262
26	8	0	3.769425	0.487502	2.703538
27	6	0	-1.169961	-1.126835	0.551735
28	6	0	-2.279325	-0.622616	1.225058
29	6	0	-1.345443	-2.096303	-0.439392
30	6	0	-3.557596	-1.074385	0.922431
31	6	0	-2.613984	-2.554808	-0.762948
32	6	0	-3.703594	-2.036678	-0.070010
33	1	0	-4.418620	-0.676667	1.444767
34	1	0	-2.750573	-3.297246	-1.538663

35	35	0	-2.035470	0.700410	2.530540
36	35	0	-5.431137	-2.645260	-0.504950
37	35	0	0.157988	-2.743980	-1.361112
38	6	0	0.555133	0.867554	-1.189911
39	8	0	1.624694	1.024881	-1.951069
40	1	0	-0.293020	0.273923	-1.630318
41	6	0	-0.086329	2.193779	-0.674416
42	6	0	-0.495903	3.046442	-1.875733
43	1	0	0.673363	2.734357	-0.092893
44	1	0	-0.942485	2.007970	-0.008702
45	1	0	0.371129	3.084320	-2.541798
46	1	0	-1.304363	2.539186	-2.416664
47	6	0	-0.931710	4.430394	-1.469423
48	6	0	0.008650	5.454501	-1.322862
49	6	0	-2.269534	4.711112	-1.179711
50	6	0	-0.375147	6.723868	-0.900338
51	1	0	1.052308	5.247433	-1.547715
52	6	0	-2.659840	5.979542	-0.757929
53	1	0	-3.012027	3.924352	-1.291390
54	6	0	-1.712849	6.990941	-0.616459
55	1	0	0.369655	7.507097	-0.796275
56	1	0	-3.705072	6.179946	-0.542333
57	1	0	-2.015619	7.980990	-0.290610

***Si*-TS2**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.571871	-0.360260	0.682231
2	6	0	-5.857287	-0.313752	0.151344
3	6	0	-6.623648	-1.474162	0.071760
4	6	0	-6.082303	-2.670990	0.534534
5	6	0	-4.801053	-2.706239	1.090947
6	6	0	-4.036904	-1.545549	1.177663
7	6	0	-3.909149	1.000402	0.647093
8	6	0	-4.914890	1.900598	-0.167726
9	6	0	-6.231444	1.092026	-0.243029
10	1	0	-7.626505	-1.446799	-0.344409
11	1	0	-6.665780	-3.584259	0.473752
12	1	0	-4.404563	-3.643098	1.469119
13	1	0	-3.059424	-1.542556	1.648585
14	1	0	-5.053971	2.856211	0.338670

15	1	0	-6.656443	1.168618	-1.248863
16	1	0	-3.720796	1.379721	1.650769
17	1	0	-6.971759	1.502655	0.451419
18	6	0	-2.524365	0.957122	-1.406652
19	6	0	-1.348998	0.854871	0.461895
20	7	0	-1.309227	0.896742	-1.832446
21	7	0	-2.613759	0.952330	-0.034353
22	7	0	-0.552212	0.853609	-0.663839
23	6	0	-3.791467	1.209899	-2.152692
24	1	0	-4.409243	0.302314	-2.200838
25	1	0	-3.574803	1.553616	-3.163737
26	8	0	-4.446150	2.257752	-1.460608
27	6	0	0.708424	0.208607	-0.749274
28	6	0	1.888778	0.921628	-0.967899
29	6	0	0.784304	-1.186494	-0.674401
30	6	0	3.109431	0.276120	-1.119583
31	6	0	1.991366	-1.857326	-0.809233
32	6	0	3.139624	-1.109066	-1.043306
33	1	0	4.017891	0.846128	-1.268940
34	1	0	2.032894	-2.937517	-0.745808
35	35	0	1.842268	2.794637	-1.026229
36	35	0	4.784087	-2.000973	-1.252717
37	35	0	-0.791122	-2.174850	-0.376828
38	6	0	-0.937378	0.641456	1.792811
39	8	0	-1.952235	0.463359	2.789191
40	1	0	-1.237175	-0.451693	2.093207
41	6	0	0.418625	1.174905	2.203936
42	6	0	1.424724	0.089567	2.625672
43	1	0	0.238668	1.879759	3.024199
44	1	0	0.832633	1.761658	1.378740
45	1	0	1.323433	-0.110811	3.699128
46	1	0	1.157259	-0.848605	2.121936
47	6	0	2.870440	0.394686	2.290339
48	6	0	3.331674	1.694841	2.066720
49	6	0	3.778512	-0.660837	2.153942
50	6	0	4.650661	1.928884	1.681478
51	1	0	2.656974	2.538360	2.176797
52	6	0	5.101092	-0.431263	1.790772
53	1	0	3.433226	-1.679717	2.317834
54	6	0	5.539190	0.867349	1.536631
55	1	0	4.981743	2.946170	1.495064
56	1	0	5.783429	-1.267697	1.679907
57	1	0	6.566099	1.049248	1.235545

M02[A]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.205362	0.566815	0.377985
2	6	0	-5.508829	0.779717	-0.063033
3	6	0	-6.525590	-0.087369	0.327039
4	6	0	-6.210123	-1.159815	1.158521
5	6	0	-4.900056	-1.359832	1.600606
6	6	0	-3.878530	-0.492834	1.219955
7	6	0	-3.271274	1.617926	-0.183228
8	6	0	-4.133375	2.383695	-1.252029
9	6	0	-5.598065	2.006426	-0.935067
10	1	0	-7.545129	0.067130	-0.013533
11	1	0	-6.991717	-1.846620	1.467847
12	1	0	-4.671064	-2.190826	2.260070
13	1	0	-2.865040	-0.647756	1.580882
14	1	0	-3.961408	3.457503	-1.175260
15	1	0	-6.149655	1.845305	-1.866513
16	1	0	-2.872180	2.272751	0.591525
17	1	0	-6.093093	2.825987	-0.403955
18	6	0	-2.249931	0.396832	-2.080341
19	6	0	-0.914915	0.652454	-0.371940
20	7	0	-1.178295	-0.251932	-2.418469
21	7	0	-2.122607	0.974356	-0.838992
22	7	0	-0.348832	-0.073176	-1.343931
23	6	0	-3.500685	0.705661	-2.835451
24	1	0	-4.320890	0.051541	-2.509475
25	1	0	-3.339899	0.576142	-3.905444
26	8	0	-3.777323	2.071305	-2.593250
27	6	0	0.782289	-0.913891	-1.146979
28	6	0	2.061203	-0.551185	-1.560763
29	6	0	0.589041	-2.120742	-0.472968
30	6	0	3.146889	-1.370719	-1.286671
31	6	0	1.660536	-2.949609	-0.179935
32	6	0	2.927887	-2.555776	-0.590705
33	1	0	4.142817	-1.085499	-1.600898
34	1	0	1.510502	-3.866906	0.374378
35	35	0	2.321640	1.059858	-2.488065
36	35	0	4.401988	-3.651807	-0.179363
37	35	0	-1.147062	-2.589606	0.054134
38	6	0	-0.268800	1.021702	0.938881

39	8	0	-1.228731	1.254774	1.909642
40	1	0	0.363447	0.159589	1.217583
41	6	0	0.630176	2.244790	0.714338
42	6	0	1.606683	2.405568	1.881364
43	1	0	0.000413	3.137260	0.612367
44	1	0	1.186216	2.129971	-0.222103
45	1	0	1.037057	2.581177	2.798512
46	1	0	2.138812	1.455456	2.018616
47	6	0	2.596124	3.521594	1.647284
48	6	0	2.645630	4.634000	2.488241
49	6	0	3.486527	3.460068	0.568698
50	6	0	3.562165	5.659958	2.265162
51	1	0	1.960166	4.693467	3.329454
52	6	0	4.401650	4.482365	0.341828
53	1	0	3.456613	2.607347	-0.107277
54	6	0	4.444239	5.586525	1.191778
55	1	0	3.586385	6.516192	2.932090
56	1	0	5.086834	4.417288	-0.497928
57	1	0	5.160840	6.382650	1.016934
58	6	0	-0.263890	-1.671508	3.036346
59	8	0	0.794535	-1.421474	2.432269
60	8	0	-1.279011	-0.902622	3.138152
61	1	0	-1.240881	0.386072	2.500223
62	6	0	-0.424362	-3.050589	3.667348
63	1	0	-1.112124	-3.022270	4.512869
64	1	0	-0.843330	-3.714243	2.902701
65	1	0	0.545342	-3.448243	3.969292

M02[C]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.109327	-0.809664	-0.031734
2	6	0	5.336091	-1.395943	-0.332304
3	6	0	6.194431	-0.788135	-1.245351
4	6	0	5.800968	0.406282	-1.843287
5	6	0	4.575890	0.996855	-1.520904
6	6	0	3.716208	0.399553	-0.602170
7	6	0	3.337438	-1.650644	0.963474
8	6	0	4.181584	-2.971558	1.105501
9	6	0	5.551579	-2.658262	0.462330
10	1	0	7.153041	-1.238152	-1.486543

11	1	0	6.457228	0.887995	-2.561466
12	1	0	4.294190	1.938691	-1.981751
13	1	0	2.778756	0.864794	-0.308170
14	1	0	4.276333	-3.244270	2.156737
15	1	0	5.881921	-3.509225	-0.141852
16	1	0	3.174976	-1.121076	1.903144
17	1	0	6.308406	-2.502766	1.238039
18	6	0	1.827817	-2.955990	-0.518819
19	6	0	0.839528	-1.351069	0.580619
20	7	0	0.610288	-2.974999	-0.968023
21	7	0	2.004952	-1.981107	0.433660
22	7	0	0.000930	-1.970344	-0.258455
23	6	0	2.986545	-3.866781	-0.759635
24	1	0	3.701243	-3.411867	-1.459262
25	1	0	2.644590	-4.819430	-1.163562
26	8	0	3.562676	-4.106478	0.510084
27	6	0	-1.219411	-1.394206	-0.707719
28	6	0	-2.459183	-1.803185	-0.226186
29	6	0	-1.147974	-0.341994	-1.626450
30	6	0	-3.625485	-1.197640	-0.674468
31	6	0	-2.299682	0.288912	-2.071353
32	6	0	-3.523954	-0.157913	-1.589215
33	1	0	-4.587535	-1.508934	-0.289277
34	1	0	-2.240514	1.120131	-2.762151
35	35	0	-2.570089	-3.158220	1.065419
36	35	0	-5.090762	0.730315	-2.134210
37	35	0	0.535432	0.262725	-2.186184
38	6	0	0.519160	-0.159076	1.454141
39	8	0	1.608559	0.611736	1.655056
40	1	0	-0.284856	0.353303	0.879182
41	6	0	-0.139462	-0.671756	2.757044
42	6	0	-0.947924	0.474127	3.377501
43	1	0	0.671858	-0.984357	3.423789
44	1	0	-0.795696	-1.532860	2.579286
45	1	0	-1.153717	0.255939	4.430420
46	1	0	-0.327297	1.376059	3.340005
47	6	0	-2.254428	0.696569	2.650357
48	6	0	-3.368833	-0.087675	2.967115
49	6	0	-2.377138	1.656221	1.637788
50	6	0	-4.591046	0.113437	2.331610
51	1	0	-3.276978	-0.853537	3.734395
52	6	0	-3.599625	1.856561	0.998080
53	1	0	-1.502819	2.235783	1.341021
54	6	0	-4.714283	1.100947	1.356104

55	1	0	-5.449594	-0.493045	2.605448
56	1	0	-3.682847	2.603173	0.212699
57	1	0	-5.664324	1.262115	0.855627
58	6	0	3.202112	5.242593	1.186741
59	6	0	2.723633	3.887582	0.661689
60	6	0	1.204388	3.734187	0.777492
61	6	0	0.496734	4.883854	0.067836
62	6	0	0.965736	6.244257	0.588907
63	6	0	2.485217	6.388732	0.468251
64	1	0	2.983339	3.786129	-0.402546
65	1	0	3.208592	3.059717	1.192437
66	1	0	2.990992	5.308475	2.263053
67	1	0	4.287418	5.337236	1.072886
68	1	0	0.713594	4.797462	-1.006073
69	1	0	-0.586712	4.768143	0.186812
70	1	0	0.460188	7.053833	0.051669
71	1	0	0.682067	6.342738	1.645986
72	1	0	2.762515	6.373836	-0.594946
73	1	0	2.810207	7.355390	0.868402
74	1	0	0.943593	3.788039	1.853657
75	8	0	0.772084	2.517515	0.225895
76	1	0	1.182025	1.779765	0.810556

TS2[A]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.290911	0.648786	0.435288
2	6	0	-5.614060	0.710518	0.008496
3	6	0	-6.564878	-0.142597	0.563588
4	6	0	-6.165642	-1.046661	1.545503
5	6	0	-4.837031	-1.093255	1.975310
6	6	0	-3.884248	-0.239072	1.425745
7	6	0	-3.428090	1.646845	-0.303886
8	6	0	-4.366994	2.214657	-1.434906
9	6	0	-5.798299	1.777674	-1.040099
10	1	0	-7.599521	-0.105979	0.235373
11	1	0	-6.895544	-1.720555	1.982950
12	1	0	-4.542414	-1.789804	2.753867
13	1	0	-2.856377	-0.265719	1.772825
14	1	0	-4.274519	3.299920	-1.484224
15	1	0	-6.337386	1.431082	-1.927596

16	1	0	-3.061523	2.434988	0.351801
17	1	0	-6.357023	2.628276	-0.635936
18	6	0	-2.356539	0.294219	-2.072887
19	6	0	-0.984476	0.849685	-0.433644
20	7	0	-1.244500	-0.261666	-2.416412
21	7	0	-2.253134	0.993240	-0.890405
22	7	0	-0.375499	0.090879	-1.396486
23	6	0	-3.644319	0.414540	-2.816938
24	1	0	-4.408510	-0.247445	-2.385963
25	1	0	-3.498081	0.160981	-3.866691
26	8	0	-4.018964	1.776875	-2.739885
27	6	0	0.703524	-0.792019	-1.124559
28	6	0	1.995625	-0.566790	-1.596501
29	6	0	0.454516	-1.954598	-0.386617
30	6	0	3.029616	-1.447359	-1.303105
31	6	0	1.468349	-2.848483	-0.079907
32	6	0	2.750483	-2.573518	-0.538882
33	1	0	4.030277	-1.257391	-1.669783
34	1	0	1.262620	-3.734313	0.507441
35	35	0	2.363305	0.930062	-2.667046
36	35	0	4.149994	-3.766014	-0.130486
37	35	0	-1.293596	-2.297483	0.213190
38	6	0	-0.369904	1.286672	0.782762
39	8	0	-1.292710	1.896249	1.661862
40	1	0	0.133988	0.142695	1.498611
41	6	0	0.876388	2.154563	0.575703
42	6	0	1.969318	1.940948	1.630673
43	1	0	0.547544	3.202385	0.605672
44	1	0	1.299479	1.992879	-0.420601
45	1	0	1.520921	2.011826	2.628001
46	1	0	2.364837	0.922821	1.536547
47	6	0	3.084450	2.947196	1.489182
48	6	0	3.282280	3.945918	2.443983
49	6	0	3.927554	2.916313	0.372322
50	6	0	4.298290	4.887850	2.295793
51	1	0	2.632442	3.982381	3.314419
52	6	0	4.943040	3.854942	0.220016
53	1	0	3.770559	2.161301	-0.395621
54	6	0	5.133656	4.844031	1.183759
55	1	0	4.437053	5.655331	3.051066
56	1	0	5.587789	3.816416	-0.652828
57	1	0	5.926076	5.576183	1.065594
58	6	0	-0.333907	-0.963443	3.135157
59	8	0	0.554121	-0.693736	2.233118

60	8	0	-1.320973	-0.258127	3.374605
61	1	0	-1.391421	1.275938	2.415523
62	6	0	-0.117054	-2.272330	3.856020
63	1	0	-0.730327	-2.324638	4.754289
64	1	0	-0.413318	-3.068423	3.164506
65	1	0	0.938462	-2.409541	4.094028

TS2^{C}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.380147	0.207836	0.431511
2	6	0	5.695428	0.050824	0.002732
3	6	0	6.344648	1.093101	-0.654122
4	6	0	5.654279	2.283784	-0.866597
5	6	0	4.342358	2.438900	-0.411986
6	6	0	3.686847	1.403262	0.252422
7	6	0	3.862183	-1.062634	1.071691
8	6	0	5.000131	-2.123917	0.830809
9	6	0	6.232284	-1.309228	0.369221
10	1	0	7.368601	0.978443	-0.997801
11	1	0	6.143950	3.102827	-1.384236
12	1	0	3.825698	3.381482	-0.567229
13	1	0	2.673254	1.553050	0.633704
14	1	0	5.197348	-2.669359	1.753730
15	1	0	6.729437	-1.824274	-0.458788
16	1	0	3.636445	-0.939944	2.128259
17	1	0	6.961524	-1.231227	1.182302
18	6	0	2.668303	-2.139545	-0.801488
19	6	0	1.319975	-1.180206	0.651234
20	7	0	1.499682	-2.292545	-1.326521
21	7	0	2.614720	-1.488369	0.410632
22	7	0	0.655388	-1.699236	-0.413119
23	6	0	3.996510	-2.645844	-1.254094
24	1	0	4.568091	-1.845476	-1.745379
25	1	0	3.865173	-3.472209	-1.952420
26	8	0	4.652329	-3.135702	-0.102523
27	6	0	-0.617271	-1.287497	-0.887681
28	6	0	-1.740814	-2.105857	-0.793759
29	6	0	-0.720558	-0.053730	-1.535779
30	6	0	-2.967996	-1.687643	-1.292317
31	6	0	-1.936112	0.385903	-2.043441

32	6	0	-3.045168	-0.440783	-1.903202
33	1	0	-3.843679	-2.317487	-1.200152
34	1	0	-2.015421	1.348660	-2.533812
35	35	0	-1.583164	-3.779895	0.033867
36	35	0	-4.709623	0.149074	-2.557913
37	35	0	0.823530	0.993742	-1.727580
38	6	0	0.741388	-0.389300	1.725028
39	8	0	1.716149	-0.085747	2.707774
40	1	0	0.525119	0.809331	1.327417
41	6	0	-0.492854	-1.009377	2.380732
42	6	0	-1.261896	0.026965	3.231047
43	1	0	-0.165375	-1.848341	3.007098
44	1	0	-1.164135	-1.432280	1.631371
45	1	0	-1.091906	-0.153967	4.295582
46	1	0	-0.848865	1.020637	3.012833
47	6	0	-2.746297	0.031321	2.949457
48	6	0	-3.690314	-0.113266	3.966495
49	6	0	-3.207346	0.188990	1.636465
50	6	0	-5.055802	-0.100583	3.683841
51	1	0	-3.351410	-0.238646	4.991451
52	6	0	-4.567313	0.204026	1.347239
53	1	0	-2.481653	0.314664	0.834243
54	6	0	-5.498847	0.056931	2.374425
55	1	0	-5.774133	-0.217541	4.489777
56	1	0	-4.898319	0.331105	0.320436
57	1	0	-6.561444	0.066411	2.153288
58	6	0	0.388936	5.411280	-0.062386
59	6	0	1.079287	4.118194	0.374338
60	6	0	0.220090	3.271880	1.326526
61	6	0	-1.165753	3.029613	0.710049
62	6	0	-1.853537	4.319134	0.256414
63	6	0	-0.965255	5.107583	-0.708162
64	1	0	1.294898	3.499339	-0.508392
65	1	0	2.039483	4.322563	0.864620
66	1	0	0.227220	6.052951	0.815653
67	1	0	1.026384	5.976294	-0.751819
68	1	0	-1.026149	2.364475	-0.154151
69	1	0	-1.791433	2.492275	1.431712
70	1	0	-2.820370	4.090856	-0.207249
71	1	0	-2.067085	4.944405	1.134681
72	1	0	-0.800383	4.508982	-1.616849
73	1	0	-1.462219	6.033323	-1.020245
74	1	0	0.051076	3.892196	2.234143
75	8	0	0.868542	2.095192	1.656933

76	1	0	1.691610	0.894646	2.728741

M2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.253550	-0.547092	0.702778
2	6	0	-5.425380	-0.902881	0.040779
3	6	0	-5.854674	-2.228513	0.034920
4	6	0	-5.094537	-3.187653	0.698361
5	6	0	-3.924499	-2.826566	1.371799
6	6	0	-3.501847	-1.500000	1.386176
7	6	0	-3.958847	0.932402	0.567019
8	6	0	-5.119658	1.479966	-0.353627
9	6	0	-6.088778	0.293455	-0.588888
10	1	0	-6.766838	-2.510553	-0.483083
11	1	0	-5.414044	-4.225008	0.695811
12	1	0	-3.344252	-3.584724	1.888226
13	1	0	-2.587277	-1.212733	1.895044
14	1	0	-5.623507	2.298960	0.160410
15	1	0	-6.269739	0.164950	-1.661694
16	1	0	-3.977992	1.427506	1.538265
17	1	0	-7.061167	0.492793	-0.127893
18	6	0	-2.474923	1.261860	-1.387494
19	6	0	-1.387014	1.196214	0.559746
20	7	0	-1.251991	1.346463	-1.762865
21	7	0	-2.658670	1.205558	-0.031293
22	7	0	-0.503114	1.328844	-0.552919
23	6	0	-3.702238	1.274303	-2.233896
24	1	0	-4.056372	0.244413	-2.395631
25	1	0	-3.496152	1.734268	-3.200055
26	8	0	-4.672778	2.057067	-1.567359
27	6	0	0.692248	0.567624	-0.696808
28	6	0	1.934167	1.200049	-0.808865
29	6	0	0.679697	-0.826811	-0.831541
30	6	0	3.105675	0.497031	-1.068502
31	6	0	1.829066	-1.561074	-1.084612
32	6	0	3.032405	-0.878472	-1.216927
33	1	0	4.053070	1.015580	-1.141060
34	1	0	1.785508	-2.638510	-1.185031
35	35	0	2.053626	3.061315	-0.572443
36	35	0	4.601017	-1.848330	-1.601725

37	35	0	-0.949662	-1.747529	-0.618489
38	6	0	-1.056243	1.190351	1.862937
39	8	0	-2.069457	1.128736	2.816673
40	1	0	-1.877600	0.401186	3.422691
41	6	0	0.360854	1.268528	2.331250
42	6	0	1.021515	-0.106725	2.562184
43	1	0	0.392635	1.871566	3.246301
44	1	0	0.925268	1.828202	1.580832
45	1	0	0.807199	-0.459373	3.579979
46	1	0	0.551870	-0.832367	1.885670
47	6	0	2.516385	-0.144803	2.321636
48	6	0	3.310062	1.004403	2.298289
49	6	0	3.129916	-1.379457	2.080767
50	6	0	4.672932	0.922073	2.012730
51	1	0	2.867954	1.978928	2.482764
52	6	0	4.489933	-1.467599	1.809635
53	1	0	2.521459	-2.281427	2.089898
54	6	0	5.266558	-0.310504	1.760855
55	1	0	5.269022	1.829300	1.984815
56	1	0	4.940609	-2.434597	1.609230
57	1	0	6.324981	-0.372467	1.528338

TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.318522	4.115862	0.936537
2	6	0	-0.997839	5.052517	0.150526
3	6	0	-2.155115	5.665331	0.619059
4	6	0	-2.623296	5.338647	1.891174
5	6	0	-1.930023	4.425077	2.684473
6	6	0	-0.771357	3.807235	2.215682
7	6	0	0.836999	3.517110	0.150378
8	6	0	1.044091	4.574844	-0.969876
9	6	0	-0.344054	5.213459	-1.193697
10	1	0	-2.685342	6.385441	0.002747
11	1	0	-3.527952	5.804432	2.269207
12	1	0	-2.297353	4.188268	3.677836
13	1	0	-0.243133	3.086774	2.826742
14	1	0	1.728401	5.329603	-0.576005
15	1	0	-0.921161	4.665215	-1.948704
16	1	0	1.748979	3.330717	0.722089

17	1	0	-0.269336	6.250736	-1.527965
18	6	0	0.233043	2.153785	-1.874947
19	6	0	-0.079509	1.127533	0.049338
20	7	0	-0.460063	1.119240	-2.206211
21	7	0	0.429101	2.266636	-0.517080
22	7	0	-0.700346	0.457510	-0.999083
23	6	0	0.892127	3.111574	-2.821975
24	1	0	0.142036	3.591737	-3.462280
25	1	0	1.581410	2.540164	-3.445670
26	8	0	1.669912	4.053434	-2.116241
27	6	0	-1.964329	-0.194870	-0.930757
28	6	0	-2.100900	-1.547292	-1.245622
29	6	0	-3.129087	0.524047	-0.629611
30	6	0	-3.339943	-2.175624	-1.266777
31	6	0	-4.378699	-0.078034	-0.635121
32	6	0	-4.466484	-1.425818	-0.964835
33	1	0	-3.419414	-3.228618	-1.504809
34	1	0	-5.266527	0.492639	-0.392757
35	35	0	-0.567911	-2.561863	-1.638505
36	35	0	-6.155609	-2.255491	-0.997414
37	35	0	-2.995259	2.347553	-0.175753
38	6	0	0.255008	0.562582	1.283044
39	8	0	0.818060	1.300431	2.289738
40	6	0	-0.374794	-0.728291	1.691329
41	6	0	-1.756436	-0.543747	2.350458
42	1	0	0.303618	-1.244193	2.377374
43	1	0	-0.461484	-1.361961	0.805543
44	1	0	-1.617811	-0.307062	3.411977
45	1	0	-2.246239	0.336189	1.912626
46	6	0	-2.682432	-1.731834	2.196286
47	6	0	-4.057668	-1.546403	2.382730
48	6	0	-2.228644	-3.005258	1.845755
49	6	0	-4.954280	-2.593766	2.211378
50	1	0	-4.424531	-0.557508	2.649846
51	6	0	-3.126495	-4.057594	1.663424
52	1	0	-1.168520	-3.186616	1.691767
53	6	0	-4.491042	-3.855338	1.838968
54	1	0	-6.018184	-2.421993	2.342384
55	1	0	-2.753753	-5.036559	1.377372
56	1	0	-5.191687	-4.669610	1.684228
57	1	0	1.774970	1.417231	2.124596
58	7	0	3.724874	0.925929	-0.024901
59	16	0	4.530321	0.626562	1.417001
60	8	0	5.946716	0.859994	1.212489

61	8	0	3.757669	1.428582	2.364488
62	16	0	4.044760	0.318538	-1.566637
63	8	0	2.904379	0.774660	-2.341413
64	8	0	5.396515	0.721703	-1.910260
65	6	0	3.995458	-1.452407	-1.471131
66	6	0	2.821878	-2.081133	-1.057532
67	6	0	5.129606	-2.164319	-1.846219
68	6	0	2.802170	-3.469335	-1.002512
69	1	0	1.953558	-1.491727	-0.784874
70	6	0	5.084153	-3.556055	-1.806837
71	1	0	6.019488	-1.629306	-2.160041
72	6	0	3.927339	-4.203416	-1.381418
73	1	0	1.903313	-3.979172	-0.667700
74	1	0	5.954196	-4.131420	-2.104375
75	1	0	3.899580	-5.287784	-1.343686
76	6	0	4.274542	-1.077598	1.832651
77	6	0	5.237103	-2.014180	1.469988
78	6	0	3.099544	-1.434033	2.488622
79	6	0	4.997780	-3.354887	1.755044
80	1	0	6.149898	-1.692138	0.979456
81	6	0	2.876496	-2.777442	2.768794
82	1	0	2.392665	-0.666348	2.785275
83	6	0	3.819840	-3.733505	2.396232
84	1	0	5.732007	-4.102565	1.474603
85	1	0	1.971072	-3.077283	3.287054
86	1	0	3.639764	-4.781126	2.615229
87	9	0	2.148348	0.437229	0.367345

TS3-CH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.101746	-3.217300	1.411384
2	6	0	4.358773	-3.570496	0.909216
3	6	0	5.513509	-3.314954	1.639786
4	6	0	5.398221	-2.700176	2.886097
5	6	0	4.143853	-2.365583	3.394834
6	6	0	2.983814	-2.624020	2.665069
7	6	0	2.023990	-3.533336	0.387830
8	6	0	2.753897	-4.540196	-0.543984
9	6	0	4.248909	-4.165525	-0.466937
10	1	0	6.487579	-3.588980	1.245136

11	1	0	6.290086	-2.487741	3.467118
12	1	0	4.067297	-1.899089	4.371684
13	1	0	2.008547	-2.367195	3.059956
14	1	0	2.612127	-5.534132	-0.113309
15	1	0	4.513675	-3.404125	-1.212397
16	1	0	1.102392	-3.943224	0.800906
17	1	0	4.898331	-5.028148	-0.631899
18	6	0	2.115108	-2.213119	-1.737997
19	6	0	1.392223	-1.071380	0.008074
20	7	0	2.190125	-0.986439	-2.129343
21	7	0	1.692295	-2.344394	-0.434627
22	7	0	1.747384	-0.243779	-1.045718
23	6	0	2.367063	-3.423078	-2.588028
24	1	0	3.362299	-3.358082	-3.044309
25	1	0	1.624817	-3.452583	-3.388830
26	8	0	2.200149	-4.603659	-1.835873
27	6	0	2.313803	1.052004	-0.910687
28	6	0	1.619390	2.188857	-1.330245
29	6	0	3.600149	1.200604	-0.381105
30	6	0	2.188546	3.452393	-1.214117
31	6	0	4.186533	2.452494	-0.255749
32	6	0	3.464073	3.563850	-0.675760
33	1	0	1.641711	4.330565	-1.533685
34	1	0	5.181398	2.559217	0.157767
35	35	0	-0.119427	1.985065	-1.990110
36	35	0	4.235975	5.275331	-0.491608
37	35	0	4.541097	-0.332284	0.185268
38	6	0	0.698022	-0.736138	1.155493
39	8	0	0.221086	-1.765062	1.936504
40	6	0	0.137913	0.581822	1.368485
41	6	0	-0.352116	0.927006	2.767444
42	1	0	-0.820185	0.536605	0.656807
43	1	0	0.725445	1.389626	0.929784
44	1	0	-0.684979	0.013323	3.271116
45	1	0	0.497512	1.299299	3.354977
46	6	0	-1.468711	1.951866	2.807317
47	6	0	-2.153416	2.147773	4.012337
48	6	0	-1.845046	2.714915	1.698234
49	6	0	-3.195339	3.062869	4.109196
50	1	0	-1.864171	1.564882	4.884439
51	6	0	-2.890771	3.634756	1.793046
52	1	0	-1.338205	2.598813	0.743135
53	6	0	-3.571324	3.810707	2.993725
54	1	0	-3.713395	3.193490	5.054209

55	1	0	-3.173004	4.211983	0.917448
56	1	0	-4.383947	4.527045	3.062669
57	1	0	-0.397423	-2.286333	1.385886
58	7	0	-2.323081	-1.084957	-1.572143
59	16	0	-2.690124	-2.404365	-0.602423
60	8	0	-3.430904	-3.360514	-1.406349
61	8	0	-1.393528	-2.785082	-0.038404
62	16	0	-3.433654	-0.195745	-2.489613
63	8	0	-2.694986	0.988360	-2.891689
64	8	0	-3.962466	-1.106218	-3.490313
65	6	0	-4.765924	0.314626	-1.436784
66	6	0	-4.499346	1.128562	-0.336413
67	6	0	-6.054947	-0.083262	-1.774693
68	6	0	-5.564955	1.535850	0.456364
69	1	0	-3.479525	1.407725	-0.092009
70	6	0	-7.113730	0.354636	-0.982862
71	1	0	-6.211333	-0.719228	-2.639312
72	6	0	-6.867551	1.156747	0.128008
73	1	0	-5.368805	2.146935	1.332402
74	1	0	-8.128573	0.064641	-1.233574
75	1	0	-7.696046	1.485779	0.747535
76	6	0	-3.727448	-1.868848	0.737419
77	6	0	-5.087555	-2.154843	0.664614
78	6	0	-3.174677	-1.174290	1.811062
79	6	0	-5.915363	-1.718769	1.694491
80	1	0	-5.479007	-2.704233	-0.184937
81	6	0	-4.014498	-0.746713	2.832477
82	1	0	-2.110649	-0.975072	1.846184
83	6	0	-5.380641	-1.015570	2.771380
84	1	0	-6.979181	-1.926361	1.650738
85	1	0	-3.599990	-0.189886	3.666551
86	1	0	-6.033201	-0.673166	3.568197
87	9	0	-1.671965	0.003489	-0.330929

TS3-OH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.335817	3.647032	1.036909
2	6	0	-0.154125	4.703719	0.263198
3	6	0	-1.173666	5.522498	0.736090
4	6	0	-1.702915	5.273427	2.001219

5	6	0	-1.199117	4.235216	2.784053
6	6	0	-0.172405	3.417204	2.313214
7	6	0	1.385693	2.871623	0.256223
8	6	0	1.768959	3.885542	-0.857179
9	6	0	0.512425	4.751134	-1.082289
10	1	0	-1.551669	6.338715	0.127385
11	1	0	-2.503866	5.898443	2.383296
12	1	0	-1.609616	4.061069	3.773505
13	1	0	0.221989	2.616685	2.926126
14	1	0	2.569051	4.515592	-0.458078
15	1	0	-0.157573	4.305040	-1.827651
16	1	0	2.247363	2.552017	0.843293
17	1	0	0.761403	5.759232	-1.420989
18	6	0	0.583575	1.632954	-1.772615
19	6	0	-0.025150	0.740962	0.158998
20	7	0	-0.342046	0.796702	-2.103394
21	7	0	0.814199	1.679542	-0.417024
22	7	0	-0.754259	0.221629	-0.913027
23	6	0	1.374047	2.484077	-2.720915
24	1	0	0.695788	3.102403	-3.320089
25	1	0	1.950158	1.840126	-3.383347
26	8	0	2.305968	3.272170	-2.006704
27	6	0	-2.125141	-0.158143	-0.891108
28	6	0	-2.510183	-1.474067	-1.150633
29	6	0	-3.126581	0.798115	-0.688717
30	6	0	-3.851700	-1.836897	-1.205703
31	6	0	-4.471355	0.462644	-0.733881
32	6	0	-4.814024	-0.858399	-1.001464
33	1	0	-4.134935	-2.864154	-1.397056
34	1	0	-5.234851	1.212340	-0.567647
35	35	0	-1.177543	-2.770594	-1.385211
36	35	0	-6.637384	-1.326407	-1.090741
37	35	0	-2.630197	2.578070	-0.307415
38	6	0	0.034145	0.264419	1.450016
39	8	0	1.008824	0.699232	2.263613
40	6	0	-0.928736	-0.761603	1.943766
41	6	0	-2.245961	-0.166183	2.474155
42	1	0	-0.418266	-1.348443	2.712020
43	1	0	-1.125757	-1.450679	1.116767
44	1	0	-2.113531	0.131307	3.522038
45	1	0	-2.467086	0.762150	1.933008
46	6	0	-3.443662	-1.083810	2.348015
47	6	0	-3.326368	-2.454503	2.112814
48	6	0	-4.729023	-0.534464	2.438438

49	6	0	-4.461724	-3.251983	1.959764
50	1	0	-2.345886	-2.914643	2.030278
51	6	0	-5.861178	-1.325132	2.292016
52	1	0	-4.833624	0.535339	2.609164
53	6	0	-5.730587	-2.691933	2.044642
54	1	0	-4.346661	-4.314470	1.767717
55	1	0	-6.847369	-0.874392	2.348333
56	1	0	-6.613555	-3.308536	1.909103
57	1	0	1.882352	0.484216	1.789350
58	7	0	2.520014	-0.810588	-0.814584
59	16	0	3.977774	-0.457942	-1.692238
60	8	0	4.606779	-1.713401	-2.073932
61	8	0	3.553721	0.490095	-2.706116
62	16	0	2.286056	-2.389652	-0.173105
63	8	0	1.232459	-2.235242	0.811442
64	8	0	2.103014	-3.239374	-1.335943
65	6	0	3.759732	-2.863534	0.692509
66	6	0	3.958786	-2.366710	1.979115
67	6	0	4.656485	-3.732911	0.078451
68	6	0	5.114363	-2.736681	2.658386
69	1	0	3.224923	-1.703412	2.421957
70	6	0	5.804611	-4.097813	0.775930
71	1	0	4.455508	-4.090845	-0.924745
72	6	0	6.033686	-3.595322	2.056643
73	1	0	5.294497	-2.357658	3.658501
74	1	0	6.519072	-4.774047	0.319418
75	1	0	6.932433	-3.881823	2.593423
76	6	0	5.028656	0.393396	-0.548664
77	6	0	5.961670	-0.328857	0.186014
78	6	0	4.884893	1.774386	-0.437078
79	6	0	6.772393	0.364379	1.080372
80	1	0	6.056202	-1.402307	0.052766
81	6	0	5.706375	2.448597	0.458920
82	1	0	4.152413	2.291658	-1.052790
83	6	0	6.641343	1.744205	1.218341
84	1	0	7.508833	-0.177155	1.664601
85	1	0	5.621749	3.525412	0.562475
86	1	0	7.277830	2.277827	1.916813
87	9	0	2.728330	-0.000138	0.722656

M3

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	-3.672274	-1.021221	0.533805
2	6	0	-3.889223	-1.652038	-0.697419
3	6	0	-3.622536	-3.006603	-0.856147
4	6	0	-3.162297	-3.734119	0.240614
5	6	0	-3.009656	-3.119738	1.483506
6	6	0	-3.269951	-1.758956	1.643679
7	6	0	-3.961948	0.462627	0.405262
8	6	0	-4.872595	0.500673	-0.853575
9	6	0	-4.415558	-0.689447	-1.725183
10	1	0	-3.784994	-3.491045	-1.814009
11	1	0	-2.950271	-4.792915	0.133753
12	1	0	-2.688976	-3.705424	2.338844
13	1	0	-3.146161	-1.290865	2.611377
14	1	0	-5.892416	0.323409	-0.505351
15	1	0	-3.615419	-0.411358	-2.421544
16	1	0	-4.401985	0.948496	1.273486
17	1	0	-5.237155	-1.095011	-2.318716
18	6	0	-2.523572	1.717680	-1.248485
19	6	0	-1.475475	1.146806	0.571403
20	7	0	-1.264186	1.873472	-1.526931
21	7	0	-2.701564	1.215965	0.023661
22	7	0	-0.618044	1.506638	-0.389396
23	6	0	-3.684662	2.086111	-2.122828
24	1	0	-3.583721	1.603010	-3.101056
25	1	0	-3.678591	3.168119	-2.273771
26	8	0	-4.890272	1.762810	-1.476116
27	6	0	0.741894	1.075630	-0.533255
28	6	0	1.827033	1.889880	-0.228093
29	6	0	0.948063	-0.203092	-1.061874
30	6	0	3.120537	1.431275	-0.442263
31	6	0	2.231794	-0.665277	-1.305574
32	6	0	3.303275	0.162836	-0.985948
33	1	0	3.969708	2.053856	-0.189470
34	1	0	2.395024	-1.658422	-1.704756
35	35	0	1.533572	3.569056	0.543543
36	35	0	5.047644	-0.464686	-1.271075
37	35	0	-0.536979	-1.311879	-1.410177
38	6	0	-1.149455	1.137823	2.084899
39	8	0	-2.261088	0.751507	2.800444
40	6	0	0.085631	0.366736	2.483666
41	6	0	-0.008797	-1.129464	2.171076
42	1	0	0.216749	0.559172	3.552108

43	1	0	0.929842	0.833630	1.971708
44	1	0	-0.441754	-1.652471	3.031641
45	1	0	-0.717816	-1.296430	1.351635
46	6	0	1.301605	-1.773384	1.771448
47	6	0	1.263963	-2.949409	1.014634
48	6	0	2.543529	-1.229761	2.104967
49	6	0	2.439199	-3.552224	0.578205
50	1	0	0.299874	-3.375612	0.745445
51	6	0	3.722463	-1.832990	1.670663
52	1	0	2.605164	-0.327424	2.707388
53	6	0	3.674164	-2.988994	0.897367
54	1	0	2.392932	-4.459079	-0.016683
55	1	0	4.680228	-1.388498	1.923065
56	1	0	4.592512	-3.446486	0.544157
57	1	0	-2.720594	1.549481	3.101818
58	9	0	-0.931551	2.477715	2.329495

M3-CH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.239778	0.712431	-0.475967
2	6	0	5.179903	-0.300498	-0.693374
3	6	0	5.823683	-0.404052	-1.920236
4	6	0	5.516391	0.517926	-2.919314
5	6	0	4.592328	1.538730	-2.691668
6	6	0	3.946790	1.650208	-1.461581
7	6	0	3.716333	0.627047	0.937532
8	6	0	4.808924	-0.217198	1.643316
9	6	0	5.368373	-1.143012	0.542598
10	1	0	6.563413	-1.179352	-2.092861
11	1	0	6.015477	0.451977	-3.880570
12	1	0	4.386384	2.261356	-3.474027
13	1	0	3.246947	2.457495	-1.271003
14	1	0	5.591104	0.479447	1.952367
15	1	0	4.796020	-2.075113	0.462080
16	1	0	3.522873	1.587583	1.416950
17	1	0	6.408405	-1.415113	0.732210
18	6	0	2.268131	-1.276969	1.799288
19	6	0	1.288619	0.067093	0.392893
20	7	0	1.064793	-1.757023	1.663552
21	7	0	2.447400	-0.155168	1.026838

22	7	0	0.466822	-0.904564	0.789929
23	6	0	3.371130	-1.810126	2.663314
24	1	0	3.769521	-2.733641	2.225315
25	1	0	2.970567	-2.045898	3.650712
26	8	0	4.362041	-0.826315	2.833730
27	6	0	-0.916054	-1.045891	0.478567
28	6	0	-1.856639	-0.167059	1.016088
29	6	0	-1.333162	-2.071716	-0.369145
30	6	0	-3.208198	-0.346270	0.761152
31	6	0	-2.679856	-2.250643	-0.653262
32	6	0	-3.603632	-1.387926	-0.070391
33	1	0	-3.934590	0.333886	1.187382
34	1	0	-3.000011	-3.040218	-1.321661
35	35	0	-1.318968	1.326088	2.017157
36	35	0	-5.427789	-1.593187	-0.457614
37	35	0	-0.043286	-3.152301	-1.194954
38	6	0	0.925584	1.206090	-0.452767
39	8	0	1.345214	2.407124	0.056728
40	6	0	0.200609	1.063324	-1.564519
41	6	0	-0.356314	2.259367	-2.289369
42	1	0	-0.049587	0.057418	-1.894859
43	1	0	0.441509	2.987394	-2.468118
44	1	0	-0.763865	1.958102	-3.256064
45	6	0	-1.433005	2.880466	-1.414938
46	6	0	-1.183698	4.056016	-0.700364
47	6	0	-2.662386	2.236521	-1.251108
48	6	0	-2.139299	4.567415	0.177935
49	1	0	-0.244246	4.584367	-0.850174
50	6	0	-3.624103	2.758793	-0.391995
51	1	0	-2.870110	1.321794	-1.803365
52	6	0	-3.359596	3.917732	0.336163
53	1	0	-1.932702	5.480991	0.725796
54	1	0	-4.584856	2.260601	-0.295216
55	1	0	-4.106690	4.319195	1.012383
56	1	0	0.571003	2.870758	0.423144

TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.706689	-1.009782	0.554826
2	6	0	-3.875702	-1.693999	-0.655405

3	6	0	-3.589832	-3.051009	-0.745014
4	6	0	-3.155412	-3.722785	0.397312
5	6	0	-3.046598	-3.053328	1.616125
6	6	0	-3.327127	-1.689723	1.709224
7	6	0	-4.000395	0.462812	0.347945
8	6	0	-4.876635	0.440024	-0.932350
9	6	0	-4.378718	-0.779318	-1.739840
10	1	0	-3.717423	-3.580579	-1.684161
11	1	0	-2.929738	-4.782812	0.344869
12	1	0	-2.746270	-3.598483	2.505053
13	1	0	-3.247230	-1.176263	2.659743
14	1	0	-5.904248	0.265169	-0.606975
15	1	0	-3.558025	-0.519670	-2.420407
16	1	0	-4.437643	0.997746	1.188197
17	1	0	-5.174516	-1.218661	-2.344250
18	6	0	-2.527853	1.666867	-1.321980
19	6	0	-1.511116	1.078802	0.501436
20	7	0	-1.257486	1.804080	-1.582896
21	7	0	-2.727600	1.177468	-0.055576
22	7	0	-0.633708	1.427612	-0.441225
23	6	0	-3.673770	2.005817	-2.226447
24	1	0	-3.543288	1.502770	-3.191286
25	1	0	-3.678410	3.084440	-2.400711
26	8	0	-4.890158	1.678861	-1.602411
27	6	0	0.734640	1.017703	-0.554794
28	6	0	1.794180	1.857486	-0.229844
29	6	0	0.974132	-0.254803	-1.080664
30	6	0	3.099835	1.436687	-0.443441
31	6	0	2.271178	-0.680708	-1.320781
32	6	0	3.318003	0.178958	-1.000546
33	1	0	3.931754	2.078203	-0.180504
34	1	0	2.463021	-1.668371	-1.721199
35	35	0	1.435135	3.502911	0.582770
36	35	0	5.079307	-0.390275	-1.297537
37	35	0	-0.484031	-1.403018	-1.409295
38	6	0	-1.270531	0.943737	1.994345
39	8	0	-2.343031	0.904839	2.710209
40	6	0	0.022929	0.386281	2.476019
41	6	0	0.025937	-1.134820	2.200513
42	1	0	0.089222	0.613483	3.541277
43	1	0	0.845143	0.889275	1.965864
44	1	0	-0.365118	-1.649104	3.085092
45	1	0	-0.679801	-1.376867	1.395041
46	6	0	1.373034	-1.700584	1.809195

47	6	0	1.402289	-2.897633	1.086086
48	6	0	2.579732	-1.079289	2.133624
49	6	0	2.611746	-3.451266	0.679852
50	1	0	0.465309	-3.385008	0.826239
51	6	0	3.792747	-1.634234	1.729719
52	1	0	2.588458	-0.158713	2.711298
53	6	0	3.812297	-2.815958	0.994860
54	1	0	2.618159	-4.377013	0.113228
55	1	0	4.723461	-1.133440	1.977473
56	1	0	4.756786	-3.237074	0.666556
57	1	0	-2.065027	2.100622	2.829605
58	9	0	-1.170636	2.667157	2.321974

TS4[A]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.000855	-2.163663	0.425286
2	6	0	-2.801826	-2.962996	-0.708916
3	6	0	-2.223303	-4.220071	-0.587130
4	6	0	-1.901482	-4.689444	0.687456
5	6	0	-2.182554	-3.926314	1.820539
6	6	0	-2.730780	-2.649403	1.700598
7	6	0	-3.612291	-0.847708	0.001707
8	6	0	-4.314825	-1.256800	-1.316739
9	6	0	-3.362496	-2.302310	-1.943416
10	1	0	-2.058662	-4.841548	-1.462091
11	1	0	-1.461951	-5.675068	0.800845
12	1	0	-1.967966	-4.326627	2.805874
13	1	0	-2.931137	-2.048635	2.579950
14	1	0	-5.249301	-1.746412	-1.034591
15	1	0	-2.562583	-1.831648	-2.529374
16	1	0	-4.269693	-0.357435	0.718464
17	1	0	-3.889724	-2.994733	-2.602053
18	6	0	-2.470473	0.640977	-1.699825
19	6	0	-1.365612	0.421697	0.163436
20	7	0	-1.306289	1.171108	-1.936131
21	7	0	-2.544286	0.138638	-0.418159
22	7	0	-0.634253	1.032413	-0.770205
23	6	0	-3.596777	0.529368	-2.681715
24	1	0	-3.225922	0.038905	-3.590165
25	1	0	-3.944304	1.529474	-2.950900

26	8	0	-4.682747	-0.154355	-2.109240
27	6	0	0.791348	1.080402	-0.781660
28	6	0	1.512300	2.233618	-0.495377
29	6	0	1.452062	-0.113650	-1.091228
30	6	0	2.899787	2.167164	-0.416186
31	6	0	2.831707	-0.195354	-1.017229
32	6	0	3.534419	0.950782	-0.651245
33	1	0	3.474518	3.051776	-0.171440
34	1	0	3.344357	-1.133314	-1.201257
35	35	0	0.623019	3.858950	-0.244939
36	35	0	5.400823	0.844761	-0.483257
37	35	0	0.437466	-1.620711	-1.599912
38	6	0	-1.063060	0.284786	1.670115
39	8	0	-2.083053	0.154590	2.379259
40	6	0	0.279547	-0.234858	2.112149
41	6	0	0.470088	-1.744725	1.884073
42	1	0	0.351837	0.027462	3.170159
43	1	0	1.053072	0.325434	1.585995
44	1	0	0.091861	-2.293256	2.753241
45	1	0	-0.135766	-2.084043	1.037147
46	6	0	1.914327	-2.112021	1.608382
47	6	0	2.199106	-3.201559	0.780383
48	6	0	2.979799	-1.372031	2.128837
49	6	0	3.513377	-3.522167	0.450526
50	1	0	1.377673	-3.784400	0.370327
51	6	0	4.296186	-1.689711	1.802407
52	1	0	2.787399	-0.528997	2.787129
53	6	0	4.566441	-2.758446	0.951206
54	1	0	3.715882	-4.365169	-0.202623
55	1	0	5.109155	-1.093119	2.203196
56	1	0	5.590850	-2.998793	0.685804
57	1	0	-3.121495	1.072761	2.158642
58	9	0	-0.610394	2.011773	1.788995
59	6	0	-3.654586	2.901421	1.525438
60	8	0	-3.931628	1.732421	1.971052
61	8	0	-2.486604	3.310789	1.284164
62	1	0	-1.587120	2.688849	1.569481
63	6	0	-4.800628	3.826355	1.302383
64	1	0	-5.001265	4.335847	2.250147
65	1	0	-4.539292	4.573164	0.555112
66	1	0	-5.690312	3.265857	1.019867

M4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.978211	0.644647	0.824732
2	6	0	4.202711	1.473044	-0.282295
3	6	0	4.170597	2.854202	-0.139550
4	6	0	3.929308	3.393712	1.123829
5	6	0	3.751653	2.566176	2.232981
6	6	0	3.778013	1.178463	2.095251
7	6	0	4.050998	-0.799635	0.384391
8	6	0	4.917932	-0.695430	-0.894190
9	6	0	4.501275	0.657256	-1.515790
10	1	0	4.349822	3.502960	-0.991182
11	1	0	3.907764	4.470917	1.251338
12	1	0	3.606165	3.004767	3.214482
13	1	0	3.663232	0.536308	2.961880
14	1	0	5.959573	-0.639423	-0.572121
15	1	0	3.595441	0.560034	-2.129691
16	1	0	4.407823	-1.520339	1.119480
17	1	0	5.284264	1.083040	-2.145459
18	6	0	2.470888	-1.742422	-1.365102
19	6	0	1.510907	-1.043678	0.456967
20	7	0	1.192038	-1.823648	-1.604251
21	7	0	2.707125	-1.258708	-0.104059
22	7	0	0.608526	-1.374566	-0.465396
23	6	0	3.583664	-2.039174	-2.324206
24	1	0	3.455725	-1.410009	-3.214161
25	1	0	3.533187	-3.085204	-2.633484
26	8	0	4.830796	-1.842073	-1.706303
27	6	0	-0.786545	-1.069672	-0.489578
28	6	0	-1.719491	-1.824793	0.216081
29	6	0	-1.204408	0.015758	-1.263247
30	6	0	-3.068703	-1.508321	0.145184
31	6	0	-2.550627	0.332037	-1.362776
32	6	0	-3.466325	-0.440598	-0.655702
33	1	0	-3.796264	-2.083344	0.704475
34	1	0	-2.873263	1.183243	-1.949243
35	35	0	-1.129065	-3.211132	1.331386
36	35	0	-5.286944	-0.002646	-0.746695
37	35	0	0.077252	1.094799	-2.112883
38	6	0	1.322168	-0.743815	1.945313
39	8	0	2.115824	-1.292896	2.664753
40	6	0	0.197216	0.147453	2.368054

41	6	0	0.174442	1.480133	1.599777
42	1	0	0.280325	0.277662	3.448550
43	1	0	-0.724251	-0.417155	2.183222
44	1	0	0.752277	2.221069	2.162109
45	1	0	0.706312	1.376456	0.642131
46	6	0	-1.211608	2.015579	1.299314
47	6	0	-1.338884	3.025688	0.338743
48	6	0	-2.365409	1.538584	1.923074
49	6	0	-2.589892	3.515603	-0.018688
50	1	0	-0.447196	3.413777	-0.146585
51	6	0	-3.620830	2.034986	1.572985
52	1	0	-2.304049	0.780538	2.698825
53	6	0	-3.739058	3.012227	0.590807
54	1	0	-2.670084	4.290905	-0.774128
55	1	0	-4.508491	1.643651	2.059967
56	1	0	-4.717793	3.384562	0.306484

M04[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.867673	4.195177	-0.553223
2	6	0	1.821059	5.070036	-1.072154
3	6	0	1.543713	6.430585	-1.141680
4	6	0	0.301997	6.888078	-0.699957
5	6	0	-0.651467	6.000756	-0.197722
6	6	0	-0.374549	4.636704	-0.116373
7	6	0	1.405186	2.781374	-0.587165
8	6	0	2.579368	2.848437	-1.612108
9	6	0	3.056703	4.309261	-1.492953
10	1	0	2.274378	7.124800	-1.545735
11	1	0	0.069392	7.946671	-0.757500
12	1	0	-1.615356	6.375861	0.130105
13	1	0	-1.113642	3.932424	0.257104
14	1	0	3.356596	2.124407	-1.365011
15	1	0	3.488733	4.648638	-2.437413
16	1	0	1.778260	2.444308	0.382770
17	1	0	3.831433	4.376360	-0.720376
18	6	0	0.057629	1.779320	-2.366558
19	6	0	-0.397173	0.977594	-0.392579
20	7	0	-0.899181	0.923513	-2.576248
21	7	0	0.378279	1.846680	-1.043062

22	7	0	-1.167898	0.426877	-1.338983
23	6	0	0.845332	2.629640	-3.307776
24	1	0	0.470425	3.662381	-3.269133
25	1	0	0.739720	2.247256	-4.323264
26	8	0	2.203983	2.534285	-2.953590
27	6	0	-2.229326	-0.503627	-1.172228
28	6	0	-2.186506	-1.751663	-1.802280
29	6	0	-3.342445	-0.151841	-0.402860
30	6	0	-3.215782	-2.663325	-1.593719
31	6	0	-4.369020	-1.059300	-0.180895
32	6	0	-4.280394	-2.313390	-0.773273
33	1	0	-3.177815	-3.634673	-2.070008
34	1	0	-5.216516	-0.785657	0.435410
35	35	0	-0.797275	-2.209274	-2.961188
36	35	0	-5.656303	-3.565447	-0.481705
37	35	0	-3.483668	1.566985	0.345658
38	6	0	-0.430601	0.899212	1.135545
39	8	0	-0.184706	1.945256	1.687610
40	6	0	-0.727914	-0.383982	1.855607
41	6	0	-1.155026	-0.140406	3.306805
42	1	0	0.210516	-0.947163	1.808278
43	1	0	-1.455381	-0.985468	1.302345
44	1	0	-1.128707	-1.104492	3.823809
45	1	0	-0.418024	0.509627	3.786119
46	6	0	-2.533975	0.462558	3.423223
47	6	0	-2.706340	1.824026	3.678881
48	6	0	-3.665777	-0.334182	3.226796
49	6	0	-3.983144	2.380089	3.727624
50	1	0	-1.830439	2.450009	3.824825
51	6	0	-4.942928	0.217273	3.279591
52	1	0	-3.542515	-1.398469	3.034300
53	6	0	-5.104377	1.579401	3.525502
54	1	0	-4.101967	3.440687	3.926894
55	1	0	-5.812837	-0.417233	3.134557
56	1	0	-6.098881	2.012058	3.566909
57	7	0	2.241519	-0.154854	0.542445
58	16	0	3.751820	0.384540	0.773598
59	8	0	4.585950	0.335891	-0.434471
60	8	0	3.627885	1.673792	1.461954
61	16	0	1.913999	-1.206260	-0.648420
62	8	0	0.615595	-1.793062	-0.274598
63	8	0	1.992703	-0.588698	-1.976866
64	6	0	3.111474	-2.522957	-0.572909
65	6	0	2.985916	-3.460979	0.449472

66	6	0	4.168761	-2.553908	-1.474150
67	6	0	3.946759	-4.457595	0.568185
68	1	0	2.146123	-3.401612	1.134345
69	6	0	5.119957	-3.565182	-1.351332
70	1	0	4.236783	-1.789892	-2.240422
71	6	0	5.009988	-4.509499	-0.333162
72	1	0	3.867972	-5.192096	1.362799
73	1	0	5.950085	-3.610520	-2.048523
74	1	0	5.758447	-5.290051	-0.238438
75	6	0	4.464700	-0.775608	1.928497
76	6	0	5.590760	-1.500317	1.562192
77	6	0	3.837946	-0.966654	3.158418
78	6	0	6.099978	-2.446143	2.450661
79	1	0	6.036612	-1.334218	0.587480
80	6	0	4.356018	-1.909670	4.037469
81	1	0	2.955268	-0.386478	3.410705
82	6	0	5.484861	-2.650478	3.681745
83	1	0	6.972850	-3.028211	2.172994
84	1	0	3.881557	-2.069790	5.000123
85	1	0	5.882920	-3.389328	4.370019

M04[b]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.084735	1.081387	-0.530850
2	6	0	5.432106	0.834799	-0.786200
3	6	0	6.139816	1.676518	-1.638179
4	6	0	5.473919	2.748973	-2.230304
5	6	0	4.118710	2.977251	-1.980874
6	6	0	3.407962	2.141668	-1.121620
7	6	0	3.535757	0.047573	0.424000
8	6	0	4.604576	-1.089434	0.424504
9	6	0	5.902049	-0.393051	-0.041414
10	1	0	7.189550	1.495323	-1.849279
11	1	0	6.012913	3.408512	-2.903024
12	1	0	3.616740	3.809810	-2.462615
13	1	0	2.348076	2.292856	-0.931830
14	1	0	4.675680	-1.516529	1.425609
15	1	0	6.499642	-1.075187	-0.652602
16	1	0	3.375328	0.417368	1.435904
17	1	0	6.508226	-0.111707	0.826621

18	6	0	2.213795	-1.328219	-1.123032
19	6	0	1.004337	-0.247915	0.324241
20	7	0	0.990437	-1.580203	-1.478196
21	7	0	2.259633	-0.473634	-0.057235
22	7	0	0.242599	-0.869163	-0.583329
23	6	0	3.522874	-1.884318	-1.582955
24	1	0	4.048334	-1.167621	-2.227885
25	1	0	3.363131	-2.813581	-2.129534
26	8	0	4.258534	-2.191512	-0.413126
27	6	0	-1.172510	-0.860554	-0.678530
28	6	0	-1.910604	-2.041567	-0.540568
29	6	0	-1.842754	0.342166	-0.924271
30	6	0	-3.299618	-2.007135	-0.612403
31	6	0	-3.227819	0.386832	-0.995368
32	6	0	-3.938880	-0.793513	-0.827583
33	1	0	-3.867578	-2.921260	-0.494419
34	1	0	-3.733186	1.327962	-1.169532
35	35	0	-1.071719	-3.685954	-0.260668
36	35	0	-5.820238	-0.739926	-0.888967
37	35	0	-0.894831	1.951461	-1.126218
38	6	0	0.649878	0.719881	1.443781
39	8	0	1.329349	1.718189	1.496723
40	6	0	-0.488527	0.398042	2.366776
41	6	0	-0.982135	1.639153	3.114213
42	1	0	-0.085256	-0.360841	3.044453
43	1	0	-1.294411	-0.095059	1.812146
44	1	0	-1.687674	1.308217	3.882547
45	1	0	-0.134173	2.101388	3.626412
46	6	0	-1.648134	2.648301	2.208608
47	6	0	-0.985442	3.815579	1.822011
48	6	0	-2.935719	2.415620	1.717014
49	6	0	-1.592153	4.727148	0.961744
50	1	0	0.020089	3.996649	2.190118
51	6	0	-3.548832	3.328833	0.862275
52	1	0	-3.468021	1.513362	2.013888
53	6	0	-2.875699	4.486340	0.477882
54	1	0	-1.061616	5.628782	0.671322
55	1	0	-4.556837	3.139003	0.503040
56	1	0	-3.350858	5.198539	-0.189273
57	6	0	1.869386	-2.087743	2.435872
58	8	0	2.363164	-0.977960	2.768740
59	8	0	0.800635	-2.240111	1.788263
60	6	0	2.665692	-3.349700	2.773046
61	1	0	1.995221	-4.181594	2.995128

62	1	0	3.252852	-3.621981	1.888225
63	1	0	3.348688	-3.173098	3.605080

M04[c]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.841973	1.331534	0.303170
2	6	0	-4.944365	0.677949	-0.263532
3	6	0	-6.028914	0.321482	0.525650
4	6	0	-5.998958	0.623373	1.886292
5	6	0	-4.908333	1.287749	2.446473
6	6	0	-3.823035	1.662509	1.655188
7	6	0	-2.899362	1.773390	-0.789836
8	6	0	-3.833570	1.741722	-2.030823
9	6	0	-4.785707	0.561079	-1.756316
10	1	0	-6.890856	-0.171004	0.086670
11	1	0	-6.842443	0.353844	2.513745
12	1	0	-4.914387	1.540772	3.501583
13	1	0	-3.000275	2.223065	2.085500
14	1	0	-4.411389	2.668105	-1.997802
15	1	0	-4.329893	-0.404803	-2.010839
16	1	0	-2.445151	2.751426	-0.618995
17	1	0	-5.721562	0.651344	-2.310341
18	6	0	-1.425467	0.430169	-2.362827
19	6	0	-0.730099	0.478107	-0.309379
20	7	0	-0.263602	-0.155788	-2.388744
21	7	0	-1.746124	0.853987	-1.091288
22	7	0	0.156605	-0.128230	-1.096615
23	6	0	-2.351921	0.647556	-3.516857
24	1	0	-2.943042	-0.261746	-3.686027
25	1	0	-1.766085	0.851454	-4.413891
26	8	0	-3.160229	1.769494	-3.265853
27	6	0	1.546394	-0.328666	-0.822653
28	6	0	2.389292	0.784788	-0.818478
29	6	0	2.084799	-1.599242	-0.648712
30	6	0	3.753689	0.652261	-0.633334
31	6	0	3.448699	-1.756434	-0.445451
32	6	0	4.264410	-0.629355	-0.443066
33	1	0	4.396366	1.522535	-0.596990
34	1	0	3.869196	-2.743214	-0.297533
35	35	0	1.655948	2.504753	-1.067040

36	35	0	6.104787	-0.843337	-0.159661
37	35	0	0.966735	-3.101442	-0.680030
38	6	0	-0.635284	0.657036	1.195696
39	8	0	-0.753871	1.793058	1.600415
40	6	0	-0.489086	-0.575250	2.037044
41	6	0	-1.841922	-1.078129	2.581065
42	1	0	0.162254	-0.285562	2.862411
43	1	0	0.022544	-1.360866	1.471276
44	1	0	-1.602751	-1.791752	3.376638
45	1	0	-2.355163	-0.241903	3.070190
46	6	0	-2.793841	-1.744588	1.607413
47	6	0	-2.447990	-2.100778	0.302648
48	6	0	-4.075250	-2.074404	2.059984
49	6	0	-3.359309	-2.740871	-0.537305
50	1	0	-1.444637	-1.931136	-0.069113
51	6	0	-4.983400	-2.724566	1.232726
52	1	0	-4.362393	-1.812952	3.075477
53	6	0	-4.633979	-3.051791	-0.076762
54	1	0	-3.056296	-3.015990	-1.543905
55	1	0	-5.972185	-2.968693	1.608626
56	1	0	-5.343467	-3.558072	-0.722968
57	6	0	3.194451	1.204297	2.252079
58	8	0	1.985649	0.817400	2.181717
59	8	0	3.566903	2.367618	1.947675
60	6	0	4.231343	0.219324	2.764165
61	1	0	5.214031	0.440006	2.346574
62	1	0	4.292680	0.318328	3.852239
63	1	0	3.937412	-0.806222	2.532250
64	11	0	1.402037	2.960188	1.870923

M04[d]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.806276	1.583129	0.306185
2	6	0	-5.013915	1.206429	-0.296750
3	6	0	-6.168513	1.083835	0.462934
4	6	0	-6.104416	1.345971	1.830530
5	6	0	-4.907183	1.740374	2.426574
6	6	0	-3.746732	1.876149	1.665641
7	6	0	-2.763207	1.827284	-0.759180
8	6	0	-3.655092	2.040493	-2.012392

9	6	0	-4.851335	1.092906	-1.789138
10	1	0	-7.107949	0.804645	-0.003961
11	1	0	-7.001368	1.260130	2.435660
12	1	0	-4.882438	1.969200	3.486892
13	1	0	-2.829206	2.228378	2.123809
14	1	0	-4.013418	3.070858	-1.958421
15	1	0	-4.613655	0.056225	-2.061780
16	1	0	-2.105055	2.672475	-0.547779
17	1	0	-5.731146	1.400368	-2.356635
18	6	0	-1.621021	0.212231	-2.353869
19	6	0	-0.947972	0.062431	-0.296713
20	7	0	-0.633631	-0.635047	-2.384442
21	7	0	-1.841931	0.679466	-1.076714
22	7	0	-0.227439	-0.727692	-1.091184
23	6	0	-2.444624	0.675464	-3.513940
24	1	0	-3.231568	-0.060128	-3.721843
25	1	0	-1.806858	0.758417	-4.394844
26	8	0	-2.965659	1.950499	-3.235184
27	6	0	1.056686	-1.297377	-0.818773
28	6	0	2.166413	-0.451686	-0.780240
29	6	0	1.231921	-2.671250	-0.686561
30	6	0	3.442700	-0.955578	-0.596888
31	6	0	2.500505	-3.197983	-0.488469
32	6	0	3.588287	-2.331998	-0.448907
33	1	0	4.295564	-0.292266	-0.524915
34	1	0	2.637836	-4.265468	-0.371472
35	35	0	1.933418	1.410775	-0.935886
36	35	0	5.302695	-3.040710	-0.173725
37	35	0	-0.250954	-3.813178	-0.763229
38	6	0	-0.854194	0.189465	1.214323
39	8	0	-0.749706	1.316473	1.645925
40	6	0	-1.003885	-1.061099	2.029276
41	6	0	-2.440283	-1.240320	2.563043
42	1	0	-0.307315	-0.946214	2.860697
43	1	0	-0.686609	-1.934095	1.449409
44	1	0	-2.379803	-1.997711	3.351673
45	1	0	-2.747827	-0.311402	3.058197
46	6	0	-3.515480	-1.655503	1.578419
47	6	0	-3.258576	-2.039299	0.261943
48	6	0	-4.837770	-1.711016	2.031641
49	6	0	-4.287770	-2.445619	-0.587930
50	1	0	-2.243305	-2.079323	-0.111986
51	6	0	-5.866440	-2.125734	1.194287
52	1	0	-5.059651	-1.423842	3.056605

53	6	0	-5.598680	-2.485665	-0.125639
54	1	0	-4.052859	-2.751105	-1.604033
55	1	0	-6.884022	-2.160302	1.570863
56	1	0	-6.402301	-2.809190	-0.778953
57	6	0	2.989572	-0.162067	2.252104
58	8	0	1.724495	-0.247975	2.177878
59	8	0	3.630446	0.886701	1.979662
60	6	0	3.763013	-1.380128	2.728684
61	1	0	4.757357	-1.408537	2.280385
62	1	0	3.883949	-1.307942	3.813966
63	1	0	3.215821	-2.297695	2.505235
64	11	0	1.648298	1.988465	1.921907
65	6	0	4.155080	4.378900	-0.524875
66	6	0	3.741381	4.023410	0.891349
67	6	0	1.679678	5.123278	0.530134
68	6	0	2.119525	5.442224	-0.888295
69	1	0	3.888114	3.553087	-1.202634
70	1	0	4.078594	4.800964	1.589684
71	1	0	0.600365	4.955294	0.586846
72	1	0	1.687167	6.386704	-1.226492
73	8	0	3.523457	5.573925	-0.947762
74	8	0	2.311088	3.922576	0.970097
75	1	0	1.784862	4.637107	-1.565251
76	1	0	1.954937	5.947721	1.201288
77	1	0	4.136443	3.050607	1.197138
78	1	0	5.233148	4.544294	-0.578552

TS5[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.825878	4.403735	0.154199
2	6	0	-1.862790	5.707044	-0.334114
3	6	0	-2.860373	6.577548	0.096434
4	6	0	-3.809740	6.116266	1.005725
5	6	0	-3.769259	4.803331	1.481016
6	6	0	-2.769732	3.930183	1.059338
7	6	0	-0.667619	3.642610	-0.446717
8	6	0	-0.161089	4.549942	-1.621290
9	6	0	-0.735127	5.951288	-1.307734
10	1	0	-2.904686	7.596344	-0.276503
11	1	0	-4.595927	6.783757	1.344516

12	1	0	-4.522161	4.462385	2.184060
13	1	0	-2.722274	2.903722	1.414025
14	1	0	0.927628	4.532105	-1.648643
15	1	0	-1.055811	6.437853	-2.233592
16	1	0	0.126201	3.438542	0.270487
17	1	0	0.037156	6.583666	-0.857153
18	6	0	-1.773189	2.262353	-2.161844
19	6	0	-1.071795	1.126428	-0.439424
20	7	0	-2.143629	1.040485	-2.410843
21	7	0	-1.123042	2.351553	-0.964220
22	7	0	-1.707049	0.347871	-1.320157
23	6	0	-1.832664	3.503635	-2.989466
24	1	0	-2.622661	4.174089	-2.623365
25	1	0	-2.026399	3.252412	-4.031911
26	8	0	-0.551216	4.092104	-2.910583
27	6	0	-1.989684	-1.040342	-1.199717
28	6	0	-1.295796	-1.953673	-1.993824
29	6	0	-2.892220	-1.493058	-0.236162
30	6	0	-1.533410	-3.316566	-1.862184
31	6	0	-3.141904	-2.850192	-0.096007
32	6	0	-2.463130	-3.741089	-0.920351
33	1	0	-0.978941	-4.026525	-2.462759
34	1	0	-3.827238	-3.203663	0.664014
35	35	0	0.044498	-1.342925	-3.143953
36	35	0	-2.774871	-5.584892	-0.699893
37	35	0	-3.657370	-0.291836	0.986610
38	6	0	-0.504394	0.783675	0.925802
39	8	0	-0.522362	1.719700	1.739471
40	6	0	0.061283	-0.499792	1.071554
41	6	0	0.330741	-0.980444	2.484213
42	1	0	1.221004	-0.322544	0.248160
43	1	0	-0.294271	-1.278433	0.401870
44	1	0	0.953569	-1.879953	2.437905
45	1	0	0.875312	-0.216082	3.049116
46	6	0	-0.985014	-1.294851	3.163284
47	6	0	-1.639875	-0.329955	3.933068
48	6	0	-1.617396	-2.522999	2.944866
49	6	0	-2.895590	-0.589094	4.477266
50	1	0	-1.164864	0.635455	4.079885
51	6	0	-2.871154	-2.785014	3.491306
52	1	0	-1.122261	-3.277787	2.335943
53	6	0	-3.515635	-1.817266	4.259245
54	1	0	-3.390973	0.170735	5.074431
55	1	0	-3.342317	-3.749691	3.322472

56	1	0	-4.492154	-2.020279	4.687673
57	7	0	2.165574	-0.311593	-0.589579
58	16	0	2.848944	1.148198	-0.880929
59	8	0	3.800200	1.085659	-1.979428
60	8	0	1.712116	2.071953	-0.938525
61	16	0	2.873317	-1.771025	-0.886380
62	8	0	1.932953	-2.718785	-0.293933
63	8	0	3.261563	-1.915451	-2.279635
64	6	0	4.357535	-1.745184	0.093130
65	6	0	4.236559	-1.672014	1.480229
66	6	0	5.593253	-1.728145	-0.540387
67	6	0	5.389736	-1.590940	2.248772
68	1	0	3.252820	-1.668286	1.941587
69	6	0	6.744236	-1.653657	0.243700
70	1	0	5.636622	-1.768091	-1.623346
71	6	0	6.641075	-1.586370	1.629698
72	1	0	5.314965	-1.524912	3.329065
73	1	0	7.719468	-1.645525	-0.231686
74	1	0	7.539993	-1.524526	2.235073
75	6	0	3.747944	1.529247	0.609175
76	6	0	5.136367	1.540794	0.582434
77	6	0	3.025938	1.738741	1.782986
78	6	0	5.824174	1.768165	1.772631
79	1	0	5.655908	1.366666	-0.353673
80	6	0	3.726295	1.951555	2.964864
81	1	0	1.936940	1.732897	1.769631
82	6	0	5.122044	1.967065	2.957944
83	1	0	6.909199	1.778205	1.771964
84	1	0	3.183386	2.115353	3.889925
85	1	0	5.662270	2.137771	3.883721

TS5[b]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.296775	1.039067	-0.230897
2	6	0	5.625979	0.721743	-0.500492
3	6	0	6.472534	1.686541	-1.038374
4	6	0	5.961904	2.955406	-1.305228
5	6	0	4.625138	3.261411	-1.037443
6	6	0	3.775782	2.301531	-0.491489
7	6	0	3.575292	-0.155965	0.345507

8	6	0	4.542430	-1.363551	0.092433
9	6	0	5.925659	-0.709763	-0.126139
10	1	0	7.510714	1.453420	-1.255726
11	1	0	6.609987	3.714766	-1.731204
12	1	0	4.247155	4.254935	-1.255265
13	1	0	2.733519	2.518023	-0.272439
14	1	0	4.509958	-2.032876	0.951079
15	1	0	6.480389	-1.256414	-0.894100
16	1	0	3.352438	-0.055669	1.408019
17	1	0	6.514157	-0.753071	0.796769
18	6	0	2.230736	-1.028430	-1.528159
19	6	0	1.056388	-0.168372	0.090055
20	7	0	0.996507	-1.205143	-1.900987
21	7	0	2.301304	-0.381242	-0.329386
22	7	0	0.277943	-0.649352	-0.879172
23	6	0	3.518946	-1.538705	-2.083180
24	1	0	4.115556	-0.715458	-2.498929
25	1	0	3.331897	-2.280805	-2.858598
26	8	0	4.169873	-2.185928	-1.008523
27	6	0	-1.140418	-0.629584	-0.938696
28	6	0	-1.848162	-1.815853	-0.744015
29	6	0	-1.826029	0.568897	-1.127458
30	6	0	-3.235187	-1.822127	-0.792327
31	6	0	-3.212981	0.579645	-1.185188
32	6	0	-3.895841	-0.619653	-1.025465
33	1	0	-3.786826	-2.738773	-0.627348
34	1	0	-3.743966	1.513368	-1.318952
35	35	0	-0.902987	-3.369145	-0.284707
36	35	0	-5.777981	-0.599400	-1.059862
37	35	0	-0.886429	2.188307	-1.166572
38	6	0	0.685412	0.580558	1.359003
39	8	0	1.481025	1.463931	1.667650
40	6	0	-0.455910	0.116826	2.086422
41	6	0	-1.028335	1.125338	3.074980
42	1	0	0.011948	-0.958049	2.701889
43	1	0	-1.213132	-0.364338	1.465538
44	1	0	-1.745491	0.618761	3.728743
45	1	0	-0.220875	1.506071	3.706595
46	6	0	-1.701100	2.271504	2.352406
47	6	0	-1.039857	3.486121	2.150453
48	6	0	-2.977193	2.107883	1.804061
49	6	0	-1.642079	4.513060	1.426378
50	1	0	-0.040895	3.614391	2.557062
51	6	0	-3.583897	3.133529	1.083770

52	1	0	-3.501609	1.164309	1.947372
53	6	0	-2.915859	4.340879	0.890003
54	1	0	-1.114879	5.451483	1.281439
55	1	0	-4.582958	2.991332	0.679725
56	1	0	-3.387340	5.142608	0.330344
57	6	0	1.214637	-2.684430	2.550863
58	8	0	1.929857	-2.104158	1.714297
59	8	0	0.283284	-2.131809	3.232313
60	6	0	1.407483	-4.176404	2.774649
61	1	0	0.875839	-4.515549	3.666229
62	1	0	1.012617	-4.706004	1.897271
63	1	0	2.474595	-4.406843	2.846802

TS5[c]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.270406	1.037040	-0.432672
2	6	0	-5.145858	1.070539	0.657878
3	6	0	-5.466531	2.282568	1.256850
4	6	0	-4.903921	3.452673	0.748497
5	6	0	-4.049063	3.416735	-0.354205
6	6	0	-3.727601	2.204554	-0.962561
7	6	0	-4.099420	-0.386587	-0.901508
8	6	0	-5.349251	-1.083148	-0.307720
9	6	0	-5.642411	-0.312874	0.998328
10	1	0	-6.151120	2.320081	2.098219
11	1	0	-5.147897	4.406283	1.205024
12	1	0	-3.644634	4.341633	-0.752207
13	1	0	-3.084073	2.176401	-1.836451
14	1	0	-6.167223	-0.914905	-1.011168
15	1	0	-5.081450	-0.722157	1.848086
16	1	0	-3.991439	-0.514930	-1.979698
17	1	0	-6.701348	-0.345784	1.260947
18	6	0	-2.948836	-2.207428	0.453911
19	6	0	-1.644464	-0.628622	-0.280341
20	7	0	-1.762218	-2.526380	0.886669
21	7	0	-2.914646	-1.040107	-0.270651
22	7	0	-0.963534	-1.526101	0.425452
23	6	0	-4.238400	-2.935874	0.686062
24	1	0	-4.547273	-2.806744	1.730693
25	1	0	-4.089891	-4.001390	0.503541

26	8	0	-5.215986	-2.484184	-0.219291
27	6	0	0.451258	-1.596954	0.587301
28	6	0	1.226817	-2.208743	-0.393605
29	6	0	1.068496	-1.032807	1.701998
30	6	0	2.602650	-2.293298	-0.265507
31	6	0	2.448566	-1.073563	1.834790
32	6	0	3.195452	-1.711329	0.848959
33	1	0	3.204880	-2.759540	-1.035350
34	1	0	2.931666	-0.615574	2.688815
35	35	0	0.404195	-2.798535	-1.981823
36	35	0	5.066652	-1.736190	0.996405
37	35	0	0.028879	-0.173539	3.004910
38	6	0	-1.102907	0.570082	-1.035926
39	8	0	-1.284805	0.528561	-2.263538
40	6	0	-0.342744	1.481343	-0.270610
41	6	0	-0.067416	2.871481	-0.813132
42	1	0	0.806251	0.890757	-0.621367
43	1	0	-0.512131	1.400292	0.800480
44	1	0	0.001918	2.826141	-1.905725
45	1	0	-0.919749	3.525221	-0.581121
46	6	0	1.204902	3.478161	-0.253496
47	6	0	1.619931	3.232061	1.059889
48	6	0	1.986479	4.313965	-1.055451
49	6	0	2.779654	3.820669	1.559440
50	1	0	1.060005	2.555388	1.700511
51	6	0	3.148399	4.899394	-0.559379
52	1	0	1.685561	4.500638	-2.083239
53	6	0	3.547153	4.657351	0.752468
54	1	0	3.086897	3.619343	2.580933
55	1	0	3.745715	5.538922	-1.201121
56	1	0	4.453281	5.109755	1.141436
57	6	0	2.689980	1.056743	-1.945176
58	8	0	1.757623	0.378848	-1.318215
59	8	0	2.593887	1.295648	-3.152498
60	6	0	3.902362	1.435809	-1.138778
61	1	0	4.386928	0.518457	-0.788570
62	1	0	4.597305	2.021619	-1.737711
63	1	0	3.593941	1.999677	-0.254833
64	11	0	0.675750	0.068833	-3.379283

TS5[d]

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	-3.806985	1.348738	-0.481091
2	6	0	-4.657626	1.357850	-1.590701
3	6	0	-5.794088	0.558879	-1.604540
4	6	0	-6.060561	-0.247128	-0.498843
5	6	0	-5.216500	-0.244099	0.612281
6	6	0	-4.081382	0.564187	0.635078
7	6	0	-2.651922	2.289404	-0.714515
8	6	0	-3.173369	3.190118	-1.865285
9	6	0	-4.163777	2.306384	-2.652949
10	1	0	-6.464049	0.566678	-2.458532
11	1	0	-6.943558	-0.877861	-0.495671
12	1	0	-5.445071	-0.866488	1.470456
13	1	0	-3.444889	0.583876	1.515054
14	1	0	-3.721544	4.010219	-1.397328
15	1	0	-3.665694	1.751541	-3.456704
16	1	0	-2.322450	2.845472	0.164330
17	1	0	-4.956267	2.900367	-3.112408
18	6	0	-0.848313	1.818371	-2.440858
19	6	0	-0.779213	0.564143	-0.663111
20	7	0	0.156022	1.011896	-2.636776
21	7	0	-1.453830	1.568997	-1.234968
22	7	0	0.175885	0.232572	-1.523607
23	6	0	-1.327991	2.920193	-3.336302
24	1	0	-1.846378	2.498354	-4.205432
25	1	0	-0.466906	3.485805	-3.696057
26	8	0	-2.137886	3.806407	-2.601692
27	6	0	1.258912	-0.672077	-1.321130
28	6	0	2.425691	-0.208943	-0.719748
29	6	0	1.172077	-1.990822	-1.757473
30	6	0	3.519227	-1.045318	-0.566117
31	6	0	2.251158	-2.847287	-1.606713
32	6	0	3.410719	-2.358373	-1.015580
33	1	0	4.427742	-0.695016	-0.091276
34	1	0	2.183460	-3.879508	-1.925812
35	35	0	2.473680	1.557094	-0.060180
36	35	0	4.860424	-3.524142	-0.768350
37	35	0	-0.437457	-2.609510	-2.493675
38	6	0	-0.964244	0.090011	0.771024
39	8	0	-0.910421	1.014541	1.585103
40	6	0	-1.076602	-1.319229	1.001835
41	6	0	-1.542709	-1.753870	2.391883
42	1	0	0.086873	-1.722869	0.992879

43	1	0	-1.536594	-1.839015	0.156930
44	1	0	-0.899062	-2.583744	2.707077
45	1	0	-1.357678	-0.936266	3.094940
46	6	0	-2.985579	-2.200820	2.489601
47	6	0	-3.503053	-3.151305	1.602999
48	6	0	-3.805751	-1.737405	3.520514
49	6	0	-4.800968	-3.630402	1.748424
50	1	0	-2.876992	-3.539676	0.803062
51	6	0	-5.105033	-2.220431	3.675580
52	1	0	-3.416823	-1.003011	4.221466
53	6	0	-5.606325	-3.170769	2.789691
54	1	0	-5.181932	-4.373210	1.054790
55	1	0	-5.722667	-1.855408	4.490067
56	1	0	-6.614547	-3.553147	2.910136
57	6	0	2.009895	-1.719438	2.053051
58	8	0	1.310000	-2.461945	1.304823
59	8	0	1.702404	-0.541815	2.364053
60	6	0	3.290996	-2.315403	2.605456
61	1	0	3.984586	-1.526626	2.899272
62	1	0	3.046471	-2.913404	3.488219
63	1	0	3.749122	-2.979785	1.870793
64	11	0	1.073109	1.463181	2.623644
65	6	0	3.890068	4.617322	1.463327
66	6	0	3.151431	4.018171	2.646704
67	6	0	1.100265	4.612412	1.631241
68	6	0	1.871531	5.197932	0.461532
69	1	0	4.079616	3.834847	0.711290
70	1	0	3.027012	4.770751	3.435588
71	1	0	0.153230	4.170465	1.308038
72	1	0	1.336512	6.046984	0.030555
73	8	0	3.132154	5.666580	0.893131
74	8	0	1.859473	3.558666	2.230744
75	1	0	1.998416	4.425418	-0.315235
76	1	0	0.904382	5.388387	2.382339
77	1	0	3.680932	3.150869	3.050398
78	1	0	4.845707	5.039847	1.780445

M05[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.358042	4.097697	0.127189

2	6	0	-2.578499	5.385766	-0.353592
3	6	0	-3.715360	6.087842	0.036792
4	6	0	-4.618660	5.474921	0.902545
5	6	0	-4.390476	4.180322	1.376031
6	6	0	-3.250230	3.476249	0.995265
7	6	0	-1.069532	3.535379	-0.430080
8	6	0	-0.661502	4.532881	-1.569267
9	6	0	-1.461598	5.821282	-1.269430
10	1	0	-3.899733	7.092143	-0.333255
11	1	0	-5.513007	6.008106	1.209512
12	1	0	-5.107377	3.722108	2.049682
13	1	0	-3.045638	2.471932	1.357285
14	1	0	0.415961	4.690665	-1.548117
15	1	0	-1.810884	6.270273	-2.204137
16	1	0	-0.293365	3.440736	0.326799
17	1	0	-0.819237	6.557997	-0.775027
18	6	0	-1.884652	2.037341	-2.207721
19	6	0	-1.099400	0.980622	-0.461557
20	7	0	-2.080148	0.782593	-2.482675
21	7	0	-1.292839	2.197336	-0.985528
22	7	0	-1.594703	0.138258	-1.380320
23	6	0	-2.090404	3.269841	-3.024924
24	1	0	-2.987597	3.809442	-2.691003
25	1	0	-2.197256	3.010094	-4.078060
26	8	0	-0.916534	4.041927	-2.880713
27	6	0	-1.715102	-1.272203	-1.267424
28	6	0	-0.903950	-2.102617	-2.040589
29	6	0	-2.593784	-1.828124	-0.335598
30	6	0	-0.952385	-3.482092	-1.878919
31	6	0	-2.659425	-3.203250	-0.168746
32	6	0	-1.828260	-4.009233	-0.938110
33	1	0	-0.301212	-4.122028	-2.460561
34	1	0	-3.324050	-3.629236	0.571891
35	35	0	0.310401	-1.353889	-3.251401
36	35	0	-1.869747	-5.871614	-0.658263
37	35	0	-3.624583	-0.730837	0.781130
38	6	0	-0.591619	0.711978	0.934405
39	8	0	-0.767654	1.676946	1.738086
40	6	0	-0.001161	-0.506774	1.175511
41	6	0	0.246012	-0.919926	2.603642
42	1	0	1.484381	0.014684	-0.030667
43	1	0	0.025544	-1.282301	0.417566
44	1	0	1.002961	-1.709961	2.651150
45	1	0	0.603584	-0.064088	3.185779

46	6	0	-1.060754	-1.423059	3.184539
47	6	0	-1.917111	-0.553858	3.866271
48	6	0	-1.480916	-2.734797	2.948786
49	6	0	-3.163416	-0.991844	4.308654
50	1	0	-1.606587	0.476206	4.014986
51	6	0	-2.726319	-3.173973	3.391044
52	1	0	-0.827030	-3.416243	2.406865
53	6	0	-3.573459	-2.301915	4.071594
54	1	0	-3.818732	-0.306174	4.837867
55	1	0	-3.032673	-4.200535	3.207038
56	1	0	-4.544213	-2.642734	4.417495
57	7	0	2.222942	0.190978	-0.752794
58	16	0	2.843510	1.746953	-0.683008
59	8	0	3.963801	1.812987	-1.601952
60	8	0	1.676418	2.605326	-0.831669
61	16	0	3.113065	-1.195521	-1.110501
62	8	0	2.217721	-2.261088	-0.681845
63	8	0	3.594901	-1.112416	-2.473031
64	6	0	4.507767	-1.138863	-0.017983
65	6	0	4.297475	-1.368038	1.340545
66	6	0	5.758715	-0.829366	-0.537728
67	6	0	5.384238	-1.289738	2.201583
68	1	0	3.301702	-1.599262	1.707680
69	6	0	6.840104	-0.760536	0.338468
70	1	0	5.865934	-0.646416	-1.601314
71	6	0	6.651458	-0.990213	1.698867
72	1	0	5.243639	-1.458335	3.263757
73	1	0	7.827978	-0.527581	-0.044296
74	1	0	7.497610	-0.933521	2.376244
75	6	0	3.441486	1.924471	0.979885
76	6	0	4.812851	2.012967	1.186848
77	6	0	2.518626	1.940465	2.026252
78	6	0	5.281148	2.110858	2.494309
79	1	0	5.488568	1.995792	0.338694
80	6	0	3.008962	2.028871	3.325226
81	1	0	1.443030	1.905649	1.847005
82	6	0	4.382423	2.111025	3.557688
83	1	0	6.348219	2.178994	2.678451
84	1	0	2.311906	2.044683	4.156592
85	1	0	4.752436	2.182155	4.575504

M05[b]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.211376	-1.415865	0.166389
2	6	0	-5.549873	-1.289270	-0.191119
3	6	0	-6.254336	-2.403361	-0.640248
4	6	0	-5.591799	-3.625673	-0.725128
5	6	0	-4.246238	-3.739764	-0.363266
6	6	0	-3.537862	-2.631656	0.093641
7	6	0	-3.644667	-0.090134	0.618496
8	6	0	-4.762815	0.959766	0.276204
9	6	0	-6.036368	0.126349	-0.001333
10	1	0	-7.299610	-2.321526	-0.923254
11	1	0	-6.127513	-4.501766	-1.077114
12	1	0	-3.752851	-4.703746	-0.434044
13	1	0	-2.495496	-2.684649	0.400392
14	1	0	-4.891344	1.649906	1.110479
15	1	0	-6.560282	0.529000	-0.873895
16	1	0	-3.380545	-0.092079	1.677508
17	1	0	-6.725059	0.191240	0.847396
18	6	0	-2.437204	0.759327	-1.375308
19	6	0	-1.151806	0.095405	0.259656
20	7	0	-1.231523	0.943029	-1.828135
21	7	0	-2.424186	0.226856	-0.117040
22	7	0	-0.442098	0.505784	-0.797145
23	6	0	-3.773438	1.167965	-1.901890
24	1	0	-4.335047	0.297940	-2.268990
25	1	0	-3.662991	1.894961	-2.706130
26	8	0	-4.431590	1.805386	-0.821423
27	6	0	0.965024	0.378454	-0.949039
28	6	0	1.781270	1.506363	-0.925327
29	6	0	1.541894	-0.886149	-1.073811
30	6	0	3.160899	1.388172	-1.023296
31	6	0	2.917253	-1.025817	-1.183347
32	6	0	3.707595	0.116367	-1.148448
33	1	0	3.793144	2.266041	-0.982655
34	1	0	3.364247	-2.007721	-1.264035
35	35	0	0.999885	3.184753	-0.619729
36	35	0	5.577637	-0.076530	-1.243813
37	35	0	0.462177	-2.419849	-1.040682
38	6	0	-0.659065	-0.458628	1.568020
39	8	0	-1.274399	-1.494654	1.964279
40	6	0	0.369418	0.268401	2.112765
41	6	0	1.186187	-0.295837	3.241856

42	1	0	-1.352468	1.844130	2.362185
43	1	0	0.760321	1.127405	1.572620
44	1	0	1.572012	0.491246	3.897313
45	1	0	0.553994	-0.960334	3.839365
46	6	0	2.335134	-1.085377	2.643947
47	6	0	2.081176	-2.335216	2.065538
48	6	0	3.625727	-0.559216	2.567923
49	6	0	3.103962	-3.049865	1.449974
50	1	0	1.063536	-2.720059	2.084110
51	6	0	4.650886	-1.269824	1.944962
52	1	0	3.828127	0.417172	3.001968
53	6	0	4.394183	-2.520209	1.388614
54	1	0	2.892173	-4.019074	1.006112
55	1	0	5.647135	-0.842452	1.883363
56	1	0	5.192494	-3.073763	0.902672
57	6	0	-1.616526	3.546897	1.553654
58	8	0	-0.617455	4.025309	2.033474
59	8	0	-2.047826	2.308972	1.848197
60	6	0	-2.485098	4.217270	0.522246
61	1	0	-2.610320	5.270760	0.785083
62	1	0	-1.938882	4.164744	-0.430412
63	1	0	-3.442275	3.706458	0.403820

M5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.346753	0.998241	-0.330070
2	6	0	-5.341928	0.714235	0.609162
3	6	0	-5.919960	1.739542	1.348042
4	6	0	-5.486289	3.046564	1.131683
5	6	0	-4.498916	3.324739	0.185232
6	6	0	-3.917834	2.302004	-0.562820
7	6	0	-3.901616	-0.270636	-1.020430
8	6	0	-5.057085	-1.251041	-0.690622
9	6	0	-5.641278	-0.762545	0.652629
10	1	0	-6.699380	1.528876	2.074318
11	1	0	-5.930026	3.858825	1.699120
12	1	0	-4.184072	4.350717	0.024404
13	1	0	-3.155758	2.489634	-1.313919
14	1	0	-5.811399	-1.122966	-1.469916
15	1	0	-5.134059	-1.226675	1.506931

16	1	0	-3.696998	-0.141800	-2.083305
17	1	0	-6.704984	-0.994539	0.740910
18	6	0	-2.543529	-2.081476	0.122127
19	6	0	-1.450330	-0.257001	-0.394833
20	7	0	-1.328219	-2.311540	0.522714
21	7	0	-2.661866	-0.833689	-0.434299
22	7	0	-0.661868	-1.161664	0.196693
23	6	0	-3.718751	-3.007512	0.187108
24	1	0	-4.121689	-3.035030	1.207197
25	1	0	-3.396426	-4.015676	-0.078012
26	8	0	-4.688333	-2.614491	-0.756158
27	6	0	0.754157	-1.112282	0.307438
28	6	0	1.546321	-1.336458	-0.818604
29	6	0	1.365162	-0.845391	1.529014
30	6	0	2.929307	-1.314973	-0.725970
31	6	0	2.748552	-0.790889	1.639088
32	6	0	3.511326	-1.028356	0.502888
33	1	0	3.538550	-1.484175	-1.605194
34	1	0	3.216451	-0.550969	2.585258
35	35	0	0.736195	-1.560432	-2.492990
36	35	0	5.385250	-0.899538	0.604186
37	35	0	0.291734	-0.452902	3.017033
38	6	0	-1.064521	1.029228	-1.068798
39	8	0	-1.602658	1.183045	-2.211421
40	6	0	-0.212478	1.796775	-0.328397
41	6	0	0.431212	3.038118	-0.868270
42	1	0	0.075041	1.464630	0.665198
43	1	0	0.105598	3.160585	-1.907309
44	1	0	0.120304	3.936871	-0.319187
45	6	0	1.940326	2.914606	-0.795309
46	6	0	2.590502	1.909296	-1.520058
47	6	0	2.702872	3.735693	0.035494
48	6	0	3.966240	1.736064	-1.417603
49	1	0	1.992879	1.240520	-2.138269
50	6	0	4.081382	3.556557	0.150919
51	1	0	2.208716	4.518062	0.606261
52	6	0	4.717656	2.553874	-0.573189
53	1	0	4.460028	0.950300	-1.983893
54	1	0	4.656494	4.199315	0.810739
55	1	0	5.788566	2.401993	-0.479584

TS6*R*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.377546	-1.165938	-2.345717
2	6	0	-3.536039	-1.791379	-1.875538
3	6	0	-4.731831	-1.088076	-1.790599
4	6	0	-4.752897	0.247222	-2.186878
5	6	0	-3.599055	0.862676	-2.668826
6	6	0	-2.397007	0.164067	-2.753126
7	6	0	-1.258514	-2.175915	-2.474206
8	6	0	-2.031849	-3.523491	-2.428738
9	6	0	-3.274057	-3.240637	-1.563637
10	1	0	-5.637658	-1.574034	-1.438750
11	1	0	-5.678887	0.812170	-2.132955
12	1	0	-3.639598	1.898767	-2.988610
13	1	0	-1.495543	0.635923	-3.130966
14	1	0	-2.352393	-3.733672	-3.451814
15	1	0	-3.035740	-3.355265	-0.498550
16	1	0	-0.667585	-2.042279	-3.381683
17	1	0	-4.103469	-3.909196	-1.805543
18	6	0	0.021029	-3.280766	-0.584657
19	6	0	0.575281	-1.222416	-1.003390
20	7	0	1.014118	-3.043427	0.220012
21	7	0	-0.275281	-2.187886	-1.360370
22	7	0	1.345667	-1.750466	-0.051754
23	6	0	-0.728970	-4.562386	-0.742900
24	1	0	-1.512305	-4.630888	0.021919
25	1	0	-0.043123	-5.400414	-0.612661
26	8	0	-1.249573	-4.636643	-2.051147
27	6	0	2.561160	-1.205442	0.456610
28	6	0	3.696322	-1.168779	-0.354020
29	6	0	2.618507	-0.697738	1.752501
30	6	0	4.890050	-0.653575	0.127736
31	6	0	3.801832	-0.163388	2.246905
32	6	0	4.921984	-0.156862	1.424777
33	1	0	5.767590	-0.618680	-0.503887
34	1	0	3.841213	0.251720	3.246052
35	35	0	3.601636	-1.769513	-2.127511
36	35	0	6.533486	0.572312	2.069669
37	35	0	1.031975	-0.615673	2.737789
38	6	0	0.745949	0.127377	-1.632000
39	8	0	0.680977	0.165656	-2.878563
40	6	0	0.929717	1.161045	-0.707785
41	6	0	1.405263	2.499514	-1.183888

42	1	0	1.088053	0.922283	0.335342
43	1	0	1.015652	2.693422	-2.188843
44	1	0	1.071228	3.294597	-0.509272
45	6	0	2.923629	2.447327	-1.211861
46	6	0	3.578703	1.789149	-2.259355
47	6	0	3.681748	2.969377	-0.161744
48	6	0	4.966553	1.682877	-2.265813
49	1	0	2.985488	1.348531	-3.057288
50	6	0	5.071094	2.864278	-0.167787
51	1	0	3.177692	3.467538	0.662762
52	6	0	5.717752	2.223083	-1.222001
53	1	0	5.462554	1.171584	-3.086034
54	1	0	5.648055	3.270258	0.657431
55	1	0	6.800497	2.137565	-1.224046
56	7	0	-2.628611	0.806195	0.523777
57	16	0	-2.740962	2.414684	1.104139
58	8	0	-3.915721	2.456387	1.968678
59	8	0	-1.464589	2.906039	1.590028
60	16	0	-2.479685	-0.409198	1.707911
61	8	0	-1.936235	-1.560682	0.993423
62	8	0	-1.814275	0.090207	2.905375
63	6	0	-4.163491	-0.766317	2.151936
64	6	0	-4.849316	-1.752347	1.451014
65	6	0	-4.731696	-0.097894	3.233615
66	6	0	-6.150629	-2.063485	1.829965
67	1	0	-4.360498	-2.267543	0.634663
68	6	0	-6.033456	-0.420328	3.601715
69	1	0	-4.162775	0.658141	3.761564
70	6	0	-6.741194	-1.395440	2.900392
71	1	0	-6.698006	-2.833196	1.295971
72	1	0	-6.494554	0.089032	4.440771
73	1	0	-7.756157	-1.641721	3.195217
74	6	0	-3.116429	3.241927	-0.418205
75	6	0	-4.437462	3.576655	-0.691177
76	6	0	-2.071442	3.567593	-1.276650
77	6	0	-4.716385	4.268534	-1.867241
78	1	0	-5.217973	3.307317	0.012394
79	6	0	-2.364371	4.259525	-2.446960
80	1	0	-1.059415	3.274754	-1.024915
81	6	0	-3.682925	4.610820	-2.738306
82	1	0	-5.738856	4.547178	-2.099016
83	1	0	-1.564023	4.525499	-3.129438
84	1	0	-3.906282	5.155196	-3.650143
85	9	0	-1.089693	0.882997	-0.178847

TS6*S*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.282103	4.752477	0.537496
2	6	0	0.421549	5.903701	0.193013
3	6	0	-0.176570	7.152616	0.334976
4	6	0	-1.482187	7.221296	0.816526
5	6	0	-2.182480	6.059935	1.152366
6	6	0	-1.586074	4.808272	1.019026
7	6	0	0.560286	3.518432	0.294438
8	6	0	1.780989	4.038877	-0.546875
9	6	0	1.805455	5.564306	-0.301183
10	1	0	0.361809	8.057028	0.067540
11	1	0	-1.962949	8.188144	0.927430
12	1	0	-3.199197	6.135051	1.523959
13	1	0	-2.111017	3.892881	1.277235
14	1	0	2.694000	3.543351	-0.218271
15	1	0	2.084023	6.086794	-1.220956
16	1	0	0.877297	3.038684	1.222155
17	1	0	2.558019	5.812286	0.455582
18	6	0	-0.348606	2.622831	-1.817707
19	6	0	-0.845474	1.433606	-0.057569
20	7	0	-1.086041	1.657682	-2.283631
21	7	0	-0.191588	2.523247	-0.464359
22	7	0	-1.398220	0.934613	-1.167711
23	6	0	0.407097	3.715480	-2.498996
24	1	0	-0.110946	4.676253	-2.370810
25	1	0	0.509080	3.499726	-3.562299
26	8	0	1.700917	3.727104	-1.932011
27	6	0	-2.303713	-0.158167	-1.237435
28	6	0	-1.850751	-1.402242	-1.674373
29	6	0	-3.613953	-0.010486	-0.787727
30	6	0	-2.709062	-2.494030	-1.685412
31	6	0	-4.488236	-1.087360	-0.798919
32	6	0	-4.017577	-2.315060	-1.250219
33	1	0	-2.354260	-3.468190	-1.997343
34	1	0	-5.501124	-0.978609	-0.434717
35	35	0	-0.024896	-1.599802	-2.033605
36	35	0	-5.183109	-3.793508	-1.229497
37	35	0	-4.179549	1.638780	-0.089047

38	6	0	-1.010746	0.974987	1.364161
39	8	0	-1.091365	1.890037	2.215370
40	6	0	-1.011246	-0.408125	1.533630
41	6	0	-1.405347	-1.021734	2.839312
42	1	0	-1.021768	-1.054659	0.668117
43	1	0	-0.769313	-1.884238	3.062994
44	1	0	-1.288681	-0.282321	3.636199
45	6	0	-2.855938	-1.440732	2.700266
46	6	0	-3.205442	-2.763117	2.420584
47	6	0	-3.860554	-0.467302	2.727823
48	6	0	-4.534085	-3.113774	2.187575
49	1	0	-2.424608	-3.519042	2.386335
50	6	0	-5.188255	-0.814490	2.498650
51	1	0	-3.582275	0.569196	2.907746
52	6	0	-5.529454	-2.140110	2.226487
53	1	0	-4.790404	-4.144298	1.961758
54	1	0	-5.958118	-0.048088	2.524898
55	1	0	-6.564536	-2.411906	2.041210
56	7	0	2.637349	-0.846925	1.054464
57	16	0	3.007589	-0.143116	-0.457794
58	8	0	2.901434	-1.082371	-1.568549
59	8	0	2.257417	1.104398	-0.489486
60	16	0	2.588904	-2.559136	1.203295
61	8	0	2.393522	-2.780569	2.624808
62	8	0	1.682466	-3.155981	0.239206
63	6	0	4.258614	-2.950493	0.761566
64	6	0	5.279427	-2.595943	1.642918
65	6	0	4.506219	-3.564529	-0.461376
66	6	0	6.591841	-2.864326	1.276397
67	1	0	5.040172	-2.117262	2.587204
68	6	0	5.827134	-3.840539	-0.806107
69	1	0	3.676189	-3.802236	-1.117524
70	6	0	6.861837	-3.488399	0.057556
71	1	0	7.404669	-2.589949	1.939992
72	1	0	6.045869	-4.326948	-1.750704
73	1	0	7.889588	-3.700094	-0.220305
74	6	0	4.727400	0.208031	-0.198096
75	6	0	5.662229	-0.370342	-1.047203
76	6	0	5.093203	1.041375	0.857981
77	6	0	7.011700	-0.103604	-0.828332
78	1	0	5.332195	-1.022040	-1.848562
79	6	0	6.442877	1.297441	1.062323
80	1	0	4.333728	1.460007	1.510873
81	6	0	7.398649	0.724944	0.220554

82	1	0	7.758222	-0.550016	-1.476809
83	1	0	6.751508	1.938701	1.880766
84	1	0	8.451633	0.926130	0.388959
85	9	0	1.057124	-0.502580	1.287767

M6*R*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.325930	0.864287	0.041217
2	6	0	5.245222	0.067831	-0.651624
3	6	0	5.891302	0.565666	-1.775372
4	6	0	5.609946	1.867179	-2.189796
5	6	0	4.714813	2.667206	-1.480219
6	6	0	4.067651	2.174339	-0.349284
7	6	0	3.789098	0.105180	1.228118
8	6	0	4.867310	-0.990661	1.431231
9	6	0	5.410855	-1.274557	0.015202
10	1	0	6.611942	-0.041315	-2.314110
11	1	0	6.108666	2.270133	-3.065078
12	1	0	4.528267	3.685359	-1.803657
13	1	0	3.393403	2.809020	0.215906
14	1	0	5.659378	-0.539382	2.032386
15	1	0	4.818735	-2.036722	-0.505615
16	1	0	3.592356	0.702539	2.119964
17	1	0	6.443766	-1.626341	0.041336
18	6	0	2.316084	-1.966458	1.067020
19	6	0	1.350863	-0.117055	0.478257
20	7	0	1.099861	-2.308847	0.737043
21	7	0	2.509666	-0.614821	0.917239
22	7	0	0.518867	-1.144610	0.363383
23	6	0	3.414220	-2.862068	1.554957
24	1	0	3.803998	-3.454158	0.717826
25	1	0	3.009786	-3.548946	2.300210
26	8	0	4.410377	-2.093268	2.181211
27	6	0	-0.882896	-1.080403	0.104165
28	6	0	-1.752669	-0.682369	1.121376
29	6	0	-1.380268	-1.437457	-1.147598
30	6	0	-3.120994	-0.671997	0.900819
31	6	0	-2.745955	-1.408053	-1.390224
32	6	0	-3.597918	-1.034019	-0.355007
33	1	0	-3.799808	-0.367945	1.686869

34	1	0	-3.136096	-1.667170	-2.366711
35	35	0	-1.070528	-0.131120	2.777731
36	35	0	-5.444307	-0.971304	-0.666764
37	35	0	-0.178191	-1.855210	-2.521813
38	6	0	0.981474	1.334212	0.290701
39	8	0	1.278842	2.094866	1.172821
40	6	0	0.377449	1.747352	-1.056473
41	6	0	-0.405459	3.039168	-0.956488
42	1	0	-0.232413	0.942700	-1.480881
43	1	0	0.187373	3.774130	-0.404841
44	1	0	-0.542590	3.409053	-1.976156
45	6	0	-1.743506	2.798063	-0.292226
46	6	0	-1.885313	2.873556	1.095133
47	6	0	-2.860942	2.479904	-1.071903
48	6	0	-3.126845	2.655862	1.690919
49	1	0	-1.025081	3.122641	1.710825
50	6	0	-4.104085	2.278420	-0.481330
51	1	0	-2.759454	2.422638	-2.153108
52	6	0	-4.238464	2.364407	0.904086
53	1	0	-3.224335	2.725997	2.769856
54	1	0	-4.965336	2.043619	-1.097990
55	1	0	-5.209178	2.209653	1.365258
56	9	0	1.497624	1.889071	-1.858061

M6*S*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.768406	-0.408492	-0.244715
2	6	0	4.891178	-0.904980	-0.902299
3	6	0	5.574863	-0.101320	-1.810920
4	6	0	5.108986	1.188190	-2.051059
5	6	0	3.983821	1.679996	-1.384146
6	6	0	3.304485	0.886729	-0.464010
7	6	0	3.167231	-1.464248	0.657726
8	6	0	3.977172	-2.779073	0.342112
9	6	0	5.202609	-2.316537	-0.478571
10	1	0	6.451968	-0.476992	-2.328516
11	1	0	5.626243	1.821000	-2.764596
12	1	0	3.637038	2.689600	-1.575653
13	1	0	2.438559	1.290516	0.061316
14	1	0	4.268798	-3.260325	1.274937

15	1	0	5.370739	-2.997781	-1.318268
16	1	0	3.197803	-1.213161	1.715915
17	1	0	6.103528	-2.346266	0.141593
18	6	0	1.398254	-2.384390	-0.807880
19	6	0	0.647468	-0.971716	0.662960
20	7	0	0.140915	-2.218194	-1.114041
21	7	0	1.743541	-1.643489	0.286407
22	7	0	-0.308352	-1.332345	-0.196381
23	6	0	2.439673	-3.273478	-1.405911
24	1	0	3.043080	-2.716314	-2.136405
25	1	0	1.966578	-4.119848	-1.903847
26	8	0	3.204485	-3.761631	-0.327519
27	6	0	-1.621340	-0.796901	-0.356704
28	6	0	-2.713865	-1.367333	0.287060
29	6	0	-1.789217	0.297043	-1.207447
30	6	0	-3.987313	-0.858902	0.067299
31	6	0	-3.052774	0.816135	-1.437393
32	6	0	-4.139509	0.219843	-0.798386
33	1	0	-4.843276	-1.291888	0.569702
34	1	0	-3.190492	1.668349	-2.091093
35	35	0	-2.438690	-2.763283	1.498795
36	35	0	-5.855566	0.926624	-1.077691
37	35	0	-0.261307	1.126003	-1.924402
38	6	0	0.584895	-0.003272	1.820182
39	8	0	1.470507	-0.052741	2.632936
40	6	0	-0.586559	0.978376	1.904227
41	6	0	-0.222552	2.195035	2.729157
42	1	0	-0.872769	1.288444	0.895671
43	1	0	-1.132142	2.790708	2.851045
44	1	0	0.119877	1.879115	3.717076
45	6	0	0.853257	2.968410	1.996046
46	6	0	0.568084	3.575227	0.767992
47	6	0	2.154200	3.035811	2.499137
48	6	0	1.563300	4.247404	0.062365
49	1	0	-0.441635	3.536838	0.363403
50	6	0	3.148172	3.715164	1.799936
51	1	0	2.385139	2.551540	3.443677
52	6	0	2.853741	4.324494	0.582558
53	1	0	1.326330	4.723982	-0.883834
54	1	0	4.152548	3.769998	2.206414
55	1	0	3.628049	4.859071	0.041629
56	9	0	-1.631546	0.257360	2.453795

M06*R*[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.950378	4.703982	0.753666
2	6	0	-0.159399	5.842376	0.606769
3	6	0	-0.728331	7.102856	0.747612
4	6	0	-2.091905	7.197769	1.024794
5	6	0	-2.876550	6.051728	1.163588
6	6	0	-2.308562	4.785262	1.032967
7	6	0	-0.099476	3.468651	0.550527
8	6	0	1.155236	4.005420	-0.204233
9	6	0	1.268856	5.453920	0.305158
10	1	0	-0.125728	7.998663	0.631901
11	1	0	-2.551372	8.175602	1.127460
12	1	0	-3.936534	6.147698	1.374141
13	1	0	-2.910792	3.886508	1.134990
14	1	0	2.025243	3.387382	0.019285
15	1	0	1.753767	6.082566	-0.444813
16	1	0	0.192061	2.994629	1.491853
17	1	0	1.877014	5.484280	1.217522
18	6	0	-0.829745	2.534194	-1.596530
19	6	0	-1.429950	1.345727	0.118567
20	7	0	-1.481251	1.528912	-2.107693
21	7	0	-0.789632	2.456724	-0.236816
22	7	0	-1.836221	0.788545	-1.024249
23	6	0	-0.185571	3.715116	-2.239771
24	1	0	-0.881066	4.565128	-2.173330
25	1	0	0.011975	3.498180	-3.289783
26	8	0	1.047586	3.999039	-1.624566
27	6	0	-2.826624	-0.227055	-1.175011
28	6	0	-2.471616	-1.555495	-1.384654
29	6	0	-4.168365	0.144038	-1.090129
30	6	0	-3.470299	-2.514470	-1.525795
31	6	0	-5.172334	-0.797197	-1.236966
32	6	0	-4.799975	-2.120431	-1.460643
33	1	0	-3.207273	-3.553387	-1.681422
34	1	0	-6.214827	-0.513516	-1.169673
35	35	0	-0.665922	-2.049489	-1.416761
36	35	0	-6.148231	-3.417423	-1.670695
37	35	0	-4.596056	1.936770	-0.703680
38	6	0	-1.744942	0.930814	1.541220
39	8	0	-1.854503	1.804075	2.363851

40	6	0	-1.993884	-0.551427	1.792535
41	6	0	-1.683859	-1.003566	3.207572
42	1	0	-1.419374	-1.129586	1.063437
43	1	0	-0.801644	-0.464631	3.561069
44	1	0	-2.526111	-0.720261	3.845099
45	6	0	-1.437377	-2.495203	3.233105
46	6	0	-0.377813	-3.024713	2.486609
47	6	0	-2.244785	-3.359487	3.970040
48	6	0	-0.124962	-4.391388	2.485932
49	1	0	0.273571	-2.368195	1.912048
50	6	0	-1.996168	-4.731399	3.967566
51	1	0	-3.072652	-2.957632	4.548618
52	6	0	-0.937328	-5.249214	3.226750
53	1	0	0.713166	-4.765738	1.906925
54	1	0	-2.632387	-5.394218	4.546025
55	1	0	-0.744481	-6.317452	3.227652
56	9	0	-3.349440	-0.754261	1.538237
57	6	0	2.989545	-0.339145	4.593079
58	6	0	2.039384	-0.632685	3.431394
59	6	0	1.482341	0.648811	2.810008
60	6	0	2.614368	1.596062	2.408052
61	6	0	3.578698	1.872387	3.564081
62	6	0	4.133278	0.571874	4.147379
63	1	0	2.565047	-1.189931	2.643539
64	1	0	1.215938	-1.273045	3.764020
65	1	0	2.437077	0.152903	5.405866
66	1	0	3.377967	-1.278057	4.999324
67	1	0	3.147670	1.132520	1.568686
68	1	0	2.195481	2.535938	2.032853
69	1	0	4.390414	2.523364	3.222871
70	1	0	3.047309	2.418553	4.355682
71	1	0	4.726034	0.054389	3.379928
72	1	0	4.806632	0.786308	4.983842
73	1	0	0.834981	1.159361	3.542380
74	8	0	0.643404	0.353563	1.696412
75	1	0	1.189972	-0.112143	1.021139
76	7	0	2.353052	-0.940519	-0.163350
77	16	0	2.319589	0.047798	-1.446668
78	8	0	1.887694	-0.568859	-2.700855
79	8	0	1.564577	1.224006	-0.985009
80	16	0	2.679011	-2.533716	-0.293629
81	8	0	2.543849	-3.066432	1.063510
82	8	0	1.923086	-3.188606	-1.364114
83	6	0	4.398345	-2.628082	-0.747336

84	6	0	5.360855	-2.684269	0.255313
85	6	0	4.741706	-2.536803	-2.093238
86	6	0	6.705301	-2.644543	-0.102475
87	1	0	5.047965	-2.762865	1.291748
88	6	0	6.089287	-2.483144	-2.436934
89	1	0	3.959136	-2.490417	-2.845128
90	6	0	7.066455	-2.536500	-1.444440
91	1	0	7.470503	-2.697259	0.665269
92	1	0	6.375903	-2.398974	-3.480003
93	1	0	8.115909	-2.496119	-1.718811
94	6	0	4.011219	0.567773	-1.726508
95	6	0	4.369689	0.919261	-3.024743
96	6	0	4.935428	0.602501	-0.686548
97	6	0	5.676982	1.320539	-3.282114
98	1	0	3.633985	0.849347	-3.818831
99	6	0	6.242889	0.994912	-0.956287
100	1	0	4.644668	0.275253	0.306574
101	6	0	6.612434	1.355720	-2.250481
102	1	0	5.967900	1.592475	-4.291504
103	1	0	6.976786	1.002547	-0.156808
104	1	0	7.635116	1.655034	-2.457035

M06*S*[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.672207	3.963305	-0.356018
2	6	0	-0.341612	5.075826	-1.128698
3	6	0	-1.264723	6.101469	-1.320833
4	6	0	-2.524417	5.996975	-0.740204
5	6	0	-2.854854	4.883369	0.035044
6	6	0	-1.931130	3.862094	0.238677
7	6	0	0.466590	2.955105	-0.338489
8	6	0	1.565952	3.576505	-1.284398
9	6	0	1.059722	4.988233	-1.665769
10	1	0	-1.003759	6.966780	-1.922945
11	1	0	-3.255328	6.785323	-0.889121
12	1	0	-3.834117	4.809284	0.496831
13	1	0	-2.209329	3.019052	0.863594
14	1	0	2.498986	3.608455	-0.728719
15	1	0	1.109869	5.131276	-2.750545
16	1	0	0.870967	2.735333	0.649531

17	1	0	1.700562	5.753844	-1.217758
18	6	0	-0.053123	1.455668	-2.241150
19	6	0	-0.807900	0.724292	-0.335870
20	7	0	-0.808765	0.443389	-2.554150
21	7	0	-0.035537	1.672830	-0.894011
22	7	0	-1.264103	-0.000245	-1.360073
23	6	0	0.758569	2.331337	-3.136089
24	1	0	0.137856	3.158623	-3.513152
25	1	0	1.119058	1.734448	-3.974099
26	8	0	1.873075	2.787048	-2.416942
27	6	0	-2.261391	-1.013427	-1.348646
28	6	0	-1.899572	-2.355593	-1.434844
29	6	0	-3.602668	-0.639013	-1.301158
30	6	0	-2.888300	-3.331440	-1.370305
31	6	0	-4.598660	-1.600265	-1.231474
32	6	0	-4.215527	-2.939113	-1.243908
33	1	0	-2.622583	-4.380465	-1.416429
34	1	0	-5.641892	-1.316948	-1.173513
35	35	0	-0.103535	-2.785265	-1.677080
36	35	0	-5.549939	-4.261823	-1.099711
37	35	0	-4.049192	1.196657	-1.312471
38	6	0	-1.152131	0.662920	1.144184
39	8	0	-0.580091	1.441825	1.862077
40	6	0	-2.425392	-0.055439	1.628640
41	6	0	-2.687767	0.257545	3.095701
42	1	0	-3.245719	0.367520	1.037163
43	1	0	-3.437291	-0.465356	3.433535
44	1	0	-1.775439	0.111144	3.679540
45	6	0	-3.210842	1.671350	3.241704
46	6	0	-4.444575	2.014870	2.679136
47	6	0	-2.464391	2.662369	3.880798
48	6	0	-4.923900	3.319846	2.755954
49	1	0	-5.041341	1.253587	2.180023
50	6	0	-2.941478	3.968003	3.960506
51	1	0	-1.492999	2.409295	4.294507
52	6	0	-4.170703	4.300833	3.397338
53	1	0	-5.886119	3.568424	2.318454
54	1	0	-2.347074	4.728545	4.456286
55	1	0	-4.539518	5.319972	3.455782
56	9	0	-2.426707	-1.412017	1.401131
57	6	0	0.381701	-4.780952	2.759102
58	6	0	0.296763	-3.749464	1.632287
59	6	0	0.223563	-2.328190	2.188140
60	6	0	1.402885	-2.043021	3.114686

61	6	0	1.479343	-3.069018	4.246705
62	6	0	1.562009	-4.492492	3.690040
63	1	0	1.181041	-3.817222	0.982335
64	1	0	-0.578781	-3.929921	0.999098
65	1	0	-0.548611	-4.753023	3.343925
66	1	0	0.460383	-5.790043	2.341636
67	1	0	2.322095	-2.089483	2.512792
68	1	0	1.320392	-1.018051	3.493300
69	1	0	2.340983	-2.856923	4.889266
70	1	0	0.584708	-2.982054	4.879430
71	1	0	2.498398	-4.601832	3.126776
72	1	0	1.591927	-5.222052	4.506509
73	1	0	-0.708941	-2.232680	2.761917
74	8	0	0.141108	-1.373063	1.140313
75	1	0	1.047939	-1.215805	0.793467
76	7	0	2.732151	-0.812163	0.117332
77	16	0	3.144912	0.600443	0.797870
78	8	0	3.426823	1.656250	-0.183167
79	8	0	2.148322	0.890914	1.831271
80	16	0	2.925872	-1.075864	-1.476050
81	8	0	2.785762	-2.525507	-1.656186
82	8	0	2.064161	-0.211728	-2.290231
83	6	0	4.607515	-0.665786	-1.899655
84	6	0	5.613675	-1.570734	-1.576468
85	6	0	4.877848	0.553826	-2.512597
86	6	0	6.933268	-1.238341	-1.868008
87	1	0	5.357075	-2.514028	-1.105089
88	6	0	6.202258	0.872477	-2.801971
89	1	0	4.057303	1.234572	-2.718086
90	6	0	7.225024	-0.018937	-2.477278
91	1	0	7.732175	-1.929600	-1.620786
92	1	0	6.437087	1.819001	-3.277827
93	1	0	8.255394	0.237013	-2.704202
94	6	0	4.683546	0.275132	1.645553
95	6	0	5.886866	0.537406	0.997925
96	6	0	4.648926	-0.255486	2.932157
97	6	0	7.080589	0.238193	1.649544
98	1	0	5.883921	0.972838	0.003081
99	6	0	5.848116	-0.547089	3.574248
100	1	0	3.692198	-0.418046	3.417821
101	6	0	7.061600	-0.305706	2.931356
102	1	0	8.025281	0.433447	1.152056
103	1	0	5.835672	-0.957613	4.578652
104	1	0	7.994834	-0.535900	3.435507

M06*R*[b]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.256124	-2.010346	0.378777
2	6	0	-5.617222	-2.075571	0.093506
3	6	0	-6.236630	-3.313058	-0.058453
4	6	0	-5.469521	-4.468974	0.065629
5	6	0	-4.099577	-4.393667	0.328251
6	6	0	-3.478132	-3.158438	0.488254
7	6	0	-3.804461	-0.571157	0.501047
8	6	0	-5.010138	0.268975	-0.060545
9	6	0	-6.216931	-0.696981	-0.019653
10	1	0	-7.297253	-3.375784	-0.282171
11	1	0	-5.938221	-5.439993	-0.056809
12	1	0	-3.515956	-5.304910	0.404613
13	1	0	-2.409369	-3.091985	0.670617
14	1	0	-5.174523	1.148681	0.563084
15	1	0	-6.831544	-0.561934	-0.914801
16	1	0	-3.580973	-0.288483	1.528654
17	1	0	-6.849030	-0.471278	0.845390
18	6	0	-2.701547	-0.211605	-1.659206
19	6	0	-1.281141	-0.362430	-0.006051
20	7	0	-1.533820	-0.154943	-2.224014
21	7	0	-2.591452	-0.354740	-0.302646
22	7	0	-0.662511	-0.263151	-1.187767
23	6	0	-4.071341	-0.051229	-2.233520
24	1	0	-4.562137	-1.027210	-2.349354
25	1	0	-4.010342	0.439271	-3.204725
26	8	0	-4.777527	0.800664	-1.354717
27	6	0	0.736758	-0.252597	-1.434835
28	6	0	1.364800	0.935412	-1.798403
29	6	0	1.492576	-1.390141	-1.154581
30	6	0	2.752290	0.996450	-1.830986
31	6	0	2.874993	-1.351937	-1.187410
32	6	0	3.481013	-0.140539	-1.508467
33	1	0	3.247957	1.930883	-2.060925
34	1	0	3.464926	-2.217372	-0.909557
35	35	0	0.363312	2.457122	-2.209049
36	35	0	5.359194	-0.028734	-1.467942
37	35	0	0.616879	-2.955591	-0.562278

38	6	0	-0.794661	-0.644658	1.419925
39	8	0	-1.609874	-1.181600	2.133208
40	6	0	0.578624	-0.306752	1.972610
41	6	0	1.205849	-1.531498	2.694682
42	1	0	0.436381	0.540607	2.652389
43	1	0	1.168980	-1.335525	3.769723
44	1	0	0.595451	-2.421247	2.515696
45	6	0	2.632431	-1.804759	2.270501
46	6	0	3.009540	-3.081025	1.853179
47	6	0	3.595698	-0.788258	2.300167
48	6	0	4.317037	-3.339449	1.439475
49	1	0	2.271152	-3.877988	1.832315
50	6	0	4.895237	-1.043698	1.877875
51	1	0	3.309762	0.208816	2.632130
52	6	0	5.259981	-2.316756	1.437587
53	1	0	4.593277	-4.338718	1.116556
54	1	0	5.625594	-0.239672	1.882985
55	1	0	6.273620	-2.507369	1.098580
56	6	0	-3.557586	4.114367	0.151069
57	6	0	-2.673544	2.868018	0.145751
58	6	0	-1.319846	3.119727	0.796181
59	6	0	-1.495351	3.667347	2.211860
60	6	0	-2.363005	4.927308	2.222144
61	6	0	-3.724282	4.661419	1.571775
62	1	0	-3.167110	2.071342	0.723238
63	1	0	-2.520059	2.489975	-0.873539
64	1	0	-3.093230	4.885780	-0.478082
65	1	0	-4.532304	3.886885	-0.295802
66	1	0	-1.971668	2.881090	2.816419
67	1	0	-0.505384	3.847210	2.643150
68	1	0	-2.494135	5.294663	3.245295
69	1	0	-1.850626	5.723871	1.665605
70	1	0	-4.271031	3.923999	2.177225
71	1	0	-4.330317	5.573565	1.559741
72	1	0	-0.785454	3.878269	0.196072
73	8	0	-0.573218	1.928072	0.802869
74	1	0	0.425387	2.237479	0.777388
75	6	0	2.493494	2.521668	1.585471
76	8	0	2.100090	2.142048	2.704593
77	8	0	1.757338	2.819088	0.589121
78	6	0	3.997012	2.593812	1.315845
79	1	0	4.278636	1.738909	0.688338
80	1	0	4.244895	3.500813	0.759615
81	1	0	4.565503	2.551420	2.246567

82	9	0	1.394767	0.147536	0.974719

M06*S*[b]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.395436	-1.699524	-0.543242
2	6	0	5.730151	-1.843317	-0.177172
3	6	0	6.362825	-3.072449	-0.342571
4	6	0	5.635121	-4.138255	-0.867386
5	6	0	4.292363	-3.986184	-1.222058
6	6	0	3.657795	-2.757138	-1.062723
7	6	0	3.920348	-0.289105	-0.284891
8	6	0	5.057486	0.365203	0.578335
9	6	0	6.286595	-0.551304	0.368042
10	1	0	7.403022	-3.202101	-0.059724
11	1	0	6.114752	-5.103022	-0.996547
12	1	0	3.742701	-4.830903	-1.623512
13	1	0	2.609248	-2.630411	-1.323585
14	1	0	5.240626	1.385137	0.237090
15	1	0	6.825408	-0.672242	1.312685
16	1	0	3.755585	0.263068	-1.206580
17	1	0	6.980367	-0.094115	-0.344751
18	6	0	2.663785	-0.566138	1.805390
19	6	0	1.366638	-0.253994	0.076078
20	7	0	1.459236	-0.675028	2.277368
21	7	0	2.651282	-0.313968	0.459464
22	7	0	0.665715	-0.488731	1.190048
23	6	0	3.986957	-0.565650	2.497035
24	1	0	4.499857	-1.527624	2.361115
25	1	0	3.850205	-0.376999	3.561606
26	8	0	4.716447	0.512408	1.947953
27	6	0	-0.747896	-0.546017	1.337188
28	6	0	-1.440593	0.519418	1.904577
29	6	0	-1.439241	-1.680983	0.902760
30	6	0	-2.831298	0.495880	1.936699
31	6	0	-2.821375	-1.719888	0.927745
32	6	0	-3.496465	-0.604524	1.420374
33	1	0	-3.374545	1.349117	2.321769
34	1	0	-3.362287	-2.578187	0.548228
35	35	0	-0.526027	1.970698	2.635668
36	35	0	-5.376372	-0.599264	1.383284

37	35	0	-0.462205	-3.183326	0.318238
38	6	0	0.945130	0.021574	-1.366917
39	8	0	1.835257	0.040504	-2.185091
40	6	0	-0.514551	0.082092	-1.792526
41	6	0	-0.919746	-1.203908	-2.521223
42	1	0	-1.172338	0.311118	-0.951445
43	1	0	-0.629158	-1.053928	-3.567280
44	1	0	-0.345953	-2.060695	-2.157641
45	6	0	-2.396372	-1.492469	-2.384547
46	6	0	-2.845834	-2.807830	-2.259754
47	6	0	-3.325680	-0.446251	-2.330509
48	6	0	-4.196833	-3.079622	-2.049233
49	1	0	-2.128986	-3.624054	-2.298803
50	6	0	-4.672886	-0.719053	-2.112707
51	1	0	-2.994971	0.584285	-2.455575
52	6	0	-5.111387	-2.033701	-1.959436
53	1	0	-4.531482	-4.107343	-1.945145
54	1	0	-5.381335	0.101664	-2.054245
55	1	0	-6.160713	-2.239487	-1.773527
56	6	0	3.423904	4.323530	-0.297536
57	6	0	2.626171	3.026963	-0.138198
58	6	0	1.150279	3.246447	-0.455873
59	6	0	0.979186	3.806325	-1.866411
60	6	0	1.762798	5.109607	-2.033277
61	6	0	3.244607	4.907038	-1.702798
62	1	0	3.005718	2.280148	-0.853120
63	1	0	2.729744	2.606229	0.871998
64	1	0	3.069348	5.053131	0.442890
65	1	0	4.485094	4.150808	-0.084428
66	1	0	1.351762	3.048784	-2.570402
67	1	0	-0.089381	3.929705	-2.073912
68	1	0	1.649190	5.497019	-3.050749
69	1	0	1.347722	5.871463	-1.358855
70	1	0	3.681636	4.214112	-2.435123
71	1	0	3.792647	5.851303	-1.791340
72	1	0	0.750114	3.980189	0.269284
73	8	0	0.452097	2.035612	-0.299919
74	1	0	-0.589958	2.249710	-0.321907
75	6	0	-2.783945	2.774415	-1.022305
76	8	0	-2.482859	3.216996	-2.131956
77	8	0	-1.972808	2.393014	-0.099253
78	6	0	-4.258814	2.646928	-0.633353
79	1	0	-4.468294	1.633950	-0.275203
80	1	0	-4.475896	3.331678	0.192299

81	1	0	-4.904950	2.884611	-1.479556
82	9	0	-0.604447	1.120800	-2.686126

TS7*R*[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.165549	4.526950	0.942736
2	6	0	-0.701471	5.821417	0.724028
3	6	0	-1.525174	6.907809	1.001935
4	6	0	-2.808763	6.668922	1.490935
5	6	0	-3.262222	5.365841	1.709289
6	6	0	-2.437995	4.274313	1.442183
7	6	0	-0.108157	3.518876	0.548656
8	6	0	0.914135	4.346315	-0.298044
9	6	0	0.714420	5.794808	0.199595
10	1	0	-1.179318	7.923191	0.832637
11	1	0	-3.465408	7.506589	1.703818
12	1	0	-4.262710	5.203388	2.097010
13	1	0	-2.764802	3.253401	1.619281
14	1	0	1.927437	3.975488	-0.134685
15	1	0	0.901488	6.499683	-0.614438
16	1	0	0.360323	3.067733	1.422680
17	1	0	1.424826	6.018280	1.003993
18	6	0	-0.975192	2.638082	-1.564793
19	6	0	-1.121585	1.219158	0.087341
20	7	0	-1.562227	1.605555	-2.084815
21	7	0	-0.703082	2.442174	-0.241614
22	7	0	-1.653811	0.719652	-1.042049
23	6	0	-0.561461	3.935563	-2.173231
24	1	0	-1.302122	4.708310	-1.921223
25	1	0	-0.503779	3.834633	-3.256980
26	8	0	0.727457	4.259216	-1.704444
27	6	0	-2.635129	-0.312757	-1.189554
28	6	0	-2.296423	-1.632284	-1.471713
29	6	0	-3.979337	0.044096	-1.064222
30	6	0	-3.290681	-2.588652	-1.651255
31	6	0	-4.984180	-0.891432	-1.248527
32	6	0	-4.619233	-2.200500	-1.548717
33	1	0	-3.025472	-3.616765	-1.863133
34	1	0	-6.024671	-0.611533	-1.145244
35	35	0	-0.492986	-2.111996	-1.554800

36	35	0	-5.971010	-3.488853	-1.796010
37	35	0	-4.418426	1.798538	-0.555036
38	6	0	-1.045819	0.677960	1.525988
39	8	0	-1.110221	1.580517	2.381958
40	6	0	-1.843422	-0.604300	1.742274
41	6	0	-1.693630	-1.177839	3.148164
42	1	0	-1.598314	-1.345479	0.978504
43	1	0	-0.890668	-0.642608	3.664946
44	1	0	-2.615580	-0.941792	3.686334
45	6	0	-1.439259	-2.667474	3.156751
46	6	0	-0.473357	-3.214143	2.305375
47	6	0	-2.146388	-3.518202	4.006845
48	6	0	-0.223825	-4.581876	2.301453
49	1	0	0.103540	-2.565450	1.651327
50	6	0	-1.897176	-4.889350	4.006143
51	1	0	-2.901060	-3.104952	4.671317
52	6	0	-0.936779	-5.425160	3.151593
53	1	0	0.531186	-4.977535	1.629592
54	1	0	-2.459666	-5.539070	4.669828
55	1	0	-0.746139	-6.493886	3.148681
56	9	0	-3.176061	-0.220481	1.549078
57	6	0	2.640921	-0.295363	4.613293
58	6	0	1.864548	-0.798641	3.391894
59	6	0	1.366611	0.383105	2.560362
60	6	0	2.549788	1.255523	2.125120
61	6	0	3.295000	1.793610	3.346464
62	6	0	3.791944	0.632290	4.213698
63	1	0	2.498967	-1.434183	2.762851
64	1	0	1.027970	-1.430418	3.703022
65	1	0	1.954128	0.255582	5.270598
66	1	0	3.019365	-1.143044	5.193480
67	1	0	3.237822	0.647796	1.522336
68	1	0	2.161697	2.042849	1.469302
69	1	0	4.134026	2.426314	3.037125
70	1	0	2.620078	2.425715	3.939208
71	1	0	4.537112	0.059046	3.642589
72	1	0	4.302559	1.012090	5.104890
73	1	0	0.718159	1.009664	3.192432
74	8	0	0.580982	-0.039417	1.449958
75	1	0	1.425981	-0.361664	0.445759
76	7	0	2.193391	-0.683987	-0.398301
77	16	0	2.210611	0.323908	-1.721630
78	8	0	1.576535	-0.249801	-2.896741
79	8	0	1.681446	1.571762	-1.172982

80	16	0	2.734575	-2.256083	-0.414854
81	8	0	2.235660	-2.831567	0.826511
82	8	0	2.434841	-2.890725	-1.693005
83	6	0	4.502608	-2.125571	-0.273654
84	6	0	5.041590	-1.751755	0.954670
85	6	0	5.299975	-2.367237	-1.385547
86	6	0	6.418952	-1.601714	1.064376
87	1	0	4.390433	-1.592560	1.808920
88	6	0	6.678504	-2.210168	-1.262988
89	1	0	4.840673	-2.664897	-2.322179
90	6	0	7.234219	-1.827813	-0.044599
91	1	0	6.855649	-1.315463	2.015702
92	1	0	7.316773	-2.388101	-2.122239
93	1	0	8.309433	-1.708377	0.043619
94	6	0	3.929725	0.540175	-2.115161
95	6	0	4.367758	0.180721	-3.384041
96	6	0	4.789449	1.073494	-1.157192
97	6	0	5.712860	0.360294	-3.701798
98	1	0	3.661608	-0.234998	-4.094168
99	6	0	6.129918	1.234483	-1.482644
100	1	0	4.409574	1.348345	-0.177261
101	6	0	6.587862	0.881000	-2.753448
102	1	0	6.073821	0.088750	-4.688083
103	1	0	6.819891	1.634422	-0.747271
104	1	0	7.636561	1.012417	-3.000989

TS7*S*[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.721090	3.761838	-0.666364
2	6	0	-0.441807	4.849759	-1.489680
3	6	0	-1.389302	5.855850	-1.664878
4	6	0	-2.614202	5.748621	-1.011500
5	6	0	-2.883938	4.660487	-0.177414
6	6	0	-1.933503	3.659696	0.012291
7	6	0	0.422088	2.765937	-0.670650
8	6	0	1.424270	3.317068	-1.750360
9	6	0	0.939799	4.749633	-2.079415
10	1	0	-1.177721	6.706004	-2.306999
11	1	0	-3.365655	6.520099	-1.148226
12	1	0	-3.834812	4.592241	0.341815

13	1	0	-2.123416	2.824191	0.681243
14	1	0	2.432203	3.302977	-1.343142
15	1	0	0.965018	4.917138	-3.161399
16	1	0	0.880729	2.630418	0.307748
17	1	0	1.610534	5.487237	-1.627291
18	6	0	-0.372227	1.215348	-2.417243
19	6	0	-0.713738	0.480153	-0.390834
20	7	0	-1.124469	0.172685	-2.580572
21	7	0	-0.110990	1.448594	-1.093819
22	7	0	-1.331811	-0.278872	-1.308123
23	6	0	0.265508	2.108228	-3.429774
24	1	0	-0.386532	2.967434	-3.646427
25	1	0	0.439232	1.551049	-4.350808
26	8	0	1.512826	2.502756	-2.910953
27	6	0	-2.401752	-1.209163	-1.139318
28	6	0	-2.173750	-2.571717	-0.980893
29	6	0	-3.711030	-0.722285	-1.173195
30	6	0	-3.245932	-3.452938	-0.892705
31	6	0	-4.792665	-1.584841	-1.082810
32	6	0	-4.537192	-2.947576	-0.959452
33	1	0	-3.070355	-4.513810	-0.767124
34	1	0	-5.806278	-1.205421	-1.101466
35	35	0	-0.414006	-3.151802	-0.812704
36	35	0	-5.995069	-4.136945	-0.854792
37	35	0	-3.991368	1.138252	-1.209860
38	6	0	-0.678077	0.397696	1.176517
39	8	0	-0.414552	1.509439	1.709200
40	6	0	-1.975108	-0.290983	1.705903
41	6	0	-2.361223	0.187171	3.104079
42	1	0	-2.790014	-0.004243	1.034244
43	1	0	-2.952551	-0.619649	3.551636
44	1	0	-1.474895	0.356084	3.719909
45	6	0	-3.187322	1.452716	3.029909
46	6	0	-4.463518	1.419697	2.460493
47	6	0	-2.684019	2.674435	3.478736
48	6	0	-5.228259	2.578092	2.352935
49	1	0	-4.864040	0.475148	2.095220
50	6	0	-3.449232	3.833507	3.383893
51	1	0	-1.672663	2.713080	3.870563
52	6	0	-4.724838	3.788355	2.824831
53	1	0	-6.217714	2.532944	1.908117
54	1	0	-3.043537	4.776817	3.735797
55	1	0	-5.319782	4.693687	2.750268
56	9	0	-1.894237	-1.678603	1.658059

57	6	0	1.652790	-3.193464	3.851200
58	6	0	1.381943	-2.584685	2.473080
59	6	0	0.717629	-1.222200	2.625455
60	6	0	1.556562	-0.268744	3.466859
61	6	0	1.830997	-0.882445	4.842127
62	6	0	2.501260	-2.252325	4.710716
63	1	0	2.325126	-2.459723	1.926477
64	1	0	0.739279	-3.225105	1.861950
65	1	0	0.697642	-3.380447	4.361347
66	1	0	2.145966	-4.164031	3.739352
67	1	0	2.503621	-0.106022	2.940553
68	1	0	1.057183	0.701401	3.535005
69	1	0	2.451961	-0.203973	5.436422
70	1	0	0.881852	-0.996144	5.385165
71	1	0	3.485522	-2.124915	4.238389
72	1	0	2.674301	-2.689848	5.699553
73	1	0	-0.259426	-1.367249	3.093635
74	8	0	0.474715	-0.692645	1.298097
75	1	0	1.570992	-0.428146	0.782418
76	7	0	2.692548	-0.372624	0.195482
77	16	0	3.547399	1.039113	0.278899
78	8	0	3.833031	1.558290	-1.056166
79	8	0	2.829895	1.871474	1.238235
80	16	0	2.659257	-1.338555	-1.167347
81	8	0	2.417508	-2.688522	-0.659763
82	8	0	1.734395	-0.775989	-2.147602
83	6	0	4.290279	-1.350550	-1.873522
84	6	0	5.216369	-2.250588	-1.354232
85	6	0	4.584902	-0.514015	-2.946094
86	6	0	6.489203	-2.295331	-1.914589
87	1	0	4.934917	-2.899455	-0.531847
88	6	0	5.861551	-0.570688	-3.496287
89	1	0	3.830386	0.171897	-3.314812
90	6	0	6.809705	-1.454716	-2.978595
91	1	0	7.226940	-2.986838	-1.522051
92	1	0	6.116904	0.073035	-4.331009
93	1	0	7.802754	-1.493825	-3.415136
94	6	0	5.119694	0.618878	1.010368
95	6	0	6.217722	0.413539	0.181627
96	6	0	5.221803	0.530268	2.396953
97	6	0	7.438053	0.071314	0.758158
98	1	0	6.116698	0.527174	-0.893341
99	6	0	6.447105	0.190926	2.959759
100	1	0	4.362404	0.754071	3.019623

101	6	0	7.550726	-0.046077	2.140773
102	1	0	8.299861	-0.100004	0.121281
103	1	0	6.542798	0.121383	4.038110
104	1	0	8.504829	-0.311031	2.585004

TS7*R*[b]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.118690	-1.891781	0.550635
2	6	0	-5.427589	-2.193339	0.187644
3	6	0	-5.873925	-3.511271	0.244229
4	6	0	-4.989542	-4.504434	0.659401
5	6	0	-3.675699	-4.191514	1.018710
6	6	0	-3.228055	-2.874735	0.967076
7	6	0	-3.840967	-0.415462	0.397335
8	6	0	-5.098475	0.154611	-0.354570
9	6	0	-6.176041	-0.951083	-0.227373
10	1	0	-6.891633	-3.763074	-0.038247
11	1	0	-5.323552	-5.536042	0.700876
12	1	0	-3.002424	-4.979696	1.338733
13	1	0	-2.208019	-2.618463	1.244138
14	1	0	-5.414145	1.087842	0.113766
15	1	0	-6.710025	-1.060143	-1.176540
16	1	0	-3.690385	0.081435	1.351336
17	1	0	-6.916547	-0.670622	0.528553
18	6	0	-2.686519	-0.363202	-1.764651
19	6	0	-1.316579	-0.100131	-0.074671
20	7	0	-1.506999	-0.330988	-2.304319
21	7	0	-2.616174	-0.231666	-0.403944
22	7	0	-0.670345	-0.175283	-1.246936
23	6	0	-4.036617	-0.416008	-2.399276
24	1	0	-4.448200	-1.434102	-2.359377
25	1	0	-3.969689	-0.096712	-3.439175
26	8	0	-4.841275	0.511701	-1.701756
27	6	0	0.731431	-0.232409	-1.465436
28	6	0	1.439447	0.910509	-1.817632
29	6	0	1.398167	-1.425613	-1.195847
30	6	0	2.828358	0.892017	-1.778447
31	6	0	2.780245	-1.468307	-1.155037
32	6	0	3.469119	-0.285425	-1.410737
33	1	0	3.389594	1.793885	-1.986960

34	1	0	3.305538	-2.374188	-0.875519
35	35	0	0.519253	2.457498	-2.318727
36	35	0	5.343373	-0.285767	-1.233117
37	35	0	0.379889	-2.963681	-0.805371
38	6	0	-0.872769	0.141728	1.391434
39	8	0	-1.774157	0.127225	2.208157
40	6	0	0.554898	-0.014324	1.887166
41	6	0	0.815335	-1.441647	2.407040
42	1	0	0.689818	0.746547	2.660447
43	1	0	0.509447	-1.473978	3.457599
44	1	0	0.186585	-2.162989	1.874253
45	6	0	2.262428	-1.859255	2.234099
46	6	0	2.559996	-3.173444	1.870512
47	6	0	3.313693	-0.943833	2.379488
48	6	0	3.874349	-3.566216	1.618570
49	1	0	1.753846	-3.892942	1.755408
50	6	0	4.622298	-1.333094	2.114381
51	1	0	3.104340	0.088213	2.656668
52	6	0	4.908286	-2.640857	1.722826
53	1	0	4.085100	-4.591841	1.330691
54	1	0	5.422498	-0.604172	2.202035
55	1	0	5.930038	-2.933823	1.502321
56	6	0	-3.433429	4.207141	0.174391
57	6	0	-2.548775	2.962673	0.093496
58	6	0	-1.199242	3.202475	0.766986
59	6	0	-1.392656	3.616547	2.225441
60	6	0	-2.281950	4.858188	2.328912
61	6	0	-3.628430	4.635773	1.631967
62	1	0	-3.052549	2.139769	0.622073
63	1	0	-2.383528	2.644417	-0.944843
64	1	0	-2.955576	5.025061	-0.381426
65	1	0	-4.400217	4.020015	-0.306101
66	1	0	-1.855037	2.773901	2.758303
67	1	0	-0.408274	3.780543	2.676075
68	1	0	-2.436839	5.131877	3.377648
69	1	0	-1.771473	5.706793	1.853275
70	1	0	-4.180208	3.847900	2.164074
71	1	0	-4.240690	5.542395	1.682919
72	1	0	-0.703350	4.035268	0.233171
73	8	0	-0.371715	2.071243	0.650384
74	1	0	0.693999	2.436406	0.647837
75	6	0	2.647024	2.627776	1.494101
76	8	0	2.258722	2.311320	2.626153
77	8	0	1.893095	2.907416	0.491013

78	6	0	4.138660	2.644493	1.190182
79	1	0	4.401427	1.691688	0.714328
80	1	0	4.386058	3.444512	0.489548
81	1	0	4.717278	2.744206	2.109175
82	9	0	1.447704	0.282600	0.887352

TS7*S*[b]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.289243	-1.688653	0.595231
2	6	0	-5.602202	-1.962978	0.224979
3	6	0	-6.136198	-3.227537	0.458978
4	6	0	-5.333884	-4.196956	1.056661
5	6	0	-4.014666	-3.912992	1.420229
6	6	0	-3.479577	-2.648646	1.191599
7	6	0	-3.917338	-0.266702	0.248941
8	6	0	-5.106416	0.256165	-0.635455
9	6	0	-6.255254	-0.754596	-0.398789
10	1	0	-7.158658	-3.457451	0.175093
11	1	0	-5.737243	-5.187724	1.239062
12	1	0	-3.406366	-4.682139	1.884149
13	1	0	-2.454617	-2.415397	1.470966
14	1	0	-5.378963	1.266002	-0.326608
15	1	0	-6.760408	-0.971377	-1.345116
16	1	0	-3.771289	0.347539	1.133866
17	1	0	-7.002944	-0.324604	0.275175
18	6	0	-2.668938	-0.577834	-1.846781
19	6	0	-1.372741	-0.141120	-0.141724
20	7	0	-1.464727	-0.673130	-2.321877
21	7	0	-2.657233	-0.256760	-0.514641
22	7	0	-0.672701	-0.407463	-1.249481
23	6	0	-3.994217	-0.663781	-2.528920
24	1	0	-4.457317	-1.646083	-2.361235
25	1	0	-3.872892	-0.502426	-3.599936
26	8	0	-4.774933	0.391581	-2.008146
27	6	0	0.740084	-0.492340	-1.382600
28	6	0	1.468484	0.567885	-1.910335
29	6	0	1.393318	-1.655346	-0.963806
30	6	0	2.858867	0.515851	-1.906170
31	6	0	2.774543	-1.724016	-0.951608
32	6	0	3.485737	-0.610314	-1.395908

33	1	0	3.431600	1.365240	-2.255541
34	1	0	3.286156	-2.602975	-0.578137
35	35	0	0.591998	2.047159	-2.631128
36	35	0	5.363429	-0.641928	-1.294604
37	35	0	0.363014	-3.145608	-0.447169
38	6	0	-0.944924	0.257730	1.277780
39	8	0	-1.842588	0.364155	2.089754
40	6	0	0.505901	0.141513	1.725813
41	6	0	0.777113	-1.188481	2.428925
42	1	0	1.195681	0.314415	0.897635
43	1	0	0.443406	-1.058803	3.464624
44	1	0	0.167069	-1.988533	1.999801
45	6	0	2.236958	-1.574444	2.348219
46	6	0	2.607064	-2.915102	2.233076
47	6	0	3.233898	-0.591049	2.327769
48	6	0	3.944069	-3.271373	2.064025
49	1	0	1.839888	-3.684830	2.246322
50	6	0	4.567575	-0.946931	2.152801
51	1	0	2.964228	0.457290	2.443451
52	6	0	4.926502	-2.286256	2.008425
53	1	0	4.215078	-4.318241	1.965967
54	1	0	5.327698	-0.172013	2.119451
55	1	0	5.966095	-2.558119	1.855649
56	6	0	-3.357023	4.393099	0.268693
57	6	0	-2.572572	3.090229	0.093956
58	6	0	-1.110822	3.278071	0.491081
59	6	0	-0.989931	3.781605	1.928056
60	6	0	-1.769105	5.085870	2.109016
61	6	0	-3.236004	4.915234	1.704026
62	1	0	-3.003080	2.322366	0.753150
63	1	0	-2.627634	2.717280	-0.938242
64	1	0	-2.957362	5.146683	-0.423227
65	1	0	-4.408931	4.244996	-0.000578
66	1	0	-1.391877	3.004883	2.592842
67	1	0	0.071275	3.897285	2.173566
68	1	0	-1.698042	5.431225	3.145420
69	1	0	-1.315028	5.868750	1.485499
70	1	0	-3.712938	4.197892	2.386290
71	1	0	-3.777325	5.861858	1.807655
72	1	0	-0.672368	4.036132	-0.185312
73	8	0	-0.399340	2.075559	0.301922
74	1	0	0.682309	2.292629	0.343463
75	6	0	2.794048	2.818890	1.079026
76	8	0	2.478203	3.371158	2.129498

77	8	0	1.992693	2.402515	0.154629
78	6	0	4.267321	2.580574	0.750015
79	1	0	4.425430	1.537463	0.458052
80	1	0	4.551522	3.200796	-0.105871
81	1	0	4.897608	2.832147	1.603579
82	9	0	0.700288	1.150131	2.639996

M07*R*[b]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.043317	-1.772055	0.670584
2	6	0	-5.342835	-2.144644	0.341953
3	6	0	-5.774831	-3.443674	0.597573
4	6	0	-4.888134	-4.345661	1.182068
5	6	0	-3.589860	-3.956261	1.523481
6	6	0	-3.157883	-2.657149	1.273217
7	6	0	-3.776821	-0.330532	0.314743
8	6	0	-5.049423	0.121566	-0.490768
9	6	0	-6.106731	-0.983811	-0.243927
10	1	0	-6.785426	-3.750547	0.344799
11	1	0	-5.211656	-5.362226	1.381831
12	1	0	-2.919009	-4.669031	1.991831
13	1	0	-2.165636	-2.320607	1.559217
14	1	0	-5.388580	1.094499	-0.132284
15	1	0	-6.619745	-1.223215	-1.180955
16	1	0	-3.584411	0.272793	1.201726
17	1	0	-6.868614	-0.628478	0.457273
18	6	0	-2.638262	-0.499726	-1.862601
19	6	0	-1.280578	0.027574	-0.212279
20	7	0	-1.469953	-0.443675	-2.423505
21	7	0	-2.567180	-0.223161	-0.521005
22	7	0	-0.644571	-0.118091	-1.387464
23	6	0	-3.992645	-0.666505	-2.465764
24	1	0	-4.383158	-1.678315	-2.288813
25	1	0	-3.949892	-0.480491	-3.538722
26	8	0	-4.807002	0.327085	-1.874929
27	6	0	0.763381	-0.187090	-1.549368
28	6	0	1.518871	0.955002	-1.780305
29	6	0	1.395123	-1.410449	-1.326345
30	6	0	2.902696	0.906297	-1.661977
31	6	0	2.769784	-1.481750	-1.178228

32	6	0	3.494310	-0.300752	-1.308099
33	1	0	3.492032	1.806431	-1.784919
34	1	0	3.256067	-2.415637	-0.918034
35	35	0	0.653764	2.562752	-2.196892
36	35	0	5.346956	-0.344876	-0.965092
37	35	0	0.340023	-2.963271	-1.203139
38	6	0	-0.822715	0.678094	1.235382
39	8	0	-1.793008	0.605142	2.058698
40	6	0	0.499683	0.097406	1.778747
41	6	0	0.487367	-1.400621	2.048458
42	1	0	0.699680	0.677633	2.684365
43	1	0	-0.035326	-1.567971	2.996400
44	1	0	-0.103777	-1.906568	1.275576
45	6	0	1.869241	-2.030613	2.052431
46	6	0	1.999065	-3.384037	1.728323
47	6	0	3.033189	-1.297486	2.317863
48	6	0	3.252486	-3.982570	1.620178
49	1	0	1.106189	-3.969330	1.525573
50	6	0	4.286971	-1.889706	2.195919
51	1	0	2.967936	-0.246706	2.584986
52	6	0	4.404318	-3.230882	1.836601
53	1	0	3.326848	-5.033589	1.357820
54	1	0	5.177487	-1.295003	2.375857
55	1	0	5.383928	-3.686780	1.732646
56	6	0	-3.334132	4.277034	0.021333
57	6	0	-2.554848	2.959140	0.041752
58	6	0	-1.244038	3.137421	0.803710
59	6	0	-1.476809	3.631525	2.229488
60	6	0	-2.261536	4.945966	2.206442
61	6	0	-3.579946	4.788462	1.443736
62	1	0	-3.152470	2.196166	0.550887
63	1	0	-2.342504	2.611206	-0.978244
64	1	0	-2.760485	5.028950	-0.537668
65	1	0	-4.281908	4.143055	-0.510804
66	1	0	-2.022748	2.858376	2.777644
67	1	0	-0.504143	3.757440	2.718791
68	1	0	-2.450084	5.290463	3.228189
69	1	0	-1.658425	5.723683	1.717159
70	1	0	-4.218980	4.071582	1.977245
71	1	0	-4.121697	5.739753	1.415532
72	1	0	-0.664208	3.906753	0.266958
73	8	0	-0.380397	2.003639	0.751794
74	1	0	1.267472	2.603378	0.758517
75	6	0	2.939363	2.636916	1.648210

76	8	0	2.489909	2.275723	2.715643
77	8	0	2.185052	2.939537	0.593111
78	6	0	4.410303	2.747309	1.348729
79	1	0	4.714330	1.834739	0.823453
80	1	0	4.613873	3.597137	0.695682
81	1	0	4.973117	2.826195	2.277327
82	9	0	1.537616	0.387348	0.894906

M07*S*[b]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.090977	-1.655088	-0.739394
2	6	0	5.366675	-2.077640	-0.381583
3	6	0	5.801973	-3.348715	-0.749588
4	6	0	4.944181	-4.169047	-1.478684
5	6	0	3.674301	-3.723546	-1.857241
6	6	0	3.238169	-2.452813	-1.494030
7	6	0	3.812392	-0.257219	-0.248641
8	6	0	5.077993	0.128424	0.605261
9	6	0	6.116554	-0.993596	0.349917
10	1	0	6.794683	-3.694263	-0.476711
11	1	0	5.271129	-5.162221	-1.769558
12	1	0	3.032026	-4.367868	-2.448686
13	1	0	2.277173	-2.059156	-1.813042
14	1	0	5.448320	1.103105	0.285016
15	1	0	6.548403	-1.324757	1.300295
16	1	0	3.616058	0.420881	-1.078124
17	1	0	6.943276	-0.615355	-0.259294
18	6	0	2.657179	-0.567787	1.920651
19	6	0	1.311802	0.005455	0.284010
20	7	0	1.480922	-0.560306	2.469624
21	7	0	2.597851	-0.232701	0.591013
22	7	0	0.662351	-0.202232	1.438729
23	6	0	4.006854	-0.732553	2.533651
24	1	0	4.417864	-1.729534	2.321562
25	1	0	3.949312	-0.589891	3.612495
26	8	0	4.807059	0.297008	1.988847
27	6	0	-0.748555	-0.286032	1.570333
28	6	0	-1.518927	0.841262	1.832184
29	6	0	-1.368823	-1.511747	1.312912
30	6	0	-2.903511	0.774504	1.723039

31	6	0	-2.745219	-1.596696	1.182236
32	6	0	-3.486511	-0.429955	1.353393
33	1	0	-3.503107	1.664311	1.867264
34	1	0	-3.221631	-2.530068	0.902372
35	35	0	-0.689917	2.454216	2.287678
36	35	0	-5.341650	-0.478722	1.041418
37	35	0	-0.296109	-3.040614	1.103418
38	6	0	0.818417	0.655453	-1.118785
39	8	0	1.761915	0.615581	-1.973766
40	6	0	-0.545503	0.062353	-1.560052
41	6	0	-0.505542	-1.374147	-2.038706
42	1	0	-1.296993	0.187002	-0.774970
43	1	0	-0.054136	-1.369065	-3.037579
44	1	0	0.163156	-1.956262	-1.393456
45	6	0	-1.876154	-2.021936	-2.030591
46	6	0	-2.008035	-3.395209	-1.808537
47	6	0	-3.039637	-1.256294	-2.175653
48	6	0	-3.265168	-3.984879	-1.695962
49	1	0	-1.115056	-4.003958	-1.693862
50	6	0	-4.297365	-1.842124	-2.061892
51	1	0	-2.956635	-0.190926	-2.370375
52	6	0	-4.415514	-3.207365	-1.810501
53	1	0	-3.345405	-5.051950	-1.512122
54	1	0	-5.186826	-1.227216	-2.159636
55	1	0	-5.395595	-3.663076	-1.711107
56	6	0	3.228946	4.328677	0.119900
57	6	0	2.493342	2.986561	0.085131
58	6	0	1.171482	3.133125	-0.663108
59	6	0	1.371521	3.650685	-2.085023
60	6	0	2.117442	4.987934	-2.049855
61	6	0	3.446013	4.864846	-1.298049
62	1	0	3.113746	2.255821	-0.443323
63	1	0	2.303532	2.611755	1.100161
64	1	0	2.634375	5.053496	0.692771
65	1	0	4.184868	4.220065	0.643176
66	1	0	1.933938	2.900906	-2.648915
67	1	0	0.389947	3.753092	-2.560963
68	1	0	2.287395	5.351131	-3.068294
69	1	0	1.493524	5.740493	-1.547245
70	1	0	4.104553	4.175967	-1.844652
71	1	0	3.956449	5.833152	-1.262211
72	1	0	0.571873	3.876830	-0.111556
73	8	0	0.348786	1.970368	-0.609746
74	1	0	-1.318161	2.454750	-0.838375

75	6	0	-3.029604	2.881716	-1.625605
76	8	0	-2.583826	3.361160	-2.640555
77	8	0	-2.277630	2.477835	-0.597540
78	6	0	-4.497501	2.689481	-1.333231
79	1	0	-4.671349	1.705174	-0.889788
80	1	0	-4.816870	3.439777	-0.603913
81	1	0	-5.073914	2.809541	-2.248763
82	9	0	-0.957494	0.868008	-2.615283

M7*R*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.528498	-0.737663	0.663741
2	6	0	-5.843366	-0.815458	0.215277
3	6	0	-6.653897	-1.872805	0.621539
4	6	0	-6.123206	-2.834047	1.478271
5	6	0	-4.807479	-2.733446	1.939118
6	6	0	-3.994074	-1.675914	1.540941
7	6	0	-3.827978	0.479518	0.113358
8	6	0	-4.873486	1.135619	-0.867895
9	6	0	-6.197862	0.358301	-0.660055
10	1	0	-7.681574	-1.945979	0.277814
11	1	0	-6.741941	-3.666254	1.799184
12	1	0	-4.418719	-3.482607	2.621182
13	1	0	-2.978379	-1.561966	1.906613
14	1	0	-4.984935	2.190918	-0.617592
15	1	0	-6.613567	0.066956	-1.630813
16	1	0	-3.499142	1.145227	0.911501
17	1	0	-6.942933	0.997665	-0.176593
18	6	0	-2.628719	-0.230396	-1.947360
19	6	0	-1.330725	0.002911	-0.197862
20	7	0	-1.447288	-0.530146	-2.391827
21	7	0	-2.598629	0.108965	-0.618623
22	7	0	-0.653383	-0.387139	-1.287052
23	6	0	-3.924395	-0.080143	-2.668891
24	1	0	-4.591016	-0.927496	-2.454677
25	1	0	-3.755187	-0.017805	-3.743622
26	8	0	-4.471887	1.146248	-2.230610
27	6	0	0.753557	-0.544750	-1.424808
28	6	0	1.542791	0.542916	-1.797600
29	6	0	1.353975	-1.784437	-1.208191

30	6	0	2.923200	0.420185	-1.884305
31	6	0	2.733264	-1.928971	-1.282025
32	6	0	3.498009	-0.814755	-1.607209
33	1	0	3.533565	1.270386	-2.161231
34	1	0	3.197565	-2.885858	-1.080706
35	35	0	0.726028	2.168693	-2.224966
36	35	0	5.372238	-0.981885	-1.678087
37	35	0	0.282955	-3.252079	-0.748187
38	6	0	-0.798010	0.367408	1.259746
39	8	0	-1.753289	0.741650	2.028428
40	6	0	0.030247	-0.829269	1.785942
41	6	0	0.723554	-0.484015	3.103643
42	1	0	0.772306	-1.168010	1.061629
43	1	0	0.444127	0.535628	3.390482
44	1	0	0.318938	-1.148517	3.872035
45	6	0	2.228384	-0.625855	3.035915
46	6	0	2.946285	-0.141855	1.934552
47	6	0	2.934478	-1.249963	4.065742
48	6	0	4.329060	-0.286870	1.865698
49	1	0	2.408745	0.360100	1.131615
50	6	0	4.319143	-1.392111	4.002590
51	1	0	2.391185	-1.635699	4.924714
52	6	0	5.021076	-0.914934	2.899563
53	1	0	4.866457	0.078193	0.995223
54	1	0	4.847107	-1.885515	4.812928
55	1	0	6.098717	-1.032673	2.843946
56	9	0	-0.851942	-1.895103	1.958880
57	6	0	1.410631	4.767893	1.837694
58	6	0	1.443020	3.319100	1.348330
59	6	0	0.074442	2.653263	1.461621
60	6	0	-1.008300	3.468185	0.751273
61	6	0	-1.033580	4.912176	1.259786
62	6	0	0.337130	5.573089	1.102501
63	1	0	1.741353	3.283980	0.291131
64	1	0	2.174480	2.728427	1.911133
65	1	0	1.191862	4.781826	2.914109
66	1	0	2.395202	5.229545	1.709996
67	1	0	-0.800277	3.458523	-0.324917
68	1	0	-1.971865	2.977161	0.912492
69	1	0	-1.801491	5.484887	0.729246
70	1	0	-1.313841	4.917626	2.322010
71	1	0	0.592521	5.621926	0.034516
72	1	0	0.311650	6.603499	1.472670
73	1	0	-0.212700	2.562254	2.518754

74	8	0	0.233879	1.352707	0.905607

M7*S*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.029984	0.303692	-0.643426
2	6	0	-5.213617	0.435599	-1.364691
3	6	0	-6.261367	-0.455962	-1.150819
4	6	0	-6.094626	-1.472947	-0.213203
5	6	0	-4.907464	-1.589636	0.513981
6	6	0	-3.860661	-0.692652	0.312673
7	6	0	-3.021671	1.350247	-1.053459
8	6	0	-3.667234	2.056766	-2.301566
9	6	0	-5.150731	1.615379	-2.301517
10	1	0	-7.189126	-0.365274	-1.708273
11	1	0	-6.898690	-2.182112	-0.042674
12	1	0	-4.796636	-2.377351	1.251020
13	1	0	-2.942286	-0.746020	0.894290
14	1	0	-3.564937	3.138016	-2.208282
15	1	0	-5.468696	1.383054	-3.323025
16	1	0	-2.777184	2.030322	-0.236680
17	1	0	-5.788479	2.430422	-1.943883
18	6	0	-1.582223	0.152153	-2.674357
19	6	0	-0.649932	0.455169	-0.716137
20	7	0	-0.424898	-0.425787	-2.785094
21	7	0	-1.751763	0.708196	-1.432563
22	7	0	0.136140	-0.228200	-1.553949
23	6	0	-2.651616	0.400656	-3.685337
24	1	0	-3.499729	-0.281337	-3.531626
25	1	0	-2.258103	0.265231	-4.692560
26	8	0	-3.024475	1.755607	-3.534254
27	6	0	1.428930	-0.735324	-1.264712
28	6	0	2.552866	0.072725	-1.418613
29	6	0	1.574568	-2.042147	-0.803859
30	6	0	3.805665	-0.392000	-1.041369
31	6	0	2.815843	-2.526934	-0.421612
32	6	0	3.912965	-1.679540	-0.529271
33	1	0	4.678328	0.240277	-1.145676
34	1	0	2.923167	-3.535601	-0.043990
35	35	0	2.375724	1.770420	-2.183307
36	35	0	5.602451	-2.302078	0.024356

37	35	0	0.057566	-3.148221	-0.689007
38	6	0	-0.392925	0.957566	0.771710
39	8	0	-1.488288	1.382383	1.301193
40	6	0	0.263571	-0.214261	1.598223
41	6	0	-0.166634	-0.212681	3.063790
42	1	0	-0.029273	-1.176062	1.159449
43	1	0	0.642174	-0.700937	3.619510
44	1	0	-0.274527	0.810928	3.425564
45	6	0	-1.456074	-0.964249	3.292556
46	6	0	-1.517097	-2.344900	3.080525
47	6	0	-2.607079	-0.301914	3.722989
48	6	0	-2.693173	-3.052501	3.318933
49	1	0	-0.633517	-2.873761	2.726909
50	6	0	-3.781820	-1.005337	3.970076
51	1	0	-2.575799	0.777067	3.835447
52	6	0	-3.826314	-2.385032	3.778401
53	1	0	-2.720618	-4.125949	3.157298
54	1	0	-4.667582	-0.474824	4.305750
55	1	0	-4.742152	-2.934478	3.974924
56	9	0	1.656849	-0.157445	1.533661
57	6	0	3.224160	3.850588	2.321159
58	6	0	2.606576	2.989482	1.217355
59	6	0	1.141833	2.686764	1.515599
60	6	0	0.339090	3.969183	1.718161
61	6	0	0.956090	4.834696	2.819723
62	6	0	2.426347	5.141428	2.523290
63	1	0	2.658253	3.519541	0.257157
64	1	0	3.141919	2.041023	1.095845
65	1	0	3.231363	3.282938	3.261882
66	1	0	4.268721	4.078406	2.083845
67	1	0	0.341353	4.518131	0.766131
68	1	0	-0.696087	3.699588	1.941387
69	1	0	0.386752	5.762726	2.937531
70	1	0	0.888971	4.301073	3.778262
71	1	0	2.487848	5.746995	1.608552
72	1	0	2.865001	5.737886	3.330526
73	1	0	1.101669	2.091970	2.439834
74	8	0	0.629186	1.927881	0.429462

TS8*R*

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

1	6	0	-4.296865	-1.248473	0.529795
2	6	0	-5.607382	-1.373184	0.082799
3	6	0	-6.210823	-2.628806	0.060729
4	6	0	-5.478988	-3.734250	0.488786
5	6	0	-4.164403	-3.593685	0.944612
6	6	0	-3.558507	-2.341097	0.972210
7	6	0	-3.810480	0.177919	0.443184
8	6	0	-4.992044	0.961175	-0.238740
9	6	0	-6.180796	-0.033607	-0.305245
10	1	0	-7.232765	-2.746783	-0.287594
11	1	0	-5.936678	-4.718442	0.470959
12	1	0	-3.616572	-4.467192	1.283557
13	1	0	-2.545938	-2.195090	1.340139
14	1	0	-5.240887	1.837928	0.359428
15	1	0	-6.622523	-0.022932	-1.307412
16	1	0	-3.531284	0.584610	1.418223
17	1	0	-6.968602	0.271392	0.390759
18	6	0	-2.660717	0.329524	-1.753029
19	6	0	-1.325363	0.049142	-0.009145
20	7	0	-1.481817	0.230460	-2.283957
21	7	0	-2.601709	0.239310	-0.385080
22	7	0	-0.673057	0.062674	-1.183570
23	6	0	-3.994997	0.592729	-2.366376
24	1	0	-4.555224	-0.346499	-2.482709
25	1	0	-3.883677	1.063772	-3.342871
26	8	0	-4.663508	1.498910	-1.511755
27	6	0	0.695792	-0.260151	-1.356288
28	6	0	1.634164	0.709133	-1.704087
29	6	0	1.122476	-1.578152	-1.169944
30	6	0	2.982129	0.390963	-1.812599
31	6	0	2.466227	-1.916831	-1.256059
32	6	0	3.380102	-0.917654	-1.567782
33	1	0	3.705415	1.153435	-2.073821
34	1	0	2.791203	-2.933832	-1.077099
35	35	0	1.074811	2.461604	-2.066559
36	35	0	5.211635	-1.343540	-1.648906
37	35	0	-0.140476	-2.905693	-0.746677
38	6	0	-0.691262	0.396900	1.736396
39	8	0	-1.664604	0.649527	2.467778
40	6	0	0.195189	-0.816525	2.047265
41	6	0	1.113774	-0.545355	3.249856
42	1	0	0.799089	-1.088103	1.181212
43	1	0	0.893223	0.447325	3.656661

44	1	0	0.864267	-1.277194	4.022651
45	6	0	2.576563	-0.650535	2.879800
46	6	0	3.101886	0.145641	1.853338
47	6	0	3.419002	-1.564900	3.512544
48	6	0	4.433808	0.022925	1.473095
49	1	0	2.448064	0.854689	1.349427
50	6	0	4.753893	-1.691428	3.129532
51	1	0	3.023391	-2.192102	4.307194
52	6	0	5.264048	-0.902232	2.103712
53	1	0	4.826557	0.641908	0.670778
54	1	0	5.391541	-2.414182	3.629383
55	1	0	6.299091	-1.005662	1.793053
56	9	0	-0.636879	-1.892749	2.320339
57	6	0	0.760044	5.094474	1.712770
58	6	0	1.057040	3.604886	1.536094
59	6	0	-0.205754	2.757933	1.654935
60	6	0	-1.319388	3.236346	0.722075
61	6	0	-1.592829	4.731318	0.905941
62	6	0	-0.315779	5.553827	0.726669
63	1	0	1.486716	3.426448	0.542492
64	1	0	1.789166	3.254832	2.272446
65	1	0	0.408895	5.279667	2.736998
66	1	0	1.678558	5.675818	1.583368
67	1	0	-1.014069	3.034304	-0.312363
68	1	0	-2.223613	2.653284	0.924333
69	1	0	-2.366401	5.057605	0.203401
70	1	0	-1.989463	4.905090	1.915602
71	1	0	0.057260	5.424027	-0.299471
72	1	0	-0.525521	6.620446	0.858375
73	1	0	-0.581758	2.783799	2.686398
74	8	0	0.202237	1.422122	1.354676

TS8*S*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.020930	0.482875	-0.526727
2	6	0	-5.241186	0.652154	-1.174216
3	6	0	-6.292818	-0.224453	-0.918310
4	6	0	-6.093363	-1.264583	-0.014518
5	6	0	-4.867690	-1.421491	0.638690
6	6	0	-3.816598	-0.541516	0.393770

7	6	0	-3.009562	1.511868	-0.976080
8	6	0	-3.737932	2.314546	-2.118861
9	6	0	-5.214918	1.847651	-2.091619
10	1	0	-7.249235	-0.103347	-1.418702
11	1	0	-6.900861	-1.961296	0.188424
12	1	0	-4.731800	-2.230807	1.347314
13	1	0	-2.863838	-0.640415	0.912828
14	1	0	-3.653784	3.384264	-1.925892
15	1	0	-5.552218	1.621179	-3.108623
16	1	0	-2.683940	2.153183	-0.153335
17	1	0	-5.861079	2.646356	-1.713519
18	6	0	-1.711426	0.417812	-2.790099
19	6	0	-0.718015	0.481722	-0.800477
20	7	0	-0.598046	-0.219937	-2.986284
21	7	0	-1.808553	0.860708	-1.494802
22	7	0	-0.016122	-0.169175	-1.738283
23	6	0	-2.805116	0.815034	-3.724373
24	1	0	-3.666617	0.138913	-3.622273
25	1	0	-2.459228	0.797003	-4.757756
26	8	0	-3.146326	2.150131	-3.400266
27	6	0	1.251066	-0.743647	-1.484220
28	6	0	2.406522	0.027466	-1.596092
29	6	0	1.352607	-2.055046	-1.024575
30	6	0	3.645338	-0.492699	-1.246648
31	6	0	2.576988	-2.598178	-0.663045
32	6	0	3.708103	-1.798856	-0.777184
33	1	0	4.538754	0.113541	-1.327228
34	1	0	2.644427	-3.612584	-0.291433
35	35	0	2.272279	1.788739	-2.214651
36	35	0	5.379629	-2.500124	-0.255556
37	35	0	-0.217976	-3.073915	-0.826844
38	6	0	-0.267334	1.077519	1.189374
39	8	0	-1.319949	1.459524	1.684810
40	6	0	0.351226	-0.254188	1.674954
41	6	0	0.090449	-0.525775	3.157578
42	1	0	-0.074059	-1.072982	1.088564
43	1	0	0.898735	-1.184818	3.492977
44	1	0	0.144431	0.398140	3.739069
45	6	0	-1.238290	-1.208923	3.376870
46	6	0	-1.429549	-2.513979	2.911521
47	6	0	-2.291165	-0.566940	4.028780
48	6	0	-2.637107	-3.173931	3.119680
49	1	0	-0.626203	-3.016445	2.375451
50	6	0	-3.500287	-1.224345	4.241091

51	1	0	-2.160742	0.459251	4.358188
52	6	0	-3.673149	-2.532507	3.796800
53	1	0	-2.767380	-4.189747	2.758817
54	1	0	-4.309618	-0.712888	4.752397
55	1	0	-4.614974	-3.045926	3.965338
56	9	0	1.721590	-0.244216	1.445165
57	6	0	3.697363	3.551065	2.258972
58	6	0	2.848838	2.813858	1.220654
59	6	0	1.427829	2.620916	1.728740
60	6	0	0.776893	3.945730	2.109225
61	6	0	1.625629	4.688893	3.144377
62	6	0	3.058072	4.888657	2.642134
63	1	0	2.803696	3.392572	0.289225
64	1	0	3.266406	1.831614	0.973970
65	1	0	3.790311	2.927806	3.159088
66	1	0	4.711344	3.705393	1.876406
67	1	0	0.688967	4.547279	1.194843
68	1	0	-0.236544	3.755904	2.475336
69	1	0	1.165819	5.652448	3.386395
70	1	0	1.649821	4.108922	4.077462
71	1	0	3.040900	5.542601	1.759799
72	1	0	3.661533	5.394975	3.402821
73	1	0	1.467872	1.971790	2.617905
74	8	0	0.680438	1.969114	0.692334

P*R*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.456706	1.654288	0.011399
2	8	0	1.195635	2.591437	0.160784
3	6	0	-1.038504	1.753089	-0.252457
4	6	0	-1.877295	1.090600	0.861286
5	1	0	-1.243221	1.276148	-1.218567
6	1	0	-1.219903	0.736366	1.661545
7	1	0	-2.500752	1.885411	1.279334
8	6	0	-2.739090	-0.050055	0.374572
9	6	0	-2.148393	-1.218398	-0.117751
10	6	0	-4.130479	0.045783	0.391230
11	6	0	-2.935661	-2.266892	-0.582226
12	1	0	-1.064026	-1.297024	-0.134075
13	6	0	-4.921049	-1.004399	-0.070748

14	1	0	-4.598347	0.950808	0.769371
15	6	0	-4.325279	-2.162764	-0.560106
16	1	0	-2.465116	-3.168964	-0.960793
17	1	0	-6.002548	-0.914568	-0.049701
18	1	0	-4.939487	-2.981844	-0.920153
19	9	0	-1.352590	3.087420	-0.350954
20	6	0	3.782249	-1.716870	1.033386
21	6	0	2.316273	-1.332416	0.811530
22	6	0	2.222348	0.091092	0.286931
23	6	0	3.011079	0.272635	-1.003758
24	6	0	4.477285	-0.110361	-0.783933
25	6	0	4.599822	-1.539007	-0.248983
26	1	0	1.863396	-2.006325	0.072333
27	1	0	1.738579	-1.422792	1.736862
28	1	0	4.206038	-1.081550	1.822548
29	1	0	3.844576	-2.748929	1.390949
30	1	0	2.565990	-0.375407	-1.770260
31	1	0	2.922819	1.308113	-1.343911
32	1	0	5.033230	-0.000150	-1.719648
33	1	0	4.927086	0.586105	-0.064148
34	1	0	4.232694	-2.241199	-1.009329
35	1	0	5.649719	-1.787590	-0.065094
36	1	0	2.583182	0.801070	1.040425
37	8	0	0.821782	0.365762	0.056550

PS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.146958	-0.665532	1.189781
2	8	0	0.861932	-0.700014	2.157880
3	6	0	0.483306	-1.525312	-0.031686
4	6	0	1.123098	-0.694256	-1.146914
5	1	0	1.179226	-2.289326	0.323806
6	1	0	1.281622	-1.370844	-1.992036
7	1	0	0.418536	0.078605	-1.471388
8	6	0	2.423537	-0.062724	-0.714080
9	6	0	3.638103	-0.714280	-0.934023
10	6	0	2.424747	1.169723	-0.057216
11	6	0	4.834521	-0.142391	-0.511272
12	1	0	3.645464	-1.673251	-1.446359
13	6	0	3.618827	1.743234	0.367888

14	1	0	1.480567	1.678993	0.125322
15	6	0	4.826730	1.088229	0.140207
16	1	0	5.773018	-0.656377	-0.692784
17	1	0	3.605557	2.700772	0.878331
18	1	0	5.758915	1.535469	0.469984
19	9	0	-0.639434	-2.166801	-0.535605
20	6	0	-4.228809	-0.690946	-0.291896
21	6	0	-3.031799	-0.738918	0.661772
22	6	0	-1.928445	0.187124	0.169039
23	6	0	-2.419081	1.618710	0.019462
24	6	0	-3.617393	1.670735	-0.932918
25	6	0	-4.739101	0.742185	-0.460987
26	1	0	-3.333433	-0.406792	1.663160
27	1	0	-2.637954	-1.755635	0.747827
28	1	0	-3.925526	-1.086388	-1.270833
29	1	0	-5.024948	-1.343446	0.078530
30	1	0	-2.708015	1.989481	1.010849
31	1	0	-1.599797	2.250496	-0.340299
32	1	0	-3.978761	2.699790	-1.018015
33	1	0	-3.295108	1.363863	-1.937112
34	1	0	-5.123086	1.103210	0.502285
35	1	0	-5.574591	0.768055	-1.167583
36	1	0	-1.559949	-0.172559	-0.795377
37	8	0	-0.856686	0.221713	1.135770

M0X-Act-D

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.210588	3.158635	0.035410
2	8	0	2.430549	4.283180	0.434877
3	1	0	1.398519	2.957708	-0.691979
4	6	0	2.983959	1.943915	0.469532
5	6	0	3.443559	1.112879	-0.741391
6	1	0	2.305620	1.324789	1.071954
7	1	0	3.829768	2.255623	1.090173
8	1	0	2.586434	0.936119	-1.400914
9	1	0	4.190407	1.676999	-1.312704
10	6	0	4.013408	-0.213387	-0.305919
11	6	0	3.174584	-1.325280	-0.193673
12	6	0	5.357870	-0.343448	0.048314
13	6	0	3.671269	-2.539454	0.270701

14	1	0	2.130199	-1.237786	-0.482737
15	6	0	5.858415	-1.559756	0.507367
16	1	0	6.016933	0.518372	-0.035745
17	6	0	5.014040	-2.661838	0.622193
18	1	0	2.999597	-3.388380	0.356140
19	1	0	6.907230	-1.646142	0.777095
20	1	0	5.401361	-3.609748	0.984073
21	7	0	0.055106	0.721603	-0.028470
22	16	0	-0.182172	-0.454143	1.048703
23	8	0	-0.132110	-1.811412	0.487441
24	8	0	0.671848	-0.158326	2.201225
25	16	0	-0.295863	0.501325	-1.589416
26	8	0	-0.254315	1.834224	-2.201146
27	8	0	0.503675	-0.549853	-2.227740
28	6	0	-1.996533	-0.048782	-1.655705
29	6	0	-3.003782	0.860679	-1.341492
30	6	0	-2.277160	-1.380105	-1.936089
31	6	0	-4.321973	0.422656	-1.309883
32	1	0	-2.741474	1.890473	-1.119227
33	6	0	-3.604410	-1.806579	-1.916381
34	1	0	-1.455511	-2.054545	-2.150933
35	6	0	-4.620860	-0.909095	-1.601382
36	1	0	-5.116910	1.115883	-1.053819
37	1	0	-3.841474	-2.842352	-2.138730
38	1	0	-5.652315	-1.247973	-1.575770
39	6	0	-1.875291	-0.210103	1.591240
40	6	0	-2.792726	-1.244062	1.465565
41	6	0	-2.248734	1.036179	2.090682
42	6	0	-4.116332	-1.025479	1.844203
43	1	0	-2.462569	-2.192873	1.057027
44	6	0	-3.569904	1.244128	2.468472
45	1	0	-1.510738	1.829424	2.160838
46	6	0	-4.503554	0.213893	2.343977
47	1	0	-4.845883	-1.822193	1.735576
48	1	0	-3.875695	2.211025	2.855617
49	1	0	-5.536463	0.383368	2.633057

TS1X-Act-D

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.221277	2.744925	1.901107

2	8	0	2.099109	2.928633	3.088368
3	1	0	2.127974	3.574124	1.174177
4	6	0	2.512928	1.389478	1.311724
5	6	0	3.388561	1.404057	0.065830
6	1	0	1.457723	0.965865	1.025893
7	1	0	2.846917	0.690011	2.084575
8	1	0	2.904284	1.993402	-0.720791
9	1	0	4.325360	1.919825	0.320896
10	6	0	3.699448	0.011610	-0.428319
11	6	0	3.069121	-0.508711	-1.557834
12	6	0	4.599378	-0.791319	0.278306
13	6	0	3.330624	-1.814466	-1.970438
14	1	0	2.356255	0.103132	-2.103273
15	6	0	4.863530	-2.091589	-0.134273
16	1	0	5.097021	-0.389722	1.158575
17	6	0	4.227605	-2.607188	-1.262977
18	1	0	2.823183	-2.211033	-2.844155
19	1	0	5.565415	-2.703823	0.423402
20	1	0	4.430902	-3.623579	-1.585165
21	7	0	0.017305	0.547228	0.562431
22	16	0	0.052396	-1.121419	0.144652
23	8	0	-0.027273	-1.326795	-1.292018
24	8	0	1.138288	-1.668203	0.935789
25	16	0	-0.287638	1.742167	-0.625195
26	8	0	-0.194186	2.984159	0.125541
27	8	0	0.521112	1.565519	-1.820323
28	6	0	-1.973241	1.351026	-0.984329
29	6	0	-2.944918	1.659076	-0.032705
30	6	0	-2.269313	0.727049	-2.192953
31	6	0	-4.264776	1.327368	-0.311651
32	1	0	-2.663740	2.146656	0.895279
33	6	0	-3.598778	0.412637	-2.458280
34	1	0	-1.469774	0.494890	-2.888055
35	6	0	-4.587235	0.709328	-1.520746
36	1	0	-5.041663	1.551585	0.410815
37	1	0	-3.861642	-0.065011	-3.395858
38	1	0	-5.621093	0.456939	-1.733802
39	6	0	-1.510051	-1.568429	0.860714
40	6	0	-2.556353	-1.927507	0.018125
41	6	0	-1.644574	-1.525634	2.247429
42	6	0	-3.782758	-2.253188	0.590734
43	1	0	-2.404578	-1.947153	-1.055451
44	6	0	-2.874918	-1.854035	2.801619
45	1	0	-0.801927	-1.240181	2.868711

46	6	0	-3.939841	-2.213381	1.974042
47	1	0	-4.614266	-2.536595	-0.045611
48	1	0	-3.004994	-1.829555	3.877898
49	1	0	-4.899311	-2.465474	2.414014

M1X-Act-D

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.054802	-0.094780	0.256869
2	8	0	4.086678	-0.719592	-0.116230
3	1	0	2.935859	0.108464	1.362106
4	6	0	2.002556	0.415453	-0.474946
5	6	0	0.863804	1.144879	0.165517
6	1	0	1.989876	0.283738	-1.556096
7	1	0	1.094720	1.251912	1.238068
8	1	0	0.736142	2.178099	-0.204193
9	6	0	-0.506681	0.480975	0.070177
10	6	0	-0.625062	-0.911335	0.087300
11	6	0	-1.678737	1.237934	-0.012268
12	6	0	-1.872517	-1.526423	0.039937
13	1	0	0.294780	-1.489481	0.120929
14	6	0	-2.931422	0.629983	-0.066324
15	1	0	-1.603371	2.323645	-0.037981
16	6	0	-3.034109	-0.758546	-0.038122
17	1	0	-1.941040	-2.611046	0.056789
18	1	0	-3.828270	1.240312	-0.134196
19	1	0	-4.007923	-1.237744	-0.084432

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.753605	-1.814089	0.492425
2	6	0	-4.841878	-2.585476	0.096058
3	6	0	-5.209146	-3.703252	0.841656
4	6	0	-4.468151	-4.026303	1.976339
5	6	0	-3.383865	-3.237868	2.371638
6	6	0	-3.016566	-2.115618	1.633426
7	6	0	-3.516865	-0.670172	-0.466945

8	6	0	-4.489804	-0.956050	-1.668783
9	6	0	-5.485190	-2.019586	-1.144900
10	1	0	-6.055672	-4.314543	0.542923
11	1	0	-4.739558	-4.898288	2.563151
12	1	0	-2.828597	-3.499556	3.266586
13	1	0	-2.208852	-1.453035	1.934600
14	1	0	-4.995315	-0.036085	-1.965402
15	1	0	-5.673098	-2.766326	-1.923002
16	1	0	-3.691599	0.294051	0.006108
17	1	0	-6.447171	-1.553964	-0.906208
18	6	0	-1.716295	-1.544734	-1.899670
19	6	0	-1.044170	-0.017845	-0.461660
20	7	0	-0.436345	-1.484823	-2.086674
21	7	0	-2.121483	-0.671781	-0.926699
22	7	0	-0.030935	-0.537333	-1.176267
23	6	0	-2.774444	-2.299366	-2.633156
24	1	0	-3.099679	-3.175360	-2.054767
25	1	0	-2.400648	-2.628470	-3.602594
26	8	0	-3.830786	-1.386351	-2.852949
27	6	0	1.375240	-0.357901	-1.041810
28	6	0	2.024279	0.757735	-1.570379
29	6	0	2.134000	-1.359141	-0.433812
30	6	0	3.403312	0.887647	-1.471945
31	6	0	3.515858	-1.260498	-0.344121
32	6	0	4.129688	-0.129546	-0.863742
33	1	0	3.898393	1.764930	-1.868762
34	1	0	4.090529	-2.033314	0.150103
35	35	0	1.019694	2.114132	-2.380788
36	35	0	5.999113	0.040711	-0.721267
37	35	0	1.273735	-2.850828	0.311153
38	6	0	-1.219799	1.160070	0.684115
39	8	0	-2.132345	0.810313	1.513449
40	6	0	0.162850	1.450436	1.290072
41	6	0	0.627235	0.286221	2.160739
42	1	0	0.054944	2.356280	1.892222
43	1	0	0.875192	1.688971	0.496662
44	1	0	0.097283	0.333861	3.118175
45	1	0	0.293479	-0.660254	1.710408
46	6	0	2.119148	0.182803	2.390226
47	6	0	2.648244	-1.005539	2.910307
48	6	0	3.006823	1.212404	2.069076
49	6	0	4.019505	-1.174078	3.068069
50	1	0	1.971541	-1.817591	3.164590
51	6	0	4.382233	1.051419	2.233512

52	1	0	2.626954	2.150611	1.676102
53	6	0	4.895805	-0.146293	2.719761
54	1	0	4.406865	-2.110388	3.458975
55	1	0	5.055141	1.858119	1.957569
56	1	0	5.967974	-0.279299	2.824622
57	6	0	-4.760068	4.113160	0.439980
58	6	0	-3.877813	2.888749	0.182774
59	6	0	-2.398073	3.283133	0.148707
60	6	0	-1.994423	3.959263	1.461010
61	6	0	-2.884156	5.175599	1.737597
62	6	0	-4.365699	4.794623	1.751920
63	1	0	-4.015405	2.154119	0.982578
64	1	0	-4.138815	2.414473	-0.772177
65	1	0	-4.645254	4.829883	-0.385515
66	1	0	-5.815437	3.821540	0.460681
67	1	0	-2.090449	3.226379	2.270271
68	1	0	-0.944665	4.267841	1.402899
69	1	0	-2.598040	5.639353	2.687370
70	1	0	-2.718609	5.929541	0.955247
71	1	0	-4.551376	4.102793	2.584335
72	1	0	-4.985410	5.680807	1.926598
73	1	0	-2.278967	4.029329	-0.652783
74	8	0	-1.536689	2.228686	-0.265932

TS6^{S1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.225957	-1.408262	-0.016638
2	6	0	-5.329757	-1.934659	0.652199
3	6	0	-6.611292	-1.498995	0.331269
4	6	0	-6.761576	-0.536770	-0.666184
5	6	0	-5.649002	-0.028957	-1.339343
6	6	0	-4.360661	-0.464674	-1.029422
7	6	0	-2.952060	-2.070163	0.464448
8	6	0	-3.385387	-2.847227	1.763489
9	6	0	-4.916218	-2.991472	1.644209
10	1	0	-7.477903	-1.900924	0.847982
11	1	0	-7.754895	-0.182481	-0.924003
12	1	0	-5.785265	0.718377	-2.115604
13	1	0	-3.475009	-0.063286	-1.531132
14	1	0	-2.881411	-3.813688	1.808956

15	1	0	-5.375847	-2.879846	2.630472
16	1	0	-2.542217	-2.755982	-0.277053
17	1	0	-5.174278	-3.989735	1.273859
18	6	0	-1.883446	-0.450528	1.986796
19	6	0	-0.737792	-0.794192	0.162338
20	7	0	-0.799901	0.241522	2.159264
21	7	0	-1.869882	-1.128247	0.796548
22	7	0	-0.086272	0.016952	1.011079
23	6	0	-2.985159	-0.785774	2.934206
24	1	0	-3.938386	-0.357371	2.599528
25	1	0	-2.749280	-0.423247	3.934230
26	8	0	-3.014998	-2.201040	2.976725
27	6	0	1.270092	0.452836	0.953608
28	6	0	2.312727	-0.480774	0.900105
29	6	0	1.587622	1.814191	0.997712
30	6	0	3.636648	-0.069207	0.838004
31	6	0	2.909743	2.238309	0.934610
32	6	0	3.918417	1.289067	0.842913
33	1	0	4.426233	-0.806912	0.776505
34	1	0	3.140828	3.295763	0.955600
35	35	0	1.981585	-2.324363	0.883470
36	35	0	5.711501	1.851196	0.731711
37	35	0	0.247044	3.110895	1.160916
38	6	0	-0.248558	-1.417460	-1.145272
39	8	0	-0.646048	-2.549240	-1.366067
40	6	0	0.496086	-0.550941	-2.045246
41	6	0	1.206712	-1.297888	-3.166053
42	1	0	1.152912	0.144065	-1.515067
43	1	0	0.493957	-1.955474	-3.671566
44	1	0	1.566089	-0.574079	-3.904013
45	6	0	2.363453	-2.110297	-2.628082
46	6	0	2.251107	-3.488511	-2.429281
47	6	0	3.547133	-1.475469	-2.240024
48	6	0	3.294230	-4.213079	-1.856695
49	1	0	1.328104	-3.987589	-2.710009
50	6	0	4.595035	-2.196968	-1.674524
51	1	0	3.649143	-0.401339	-2.387168
52	6	0	4.469071	-3.570254	-1.474293
53	1	0	3.187982	-5.283440	-1.707418
54	1	0	5.511847	-1.684456	-1.393928
55	1	0	5.282877	-4.134740	-1.030050
56	6	0	-2.570354	4.257756	-2.806842
57	6	0	-2.401369	2.739874	-2.902057
58	6	0	-1.820434	2.130076	-1.614680

59	6	0	-2.719161	2.534146	-0.431479
60	6	0	-2.867913	4.052186	-0.311268
61	6	0	-3.437668	4.641125	-1.605039
62	1	0	-3.377774	2.264709	-3.081853
63	1	0	-1.756399	2.467593	-3.745458
64	1	0	-1.581239	4.723424	-2.692394
65	1	0	-3.000798	4.659205	-3.731216
66	1	0	-3.710180	2.086630	-0.586531
67	1	0	-2.315237	2.096783	0.491055
68	1	0	-3.502426	4.316806	0.542392
69	1	0	-1.882413	4.505494	-0.126816
70	1	0	-4.452542	4.247275	-1.755961
71	1	0	-3.526452	5.730438	-1.525605
72	1	0	-0.836734	2.630455	-1.446218
73	8	0	-1.683399	0.763474	-1.711404
74	1	0	-0.465715	0.167672	-2.268080

P^{S1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.563255	-0.029305	-0.000220
2	8	0	0.894379	-1.192313	-0.000653
3	6	0	-0.869618	0.455333	-0.000059
4	6	0	-1.858640	-0.700236	-0.000676
5	1	0	-0.999501	1.101826	-0.875447
6	1	0	-0.999614	1.100941	0.875969
7	1	0	-1.659140	-1.334404	-0.871803
8	1	0	-1.658957	-1.335486	0.869614
9	6	0	-3.318254	-0.297918	-0.000260
10	6	0	-4.291630	-1.304490	-0.000167
11	6	0	-3.744488	1.030671	0.000005
12	6	0	-5.646002	-0.995497	0.000163
13	1	0	-3.974329	-2.344735	-0.000356
14	6	0	-5.103768	1.345974	0.000341
15	1	0	-3.019705	1.838565	-0.000041
16	6	0	-6.058700	0.336754	0.000418
17	1	0	-6.381684	-1.793932	0.000232
18	1	0	-5.412046	2.386950	0.000546
19	1	0	-7.115817	0.582192	0.000681
20	6	0	4.853384	0.031727	1.262382
21	6	0	3.322002	0.089025	1.266870

22	6	0	2.835974	0.786770	0.000279
23	6	0	3.322295	0.089997	-1.266731
24	6	0	4.853679	0.032706	-1.261938
25	6	0	5.374635	-0.660036	0.000016
26	1	0	2.911423	-0.924229	1.300328
27	1	0	2.953665	0.632044	2.143693
28	1	0	5.257497	1.052342	1.307185
29	1	0	5.206624	-0.487251	2.158615
30	1	0	2.911722	-0.923233	-1.301061
31	1	0	2.954150	0.633684	-2.143221
32	1	0	5.207128	-0.485570	-2.158494
33	1	0	5.257793	1.053359	-1.305848
34	1	0	5.040054	-1.705768	-0.000431
35	1	0	6.469247	-0.674328	0.000143
36	1	0	3.229823	1.810831	0.000720
37	8	0	1.407736	1.010732	0.000209

M07*R*^{S2}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.182785	-2.573486	0.103658
2	6	0	5.390916	-2.466982	0.802296
3	6	0	5.578100	-3.156633	1.993476
4	6	0	4.546786	-3.961510	2.473442
5	6	0	3.357698	-4.096981	1.757177
6	6	0	3.166640	-3.410173	0.558985
7	6	0	4.250130	-1.742900	-1.159248
8	6	0	5.781206	-1.597856	-1.361324
9	6	0	6.369068	-1.589222	0.065732
10	1	0	6.516119	-3.079228	2.534370
11	1	0	4.677933	-4.505001	3.403373
12	1	0	2.576483	-4.752420	2.127775
13	1	0	2.251344	-3.543509	-0.006869
14	1	0	6.113139	-2.501814	-1.876668
15	1	0	6.381389	-0.581269	0.497938
16	1	0	3.727840	-2.160062	-2.020752
17	1	0	7.393969	-1.964787	0.085321
18	6	0	4.444313	0.787743	-1.180193
19	6	0	2.508491	0.034987	-0.549167
20	7	0	3.741746	1.849419	-0.902149
21	7	0	3.720113	-0.357907	-0.963323

22	7	0	2.545557	1.358424	-0.496338
23	6	0	5.852201	0.746345	-1.691046
24	1	0	6.545293	1.038226	-0.892591
25	1	0	5.953445	1.461344	-2.509226
26	8	0	6.139965	-0.530219	-2.207220
27	6	0	1.463396	2.246207	-0.223875
28	6	0	0.473592	2.439108	-1.190187
29	6	0	1.432613	2.956776	0.973289
30	6	0	-0.532177	3.368958	-0.974760
31	6	0	0.410484	3.861400	1.216457
32	6	0	-0.554054	4.053101	0.232710
33	1	0	-1.324177	3.489075	-1.701457
34	1	0	0.366087	4.401245	2.153439
35	35	0	0.455125	1.383475	-2.734977
36	35	0	-1.967830	5.242499	0.565566
37	35	0	2.776179	2.687062	2.255553
38	6	0	1.317114	-0.882374	-0.336796
39	8	0	1.202556	-1.796012	-1.108150
40	6	0	0.473722	-0.611997	0.892386
41	6	0	-0.128743	-1.905099	1.401123
42	1	0	-0.293232	0.139944	0.675384
43	1	0	-0.502812	-2.447153	0.527926
44	1	0	0.688042	-2.499930	1.833618
45	6	0	-1.246119	-1.736642	2.399108
46	6	0	-2.241561	-2.714680	2.468712
47	6	0	-1.302080	-0.646199	3.269571
48	6	0	-3.263227	-2.618952	3.408905
49	1	0	-2.218141	-3.548680	1.770155
50	6	0	-2.334079	-0.541255	4.199094
51	1	0	-0.543682	0.129043	3.212072
52	6	0	-3.312293	-1.530262	4.278053
53	1	0	-4.031129	-3.386173	3.449253
54	1	0	-2.374188	0.317334	4.861684
55	1	0	-4.113284	-1.447050	5.006111
56	9	0	1.371813	-0.068645	1.820602
57	7	0	-1.734072	-0.447535	-1.037131
58	16	0	-2.072014	-1.377564	-2.318378
59	8	0	-3.281112	-0.963680	-3.037359
60	8	0	-0.848916	-1.584058	-3.097843
61	16	0	-2.663636	0.808660	-0.636089
62	8	0	-2.059441	1.335705	0.599845
63	8	0	-2.879429	1.762296	-1.729717
64	6	0	-4.268907	0.169801	-0.191657
65	6	0	-4.417503	-0.414947	1.061883

66	6	0	-5.303786	0.192748	-1.121258
67	6	0	-5.632142	-1.013090	1.383483
68	1	0	-3.591627	-0.392055	1.765854
69	6	0	-6.515598	-0.406297	-0.786151
70	1	0	-5.137937	0.652509	-2.088455
71	6	0	-6.675755	-1.014306	0.459148
72	1	0	-5.759049	-1.474402	2.358000
73	1	0	-7.333607	-0.402990	-1.499142
74	1	0	-7.621393	-1.484376	0.711574
75	6	0	-2.451659	-2.948461	-1.541966
76	6	0	-3.735187	-3.158968	-1.042988
77	6	0	-1.455708	-3.911658	-1.414896
78	6	0	-4.018527	-4.356332	-0.392979
79	1	0	-4.500319	-2.399357	-1.175198
80	6	0	-1.750788	-5.108375	-0.763514
81	1	0	-0.472928	-3.710003	-1.829728
82	6	0	-3.028821	-5.329589	-0.252680
83	1	0	-5.015156	-4.528945	0.001079
84	1	0	-0.985887	-5.872029	-0.662455
85	1	0	-3.255686	-6.264210	0.250768

M07*S*^{R2}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.297816	-2.112724	0.155445
2	6	0	-5.553108	-2.711938	0.257931
3	6	0	-5.881147	-3.782071	-0.566198
4	6	0	-4.941303	-4.225300	-1.496829
5	6	0	-3.698475	-3.600108	-1.609946
6	6	0	-3.360938	-2.529523	-0.782762
7	6	0	-4.190201	-0.985352	1.166767
8	6	0	-5.680043	-0.672745	1.513268
9	6	0	-6.394035	-2.019705	1.303314
10	1	0	-6.856821	-4.253600	-0.496767
11	1	0	-5.186243	-5.056342	-2.150544
12	1	0	-2.979620	-3.942770	-2.347089
13	1	0	-2.399405	-2.036796	-0.883745
14	1	0	-5.778805	-0.293588	2.531519
15	1	0	-7.431168	-1.854474	1.000751
16	1	0	-3.616463	-1.258507	2.052609
17	1	0	-6.404942	-2.587768	2.240728

18	6	0	-4.238724	0.870918	-0.416030
19	6	0	-2.365285	0.771477	0.696190
20	7	0	-3.501558	1.812306	-0.931629
21	7	0	-3.572319	0.206499	0.576761
22	7	0	-2.339918	1.730085	-0.235201
23	6	0	-5.679570	0.518415	-0.607502
24	1	0	-5.784144	-0.378481	-1.229008
25	1	0	-6.201054	1.350317	-1.080814
26	8	0	-6.227578	0.354605	0.689356
27	6	0	-1.183176	2.450451	-0.650086
28	6	0	-0.782840	3.605879	0.009886
29	6	0	-0.398748	1.896036	-1.664502
30	6	0	0.472854	4.140592	-0.240363
31	6	0	0.850884	2.428657	-1.939741
32	6	0	1.286643	3.507503	-1.175414
33	1	0	0.824216	5.001625	0.313821
34	1	0	1.501563	1.964976	-2.670324
35	35	0	-1.917896	4.374555	1.289109
36	35	0	3.061807	4.083288	-1.365285
37	35	0	-1.005313	0.378794	-2.569042
38	6	0	-1.403182	0.496734	1.849071
39	8	0	-1.901008	0.026534	2.838972
40	6	0	0.051757	0.951712	1.767831
41	6	0	0.951714	0.149731	2.676988
42	1	0	0.406467	0.921084	0.734805
43	1	0	0.613720	0.302183	3.708050
44	1	0	0.803614	-0.910413	2.448204
45	6	0	2.418358	0.511217	2.546442
46	6	0	2.899128	1.455513	1.638361
47	6	0	3.340099	-0.157489	3.361471
48	6	0	4.262928	1.727638	1.549424
49	1	0	2.227296	1.983147	0.968181
50	6	0	4.702265	0.108674	3.273618
51	1	0	2.977506	-0.901227	4.068382
52	6	0	5.169236	1.061002	2.367143
53	1	0	4.602795	2.455183	0.819133
54	1	0	5.398616	-0.423455	3.914648
55	1	0	6.231366	1.273520	2.295208
56	9	0	0.037623	2.275354	2.215207
57	7	0	1.387175	-0.710094	-0.451302
58	16	0	2.539799	-0.578911	-1.597081
59	8	0	2.040450	-0.848221	-2.945232
60	8	0	3.180375	0.716513	-1.358009
61	16	0	0.362644	-1.931803	-0.354001

62	8	0	-0.731473	-1.443849	0.530090
63	8	0	-0.083503	-2.538100	-1.612359
64	6	0	1.177287	-3.245685	0.548850
65	6	0	2.218864	-2.960268	1.425998
66	6	0	0.728202	-4.548600	0.352703
67	6	0	2.822911	-4.004525	2.119563
68	1	0	2.581758	-1.942056	1.527713
69	6	0	1.333021	-5.583956	1.059290
70	1	0	-0.069536	-4.738599	-0.357810
71	6	0	2.378865	-5.312758	1.939927
72	1	0	3.651445	-3.791180	2.787911
73	1	0	0.993853	-6.604467	0.914317
74	1	0	2.855212	-6.125301	2.479348
75	6	0	3.732588	-1.840167	-1.200680
76	6	0	3.573609	-3.111930	-1.742155
77	6	0	4.723553	-1.553413	-0.267064
78	6	0	4.435205	-4.125404	-1.331545
79	1	0	2.780742	-3.292683	-2.462145
80	6	0	5.582959	-2.573690	0.128953
81	1	0	4.801302	-0.549745	0.142237
82	6	0	5.436485	-3.855938	-0.399955
83	1	0	4.324054	-5.125057	-1.738539
84	1	0	6.362605	-2.368672	0.856066
85	1	0	6.104711	-4.650483	-0.082709

TS7*R*^{S2}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.235897	-2.596972	0.245704
2	6	0	5.462874	-2.397046	0.887219
3	6	0	5.689442	-2.924068	2.153056
4	6	0	4.676608	-3.658057	2.767354
5	6	0	3.464893	-3.882477	2.113390
6	6	0	3.235441	-3.360723	0.841403
7	6	0	4.251592	-1.934831	-1.116760
8	6	0	5.772931	-1.785597	-1.378146
9	6	0	6.409275	-1.611183	0.017779
10	1	0	6.643049	-2.774409	2.649976
11	1	0	4.838084	-4.074639	3.756352
12	1	0	2.694656	-4.477189	2.593909
13	1	0	2.303113	-3.551176	0.323000

14	1	0	6.110126	-2.733376	-1.803386
15	1	0	6.431516	-0.560238	0.330043
16	1	0	3.716014	-2.472533	-1.897294
17	1	0	7.436446	-1.980769	0.044899
18	6	0	4.395001	0.575528	-1.396356
19	6	0	2.472314	-0.148673	-0.663484
20	7	0	3.693586	1.648944	-1.176718
21	7	0	3.686916	-0.552399	-1.077411
22	7	0	2.505772	1.180395	-0.710773
23	6	0	5.783497	0.509538	-1.956563
24	1	0	6.500011	0.904414	-1.226222
25	1	0	5.832188	1.131581	-2.852083
26	8	0	6.086940	-0.808306	-2.344457
27	6	0	1.523518	2.135051	-0.314490
28	6	0	0.480590	2.481339	-1.166053
29	6	0	1.670766	2.775128	0.914270
30	6	0	-0.412337	3.482135	-0.802318
31	6	0	0.775887	3.755181	1.305419
32	6	0	-0.256624	4.090108	0.434394
33	1	0	-1.245638	3.727067	-1.446690
34	1	0	0.872471	4.236412	2.270223
35	35	0	0.263868	1.552955	-2.773354
36	35	0	-1.518486	5.374077	0.982306
37	35	0	3.071536	2.263533	2.054145
38	6	0	1.350621	-1.145549	-0.406873
39	8	0	1.354184	-2.110263	-1.171225
40	6	0	0.399592	-0.857742	0.616814
41	6	0	-0.090414	-2.062467	1.392845
42	1	0	-0.742959	-0.471639	-0.201825
43	1	0	-0.234626	-2.866141	0.663776
44	1	0	0.726792	-2.379160	2.059911
45	6	0	-1.340555	-1.907319	2.228734
46	6	0	-2.340779	-2.877603	2.143453
47	6	0	-1.472497	-0.885331	3.175727
48	6	0	-3.433742	-2.857960	3.006756
49	1	0	-2.251745	-3.667018	1.402642
50	6	0	-2.565659	-0.863094	4.038956
51	1	0	-0.714135	-0.111809	3.232467
52	6	0	-3.543143	-1.856224	3.967572
53	1	0	-4.197686	-3.625790	2.922635
54	1	0	-2.655130	-0.066837	4.771284
55	1	0	-4.388778	-1.839046	4.648551
56	9	0	0.843504	0.151291	1.469116
57	7	0	-1.811880	-0.306868	-0.857748

58	16	0	-2.144432	-1.213581	-2.200968
59	8	0	-3.303385	-0.655322	-2.889675
60	8	0	-0.906974	-1.435467	-2.934822
61	16	0	-2.704911	1.016706	-0.430564
62	8	0	-2.087644	1.446784	0.821095
63	8	0	-2.830834	1.973120	-1.524967
64	6	0	-4.331701	0.384711	-0.097367
65	6	0	-4.528026	-0.317423	1.085463
66	6	0	-5.337009	0.545122	-1.045859
67	6	0	-5.775589	-0.886883	1.321941
68	1	0	-3.715192	-0.411065	1.798125
69	6	0	-6.580052	-0.029834	-0.796057
70	1	0	-5.124309	1.085608	-1.960851
71	6	0	-6.795836	-0.745841	0.381686
72	1	0	-5.943965	-1.440465	2.240172
73	1	0	-7.377874	0.077191	-1.523277
74	1	0	-7.766944	-1.194442	0.567028
75	6	0	-2.628242	-2.786469	-1.511893
76	6	0	-3.942384	-2.961726	-1.085639
77	6	0	-1.683097	-3.804866	-1.432398
78	6	0	-4.313398	-4.194990	-0.558439
79	1	0	-4.662641	-2.154339	-1.185284
80	6	0	-2.072612	-5.038092	-0.912311
81	1	0	-0.668621	-3.617029	-1.773546
82	6	0	-3.383401	-5.231338	-0.477831
83	1	0	-5.333410	-4.347763	-0.220625
84	1	0	-1.353300	-5.848154	-0.849546
85	1	0	-3.682594	-6.194305	-0.075946

TS7*S*^{S2}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.550604	-2.378657	0.168797
2	6	0	-5.863976	-2.784197	-0.050726
3	6	0	-6.165019	-3.606182	-1.134418
4	6	0	-5.134918	-4.001319	-1.983974
5	6	0	-3.818296	-3.595455	-1.749489
6	6	0	-3.507702	-2.782885	-0.662307
7	6	0	-4.461261	-1.463352	1.370602
8	6	0	-5.955122	-1.214177	1.802955
9	6	0	-6.793762	-2.240493	1.004057

10	1	0	-7.185956	-3.928491	-1.316709
11	1	0	-5.357702	-4.634760	-2.836787
12	1	0	-3.023773	-3.923160	-2.412173
13	1	0	-2.480971	-2.487327	-0.463160
14	1	0	-6.051353	-1.363283	2.878399
15	1	0	-7.684554	-1.754283	0.592732
16	1	0	-3.865339	-1.885713	2.176554
17	1	0	-7.143865	-3.039194	1.665550
18	6	0	-4.550215	0.786729	0.352022
19	6	0	-2.529216	0.170284	0.907307
20	7	0	-3.787873	1.743167	-0.081433
21	7	0	-3.822329	-0.192240	0.971126
22	7	0	-2.531607	1.350556	0.274796
23	6	0	-6.036551	0.653983	0.344258
24	1	0	-6.359148	0.010753	-0.486573
25	1	0	-6.501052	1.634371	0.240320
26	8	0	-6.395284	0.119728	1.600308
27	6	0	-1.449446	2.017913	-0.370321
28	6	0	-0.972555	3.240791	0.090105
29	6	0	-0.963240	1.484467	-1.562980
30	6	0	0.027395	3.905357	-0.602067
31	6	0	0.017825	2.146745	-2.284314
32	6	0	0.516528	3.337835	-1.772783
33	1	0	0.426091	4.839212	-0.227193
34	1	0	0.422276	1.714605	-3.188923
35	35	0	-1.683947	3.982432	1.656941
36	35	0	1.934276	4.181724	-2.669395
37	35	0	-1.644444	-0.150025	-2.188723
38	6	0	-1.420908	-0.683187	1.509440
39	8	0	-1.708201	-1.867712	1.686647
40	6	0	-0.172358	-0.057384	1.791430
41	6	0	0.609653	-0.719145	2.906399
42	1	0	0.682033	-0.334262	0.514266
43	1	0	0.013245	-0.670060	3.831513
44	1	0	0.663213	-1.782706	2.649749
45	6	0	1.992213	-0.192062	3.230194
46	6	0	2.305420	1.172708	3.218866
47	6	0	2.964268	-1.091112	3.685368
48	6	0	3.551391	1.616006	3.658394
49	1	0	1.576074	1.887197	2.859214
50	6	0	4.211080	-0.649828	4.121636
51	1	0	2.729774	-2.153460	3.716852
52	6	0	4.508094	0.710958	4.114499
53	1	0	3.775405	2.678015	3.640219

54	1	0	4.945322	-1.368712	4.473598
55	1	0	5.475277	1.063377	4.459272
56	9	0	-0.323661	1.316814	1.989081
57	7	0	1.442056	-0.630478	-0.367704
58	16	0	2.543191	0.509314	-0.879981
59	8	0	2.472142	0.695962	-2.322294
60	8	0	2.313202	1.633480	0.018097
61	16	0	1.161594	-2.080900	-1.113372
62	8	0	-0.063153	-2.565703	-0.485764
63	8	0	1.235976	-1.981204	-2.563374
64	6	0	2.512571	-3.124559	-0.602593
65	6	0	3.046131	-2.993131	0.675377
66	6	0	2.995263	-4.066087	-1.505216
67	6	0	4.097907	-3.818627	1.053138
68	1	0	2.678865	-2.218648	1.341633
69	6	0	4.037959	-4.899723	-1.109259
70	1	0	2.569684	-4.124348	-2.501205
71	6	0	4.588988	-4.774202	0.163841
72	1	0	4.543927	-3.700139	2.035929
73	1	0	4.427687	-5.638787	-1.801277
74	1	0	5.412471	-5.415560	0.461245
75	6	0	4.131997	-0.205852	-0.540285
76	6	0	4.738221	-0.976694	-1.529019
77	6	0	4.684779	-0.053347	0.725337
78	6	0	5.935776	-1.618290	-1.230481
79	1	0	4.267892	-1.072007	-2.502764
80	6	0	5.889934	-0.690891	1.004938
81	1	0	4.180420	0.554381	1.469182
82	6	0	6.508107	-1.475075	0.033267
83	1	0	6.419681	-2.232028	-1.982934
84	1	0	6.334972	-0.577077	1.988315
85	1	0	7.442545	-1.979054	0.259807

M7*R*^{S2}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.366140	0.942199	-0.318980
2	6	0	5.359222	0.083380	-0.797718
3	6	0	5.989990	0.348928	-2.006974
4	6	0	5.610880	1.482554	-2.724700
5	6	0	4.624813	2.341294	-2.236382

6	6	0	3.990632	2.083190	-1.021955
7	6	0	3.866505	0.462895	1.023456
8	6	0	4.996881	-0.498929	1.470790
9	6	0	5.601506	-1.053583	0.162800
10	1	0	6.768785	-0.308360	-2.381850
11	1	0	6.096159	1.704814	-3.670002
12	1	0	4.353763	3.224605	-2.805373
13	1	0	3.228895	2.738265	-0.608761
14	1	0	5.749479	0.112327	1.973947
15	1	0	5.076059	-1.955446	-0.174426
16	1	0	3.644529	1.268929	1.723141
17	1	0	6.655555	-1.314572	0.280462
18	6	0	2.468885	-1.620683	1.370274
19	6	0	1.435037	0.066616	0.437201
20	7	0	1.252477	-2.044871	1.193926
21	7	0	2.623591	-0.337055	0.916165
22	7	0	0.622676	-0.981351	0.610906
23	6	0	3.613582	-2.361548	1.989359
24	1	0	4.019907	-3.085947	1.272280
25	1	0	3.258364	-2.910676	2.862675
26	8	0	4.592470	-1.451283	2.433707
27	6	0	-0.781378	-1.016833	0.396543
28	6	0	-1.639105	-0.298368	1.229581
29	6	0	-1.311033	-1.770647	-0.647908
30	6	0	-3.013407	-0.348799	1.038300
31	6	0	-2.680329	-1.822461	-0.864789
32	6	0	-3.512162	-1.107403	-0.011681
33	1	0	-3.675565	0.212029	1.684109
34	1	0	-3.085657	-2.400737	-1.685238
35	35	0	-0.943649	0.768157	2.602869
36	35	0	-5.373174	-1.153065	-0.295735
37	35	0	-0.149956	-2.680991	-1.804171
38	6	0	1.086141	1.477530	0.085424
39	8	0	1.590954	2.355221	0.866293
40	6	0	0.271632	1.626256	-0.992806
41	6	0	-0.459394	2.865103	-1.362084
42	1	0	0.020857	3.692585	-0.833095
43	1	0	-0.397147	3.052788	-2.440510
44	6	0	-1.907560	2.726169	-0.933390
45	6	0	-2.295324	3.089214	0.359163
46	6	0	-2.853050	2.154469	-1.787300
47	6	0	-3.612319	2.914833	0.776471
48	1	0	-1.551287	3.494429	1.040227
49	6	0	-4.169243	1.973136	-1.370490

50	1	0	-2.551248	1.851980	-2.786656
51	6	0	-4.554774	2.360137	-0.088599
52	1	0	-3.902278	3.209459	1.781184
53	1	0	-4.892896	1.519131	-2.040800
54	1	0	-5.580240	2.215703	0.238046
55	9	0	-0.090438	0.522745	-1.724629

M7*S*^{S2}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.416733	0.885525	-0.121755
2	6	0	5.753145	0.565390	-0.344196
3	6	0	6.480886	1.256025	-1.310084
4	6	0	5.844948	2.258525	-2.038677
5	6	0	4.504975	2.576600	-1.801176
6	6	0	3.773523	1.894997	-0.831772
7	6	0	3.824183	0.008738	0.960079
8	6	0	4.916023	-1.095782	1.209803
9	6	0	6.210987	-0.535188	0.579710
10	1	0	7.523646	1.015547	-1.495227
11	1	0	6.398058	2.801291	-2.798826
12	1	0	4.032792	3.369366	-2.372479
13	1	0	2.740107	2.135690	-0.595111
14	1	0	5.027609	-1.282743	2.278197
15	1	0	6.755072	-1.338597	0.073723
16	1	0	3.576896	0.580575	1.854834
17	1	0	6.870355	-0.138277	1.358815
18	6	0	2.602868	-1.686630	-0.359030
19	6	0	1.302417	-0.268525	0.688662
20	7	0	1.405748	-2.023700	-0.730563
21	7	0	2.582926	-0.621498	0.499703
22	7	0	0.606331	-1.121142	-0.077558
23	6	0	3.929859	-2.330856	-0.591750
24	1	0	4.511432	-1.769329	-1.335474
25	1	0	3.799415	-3.356987	-0.934769
26	8	0	4.569822	-2.366629	0.670222
27	6	0	-0.770839	-1.042304	-0.412399
28	6	0	-1.661775	-2.014564	0.039210
29	6	0	-1.232746	-0.007762	-1.225679
30	6	0	-3.002615	-1.966255	-0.315929
31	6	0	-2.571316	0.059237	-1.591977

32	6	0	-3.434471	-0.926978	-1.132248
33	1	0	-3.693947	-2.718114	0.043000
34	1	0	-2.929546	0.868122	-2.215876
35	35	0	-1.041806	-3.370002	1.171064
36	35	0	-5.254210	-0.839972	-1.615466
37	35	0	-0.043495	1.308175	-1.837618
38	6	0	0.867718	0.942676	1.449894
39	8	0	1.654078	1.945009	1.352990
40	6	0	-0.290175	0.816424	2.154470
41	6	0	-0.985799	1.913905	2.870938
42	1	0	-1.298198	1.568560	3.865823
43	1	0	-0.250450	2.711572	3.011622
44	6	0	-2.193023	2.460519	2.123682
45	6	0	-3.021570	1.616019	1.379357
46	6	0	-2.498472	3.821423	2.174660
47	6	0	-4.130551	2.120126	0.705338
48	1	0	-2.791734	0.554770	1.330590
49	6	0	-3.607553	4.329689	1.502829
50	1	0	-1.855345	4.489304	2.741994
51	6	0	-4.427936	3.479836	0.765597
52	1	0	-4.759571	1.447203	0.128341
53	1	0	-3.826552	5.392092	1.549840
54	1	0	-5.291682	3.874430	0.239720
55	9	0	-0.912021	-0.409894	2.216654