Supporting Information

Theoretical study on the mechanisms of the reactions between 1,3-dialkynes and ammonia derivatives for the formation of five-membered N-heterocycles

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Table S1. Total energies (E) and Gibbs free energies (G) of all optimized structures are calculated by M06-2X/6-31G(d, p) level in DMSO solvent. (Unit: Hartree)

	E	G		E	G
R1	-615.37049150	-615.209325			
N_R2	-111.81365677	-111.782415	**O_R2**	-131.66054618	-131.642049
N_R2-complex	-223.64618408	-223.566070	**O_R2-complex-N**	-263.33582905	-263.280828
N_M1	-727.17545262	-726.958680	**O_R2-complex-O**	-263.33158356	-263.278080
N_M2	-727.25461368	-727.037193	**O_M1**	-747.051331	-746.846427
N_M3	-839.01940939	-838.752364	**O_M2**	-747.092921	-746.888725
N_M4	-1454.52524613	-1454.068770	**O_M3**	-878.729854	-878.489149
N_M5	-1454.48961261	-1454.034559	**O_M4**	-1494.202724	-1493.773193
N_M6	-727.26070819	-727.045037	**O_M5**	-1494.172250	-1493.743462
N_M7	-727.26237965	-727.046509	**O_M6**	-747.107335	-746.903496
N_M8	-727.26614037	-727.045204	**O_M7**	-747.104529	-746.900747
N_M9	-1454.55828014	-1454.093634	**O_M8**	-747.072406	-746.866627
N_M10	-839.10972322	-838.840294	**O_M9**	-1494.173267	-1493.73886
N_M11	-839.11559957	-838.843393	**O_M10**	-878.76230862	-878.519056
N_P	-727.35101477	-727.131332	**O_P**	-747.177514	-746.970646
N_TS1	-727.16286429	-726.950882	**O_TS1**	-747.009096	-746.807898
N_TS2	-727.13827770	-726.927793	**O_TS2**	-747.006948	-746.807274
N_TS3	-839.00728216	-838.744236	**O_TS3**	-746.993084	-746.795198
N_TS4	-727.15380993	-726.943027	**O_TS4**	-878.715852	-878.477595
N_TS5	-839.00557095	-838.741160	**O_TS5-N**	-878.68392868	-878.445336
N_TS6	-1454.47685007	-1454.023438	**O_TS5-O**	-878.69381178	-878.456088
N_TS7	-1454.48618507	-1454.034418	**O_TS6**	-1494.151097	-1493.723677
N_TS8	-727.25769457	-727.040607	**O_TS7**	-1494.169534	-1493.74168
N_TS9	-727.23866390	-727.020209	**O_TS8**	-747.099470	-746.895249
N_TS10	-727.19523673	-726.980079	**O_TS9**	-747.059208	-746.855132
N_TS11	-1454.55451621	-1454.093474	**O_TS10**	-747.028924	-746.829184
N_TS12	-839.10916339	-838.841489	**O_TS11**	-1494.178083	-1493.744067
N_TS13	-839.11550124	-838.842594	**O_TS12**	-878.76030656	-878.516600

Cartesian coordinates of all stationary points:

R1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.901966	-0.000267	-0.000211
2	6	0	0.687060	-0.000289	-0.000145
3	6	0	-0.687060	-0.000356	0.000020
4	6	0	-1.901967	-0.000313	0.000121
5	6	0	-3.332894	-0.000118	0.000115
6	6	0	-4.037836	-0.878431	0.837321
7	6	0	-4.037573	0.878394	-0.837109
8	6	0	-5.427387	-0.874238	0.833473
9	1	0	-3.487734	-1.555338	1.482265
10	6	0	-5.427124	0.874595	-0.833289
11	1	0	-3.487265	1.555143	-1.482043
12	6	0	-6.123435	0.000276	0.000086
13	1	0	-5.969053	-1.554792	1.481877
14	1	0	-5.968587	1.555301	-1.481704
15	1	0	-7.208398	0.000429	0.000076
16	6	0	3.332894	-0.000091	-0.000141
17	6	0	4.037552	0.878636	0.836870
18	6	0	4.037856	-0.878644	-0.837080
19	6	0	5.427105	0.874814	0.833107
20	1	0	3.487235	1.555566	1.481607
21	6	0	5.427407	-0.874472	-0.833178
22	1	0	3.487772	-1.555712	-1.481871
23	6	0	6.123436	0.000259	0.000000
24	1	0	5.968547	1.555687	1.481364
25	1	0	5.969084	-1.555210	-1.481380
26	1	0	7.208400	0.000395	0.000054

N_R2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.735613	-0.000013
2	1	0	0.587852	0.982859	0.795207

3	1	0	0.588019	0.982851	-0.795114
4	7	0	0.000000	-0.735613	-0.000013
5	1	0	-0.587852	-0.982859	0.795207
6	1	0	-0.588019	-0.982851	-0.795114

N_R2-complex

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.557027	0.669803	-0.042439
2	1	0	-2.361859	0.986218	-0.574790
3	1	0	-1.700640	0.994814	0.912444
4	7	0	-1.537427	-0.765226	-0.105291
5	1	0	-0.575326	-1.036163	0.102801
6	1	0	-2.128662	-1.159794	0.624055
7	7	0	1.552301	-0.670467	0.017880
8	1	0	1.742978	-0.966469	-0.938226
9	1	0	2.326815	-1.008070	0.581068
10	7	0	1.534133	0.761191	0.125882
11	1	0	2.166389	1.176599	-0.555907
12	1	0	0.586444	1.045756	-0.123666

N_M1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.196945	-1.090028	0.060928
2	6	0	1.136053	-1.902426	0.075979
3	6	0	-0.208353	-1.453723	0.015591
4	6	0	-1.358959	-1.071024	-0.024664
5	6	0	-2.686679	-0.538000	-0.062610
6	6	0	-2.868181	0.854032	-0.084536
7	6	0	-3.807007	-1.382223	-0.072095
8	6	0	-4.150106	1.388817	-0.115698
9	1	0	-1.996077	1.500273	-0.076113
10	6	0	-5.085807	-0.838042	-0.103031
11	1	0	-3.663759	-2.457432	-0.054326
12	6	0	-5.260380	0.545052	-0.125238
13	1	0	-4.284298	2.465297	-0.132760
14	1	0	-5.949391	-1.494691	-0.109921

15	1	0	-6.260650	0.964809	-0.150363
16	6	0	2.223611	0.383791	0.045380
17	6	0	1.367002	1.105184	0.889004
18	6	0	3.100045	1.085312	-0.793205
19	6	0	1.382730	2.495078	0.886376
20	1	0	0.696772	0.566655	1.550824
21	6	0	3.114404	2.476917	-0.791060
22	1	0	3.754753	0.556193	-1.480163
23	6	0	2.256819	3.184515	0.047271
24	1	0	0.717086	3.041488	1.546603
25	1	0	3.791918	3.007411	-1.451743
26	1	0	2.269219	4.269381	0.047085
27	7	0	3.605699	-3.196844	0.096120
28	1	0	1.371446	-2.966275	0.138421
29	1	0	3.349093	-3.394076	-0.877993
30	7	0	3.538072	-1.764647	0.123149
31	1	0	3.955222	-1.474536	1.012901
32	1	0	4.129434	-1.313453	-0.587686

N_M2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.279320	-1.076686	0.052667
2	6	0	1.207369	-1.917142	0.054155
3	6	0	-0.137031	-1.473532	-0.000214
4	6	0	-1.295469	-1.107337	-0.041828
5	6	0	-2.627733	-0.589066	-0.069848
6	6	0	-3.742582	-1.441392	-0.112426
7	6	0	-2.830356	0.801358	-0.048976
8	6	0	-5.027537	-0.910875	-0.132675
9	1	0	-3.589678	-2.515488	-0.128679
10	6	0	-4.118278	1.322460	-0.069435
11	1	0	-1.966503	1.458358	-0.015983
12	6	0	-5.220923	0.469702	-0.111582
13	1	0	-5.882600	-1.578424	-0.165031
14	1	0	-4.262872	2.397925	-0.052535
15	1	0	-6.225733	0.878792	-0.128203
16	6	0	2.176118	0.405409	0.054246
17	6	0	1.284796	1.068131	0.905806
18	6	0	3.000560	1.157918	-0.791134
19	6	0	1.211176	2.457311	0.899531

20	1	0	0.658066	0.491253	1.577077
21	6	0	2.922273	2.547786	-0.796511
22	1	0	3.689852	0.648650	-1.457546
23	6	0	2.026727	3.200306	0.046610
24	1	0	0.520069	2.960800	1.568028
25	1	0	3.558853	3.120526	-1.462985
26	1	0	1.965698	4.283731	0.042979
27	7	0	3.575297	-1.539052	-0.023610
28	1	0	1.373432	-2.989015	0.052545
29	1	0	4.287996	-0.928492	0.351420
30	7	0	3.891388	-2.895232	0.111258
31	1	0	3.378620	-3.292521	0.900341
32	1	0	3.577435	-3.382214	-0.725280

N_M3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.734675	-0.393252	-0.695483
2	6	0	0.776415	-1.327467	-0.765236
3	6	0	-0.599143	-1.104467	-0.501095
4	6	0	-1.780580	-0.936487	-0.280210
5	6	0	-3.161119	-0.666575	-0.016744
6	6	0	-3.554270	0.624662	0.369414
7	6	0	-4.128973	-1.674421	-0.144095
8	6	0	-4.892911	0.898469	0.622467
9	1	0	-2.800703	1.399837	0.467405
10	6	0	-5.465680	-1.391190	0.110823
11	1	0	-3.822666	-2.671240	-0.443207
12	6	0	-5.850476	-0.107132	0.494377
13	1	0	-5.190356	1.898361	0.920674
14	1	0	-6.209682	-2.174344	0.009435
15	1	0	-6.894830	0.109687	0.693506
16	6	0	1.594064	1.041142	-0.386902
17	6	0	2.575637	1.702281	0.366073
18	6	0	0.492557	1.771589	-0.855103
19	6	0	2.447529	3.057042	0.656578
20	1	0	3.431874	1.156164	0.752841
21	6	0	0.369194	3.124781	-0.561701
22	1	0	-0.259335	1.275750	-1.459094
23	6	0	1.344735	3.771451	0.195703
24	1	0	3.210826	3.553084	1.246869

25	1	0	-0.487169	3.678175	-0.933487
26	1	0	1.247222	4.828219	0.421633
27	7	0	3.375547	-2.188813	-1.375793
28	1	0	1.125482	-2.330238	-1.010304
29	1	0	2.923426	-2.214065	-2.296375
30	7	0	3.128281	-0.844039	-0.935513
31	1	0	3.630483	-0.813425	0.007736
32	1	0	3.566630	-0.126411	-1.527699
33	7	0	4.238507	-1.426114	1.482848
34	1	0	5.214973	-1.702110	1.390126
35	1	0	4.155172	-0.899287	2.346976
36	7	0	3.358055	-2.560986	1.561334
37	1	0	3.218033	-2.847370	0.584643
38	1	0	3.827965	-3.323676	2.045007

N_M4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.004115	1.566606	1.422767
2	6	0	0.597538	0.399065	1.813441
3	6	0	1.903693	0.015570	1.439634
4	6	0	3.016411	-0.352799	1.105280
5	6	0	4.313925	-0.755612	0.661394
6	6	0	4.843084	-2.003332	1.031208
7	6	0	5.074226	0.089694	-0.166012
8	6	0	6.100915	-2.391205	0.585803
9	1	0	4.257456	-2.658613	1.667595
10	6	0	6.331561	-0.307835	-0.606678
11	1	0	4.668882	1.056714	-0.450566
12	6	0	6.849560	-1.547489	-0.234205
13	1	0	6.498583	-3.357297	0.880001
14	1	0	6.909943	0.353313	-1.244112
15	1	0	7.830536	-1.854889	-0.580967
16	6	0	0.715916	2.652796	0.701347
17	6	0	0.072554	3.344755	-0.333558
18	6	0	2.034944	2.993069	1.026923
19	6	0	0.743713	4.332988	-1.047333
20	1	0	-0.946847	3.082670	-0.600604
21	6	0	2.705448	3.978138	0.308109
22	1	0	2.531728	2.484913	1.845530
23	6	0	2.064079	4.646637	-0.733991

24	1	0	0.236731	4.850916	-1.854798
25	1	0	3.728036	4.230802	0.569326
26	1	0	2.589454	5.413937	-1.293216
27	7	0	-1.322370	1.808817	1.613436
28	1	0	-0.011154	-0.322356	2.346091
29	1	0	-1.670382	2.748980	1.488277
30	7	0	-2.174714	0.826054	2.114904
31	1	0	-2.600967	1.151298	2.978138
32	1	0	-2.908654	0.661346	1.427342
33	6	0	0.007668	-0.665323	-1.343318
34	6	0	-0.895697	0.323805	-1.577193
35	6	0	-2.272486	0.233280	-1.264131
36	6	0	-3.455874	0.192594	-0.979476
37	6	0	-4.810995	0.057115	-0.540705
38	6	0	-5.187803	-1.089566	0.182177
39	6	0	-5.770973	1.049682	-0.793510
40	6	0	-6.492094	-1.234061	0.638326
41	1	0	-4.443987	-1.857463	0.374336
42	6	0	-7.073813	0.895929	-0.332700
43	1	0	-5.485342	1.936084	-1.350231
44	6	0	-7.439638	-0.243046	0.383702
45	1	0	-6.770155	-2.122721	1.195757
46	1	0	-7.807856	1.670129	-0.532143
47	1	0	-8.457260	-0.357342	0.742165
48	6	0	-0.324778	-1.995521	-0.771446
49	6	0	0.254228	-3.144966	-1.324597
50	6	0	-1.189512	-2.128208	0.321943
51	6	0	-0.039916	-4.404117	-0.808902
52	1	0	0.924232	-3.047902	-2.173111
53	6	0	-1.478146	-3.389246	0.835776
54	1	0	-1.615122	-1.243572	0.784725
55	6	0	-0.909319	-4.530231	0.271502
56	1	0	0.408650	-5.286145	-1.254538
57	1	0	-2.144725	-3.478609	1.688215
58	1	0	-1.138325	-5.511114	0.675809
59	7	0	1.344701	-0.546937	-1.689395
60	1	0	-0.523767	1.247700	-2.004463
61	1	0	1.943761	-1.053038	-1.040031
62	7	0	1.801569	0.747355	-2.009976
63	1	0	2.054246	1.237968	-1.148156
64	1	0	2.642772	0.642304	-2.568610

N_M5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.401363	1.719710	1.625948
2	6	0	0.914559	0.390369	1.811470
3	6	0	2.087360	-0.111327	1.272973
4	6	0	3.050090	-0.614849	0.693374
5	6	0	4.263278	-1.077633	0.109072
6	6	0	4.708355	-2.401655	0.288819
7	6	0	5.039424	-0.210489	-0.687319
8	6	0	5.888871	-2.835076	-0.301534
9	1	0	4.116435	-3.078945	0.896176
10	6	0	6.216551	-0.656040	-1.274881
11	1	0	4.704488	0.813557	-0.829255
12	6	0	6.649888	-1.968661	-1.086653
13	1	0	6.217656	-3.858493	-0.148578
14	1	0	6.802370	0.026429	-1.883082
15	1	0	7.570627	-2.312574	-1.546006
16	6	0	1.124385	2.690312	0.746902
17	6	0	0.394402	3.527167	-0.107678
18	6	0	2.521390	2.792446	0.745549
19	6	0	1.040217	4.412137	-0.965049
20	1	0	-0.689160	3.463589	-0.088780
21	6	0	3.169147	3.679839	-0.112827
22	1	0	3.105799	2.178776	1.421874
23	6	0	2.432543	4.484741	-0.978879
24	1	0	0.455805	5.042248	-1.628430
25	1	0	4.252916	3.744981	-0.097978
26	1	0	2.937930	5.169264	-1.652707
27	7	0	-0.720929	2.171312	2.108641
28	1	0	0.381958	-0.278352	2.477105
29	1	0	-3.590569	1.100593	1.328639
30	7	0	-1.466129	1.261048	2.881332
31	1	0	-0.874383	0.762266	3.549449
32	1	0	-2.113418	1.816601	3.431314
33	6	0	-0.265248	-0.594155	-0.604962
34	6	0	-1.143503	0.550825	-0.734593
35	6	0	-2.352502	0.616206	-0.213535
36	6	0	-3.546230	0.720105	0.306868
37	6	0	-4.811445	0.336093	-0.348665
38	6	0	-4.835469	-0.245393	-1.622971
39	6	0	-6.018332	0.554235	0.322947
40	6	0	-6.043807	-0.596267	-2.210659

41	1	0	-3.899479	-0.422204	-2.146144
42	6	0	-7.228910	0.202615	-0.268286
43	1	0	-6.004053	1.002398	1.312445
44	6	0	-7.245282	-0.373115	-1.535608
45	1	0	-6.051068	-1.047225	-3.197852
46	1	0	-8.158885	0.378284	0.262688
47	1	0	-8.187723	-0.649181	-1.997204
48	6	0	-0.672089	-1.868855	0.024674
49	6	0	-0.338542	-3.073219	-0.607637
50	6	0	-1.408244	-1.894279	1.218221
51	6	0	-0.726574	-4.288983	-0.051359
52	1	0	0.196835	-3.058965	-1.552094
53	6	0	-1.796140	-3.111538	1.762133
54	1	0	-1.639495	-0.961912	1.727341
55	6	0	-1.455452	-4.310312	1.133458
56	1	0	-0.465670	-5.215464	-0.551477
57	1	0	-2.357628	-3.126781	2.690369
58	1	0	-1.759133	-5.257062	1.568279
59	7	0	0.876778	-0.603966	-1.270364
60	1	0	-0.742043	1.399085	-1.281576
61	1	0	1.575726	-1.287347	-0.969014
62	7	0	1.348059	0.551623	-1.904100
63	1	0	1.918197	1.071932	-1.231233
64	1	0	1.947175	0.254652	-2.668698

N_M6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.231036	-0.964699	-0.149917
2	6	0	1.100410	-1.915906	-0.008970
3	6	0	-0.024883	-1.633893	0.603005
4	6	0	-1.152819	-1.332016	1.198193
5	6	0	-2.331694	-0.755018	0.519018
6	6	0	-2.442691	-0.731041	-0.877880
7	6	0	-3.366573	-0.213868	1.289341
8	6	0	-3.553604	-0.158916	-1.486680
9	1	0	-1.657796	-1.178530	-1.482579
10	6	0	-4.480578	0.355277	0.678363
11	1	0	-3.292028	-0.236569	2.372974
12	6	0	-4.575985	0.388109	-0.710904
13	1	0	-3.626832	-0.146974	-2.569423

14	1	0	-5.274171	0.773725	1.289138
15	1	0	-5.443793	0.832113	-1.187489
16	6	0	1.979414	0.501896	-0.081341
17	6	0	0.790487	1.065202	-0.558038
18	6	0	2.960586	1.349620	0.448072
19	6	0	0.588328	2.441892	-0.507728
20	1	0	0.021331	0.428525	-0.982776
21	6	0	2.758343	2.724531	0.497505
22	1	0	3.880087	0.914065	0.824561
23	6	0	1.569802	3.276779	0.020942
24	1	0	-0.338716	2.859944	-0.887538
25	1	0	3.526577	3.366985	0.916285
26	1	0	1.409748	4.349318	0.064105
27	7	0	3.453943	-1.328648	-0.318259
28	1	0	1.206307	-2.918066	-0.421793
29	7	0	3.800221	-2.647990	-0.267775
30	1	0	3.088783	-3.314774	-0.555284
31	1	0	4.655169	-2.791050	-0.788983
32	1	0	-1.231275	-1.489944	2.273152

N_M7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.457491	0.241924	0.329101
2	6	0	0.522733	-0.790203	-0.175325
3	6	0	-0.699311	-1.034510	0.239535
4	6	0	-1.926526	-1.302975	0.620993
5	6	0	-3.134482	-0.609582	0.125023
6	6	0	-3.049280	0.537296	-0.675526
7	6	0	-4.396194	-1.103467	0.473827
8	6	0	-4.204466	1.165323	-1.125370
9	1	0	-2.071233	0.936938	-0.929461
10	6	0	-5.551792	-0.472856	0.021477
11	1	0	-4.467077	-1.988050	1.100783
12	6	0	-5.459448	0.662033	-0.780905
13	1	0	-4.127952	2.054148	-1.743688
14	1	0	-6.524264	-0.867559	0.298003
15	1	0	-6.359611	1.155766	-1.132440
16	6	0	2.902995	0.051928	0.025549
17	6	0	3.440700	-1.229708	-0.136924
18	6	0	3.753704	1.159164	-0.090361

19	6	0	4.796615	-1.400975	-0.409321
20	1	0	2.802524	-2.102145	-0.031438
21	6	0	5.105534	0.987228	-0.361643
22	1	0	3.336339	2.152901	0.030949
23	6	0	5.633031	-0.294561	-0.524109
24	1	0	5.198629	-2.402220	-0.526819
25	1	0	5.750345	1.855630	-0.453965
26	1	0	6.688424	-0.427921	-0.738794
27	7	0	1.138064	1.323895	0.951745
28	1	0	0.894959	-1.389959	-1.005912
29	7	0	-0.166603	1.609146	1.203982
30	1	0	-0.762118	0.823251	1.443389
31	1	0	-0.228696	2.348623	1.890690
32	1	0	-2.078338	-2.077042	1.372494

N_M8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.601706	-0.113436	0.052798
2	6	0	-0.721336	0.967605	-0.009345
3	6	0	0.594852	0.456517	0.030454
4	6	0	1.827778	1.027919	-0.031671
5	6	0	3.160668	0.447282	-0.018263
6	6	0	3.478845	-0.916097	0.152194
7	6	0	4.248739	1.332345	-0.191130
8	6	0	4.799757	-1.358183	0.141862
9	1	0	2.715476	-1.667813	0.309496
10	6	0	5.562081	0.889921	-0.200143
11	1	0	4.039760	2.390487	-0.323038
12	6	0	5.852111	-0.465899	-0.034753
13	1	0	5.000880	-2.416368	0.278288
14	1	0	6.365830	1.606857	-0.337642
15	1	0	6.878326	-0.817164	-0.041529
16	6	0	-3.077183	-0.024530	0.010284
17	6	0	-3.722572	1.195031	0.239146
18	6	0	-3.844788	-1.163702	-0.257068
19	6	0	-5.110468	1.276900	0.192183
20	1	0	-3.138681	2.080429	0.469193
21	6	0	-5.232536	-1.080240	-0.303022
22	1	0	-3.341965	-2.108473	-0.433593
23	6	0	-5.869066	0.139816	-0.080446

24	1	0	-5.599975	2.228520	0.371947
25	1	0	-5.818545	-1.968391	-0.516591
26	1	0	-6.951775	0.204134	-0.117989
27	7	0	-1.045982	-1.323444	0.145353
28	1	0	-0.967389	2.010246	-0.127151
29	7	0	0.380155	-1.020575	0.147068
30	1	0	0.781899	-1.386439	1.017072
31	1	0	0.827764	-1.525054	-0.626446
32	1	0	1.798131	2.109666	-0.127447

N_M9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.263899	-1.144593	0.254308
2	6	0	-2.459048	-1.543448	-0.825711
3	6	0	-1.135090	-1.593291	-0.373608
4	6	0	0.061441	-1.884040	-0.983776
5	6	0	1.391356	-2.100204	-0.425686
6	6	0	2.372970	-2.644546	-1.285492
7	6	0	1.799156	-1.797677	0.888432
8	6	0	3.672175	-2.871674	-0.864064
9	1	0	2.090608	-2.886864	-2.306666
10	6	0	3.108294	-2.023916	1.307988
11	1	0	1.128284	-1.330300	1.599575
12	6	0	4.055003	-2.558965	0.442854
13	1	0	4.394504	-3.289367	-1.558999
14	1	0	3.388034	-1.757940	2.323320
15	1	0	5.075892	-2.718980	0.774155
16	6	0	-4.727737	-0.950429	0.205613
17	6	0	-5.371618	-0.761353	-1.021015
18	6	0	-5.479765	-0.931258	1.385106
19	6	0	-6.747963	-0.565133	-1.069229
20	1	0	-4.788948	-0.744047	-1.936749
21	6	0	-6.855901	-0.735060	1.335175
22	1	0	-4.975312	-1.075681	2.334673
23	6	0	-7.493278	-0.553246	0.108597
24	1	0	-7.237871	-0.416094	-2.025934
25	1	0	-7.433221	-0.725701	2.254032
26	1	0	-8.567070	-0.400313	0.071124
27	7	0	-2.631777	-0.938396	1.401821
28	1	0	-2.781580	-1.792948	-1.823764

29	7	0	-1.243928	-1.195604	1.059463
30	1	0	-0.716444	-0.308316	1.216921
31	1	0	-0.867357	-1.913165	1.689541
32	1	0	-0.045615	-2.145726	-2.033370
33	6	0	3.247072	1.099007	-0.115657
34	6	0	2.365800	1.433120	0.928108
35	6	0	1.071056	1.450504	0.400946
36	6	0	-0.171702	1.720697	0.925675
37	6	0	-1.432914	1.997790	0.243206
38	6	0	-2.421263	2.703557	0.965681
39	6	0	-1.756876	1.627646	-1.076729
40	6	0	-3.641289	3.038850	0.401887
41	1	0	-2.205663	2.993382	1.990734
42	6	0	-2.984697	1.967726	-1.641745
43	1	0	-1.092320	1.011588	-1.672117
44	6	0	-3.933679	2.677132	-0.915794
45	1	0	-4.371250	3.585296	0.991615
46	1	0	-3.200433	1.653987	-2.659035
47	1	0	-4.890629	2.931320	-1.359630
48	6	0	4.714836	0.981972	0.004216
49	6	0	5.312319	0.853543	1.261677
50	6	0	5.518746	0.972784	-1.140790
51	6	0	6.692716	0.723489	1.373677
52	1	0	4.693178	0.833124	2.153004
53	6	0	6.898524	0.841767	-1.027284
54	1	0	5.050939	1.071900	-2.114628
55	6	0	7.489084	0.717816	0.229640
56	1	0	7.146761	0.620207	2.353834
57	1	0	7.515072	0.837951	-1.920319
58	1	0	8.566010	0.615468	0.317350
59	7	0	2.687806	0.891898	-1.299121
60	1	0	2.621005	1.687183	1.944235
61	7	0	1.273780	1.074569	-1.028405
62	1	0	0.887552	1.779040	-1.669043
63	1	0	0.796595	0.171405	-1.224780
64	1	0	-0.144861	1.994916	1.977373

N_M10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.612190	-0.342537	-0.156306

2	6	0	0.739105	-1.263837	0.427844
3	6	0	-0.577704	-0.817996	0.172521
4	6	0	-1.807738	-1.337935	0.454155
5	6	0	-3.132321	-0.836623	0.134037
6	6	0	-3.437665	0.467334	-0.312523
7	6	0	-4.224741	-1.720444	0.289873
8	6	0	-4.745553	0.844530	-0.607691
9	1	0	-2.669321	1.225797	-0.402104
10	6	0	-5.525687	-1.339984	-0.000227
11	1	0	-4.027995	-2.729563	0.642653
12	6	0	-5.800716	-0.050707	-0.461230
13	1	0	-4.936712	1.858264	-0.947453
14	1	0	-6.332417	-2.055069	0.131481
15	1	0	-6.817149	0.249433	-0.692552
16	6	0	3.089843	-0.415623	-0.136324
17	6	0	3.740171	-1.597828	0.231554
18	6	0	3.856395	0.700412	-0.491224
19	6	0	5.129758	-1.662039	0.250752
20	1	0	3.157604	-2.475663	0.492012
21	6	0	5.245660	0.635081	-0.472633
22	1	0	3.350589	1.616819	-0.776797
23	6	0	5.886550	-0.545518	-0.100493
24	1	0	5.622553	-2.585851	0.536165
25	1	0	5.829851	1.507559	-0.747216
26	1	0	6.970526	-0.595961	-0.085437
27	7	0	1.033256	0.686486	-0.776102
28	1	0	0.993899	-2.155437	0.977876
29	7	0	-0.380195	0.467372	-0.525752
30	1	0	-0.667679	1.306503	0.141666
31	1	0	-0.903413	0.525226	-1.403965
32	1	0	-1.780510	-2.304915	0.948617
33	7	0	0.260458	3.450666	0.417164
34	1	0	0.724473	4.053484	1.092597
35	1	0	0.973462	2.858147	-0.007733
36	7	0	-0.625254	2.552634	1.100270
37	1	0	-0.276410	2.279150	2.019015
38	1	0	-1.514503	3.024258	1.239596

N_M11

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

1	6	0	1.425103	-0.350543	-0.297900
2	6	0	0.517278	-1.146251	0.423324
3	6	0	-0.781288	-0.675722	0.082831
4	6	0	-2.033883	-1.180606	0.419966
5	6	0	-3.323294	-0.632409	0.120818
6	6	0	-3.567157	0.687800	-0.343599
7	6	0	-4.481490	-1.433364	0.322167
8	6	0	-4.854927	1.142301	-0.614472
9	1	0	-2.750239	1.394775	-0.435954
10	6	0	-5.757981	-0.972394	0.051210
11	1	0	-4.346833	-2.446069	0.695675
12	6	0	-5.966629	0.323954	-0.434277
13	1	0	-4.986838	2.163251	-0.964308
14	1	0	-6.606324	-1.631583	0.217848
15	1	0	-6.966384	0.683458	-0.653096
16	6	0	2.901862	-0.429934	-0.280591
17	6	0	3.565842	-1.155450	0.714024
18	6	0	3.657310	0.234178	-1.254702
19	6	0	4.956201	-1.223053	0.729877
20	1	0	2.991077	-1.658961	1.485597
21	6	0	5.046514	0.169784	-1.235041
22	1	0	3.140129	0.793357	-2.027840
23	6	0	5.700904	-0.560909	-0.243854
24	1	0	5.458740	-1.788033	1.508499
25	1	0	5.620049	0.687012	-1.997757
26	1	0	6.784804	-0.612437	-0.229925
27	7	0	0.827012	0.608468	-1.003319
28	1	0	0.732563	-2.021851	1.017098
29	7	0	-0.525119	0.457383	-0.697404
30	1	0	-0.213005	1.789433	0.876308
31	1	0	-1.172262	0.766705	-1.410817
32	1	0	-2.017690	-2.125631	0.954260
33	7	0	1.582756	2.694239	1.016550
34	1	0	2.409730	2.561229	1.594917
35	1	0	1.771069	2.283172	0.098180
36	7	0	0.556515	1.848085	1.563675
37	1	0	0.836845	0.864764	1.725923
38	1	0	0.200236	2.255902	2.430188

N_P

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

1	6	0	1.442932	0.070958	-0.379943
2	6	0	0.580019	1.174817	-0.162594
3	6	0	-0.649180	0.768729	-0.637652
4	6	0	-1.978509	1.459662	-0.707060
5	6	0	-3.096852	0.616107	-0.128651
6	6	0	-4.116710	0.121081	-0.941001
7	6	0	-3.103243	0.302481	1.234534
8	6	0	-5.131437	-0.670581	-0.402355
9	1	0	-4.119252	0.358838	-2.001530
10	6	0	-4.114631	-0.483852	1.774557
11	1	0	-2.305432	0.678437	1.870662
12	6	0	-5.133063	-0.973327	0.955646
13	1	0	-5.919171	-1.048410	-1.046394
14	1	0	-4.110157	-0.716768	2.834738
15	1	0	-5.922008	-1.588063	1.376758
16	6	0	2.877195	-0.050308	-0.058590
17	6	0	3.589482	1.041225	0.448680
18	6	0	3.550042	-1.262525	-0.256308
19	6	0	4.942849	0.924264	0.752882
20	1	0	3.086405	1.990783	0.603915
21	6	0	4.902031	-1.377497	0.046462
22	1	0	2.999913	-2.111589	-0.648551
23	6	0	5.604797	-0.284909	0.553200
24	1	0	5.480772	1.781480	1.145456
25	1	0	5.408974	-2.324274	-0.111885
26	1	0	6.659908	-0.375801	0.790061
27	7	0	0.785001	-0.940979	-0.945357
28	1	0	0.806062	2.132225	0.281308
29	7	0	-0.468786	-0.494659	-1.090024
30	1	0	-1.171746	-1.100870	-1.488857
31	1	0	-1.892467	2.403665	-0.161294
32	1	0	-2.209636	1.711864	-1.747558

N-TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.021153	1.116832	0.015754
2	6	0	0.857603	1.755664	0.007798
3	6	0	-0.436685	1.226954	-0.016804
4	6	0	-1.593019	0.839652	-0.014737

5	6	0	-2.919714	0.301937	0.001345
6	6	0	-4.028537	1.106798	-0.306219
7	6	0	-3.125699	-1.049032	0.327577
8	6	0	-5.310508	0.569311	-0.290002
9	1	0	-3.870792	2.150439	-0.557694
10	6	0	-4.410390	-1.578066	0.348238
11	1	0	-2.269210	-1.671124	0.567764
12	6	0	-5.505028	-0.771597	0.038497
13	1	0	-6.160651	1.198217	-0.533290
14	1	0	-4.559126	-2.622212	0.603497
15	1	0	-6.507324	-1.187194	0.053154
16	6	0	2.465581	-0.278708	-0.026604
17	6	0	1.505917	-1.304514	-0.079409
18	6	0	3.822948	-0.637507	-0.017294
19	6	0	1.893047	-2.636957	-0.116479
20	1	0	0.453376	-1.044418	-0.092055
21	6	0	4.205384	-1.975548	-0.055422
22	1	0	4.606484	0.113207	0.017512
23	6	0	3.244872	-2.980877	-0.103745
24	1	0	1.134917	-3.412631	-0.157882
25	1	0	5.260551	-2.228326	-0.047638
26	1	0	3.545302	-4.023005	-0.132367
27	7	0	2.643076	3.504052	0.071022
28	1	0	1.373290	2.984684	0.017368
29	1	0	2.714162	3.777746	1.052926
30	7	0	3.163612	2.169347	0.053560
31	1	0	3.735172	2.055280	-0.787116
32	1	0	3.775483	1.969497	0.848788

N-TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.243842	-1.066916	0.068294
2	6	0	1.177797	-1.891177	0.062562
3	6	0	-0.166286	-1.438361	0.008264
4	6	0	-1.322631	-1.070806	-0.031335
5	6	0	-2.659589	-0.561719	-0.065433
6	6	0	-2.872236	0.826324	-0.050031
7	6	0	-3.763019	-1.427356	-0.108293
8	6	0	-4.165225	1.334423	-0.076649
9	1	0	-2.014793	1.491270	-0.015714

10	6	0	-5.052958	-0.909860	-0.135618
11	1	0	-3.597800	-2.499579	-0.119593
12	6	0	-5.257876	0.469151	-0.120094
13	1	0	-4.321568	2.408108	-0.064088
14	1	0	-5.901598	-1.585161	-0.169434
15	1	0	-6.266510	0.868479	-0.142010
16	6	0	2.206140	0.414958	0.060584
17	6	0	1.342469	1.108488	0.916453
18	6	0	3.031823	1.140608	-0.806781
19	6	0	1.302854	2.498919	0.899587
20	1	0	0.710669	0.552074	1.600519
21	6	0	2.990062	2.531361	-0.822059
22	1	0	3.690160	0.623296	-1.500007
23	6	0	2.125632	3.213441	0.030702
24	1	0	0.633423	3.025371	1.572226
25	1	0	3.628539	3.081261	-1.505437
26	1	0	2.093872	4.297915	0.019300
27	7	0	3.646544	-3.186089	0.030100
28	1	0	1.382025	-2.957476	0.065635
29	1	0	4.466592	-3.267719	-0.579658
30	7	0	3.545181	-1.637784	0.138554
31	1	0	3.918645	-2.193387	1.010120
32	1	0	4.271496	-1.106211	-0.333351

N-TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.938737	-1.178057	-0.209464
2	6	0	0.763578	-1.843170	-0.212457
3	6	0	-0.521960	-1.282993	-0.143612
4	6	0	-1.677468	-0.891531	-0.098594
5	6	0	-3.004034	-0.355827	-0.049406
6	6	0	-4.121105	-1.202406	0.037521
7	6	0	-3.203329	1.034573	-0.088027
8	6	0	-5.403705	-0.668201	0.085027
9	1	0	-3.969510	-2.276399	0.067391
10	6	0	-4.488139	1.561906	-0.042567
11	1	0	-2.339899	1.688994	-0.155545
12	6	0	-5.590834	0.712849	0.044814
13	1	0	-6.260191	-1.331138	0.152277
14	1	0	-4.630590	2.637188	-0.074425

15	1	0	-6.593433	1.126355	0.081546
16	6	0	2.390071	0.211601	-0.104770
17	6	0	1.489778	1.210141	0.300850
18	6	0	3.710203	0.581145	-0.406122
19	6	0	1.899042	2.534142	0.393802
20	1	0	0.468543	0.935539	0.543709
21	6	0	4.116200	1.908876	-0.308842
22	1	0	4.428124	-0.164843	-0.738122
23	6	0	3.213579	2.890561	0.091222
24	1	0	1.189955	3.292936	0.709622
25	1	0	5.140615	2.174147	-0.549321
26	1	0	3.531005	3.925243	0.167569
27	7	0	2.930469	-2.276918	-0.331713
28	1	0	1.866124	-2.890899	-0.363085
29	1	0	3.475522	-2.285555	-1.195792
30	7	0	3.807851	-2.542493	0.767358
31	1	0	4.267047	-1.666818	1.019082
32	1	0	3.194758	-2.770533	1.549319

N-TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.792638	-0.406929	-0.756941
2	6	0	0.817770	-1.336744	-0.831626
3	6	0	-0.552881	-1.107834	-0.550576
4	6	0	-1.733722	-0.940271	-0.319057
5	6	0	-3.111561	-0.667247	-0.046919
6	6	0	-3.500549	0.621569	0.353790
7	6	0	-4.086785	-1.668041	-0.180184
8	6	0	-4.837260	0.898996	0.613749
9	1	0	-2.743857	1.393187	0.456809
10	6	0	-5.421598	-1.381562	0.081942
11	1	0	-3.786927	-2.663584	-0.490247
12	6	0	-5.800893	-0.100107	0.479344
13	1	0	-5.128747	1.897633	0.922492
14	1	0	-6.168907	-2.161046	-0.025056
15	1	0	-6.843675	0.119402	0.683782
16	6	0	1.616429	1.022485	-0.418199
17	6	0	2.576204	1.684042	0.361192
18	6	0	0.510648	1.747525	-0.883084
19	6	0	2.422353	3.028621	0.685452

20	1	0	3.444003	1.144735	0.730276
21	6	0	0.360277	3.091446	-0.558434
22	1	0	-0.225443	1.255142	-1.508868
23	6	0	1.312974	3.735924	0.229163
24	1	0	3.170519	3.522207	1.297101
25	1	0	-0.500122	3.639518	-0.929302
26	1	0	1.193427	4.784707	0.480675
27	7	0	3.433213	-2.129786	-1.478601
28	1	0	1.149891	-2.340315	-1.086588
29	1	0	2.932801	-2.146644	-2.375514
30	7	0	3.154616	-0.823719	-0.951949
31	1	0	3.680806	-1.118159	0.229971
32	1	0	3.666576	-0.059344	-1.404032
33	7	0	3.145334	-1.972577	2.207940
34	1	0	3.438757	-2.708107	2.846629
35	1	0	3.263080	-1.093276	2.703624
36	1	0	3.834166	-2.721810	0.443711
37	7	0	4.039735	-1.950040	1.097283
38	1	0	5.029090	-1.942635	1.344158

N_TS5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.813227	-0.362376	-0.380116
2	6	0	0.768043	-1.202490	-0.457654
3	6	0	-0.565903	-0.820715	-0.328907
4	6	0	-1.778925	-0.648909	-0.245936
5	6	0	-3.178874	-0.411714	-0.134409
6	6	0	-3.837289	-0.553861	1.102290
7	6	0	-3.940206	-0.031649	-1.256449
8	6	0	-5.203541	-0.322695	1.207689
9	1	0	-3.262494	-0.846270	1.975183
10	6	0	-5.306115	0.196504	-1.140213
11	1	0	-3.446492	0.081924	-2.216226
12	6	0	-5.947673	0.053193	0.089686
13	1	0	-5.690571	-0.438178	2.171233
14	1	0	-5.874468	0.488429	-2.018061
15	1	0	-7.014216	0.232256	0.175968
16	6	0	1.847801	1.103276	-0.121129
17	6	0	0.853205	1.705528	0.664916
18	6	0	2.852666	1.930231	-0.649932

19	6	0	0.853648	3.076334	0.896311
20	1	0	0.077645	1.083396	1.097070
21	6	0	2.853501	3.303364	-0.417366
22	1	0	3.644339	1.513787	-1.268384
23	6	0	1.852830	3.884671	0.356117
24	1	0	0.073843	3.515456	1.511079
25	1	0	3.639415	3.917939	-0.845128
26	1	0	1.853670	4.954000	0.540165
27	7	0	2.536650	-3.407684	-0.426842
28	1	0	2.827682	-4.189389	-1.006842
29	1	0	1.551130	-3.114090	-0.589847
30	7	0	2.804970	-3.689752	0.954454
31	1	0	2.888235	-2.779196	1.406214
32	1	0	1.985852	-4.142365	1.353766
33	7	0	3.994610	-0.787210	0.578251
34	1	0	4.888611	-1.224177	0.362660
35	1	0	4.177066	0.208172	0.707016
36	7	0	3.159606	-0.952670	-0.587506
37	1	0	3.600947	-0.563224	-1.424870
38	1	0	2.990572	-2.229418	-0.668878

N_TS6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.052404	-1.559804	-1.367074
2	6	0	0.570081	-0.335596	-1.853307
3	6	0	1.679481	0.183771	-1.283578
4	6	0	2.571009	0.694801	-0.525554
5	6	0	4.035392	0.741035	-0.521701
6	6	0	4.799535	0.210736	-1.570424
7	6	0	4.686755	1.312444	0.577821
8	6	0	6.187532	0.249039	-1.513334
9	1	0	4.296905	-0.224563	-2.429692
10	6	0	6.077028	1.348279	0.632708
11	1	0	4.090023	1.733784	1.383131
12	6	0	6.829655	0.815961	-0.411477
13	1	0	6.771621	-0.163737	-2.329670
14	1	0	6.571859	1.793643	1.489636
15	1	0	7.913607	0.844046	-0.370044
16	6	0	0.846571	-2.483290	-0.535753
17	6	0	0.252964	-3.097306	0.576012

18	6	0	2.198423	-2.717037	-0.818678
19	6	0	1.006587	-3.931822	1.395940
20	1	0	-0.782478	-2.883953	0.824518
21	6	0	2.944842	-3.551737	0.003146
22	1	0	2.653421	-2.257643	-1.689643
23	6	0	2.351530	-4.156686	1.111628
24	1	0	0.545359	-4.394404	2.261533
25	1	0	3.989877	-3.733733	-0.222765
26	1	0	2.940303	-4.803477	1.753625
27	7	0	-1.210877	-1.895155	-1.568689
28	1	0	-0.032368	0.239463	-2.547341
29	1	0	-1.533100	-2.803858	-1.250762
30	7	0	-2.135951	-0.993463	-2.096962
31	1	0	-2.699653	-1.481278	-2.787573
32	1	0	-2.741403	-0.702936	-1.323424
33	6	0	0.029319	1.001605	1.469598
34	6	0	-0.835922	-0.069817	1.694046
35	6	0	-2.169443	-0.135298	1.266006
36	6	0	-3.331159	-0.232855	0.889119
37	6	0	-4.679945	-0.296057	0.428560
38	6	0	-5.180389	0.690454	-0.443794
39	6	0	-5.532804	-1.346186	0.816604
40	6	0	-6.488421	0.623301	-0.907691
41	1	0	-4.528305	1.505151	-0.746336
42	6	0	-6.839020	-1.403672	0.346439
43	1	0	-5.156490	-2.110676	1.488601
44	6	0	-7.325157	-0.422165	-0.516889
45	1	0	-6.857573	1.391866	-1.579692
46	1	0	-7.482547	-2.221176	0.656447
47	1	0	-8.345524	-0.471588	-0.882079
48	6	0	-0.400999	2.245404	0.762117
49	6	0	0.025589	3.487467	1.247288
50	6	0	-1.189918	2.211454	-0.393972
51	6	0	-0.345124	4.667474	0.608883
52	1	0	0.649012	3.513289	2.134597
53	6	0	-1.556765	3.391845	-1.035355
54	1	0	-1.501402	1.255950	-0.801315
55	6	0	-1.140808	4.623982	-0.534308
56	1	0	-0.011843	5.621948	1.004524
57	1	0	-2.163063	3.347636	-1.935178
58	1	0	-1.429690	5.542833	-1.034812
59	7	0	1.321728	1.031065	1.831258
60	1	0	-0.466753	-0.901480	2.282876
61	1	0	2.006300	1.086889	0.517730

62	7	0	1.760704	-0.176543	2.441259
63	1	0	1.612721	-0.955368	1.785628
64	1	0	2.769018	-0.086311	2.541261

N_TS7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.498742	1.597074	1.695391
2	6	0	0.997865	0.241367	1.876654
3	6	0	2.002136	-0.314686	1.162894
4	6	0	2.758069	-0.875979	0.320642
5	6	0	4.146450	-1.151387	0.004254
6	6	0	4.739015	-2.386994	0.309088
7	6	0	4.917671	-0.185042	-0.664386
8	6	0	6.066113	-2.636603	-0.025402
9	1	0	4.150109	-3.145724	0.815142
10	6	0	6.243066	-0.442080	-0.997522
11	1	0	4.462698	0.770784	-0.911315
12	6	0	6.826298	-1.668118	-0.679516
13	1	0	6.509155	-3.595711	0.225700
14	1	0	6.823644	0.320662	-1.507753
15	1	0	7.860387	-1.867661	-0.940560
16	6	0	1.219150	2.537871	0.786613
17	6	0	0.485038	3.410708	-0.028599
18	6	0	2.617668	2.565201	0.706442
19	6	0	1.127536	4.263352	-0.921169
20	1	0	-0.597798	3.394919	0.042959
21	6	0	3.260890	3.421900	-0.185176
22	1	0	3.206308	1.914434	1.344201
23	6	0	2.519114	4.265835	-1.009375
24	1	0	0.540362	4.920258	-1.555067
25	1	0	4.345604	3.429392	-0.232696
26	1	0	3.021068	4.923754	-1.711397
27	7	0	-0.596659	2.062666	2.203259
28	1	0	0.485547	-0.406551	2.580120
29	1	0	-3.516884	1.197214	1.322913
30	7	0	-1.371421	1.186728	2.968149
31	1	0	-0.813080	0.622749	3.608900
32	1	0	-1.992520	1.756513	3.531983
33	6	0	-0.352528	-0.523218	-0.856350
34	6	0	-1.246984	0.624149	-0.930519

35	6	0	-2.408310	0.695545	-0.313278
36	6	0	-3.554098	0.804730	0.305400
37	6	0	-4.866231	0.405856	-0.240252
38	6	0	-4.986270	-0.187739	-1.503818
39	6	0	-6.017148	0.620502	0.523865
40	6	0	-6.234205	-0.554490	-1.990022
41	1	0	-4.093751	-0.362748	-2.098648
42	6	0	-7.267573	0.251946	0.034360
43	1	0	-5.927900	1.078493	1.504887
44	6	0	-7.379502	-0.335979	-1.222849
45	1	0	-6.316729	-1.014331	-2.969591
46	1	0	-8.153693	0.424846	0.636541
47	1	0	-8.353167	-0.625164	-1.604587
48	6	0	-0.714521	-1.804308	-0.208200
49	6	0	-0.349709	-2.998930	-0.840105
50	6	0	-1.402857	-1.847923	1.012348
51	6	0	-0.674545	-4.224619	-0.265329
52	1	0	0.168411	-2.960603	-1.793113
53	6	0	-1.722713	-3.074979	1.579308
54	1	0	-1.640748	-0.924810	1.533194
55	6	0	-1.363236	-4.264097	0.943166
56	1	0	-0.392522	-5.144925	-0.765625
57	1	0	-2.245046	-3.105216	2.529901
58	1	0	-1.616407	-5.218480	1.393579
59	7	0	0.810008	-0.495434	-1.456725
60	1	0	-0.898291	1.468420	-1.519467
61	1	0	1.639009	-1.001733	-0.875260
62	7	0	1.224698	0.675348	-2.112918
63	1	0	1.531380	1.352489	-1.408246
64	1	0	2.042115	0.420387	-2.660377

N_TS8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.021661	-1.144449	0.238115
2	6	0	-0.817337	-1.674071	0.960670
3	6	0	0.364165	-1.725887	0.402494
4	6	0	1.541598	-1.778072	-0.174107
5	6	0	2.558023	-0.707449	-0.136656
6	6	0	2.258555	0.578331	0.332156
7	6	0	3.854162	-0.979851	-0.586539

8	6	0	3.239303	1.561590	0.362941
9	1	0	1.246588	0.803230	0.658258
10	6	0	4.836065	0.006876	-0.555884
11	1	0	4.090792	-1.972594	-0.959480
12	6	0	4.532730	1.279311	-0.078792
13	1	0	2.994462	2.554443	0.727000
14	1	0	5.838088	-0.218976	-0.906457
15	1	0	5.296643	2.049730	-0.054899
16	6	0	-2.186815	0.321650	0.080993
17	6	0	-1.520500	1.209609	0.932890
18	6	0	-3.026063	0.841767	-0.913153
19	6	0	-1.688108	2.585541	0.795834
20	1	0	-0.875805	0.819417	1.714997
21	6	0	-3.191873	2.214740	-1.048803
22	1	0	-3.537060	0.154924	-1.579377
23	6	0	-2.522922	3.093278	-0.196020
24	1	0	-1.166291	3.259654	1.467728
25	1	0	-3.840369	2.602984	-1.827948
26	1	0	-2.650251	4.165249	-0.307264
27	7	0	-2.930459	-1.913451	-0.240083
28	1	0	-0.950959	-2.050547	1.977090
29	7	0	-2.746036	-3.264230	-0.194823
30	1	0	-2.128804	-3.600460	0.541009
31	1	0	-3.640176	-3.736242	-0.184438
32	1	0	1.802686	-2.684531	-0.718711

N_TS9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.515297	-0.045196	0.293768
2	6	0	-0.655372	0.996273	-0.188083
3	6	0	0.671695	0.847002	0.043497
4	6	0	1.903332	1.360849	0.122429
5	6	0	3.140841	0.605807	-0.072315
6	6	0	3.155418	-0.655916	-0.691631
7	6	0	4.364533	1.136429	0.368258
8	6	0	4.341242	-1.367665	-0.835817
9	1	0	2.228542	-1.066352	-1.082547
10	6	0	5.550693	0.427353	0.214269
11	1	0	4.375665	2.114726	0.841808
12	6	0	5.546549	-0.832707	-0.382464

13	1	0	4.326148	-2.340640	-1.317856
14	1	0	6.483039	0.858776	0.566001
15	1	0	6.472166	-1.386421	-0.500525
16	6	0	-2.979636	-0.033641	0.066719
17	6	0	-3.647855	1.168273	-0.183169
18	6	0	-3.711387	-1.226734	0.108895
19	6	0	-5.023244	1.177736	-0.401427
20	1	0	-3.094680	2.102345	-0.189880
21	6	0	-5.083313	-1.215564	-0.110230
22	1	0	-3.189802	-2.156223	0.309859
23	6	0	-5.743170	-0.013475	-0.368247
24	1	0	-5.531348	2.117350	-0.591911
25	1	0	-5.641224	-2.146003	-0.082008
26	1	0	-6.814897	-0.006848	-0.538570
27	7	0	-0.965524	-1.118918	0.801933
28	1	0	-1.007885	1.686898	-0.945057
29	7	0	0.394181	-0.875318	0.973405
30	1	0	0.589529	-0.454927	1.881164
31	1	0	0.925857	-1.740962	0.899787
32	1	0	1.988110	2.404983	0.415653

N_TS10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.587518	-0.466916	0.237004
2	6	0	0.384644	0.269013	-0.063399
3	6	0	-0.625976	-0.636504	0.088091
4	6	0	-1.932564	-1.106130	-0.293189
5	6	0	-3.150614	-0.311817	-0.184579
6	6	0	-4.304911	-0.659950	-0.909550
7	6	0	-3.225789	0.806969	0.664908
8	6	0	-5.476031	0.078792	-0.794786
9	1	0	-4.272283	-1.523110	-1.569611
10	6	0	-4.395811	1.550694	0.770506
11	1	0	-2.351476	1.088998	1.246589
12	6	0	-5.531049	1.192439	0.044035
13	1	0	-6.351571	-0.212624	-1.367527
14	1	0	-4.423125	2.413888	1.429044
15	1	0	-6.445100	1.770657	0.130208
16	6	0	2.961156	0.031426	0.028211
17	6	0	3.212427	1.405771	-0.021779

18	6	0	4.023960	-0.868593	-0.109598
19	6	0	4.509319	1.873921	-0.210514
20	1	0	2.396102	2.110781	0.101672
21	6	0	5.317955	-0.398054	-0.298430
22	1	0	3.821021	-1.933747	-0.074331
23	6	0	5.563492	0.974043	-0.350458
24	1	0	4.696421	2.942041	-0.245697
25	1	0	6.136088	-1.102092	-0.409549
26	1	0	6.573909	1.340657	-0.499559
27	7	0	1.390838	-1.702721	0.660662
28	1	0	0.328303	1.233931	-0.542581
29	7	0	-0.021075	-1.800916	0.689039
30	1	0	-0.305862	-1.861015	1.672650
31	1	0	-1.869322	-1.753604	-1.170314
32	1	0	-1.027803	-2.399918	0.272266

N_TS11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.249738	-1.175972	0.245969
2	6	0	-2.432739	-1.566283	-0.838416
3	6	0	-1.121231	-1.609544	-0.368442
4	6	0	0.092571	-1.855018	-0.999982
5	6	0	1.409478	-2.114583	-0.432314
6	6	0	2.400915	-2.642803	-1.294137
7	6	0	1.813007	-1.840246	0.891531
8	6	0	3.698365	-2.873677	-0.870070
9	1	0	2.126465	-2.865836	-2.322094
10	6	0	3.120334	-2.074153	1.314303
11	1	0	1.137122	-1.383077	1.604639
12	6	0	4.075623	-2.587351	0.445011
13	1	0	4.424704	-3.276916	-1.569726
14	1	0	3.391646	-1.831370	2.338091
15	1	0	5.094783	-2.752697	0.778707
16	6	0	-4.710807	-0.964618	0.193432
17	6	0	-5.348244	-0.762074	-1.034402
18	6	0	-5.467976	-0.940838	1.369824
19	6	0	-6.722323	-0.548742	-1.087109
20	1	0	-4.762903	-0.750121	-1.948561
21	6	0	-6.841179	-0.727848	1.315682
22	1	0	-4.968045	-1.094015	2.320514

23	6	0	-7.472154	-0.533052	0.087413
24	1	0	-7.206719	-0.390058	-2.045145
25	1	0	-7.421777	-0.715085	2.232502
26	1	0	-8.543887	-0.367087	0.046634
27	7	0	-2.606711	-0.985211	1.383390
28	1	0	-2.746512	-1.805792	-1.842284
29	7	0	-1.232472	-1.184915	1.030627
30	1	0	-0.712249	-0.118878	1.104774
31	1	0	-0.787509	-1.821506	1.697009
32	1	0	-0.015314	-2.125904	-2.047329
33	6	0	3.208754	1.078757	-0.121725
34	6	0	2.295570	1.375809	0.941326
35	6	0	1.027668	1.320763	0.428134
36	6	0	-0.267918	1.393862	0.988381
37	6	0	-1.463825	1.904802	0.280294
38	6	0	-2.381331	2.690505	1.003845
39	6	0	-1.788624	1.611206	-1.055926
40	6	0	-3.550563	3.165246	0.426072
41	1	0	-2.160861	2.926981	2.041432
42	6	0	-2.958266	2.096624	-1.638571
43	1	0	-1.178218	0.935683	-1.646739
44	6	0	-3.846673	2.876958	-0.907096
45	1	0	-4.232713	3.768040	1.018074
46	1	0	-3.180058	1.840899	-2.670546
47	1	0	-4.760933	3.244680	-1.361097
48	6	0	4.677765	1.016351	-0.005664
49	6	0	5.279908	0.935202	1.252979
50	6	0	5.475781	1.004294	-1.155266
51	6	0	6.663931	0.844095	1.361729
52	1	0	4.667715	0.922043	2.148873
53	6	0	6.857907	0.914688	-1.043564
54	1	0	5.002585	1.068549	-2.129471
55	6	0	7.454673	0.834267	0.214625
56	1	0	7.124041	0.775462	2.341833
57	1	0	7.471985	0.908507	-1.937991
58	1	0	8.534183	0.763066	0.300135
59	7	0	2.640264	0.861973	-1.281707
60	1	0	2.544323	1.623500	1.961086
61	7	0	1.230878	0.972771	-0.999692
62	1	0	0.806221	1.661481	-1.634791
63	1	0	0.780200	0.031554	-1.188441
64	1	0	-0.223920	1.695811	2.034391

N_TS12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.608969	-0.331654	-0.160371
2	6	0	0.729258	-1.257545	0.412555
3	6	0	-0.581994	-0.802786	0.148386
4	6	0	-1.814437	-1.334403	0.425762
5	6	0	-3.135747	-0.829360	0.117253
6	6	0	-3.441714	0.474075	-0.336347
7	6	0	-4.236310	-1.702760	0.292796
8	6	0	-4.751123	0.858864	-0.614512
9	1	0	-2.667904	1.223331	-0.450625
10	6	0	-5.537665	-1.314614	0.018166
11	1	0	-4.043237	-2.711219	0.649980
12	6	0	-5.811915	-0.025936	-0.447136
13	1	0	-4.938569	1.871471	-0.960404
14	1	0	-6.347207	-2.023827	0.165271
15	1	0	-6.829243	0.279907	-0.666606
16	6	0	3.086755	-0.406393	-0.137368
17	6	0	3.734431	-1.592214	0.223330
18	6	0	3.856943	0.709202	-0.485461
19	6	0	5.123966	-1.660947	0.241134
20	1	0	3.149224	-2.469748	0.479027
21	6	0	5.246046	0.639680	-0.468724
22	1	0	3.353611	1.628829	-0.765173
23	6	0	5.884086	-0.544974	-0.104332
24	1	0	5.613950	-2.588006	0.520967
25	1	0	5.832470	1.512187	-0.738556
26	1	0	6.967916	-0.598720	-0.090551
27	7	0	1.025937	0.696661	-0.772074
28	1	0	0.978551	-2.155499	0.955349
29	7	0	-0.379543	0.483785	-0.513819
30	1	0	-0.623131	1.392061	0.279295
31	1	0	-0.917075	0.589394	-1.376814
32	1	0	-1.785231	-2.308934	0.904900
33	7	0	0.237289	3.409094	0.422616
34	1	0	0.684215	4.033552	1.089448
35	1	0	0.968744	2.870301	-0.042302
36	7	0	-0.540773	2.439484	1.137945
37	1	0	-0.107904	2.137657	2.012629
38	1	0	-1.446844	2.844705	1.360690

N_TS13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.944511	-0.176660	-0.247024
2	6	0	1.057223	-0.917322	0.563577
3	6	0	-0.228641	-0.644576	0.078211
4	6	0	-1.493064	-1.117429	0.519040
5	6	0	-2.792775	-0.818542	-0.001767
6	6	0	-3.105003	0.272337	-0.864786
7	6	0	-3.912730	-1.593445	0.420819
8	6	0	-4.415938	0.552626	-1.256339
9	1	0	-2.331973	0.955034	-1.202935
10	6	0	-5.202909	-1.311141	0.018092
11	1	0	-3.732554	-2.436543	1.083109
12	6	0	-5.483431	-0.229729	-0.832765
13	1	0	-4.595871	1.407028	-1.906421
14	1	0	-6.015435	-1.942394	0.372800
15	1	0	-6.498687	-0.011735	-1.140773
16	6	0	3.415611	-0.113620	-0.138068
17	6	0	4.124642	-1.166510	0.453202
18	6	0	4.123353	0.992937	-0.629140
19	6	0	5.512324	-1.116418	0.554817
20	1	0	3.584295	-2.036580	0.822047
21	6	0	5.510497	1.039085	-0.530187
22	1	0	3.567903	1.811528	-1.079798
23	6	0	6.209612	-0.012510	0.063417
24	1	0	6.052034	-1.941336	1.015674
25	1	0	6.044464	1.906639	-0.915408
26	1	0	7.291429	0.028480	0.141030
27	7	0	1.313278	0.524108	-1.181731
28	1	0	1.297024	-1.538265	1.412930
29	7	0	-0.021334	0.291484	-0.930909
30	1	0	-1.744481	0.684381	1.565924
31	1	0	-0.629701	0.352450	-1.735878
32	1	0	-1.444756	-1.924660	1.244948
33	7	0	-3.001310	2.289600	1.534053
34	1	0	-2.920110	3.257211	1.232701
35	1	0	-3.519827	1.779048	0.814285
36	7	0	-1.675907	1.727424	1.485757
37	1	0	-1.152141	1.910895	0.620332
38	1	0	-1.134393	2.076015	2.278650

O-R2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.011040	0.698830	0.000000
2	1	0	0.558078	0.947157	0.808317
3	1	0	0.558078	0.947157	-0.808317
4	8	0	-0.011040	-0.729944	0.000000
5	1	0	-0.950562	-0.946577	0.000000

O_R2-complex-N

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.462732	0.666673	0.035534
2	1	0	-2.032948	0.968266	-0.753361
3	1	0	-2.018424	0.875142	0.863982
4	8	0	-1.447179	-0.757004	-0.047544
5	1	0	-0.491868	-0.944483	-0.064086
6	7	0	1.591246	0.715082	0.099043
7	1	0	2.037311	0.986611	-0.776274
8	1	0	0.646754	1.110813	0.068158
9	8	0	1.346040	-0.690393	-0.074457
10	1	0	1.768689	-1.089462	0.695548

O_R2-complex-O

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.565142	-0.699521	0.139899
2	1	0	0.592893	-1.013039	0.103441
3	1	0	2.007167	-1.069033	-0.700735
4	8	0	1.467719	0.708017	-0.120430
5	1	0	1.897405	1.104952	0.646366
6	7	0	-1.565241	0.699761	-0.138579
7	1	0	-2.006273	1.067814	0.703213
8	1	0	-0.592933	1.013191	-0.102720

9	8	0	-1.467700	-0.708242	0.119107
10	1	0	-1.897722	-1.103768	-0.648221

O_M1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.182827	-1.115513	0.027311
2	6	0	1.113241	-1.917503	0.043438
3	6	0	-0.226735	-1.452088	0.001014
4	6	0	-1.374392	-1.060447	-0.031910
5	6	0	-2.698091	-0.517278	-0.063578
6	6	0	-2.869036	0.875993	-0.087582
7	6	0	-3.824485	-1.353422	-0.067397
8	6	0	-4.147115	1.420111	-0.115250
9	1	0	-1.992223	1.515862	-0.084254
10	6	0	-5.099269	-0.799837	-0.095192
11	1	0	-3.689019	-2.429602	-0.048153
12	6	0	-5.263588	0.584467	-0.119533
13	1	0	-4.273478	2.497496	-0.134272
14	1	0	-5.967701	-1.450076	-0.098129
15	1	0	-6.260831	1.011508	-0.142507
16	6	0	2.238930	0.357038	0.032521
17	6	0	1.372325	1.085507	0.859812
18	6	0	3.155619	1.050317	-0.769191
19	6	0	1.415444	2.474612	0.873862
20	1	0	0.673705	0.553992	1.497093
21	6	0	3.198296	2.441106	-0.748616
22	1	0	3.824006	0.516971	-1.439082
23	6	0	2.328351	3.156071	0.070405
24	1	0	0.741258	3.026543	1.520615
25	1	0	3.908078	2.964960	-1.379937
26	1	0	2.362224	4.240386	0.083915
27	1	0	1.329141	-2.983076	0.071814
28	7	0	3.505163	-1.808362	0.051336
29	1	0	4.018194	-1.404197	0.851466
30	1	0	4.026088	-1.487342	-0.779207
31	8	0	3.468809	-3.161212	0.107575

O_M2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.250849	-1.096675	0.054224
2	6	0	1.174990	-1.919538	0.066694
3	6	0	-0.166507	-1.461975	0.013556
4	6	0	-1.322422	-1.089912	-0.028643
5	6	0	-2.652352	-0.564594	-0.063828
6	6	0	-3.770774	-1.412459	-0.088385
7	6	0	-2.846514	0.826829	-0.069499
8	6	0	-5.052978	-0.875759	-0.117628
9	1	0	-3.622922	-2.487339	-0.083920
10	6	0	-4.131721	1.354228	-0.098763
11	1	0	-1.979042	1.479444	-0.050323
12	6	0	-5.238425	0.506045	-0.123240
13	1	0	-5.911751	-1.538916	-0.136276
14	1	0	-4.271080	2.430435	-0.102849
15	1	0	-6.241111	0.920002	-0.147117
16	6	0	2.197636	0.385688	0.053138
17	6	0	1.305005	1.073383	0.884461
18	6	0	3.065988	1.115448	-0.768645
19	6	0	1.270626	2.463714	0.878271
20	1	0	0.646986	0.514182	1.540513
21	6	0	3.027998	2.506878	-0.771881
22	1	0	3.757972	0.586653	-1.416129
23	6	0	2.129295	3.183870	0.048525
24	1	0	0.577310	2.986397	1.529474
25	1	0	3.698638	3.062178	-1.419489
26	1	0	2.099671	4.268606	0.045423
27	7	0	3.556022	-1.586480	-0.055381
28	1	0	1.348855	-2.989235	0.086060
29	1	0	4.212618	-1.100839	0.551043
30	8	0	3.674783	-2.959032	0.181461
31	1	0	3.949256	-3.324979	-0.670573

O_M3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.781049	-0.763049	-0.731809
2	6	0	0.734788	-1.597434	-0.727682
3	6	0	-0.616529	-1.205503	-0.550163

4	6	0	-1.780095	-0.898753	-0.394899
5	6	0	-3.132484	-0.479206	-0.188099
6	6	0	-4.184987	-1.405677	-0.231917
7	6	0	-3.409346	0.872932	0.069137
8	6	0	-5.491900	-0.982631	-0.020596
9	1	0	-3.967103	-2.449667	-0.430831
10	6	0	-4.719086	1.286287	0.279985
11	1	0	-2.590300	1.584628	0.101288
12	6	0	-5.761536	0.361196	0.235648
13	1	0	-6.302435	-1.703040	-0.055762
14	1	0	-4.927783	2.332131	0.479523
15	1	0	-6.783192	0.687378	0.400685
16	6	0	1.820345	0.687085	-0.482548
17	6	0	2.735777	1.510340	-1.153135
18	6	0	0.960373	1.261281	0.467310
19	6	0	2.779744	2.875993	-0.890079
20	1	0	3.407038	1.100222	-1.901892
21	6	0	1.008205	2.626885	0.725025
22	1	0	0.264132	0.628074	1.007334
23	6	0	1.916214	3.438217	0.046662
24	1	0	3.488398	3.500783	-1.423193
25	1	0	0.339105	3.055479	1.463865
26	1	0	1.952640	4.503192	0.250071
27	1	0	0.977462	-2.646955	-0.877447
28	7	0	3.107725	-1.400110	-0.960602
29	1	0	3.731889	-0.967861	-0.255093
30	1	0	3.442929	-1.117940	-1.892180
31	7	0	3.471236	-1.468669	1.770062
32	1	0	4.074762	-1.815123	2.513275
33	1	0	3.152613	-2.287296	1.239817
34	8	0	2.312411	-0.969256	2.434984
35	1	0	2.298071	-0.036612	2.183469
36	8	0	3.130821	-2.757458	-0.833256

O_M4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.090428	1.707090	-1.330844
2	6	0	-0.585939	0.518387	-1.758090
3	6	0	-1.882158	0.043447	-1.437854
4	6	0	-2.971329	-0.404328	-1.133282

5	6	0	-4.241399	-0.869525	-0.663889
6	6	0	-5.015797	-1.767246	-1.414278
7	6	0	-4.717679	-0.422047	0.580707
8	6	0	-6.242642	-2.204395	-0.928479
9	1	0	-4.647539	-2.114139	-2.373993
10	6	0	-5.946733	-0.863957	1.056832
11	1	0	-4.107755	0.265056	1.161926
12	6	0	-6.712260	-1.754525	0.305166
13	1	0	-6.835660	-2.898220	-1.515469
14	1	0	-6.307592	-0.513534	2.018374
15	1	0	-7.670506	-2.098871	0.679833
16	6	0	-0.869284	2.772706	-0.657222
17	6	0	-0.276798	3.527557	0.363861
18	6	0	-2.188195	3.053967	-1.033541
19	6	0	-0.997683	4.525324	1.012277
20	1	0	0.746746	3.315036	0.654226
21	6	0	-2.906766	4.050284	-0.380976
22	1	0	-2.645274	2.494977	-1.842687
23	6	0	-2.315789	4.785844	0.645341
24	1	0	-0.529906	5.095430	1.808418
25	1	0	-3.928467	4.259701	-0.680975
26	1	0	-2.878642	5.562980	1.152345
27	7	0	1.267991	1.999567	-1.383254
28	1	0	0.082104	-0.154397	-2.283617
29	1	0	1.491822	2.918947	-1.754834
30	6	0	0.051890	-0.675970	1.301110
31	6	0	0.959588	0.315447	1.468591
32	6	0	2.327184	0.209497	1.113222
33	6	0	3.504216	0.154055	0.805946
34	6	0	4.879206	0.016849	0.428201
35	6	0	5.328982	-1.188090	-0.136740
36	6	0	5.785862	1.073059	0.607742
37	6	0	6.659999	-1.329657	-0.509824
38	1	0	4.623459	-2.001595	-0.275296
39	6	0	7.115184	0.921689	0.231064
40	1	0	5.437530	2.004559	1.041599
41	6	0	7.556417	-0.277245	-0.327430
42	1	0	6.999772	-2.264471	-0.943792
43	1	0	7.810497	1.742438	0.373860
44	1	0	8.595161	-0.391065	-0.619435
45	6	0	0.325775	-2.012599	0.718997
46	6	0	-0.255731	-3.152135	1.289922
47	6	0	1.141226	-2.158001	-0.409933
48	6	0	-0.009760	-4.412666	0.753115

49	1	0	-0.887693	-3.046617	2.165603
50	6	0	1.384389	-3.419143	-0.943387
51	1	0	1.564450	-1.277078	-0.878186
52	6	0	0.812915	-4.550143	-0.361968
53	1	0	-0.459109	-5.288153	1.210370
54	1	0	2.014843	-3.516529	-1.821473
55	1	0	1.003758	-5.533031	-0.780576
56	7	0	-1.268090	-0.559664	1.749439
57	1	0	0.611298	1.256704	1.878829
58	1	0	-1.922611	-0.887298	1.038491
59	8	0	2.072540	1.042179	-1.998052
60	1	0	2.603854	0.701459	-1.256128
61	8	0	-1.640996	0.747064	2.088437
62	1	0	-1.854974	0.693262	3.030088

O_M5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.410803	1.603008	1.678326
2	6	0	0.965820	0.304822	1.872318
3	6	0	2.154218	-0.133549	1.310738
4	6	0	3.152851	-0.586788	0.749765
5	6	0	4.334642	-0.967540	0.052090
6	6	0	4.881835	-2.261187	0.161661
7	6	0	4.968975	-0.039505	-0.798746
8	6	0	6.022366	-2.606426	-0.554940
9	1	0	4.401609	-2.984390	0.812666
10	6	0	6.104986	-0.397945	-1.513886
11	1	0	4.564774	0.966326	-0.879109
12	6	0	6.639642	-1.681637	-1.397497
13	1	0	6.431658	-3.606965	-0.455916
14	1	0	6.577709	0.331228	-2.164280
15	1	0	7.527153	-1.957574	-1.956398
16	6	0	1.098572	2.622178	0.827031
17	6	0	0.350151	3.443610	-0.026609
18	6	0	2.487478	2.795149	0.873053
19	6	0	0.972507	4.398600	-0.824358
20	1	0	-0.727964	3.317012	-0.052888
21	6	0	3.110702	3.750745	0.074320
22	1	0	3.082372	2.184838	1.543570
23	6	0	2.357171	4.552096	-0.781702

24	1	0	0.375718	5.021018	-1.483314
25	1	0	4.187989	3.873248	0.127357
26	1	0	2.844266	5.293033	-1.406988
27	7	0	-0.738773	2.008163	2.144143
28	1	0	0.469150	-0.346150	2.581984
29	1	0	-3.463357	1.157314	1.284556
30	6	0	-0.246338	-0.857146	-0.514458
31	6	0	-0.987214	0.372624	-0.681909
32	6	0	-2.202906	0.559015	-0.203521
33	6	0	-3.403088	0.772804	0.266729
34	6	0	-4.670675	0.514703	-0.447647
35	6	0	-4.692107	-0.065380	-1.723335
36	6	0	-5.880426	0.852928	0.166933
37	6	0	-5.900330	-0.297271	-2.367857
38	1	0	-3.755462	-0.335334	-2.203335
39	6	0	-7.090394	0.620031	-0.481163
40	1	0	-5.869117	1.300786	1.156431
41	6	0	-7.103924	0.044497	-1.748818
42	1	0	-5.905655	-0.747719	-3.355078
43	1	0	-8.022108	0.887591	0.006193
44	1	0	-8.046501	-0.138830	-2.253451
45	6	0	-0.794475	-2.076152	0.111233
46	6	0	-0.623822	-3.310717	-0.527805
47	6	0	-1.493781	-2.004049	1.324252
48	6	0	-1.143138	-4.467003	0.045479
49	1	0	-0.117886	-3.363594	-1.486864
50	6	0	-2.011055	-3.165394	1.885527
51	1	0	-1.594203	-1.046997	1.827915
52	6	0	-1.836541	-4.396249	1.250984
53	1	0	-1.013220	-5.419631	-0.455665
54	1	0	-2.544113	-3.111558	2.828688
55	1	0	-2.241403	-5.298385	1.696840
56	7	0	0.918081	-0.987514	-1.112718
57	1	0	-0.476861	1.179539	-1.197231
58	1	0	1.547450	-1.757412	-0.907031
59	8	0	-1.371306	0.971434	2.874974
60	1	0	-2.107554	1.427419	3.298105
61	8	0	1.482924	0.059050	-1.788188
62	1	0	2.132437	0.429522	-1.158141

O_M6

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	2.168781	-1.035065	-0.117655
2	6	0	1.027437	-1.923249	0.186118
3	6	0	-0.078078	-1.516509	0.763347
4	6	0	-1.192805	-1.105594	1.315438
5	6	0	-2.366408	-0.613034	0.565406
6	6	0	-2.453573	-0.729379	-0.828611
7	6	0	-3.418196	-0.008286	1.261883
8	6	0	-3.561078	-0.236721	-1.508173
9	1	0	-1.651752	-1.221763	-1.373184
10	6	0	-4.528402	0.481844	0.579905
11	1	0	-3.360363	0.079931	2.343177
12	6	0	-4.602273	0.371898	-0.806551
13	1	0	-3.616535	-0.333571	-2.587715
14	1	0	-5.336066	0.951027	1.132485
15	1	0	-5.467727	0.753381	-1.338453
16	6	0	2.029309	0.445132	-0.078213
17	6	0	0.865249	1.074777	-0.531521
18	6	0	3.086628	1.228140	0.397711
19	6	0	0.762726	2.462606	-0.507764
20	1	0	0.041251	0.482632	-0.916950
21	6	0	2.982090	2.614903	0.420059
22	1	0	3.985229	0.736833	0.755936
23	6	0	1.818527	3.235970	-0.030691
24	1	0	-0.144144	2.938648	-0.866659
25	1	0	3.807089	3.211131	0.796416
26	1	0	1.734568	4.317703	-0.008396
27	7	0	3.334374	-1.481456	-0.425729
28	1	0	1.151287	-2.973349	-0.063044
29	1	0	-1.261442	-1.099444	2.402489
30	8	0	3.404723	-2.863505	-0.385909
31	1	0	4.300595	-3.049519	-0.692855

O_M7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.447813	0.268802	0.225631
2	6	0	0.518732	-0.733986	-0.341192
3	6	0	-0.682566	-1.012984	0.105719
4	6	0	-1.883293	-1.327277	0.522302

5	6	0	-3.118793	-0.625792	0.119981
6	6	0	-3.079204	0.592590	-0.570983
7	6	0	-4.360050	-1.181373	0.448009
8	6	0	-4.259509	1.229436	-0.935608
9	1	0	-2.115192	1.038618	-0.798399
10	6	0	-5.540617	-0.541163	0.081760
11	1	0	-4.396436	-2.121181	0.992110
12	6	0	-5.494239	0.665059	-0.613189
13	1	0	-4.217785	2.173693	-1.469529
14	1	0	-6.496760	-0.984677	0.340971
15	1	0	-6.413514	1.166431	-0.898099
16	6	0	2.906274	0.068750	0.009521
17	6	0	3.429466	-1.220644	-0.129396
18	6	0	3.773772	1.166437	-0.049255
19	6	0	4.796307	-1.409801	-0.319328
20	1	0	2.769670	-2.081267	-0.072909
21	6	0	5.136965	0.975189	-0.238465
22	1	0	3.364799	2.166274	0.047117
23	6	0	5.652779	-0.313813	-0.375358
24	1	0	5.190934	-2.415504	-0.420464
25	1	0	5.798730	1.833866	-0.287720
26	1	0	6.716980	-0.461715	-0.527754
27	7	0	1.112320	1.333803	0.860591
28	1	0	0.887170	-1.276485	-1.210781
29	1	0	-1.987347	-2.152562	1.225584
30	8	0	-0.251226	1.480696	0.997174
31	1	0	-0.340703	2.335744	1.437454

O_M8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.552339	-0.041449	-0.076388
2	6	0	0.731339	1.077076	-0.114285
3	6	0	-0.611782	0.642626	-0.126640
4	6	0	-1.843337	1.195425	-0.046500
5	6	0	-3.138785	0.523797	-0.031717
6	6	0	-3.380059	-0.745577	-0.592842
7	6	0	-4.229062	1.186705	0.565892
8	6	0	-4.640719	-1.333240	-0.519437
9	1	0	-2.596945	-1.262604	-1.137825
10	6	0	-5.485024	0.600565	0.629389

11	1	0	-4.072265	2.173831	0.992039
12	6	0	-5.699237	-0.671558	0.095969
13	1	0	-4.794895	-2.312446	-0.962372
14	1	0	-6.302430	1.136103	1.102559
15	1	0	-6.679633	-1.132732	0.150943
16	6	0	3.029112	-0.037215	0.001402
17	6	0	3.751467	1.070317	-0.452122
18	6	0	3.712691	-1.139850	0.525241
19	6	0	5.140229	1.078301	-0.374430
20	1	0	3.225959	1.918290	-0.879913
21	6	0	5.101550	-1.129245	0.598248
22	1	0	3.149785	-1.996206	0.882072
23	6	0	5.817800	-0.020684	0.150439
24	1	0	5.693924	1.941685	-0.728424
25	1	0	5.625048	-1.985861	1.010077
26	1	0	6.901256	-0.013215	0.209959
27	7	0	0.958453	-1.236806	-0.107333
28	1	0	1.039928	2.107557	-0.057681
29	1	0	-1.838180	2.270568	0.099971
30	8	0	-0.486389	-0.804255	-0.220498
31	1	0	-1.020731	-1.289256	0.440596

O_M9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.837883	-0.979949	0.219764
2	6	0	-3.046265	-1.888819	-0.473508
3	6	0	-1.710247	-1.707143	-0.066522
4	6	0	-0.509706	-2.280655	-0.335870
5	6	0	0.808946	-2.082559	0.258143
6	6	0	1.878672	-2.834989	-0.275004
7	6	0	1.098851	-1.228605	1.342922
8	6	0	3.156596	-2.752304	0.255050
9	1	0	1.684866	-3.492241	-1.116944
10	6	0	2.388270	-1.144815	1.862025
11	1	0	0.315871	-0.638060	1.804860
12	6	0	3.426453	-1.906319	1.332491
13	1	0	3.956995	-3.344005	-0.182553
14	1	0	2.580818	-0.474403	2.695339
15	1	0	4.428045	-1.833224	1.741862
16	6	0	-5.303665	-0.833067	0.111821

17	6	0	-5.970527	-1.317505	-1.020310
18	6	0	-6.032133	-0.188335	1.118724
19	6	0	-7.346775	-1.164287	-1.140701
20	1	0	-5.404957	-1.794884	-1.816316
21	6	0	-7.408753	-0.029844	0.989084
22	1	0	-5.517882	0.173071	2.005366
23	6	0	-8.068233	-0.516718	-0.136000
24	1	0	-7.856238	-1.543814	-2.020839
25	1	0	-7.964458	0.473245	1.776809
26	1	0	-9.142219	-0.395790	-0.236372
27	7	0	-3.218756	-0.151849	1.061617
28	1	0	-3.384173	-2.685986	-1.115651
29	1	0	-1.396569	0.199517	0.400167
30	1	0	-0.577809	-3.055748	-1.095143
31	6	0	3.817217	0.878480	-0.415974
32	6	0	3.174209	1.821899	0.383140
33	6	0	1.810761	1.822997	0.053378
34	6	0	0.689818	2.447990	0.500981
35	6	0	-0.678091	2.415851	0.008567
36	6	0	-1.648663	3.153920	0.725449
37	6	0	-1.122308	1.726509	-1.143772
38	6	0	-2.965203	3.225268	0.303906
39	1	0	-1.340316	3.685137	1.620952
40	6	0	-2.461607	1.794985	-1.552347
41	1	0	-0.430485	1.190348	-1.781939
42	6	0	-3.388418	2.547630	-0.842401
43	1	0	-3.674278	3.812896	0.878253
44	1	0	-2.765170	1.252577	-2.442256
45	1	0	-4.422566	2.600172	-1.163628
46	6	0	5.243580	0.493934	-0.351058
47	6	0	6.047779	0.951408	0.696305
48	6	0	5.785999	-0.365820	-1.313659
49	6	0	7.380739	0.561485	0.777379
50	1	0	5.629694	1.600593	1.458323
51	6	0	7.118682	-0.753412	-1.225554
52	1	0	5.161190	-0.722244	-2.123805
53	6	0	7.918388	-0.292661	-0.184585
54	1	0	7.996326	0.921377	1.594942
55	1	0	7.533618	-1.420839	-1.975423
56	1	0	8.958474	-0.594681	-0.115773
57	7	0	3.071842	0.238768	-1.309871
58	1	0	3.616307	2.450013	1.136478
59	1	0	1.140232	0.115524	-0.838305
60	1	0	0.873819	3.094184	1.352920

61	8	0	1.720346	0.882426	-1.052747
62	8	0	-1.776552	-0.585983	0.868406

O_M10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.833977	-0.220521	0.126563
2	6	0	1.075722	-1.342020	-0.210048
3	6	0	-0.276387	-0.991374	-0.042320
4	6	0	-1.490870	-1.547827	-0.312751
5	6	0	-2.802433	-0.990344	-0.004230
6	6	0	-3.048254	-0.126460	1.085469
7	6	0	-3.906248	-1.338381	-0.809313
8	6	0	-4.322347	0.380185	1.329527
9	1	0	-2.239380	0.123384	1.765285
10	6	0	-5.175339	-0.830276	-0.560795
11	1	0	-3.751292	-2.015904	-1.644780
12	6	0	-5.394049	0.043054	0.504290
13	1	0	-4.478658	1.036726	2.181063
14	1	0	-6.000326	-1.114487	-1.207196
15	1	0	-6.383838	0.443634	0.695182
16	6	0	3.307752	-0.107818	0.075133
17	6	0	4.104163	-1.256676	0.090978
18	6	0	3.917579	1.149980	0.013418
19	6	0	5.490345	-1.149432	0.039227
20	1	0	3.637929	-2.234560	0.159476
21	6	0	5.303459	1.254344	-0.034952
22	1	0	3.297182	2.039885	-0.004354
23	6	0	6.093058	0.105451	-0.023741
24	1	0	6.100360	-2.046644	0.052780
25	1	0	5.768231	2.233604	-0.087005
26	1	0	7.174365	0.188048	-0.063933
27	7	0	1.151131	0.843667	0.536107
28	1	0	1.433952	-2.287094	-0.582759
29	1	0	-1.457734	-2.488221	-0.852241
30	8	0	-0.235240	0.344641	0.473786
31	1	0	-0.830657	0.998291	-0.174990
32	7	0	-2.530293	2.592413	-0.661027
33	1	0	-2.830545	2.239617	0.249892
34	1	0	-1.997349	3.443759	-0.494101
35	8	0	-1.523873	1.670527	-1.098773

36	1	0	-1.975965	1.074743	-1.716714

O_P

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.382431	-0.432183	0.274129
2	6	0	-0.477799	0.186894	1.191453
3	6	0	0.667581	-0.526155	1.047257
4	6	0	2.034002	-0.420620	1.640003
5	6	0	3.051038	0.012814	0.601073
6	6	0	3.969480	-0.894641	0.073878
7	6	0	3.051355	1.330351	0.135882
8	6	0	4.880484	-0.490712	-0.901077
9	1	0	3.972591	-1.921770	0.428509
10	6	0	3.959511	1.735899	-0.836586
11	1	0	2.332600	2.039339	0.539723
12	6	0	4.877473	0.824324	-1.358119
13	1	0	5.592019	-1.205250	-1.302489
14	1	0	3.952517	2.762900	-1.187539
15	1	0	5.586579	1.140124	-2.116536
16	6	0	-2.785297	-0.077675	-0.014842
17	6	0	-3.424513	0.929588	0.712412
18	6	0	-3.488433	-0.746134	-1.024640
19	6	0	-4.747080	1.264903	0.435004
20	1	0	-2.892534	1.453977	1.499869
21	6	0	-4.808440	-0.410208	-1.298241
22	1	0	-2.991022	-1.526349	-1.590943
23	6	0	-5.442004	0.596372	-0.569791
24	1	0	-5.233710	2.049421	1.005064
25	1	0	-5.344319	-0.932824	-2.083788
26	1	0	-6.472560	0.858381	-0.786219
27	7	0	-0.804684	-1.431638	-0.351550
28	1	0	-0.644026	1.026057	1.847690
29	1	0	1.988795	0.301895	2.458937
30	1	0	2.317117	-1.388709	2.064335
31	8	0	0.482398	-1.491579	0.129684

O_TS1

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-1.951968	0.319691	0.007798
2	6	0	-0.770411	0.620476	0.010595
3	6	0	0.549625	1.012967	0.015566
4	6	0	1.785726	0.779334	0.005632
5	6	0	-3.334346	-0.051589	0.001109
6	6	0	-3.710858	-1.399649	0.116962
7	6	0	-4.332612	0.928780	-0.123623
8	6	0	-5.054437	-1.755112	0.107849
9	1	0	-2.940191	-2.157204	0.214380
10	6	0	-5.674127	0.566034	-0.135089
11	1	0	-4.042066	1.970473	-0.211872
12	6	0	-6.038077	-0.774889	-0.018903
13	1	0	-5.335552	-2.799249	0.198521
14	1	0	-6.437685	1.330558	-0.234805
15	1	0	-7.086300	-1.055540	-0.027121
16	6	0	2.858932	-0.197617	-0.012304
17	6	0	4.224531	0.107134	-0.057278
18	6	0	2.469999	-1.549171	0.015693
19	6	0	5.173856	-0.910703	-0.071787
20	1	0	4.568984	1.133882	-0.084238
21	6	0	3.420987	-2.559882	0.000480
22	1	0	1.411615	-1.788528	0.050279
23	6	0	4.779432	-2.244979	-0.042604
24	1	0	6.227764	-0.655109	-0.106490
25	1	0	3.101668	-3.596764	0.023036
26	1	0	5.523296	-3.034745	-0.053753
27	8	0	1.589274	3.404121	0.093852
28	1	0	0.829845	2.719447	0.071447
29	7	0	2.663405	2.557939	0.053956
30	1	0	3.213819	2.756477	-0.779515
31	1	0	3.229266	2.692822	0.891038

O_TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.240001	-1.082476	0.087234
2	6	0	1.178804	-1.910589	0.081444
3	6	0	-0.165626	-1.459572	0.022658
4	6	0	-1.318564	-1.083285	-0.022482

5	6	0	-2.649899	-0.560376	-0.062568
6	6	0	-2.844454	0.830295	-0.061972
7	6	0	-3.763495	-1.413194	-0.096608
8	6	0	-4.130872	1.354320	-0.094491
9	1	0	-1.978356	1.484251	-0.035527
10	6	0	-5.046765	-0.879653	-0.129156
11	1	0	-3.611501	-2.487386	-0.096550
12	6	0	-5.234052	0.501970	-0.128445
13	1	0	-4.273989	2.429854	-0.093756
14	1	0	-5.904166	-1.544051	-0.154967
15	1	0	-6.237692	0.913477	-0.154701
16	6	0	2.208259	0.397513	0.070333
17	6	0	1.340967	1.095220	0.919504
18	6	0	3.040039	1.116839	-0.796614
19	6	0	1.303296	2.485277	0.895658
20	1	0	0.704500	0.541794	1.601806
21	6	0	3.000289	2.507633	-0.817229
22	1	0	3.700259	0.596419	-1.485468
23	6	0	2.132236	3.194413	0.027850
24	1	0	0.630619	3.015867	1.561699
25	1	0	3.642964	3.053741	-1.499614
26	1	0	2.101924	4.278834	0.011190
27	1	0	1.381493	-2.976489	0.091889
28	7	0	3.543560	-1.653570	0.155813
29	1	0	3.878395	-2.354544	0.949906
30	1	0	4.270984	-1.135241	-0.332602
31	8	0	3.643582	-3.100941	-0.103087

O_TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.932668	-1.173865	-0.160021
2	6	0	0.748938	-1.827636	-0.158619
3	6	0	-0.532766	-1.260833	-0.111224
4	6	0	-1.688517	-0.869184	-0.069662
5	6	0	-3.018196	-0.342290	-0.013844
6	6	0	-4.130472	-1.170968	-0.235483
7	6	0	-3.225522	1.019108	0.265135
8	6	0	-5.416807	-0.646725	-0.181608
9	1	0	-3.971456	-2.222661	-0.449724
10	6	0	-4.514169	1.535632	0.322157

11	1	0	-2.366385	1.659838	0.436698
12	6	0	-5.612048	0.705153	0.098073
13	1	0	-6.269695	-1.294101	-0.357285
14	1	0	-4.663974	2.588039	0.539914
15	1	0	-6.617491	1.110949	0.141881
16	6	0	2.410060	0.209763	-0.112536
17	6	0	1.484008	1.262151	-0.035634
18	6	0	3.778759	0.516430	-0.153364
19	6	0	1.917322	2.581670	-0.007604
20	1	0	0.423712	1.034778	-0.002773
21	6	0	4.205912	1.840477	-0.128673
22	1	0	4.513462	-0.281582	-0.189574
23	6	0	3.279404	2.877905	-0.055710
24	1	0	1.188270	3.383730	0.051016
25	1	0	5.268114	2.060571	-0.162473
26	1	0	3.615439	3.909411	-0.033989
27	7	0	2.892238	-2.290908	-0.281804
28	1	0	1.839511	-2.908908	-0.303778
29	1	0	3.482162	-2.286316	-1.118123
30	8	0	3.797159	-2.454888	0.787324
31	1	0	3.223964	-2.619029	1.553949

O_TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.859946	-0.365637	-0.686525
2	6	0	0.923919	-1.332899	-0.788325
3	6	0	-0.464036	-1.112255	-0.596224
4	6	0	-1.654576	-0.935891	-0.429790
5	6	0	-3.041286	-0.663548	-0.206777
6	6	0	-4.016083	-1.652471	-0.413148
7	6	0	-3.439191	0.611092	0.229510
8	6	0	-5.358105	-1.368432	-0.187387
9	1	0	-3.709823	-2.637428	-0.749708
10	6	0	-4.782926	0.886110	0.452831
11	1	0	-2.683293	1.373943	0.388347
12	6	0	-5.745923	-0.101100	0.245507
13	1	0	-6.104622	-2.139222	-0.349166
14	1	0	-5.080756	1.873819	0.789552
15	1	0	-6.794349	0.116509	0.420923
16	6	0	1.613151	1.046082	-0.309741

17	6	0	2.192325	2.088898	-1.042668
18	6	0	0.810659	1.355692	0.795490
19	6	0	1.968287	3.414561	-0.681608
20	1	0	2.797178	1.869282	-1.918421
21	6	0	0.588586	2.680998	1.155006
22	1	0	0.366947	0.549288	1.370838
23	6	0	1.166591	3.713214	0.417581
24	1	0	2.416275	4.213661	-1.263080
25	1	0	-0.030994	2.908884	2.016453
26	1	0	0.992397	4.746722	0.698849
27	1	0	1.282043	-2.318569	-1.067171
28	7	0	3.230819	-0.725654	-0.824172
29	1	0	3.683382	-1.052284	0.445736
30	1	0	3.766592	0.026482	-1.265263
31	7	0	3.945601	-1.995032	1.161153
32	1	0	4.875768	-2.056460	1.572081
33	1	0	3.829690	-2.640003	0.351800
34	8	0	2.971009	-2.282210	2.124216
35	1	0	2.707169	-1.422341	2.483484
36	8	0	3.494418	-1.962036	-1.375030

O_TS5-N

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.770620	-0.397455	-0.463738
2	6	0	0.698548	-1.206374	-0.528422
3	6	0	-0.623772	-0.808503	-0.374534
4	6	0	-1.834395	-0.624449	-0.268695
5	6	0	-3.228282	-0.368966	-0.134761
6	6	0	-4.007377	-0.010487	-1.251855
7	6	0	-3.863063	-0.469863	1.118431
8	6	0	-5.367881	0.236892	-1.114755
9	1	0	-3.531575	0.071860	-2.223768
10	6	0	-5.224444	-0.220888	1.243608
11	1	0	-3.274673	-0.745504	1.987674
12	6	0	-5.986552	0.133916	0.130810
13	1	0	-5.949864	0.512699	-1.988859
14	1	0	-5.693623	-0.305597	2.219152
15	1	0	-7.049100	0.327428	0.233290
16	6	0	1.893669	1.057236	-0.171592
17	6	0	0.861770	1.735992	0.498595

18	6	0	3.030004	1.799700	-0.540195
19	6	0	0.955564	3.095457	0.768308
20	1	0	-0.018511	1.183065	0.805082
21	6	0	3.123881	3.162306	-0.264365
22	1	0	3.858882	1.328467	-1.062682
23	6	0	2.086600	3.818859	0.389312
24	1	0	0.142367	3.594035	1.286713
25	1	0	4.012510	3.707914	-0.565405
26	1	0	2.158401	4.879606	0.605615
27	7	0	2.487481	-3.468653	-0.240093
28	1	0	2.926098	-4.324875	-0.577879
29	1	0	1.478241	-3.443148	-0.427907
30	8	0	2.655039	-3.399223	1.155575
31	1	0	3.158453	-2.575748	1.288973
32	7	0	3.064669	-1.056525	-0.717868
33	1	0	3.562926	-0.672918	-1.523188
34	1	0	2.837059	-2.383405	-0.701948
35	8	0	3.961066	-0.976297	0.392683
36	1	0	3.879169	-0.073717	0.747884

O_TS5-O

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.286433	-3.619907	1.428285
2	1	0	-3.202874	-4.031320	1.603122
3	1	0	-1.637639	-4.389446	1.596794
4	8	0	-2.264505	-3.435102	0.002826
5	1	0	-1.432352	-2.649105	-0.135262
6	7	0	-3.181578	-1.057187	-0.221562
7	1	0	-3.870800	-0.675432	0.430675
8	1	0	-3.016438	-2.140822	-0.077315
9	8	0	-3.787562	-0.881499	-1.493781
10	1	0	-3.101284	-1.174564	-2.117201
11	6	0	-1.857441	-0.405139	-0.108604
12	6	0	-0.847178	-1.297592	-0.186947
13	6	0	0.509688	-0.932988	-0.172726
14	6	0	1.712950	-0.730720	-0.170749
15	6	0	3.101870	-0.385986	-0.153703
16	6	0	3.488943	0.963632	-0.208739
17	6	0	4.091802	-1.378463	-0.073558
18	6	0	4.834795	1.308515	-0.184765

19	1	0	2.721712	1.729208	-0.271905
20	6	0	5.436287	-1.026385	-0.046188
21	1	0	3.793410	-2.420831	-0.031357
22	6	0	5.810646	0.315513	-0.102619
23	1	0	5.124332	2.353401	-0.228401
24	1	0	6.194290	-1.800132	0.019242
25	1	0	6.861077	0.587186	-0.082681
26	6	0	-1.904450	1.061088	0.068666
27	6	0	-0.811406	1.731720	0.640650
28	6	0	-3.032001	1.813942	-0.297479
29	6	0	-0.842411	3.108690	0.826619
30	1	0	0.058652	1.165236	0.950458
31	6	0	-3.059684	3.191880	-0.102162
32	1	0	-3.883760	1.330385	-0.764164
33	6	0	-1.965625	3.846781	0.456246
34	1	0	0.011920	3.605878	1.275206
35	1	0	-3.940176	3.754563	-0.395268
36	1	0	-1.988159	4.921331	0.604998

O_TS6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.582960	-1.571782	-1.069243
2	6	0	0.094554	-0.454986	-1.577970
3	6	0	1.285090	-0.037505	-1.060939
4	6	0	2.372429	0.397879	-0.564513
5	6	0	3.780918	0.098022	-0.859254
6	6	0	4.153913	-0.609132	-2.011710
7	6	0	4.772790	0.510366	0.036870
8	6	0	5.491432	-0.895118	-2.258157
9	1	0	3.385612	-0.925430	-2.712284
10	6	0	6.111875	0.221557	-0.211427
11	1	0	4.479179	1.051951	0.930824
12	6	0	6.474425	-0.480627	-1.358852
13	1	0	5.769048	-1.442715	-3.153158
14	1	0	6.872471	0.545856	0.491637
15	1	0	7.518324	-0.704246	-1.553572
16	6	0	-0.031268	-2.452662	-0.018270
17	6	0	-0.851298	-2.892822	1.027305
18	6	0	1.308023	-2.857918	-0.067122
19	6	0	-0.333816	-3.718123	2.019535

20	1	0	-1.876611	-2.543427	1.088976
21	6	0	1.818380	-3.686413	0.925182
22	1	0	1.940704	-2.539663	-0.889016
23	6	0	1.000756	-4.114978	1.969679
24	1	0	-0.970979	-4.043394	2.834713
25	1	0	2.854956	-4.002494	0.879431
26	1	0	1.403859	-4.759443	2.743938
27	7	0	-1.767255	-1.938036	-1.556488
28	1	0	-0.369009	0.102803	-2.384790
29	1	0	-2.310421	-2.692327	-1.152709
30	6	0	0.554721	1.571648	1.562108
31	6	0	-0.228229	0.483586	1.875989
32	6	0	-1.561282	0.325478	1.463613
33	6	0	-2.678783	0.115949	1.019726
34	6	0	-3.939735	-0.109221	0.393148
35	6	0	-4.535708	0.903929	-0.379812
36	6	0	-4.587117	-1.352382	0.496481
37	6	0	-5.737461	0.671161	-1.035178
38	1	0	-4.037767	1.865656	-0.460940
39	6	0	-5.788039	-1.578336	-0.168277
40	1	0	-4.150372	-2.133123	1.112263
41	6	0	-6.366885	-0.570844	-0.937208
42	1	0	-6.186297	1.461301	-1.628973
43	1	0	-6.275040	-2.544378	-0.080283
44	1	0	-7.304706	-0.749032	-1.452849
45	6	0	0.064120	2.773379	0.825866
46	6	0	0.517976	4.038681	1.219877
47	6	0	-0.810923	2.681926	-0.264235
48	6	0	0.089395	5.186588	0.560039
49	1	0	1.208084	4.109785	2.053618
50	6	0	-1.235031	3.831440	-0.926029
51	1	0	-1.151598	1.708578	-0.598345
52	6	0	-0.791963	5.086920	-0.514387
53	1	0	0.443680	6.159376	0.886296
54	1	0	-1.909516	3.743927	-1.772505
55	1	0	-1.126458	5.980860	-1.031376
56	7	0	1.898889	1.630719	1.765834
57	1	0	0.239326	-0.345552	2.394471
58	1	0	2.206297	1.162680	0.461266
59	8	0	2.325230	0.474449	2.488123
60	1	0	3.093613	0.802818	2.969207
61	8	0	-2.482224	-1.074583	-2.346327
62	1	0	-2.393640	-1.412033	-3.252636

O_TS7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.498382	1.567309	1.689306
2	6	0	1.007040	0.223615	1.860429
3	6	0	2.050124	-0.299665	1.168071
4	6	0	2.837188	-0.818726	0.335317
5	6	0	4.211614	-1.092211	-0.027695
6	6	0	5.022512	-1.937695	0.746241
7	6	0	4.750303	-0.519945	-1.191740
8	6	0	6.336643	-2.191852	0.368391
9	1	0	4.611563	-2.387200	1.644570
10	6	0	6.068813	-0.768020	-1.556484
11	1	0	4.119445	0.119214	-1.803704
12	6	0	6.867842	-1.607159	-0.780550
13	1	0	6.951687	-2.846093	0.978638
14	1	0	6.472123	-0.310986	-2.454777
15	1	0	7.894351	-1.806631	-1.070083
16	6	0	1.177298	2.548900	0.791978
17	6	0	0.407499	3.449418	0.041019
18	6	0	2.572715	2.585176	0.658785
19	6	0	1.012323	4.343063	-0.836160
20	1	0	-0.671940	3.426069	0.150653
21	6	0	3.176106	3.477640	-0.226542
22	1	0	3.189313	1.920810	1.253177
23	6	0	2.399097	4.353164	-0.980898
24	1	0	0.399289	5.024258	-1.417336
25	1	0	4.257129	3.488347	-0.320443
26	1	0	2.869801	5.041061	-1.675588
27	7	0	-0.602927	2.004836	2.215987
28	1	0	0.511096	-0.393047	2.600750
29	1	0	-3.544829	1.071989	1.440709
30	6	0	-0.342734	-0.553480	-0.760261
31	6	0	-1.209223	0.610279	-0.782344
32	6	0	-2.384109	0.656813	-0.186520
33	6	0	-3.546941	0.737721	0.402628
34	6	0	-4.846161	0.389836	-0.205587
35	6	0	-4.932094	-0.139033	-1.499854
36	6	0	-6.017631	0.587760	0.531129
37	6	0	-6.168842	-0.458292	-2.044440
38	1	0	-4.023024	-0.302007	-2.072584

39	6	0	-7.256511	0.266935	-0.017307
40	1	0	-5.954040	0.994755	1.536287
41	6	0	-7.335406	-0.255873	-1.305266
42	1	0	-6.225846	-0.868492	-3.047480
43	1	0	-8.159677	0.425893	0.562842
44	1	0	-8.300531	-0.506830	-1.733057
45	6	0	-0.723351	-1.861438	-0.189242
46	6	0	-0.403019	-3.027373	-0.894997
47	6	0	-1.386566	-1.950131	1.043061
48	6	0	-0.750560	-4.272451	-0.378711
49	1	0	0.093608	-2.950482	-1.856790
50	6	0	-1.728483	-3.196850	1.549575
51	1	0	-1.586546	-1.048203	1.613671
52	6	0	-1.415391	-4.358045	0.840782
53	1	0	-0.505256	-5.171649	-0.933351
54	1	0	-2.230731	-3.266023	2.508689
55	1	0	-1.686797	-5.328285	1.244022
56	7	0	0.815312	-0.532196	-1.385259
57	1	0	-0.835995	1.484333	-1.307663
58	1	0	1.667029	-1.013257	-0.855837
59	8	0	-1.253180	0.996128	2.946219
60	1	0	-1.963377	1.475178	3.389624
61	8	0	1.233767	0.667312	-1.941153
62	1	0	1.629914	1.174951	-1.203250

O_TS8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.836813	1.249495	0.203818
2	6	0	0.654977	1.565278	1.067698
3	6	0	-0.555039	1.643266	0.583331
4	6	0	-1.769074	1.701202	0.089747
5	6	0	-2.679923	0.545090	-0.037437
6	6	0	-2.229579	-0.768923	0.146195
7	6	0	-4.024617	0.761157	-0.355903
8	6	0	-3.108935	-1.837653	0.027537
9	1	0	-1.180612	-0.945810	0.369638
10	6	0	-4.905107	-0.311112	-0.475080
11	1	0	-4.380715	1.776519	-0.506787
12	6	0	-4.451362	-1.613245	-0.281649
13	1	0	-2.745841	-2.850509	0.170182

14	1	0	-5.946375	-0.127103	-0.719718
15	1	0	-5.136477	-2.449389	-0.375959
16	6	0	2.289408	-0.160719	0.084008
17	6	0	1.724622	-1.150009	0.895129
18	6	0	3.288027	-0.521663	-0.831354
19	6	0	2.145801	-2.474414	0.793727
20	1	0	0.955213	-0.884440	1.613377
21	6	0	3.704601	-1.842452	-0.930773
22	1	0	3.726464	0.241456	-1.464868
23	6	0	3.134990	-2.825047	-0.119089
24	1	0	1.698642	-3.229448	1.432050
25	1	0	4.475270	-2.109463	-1.646878
26	1	0	3.461821	-3.856506	-0.201230
27	7	0	2.498063	2.143209	-0.429473
28	1	0	0.834755	1.719010	2.131976
29	1	0	-2.144591	2.666342	-0.247300
30	8	0	1.995244	3.414671	-0.244144
31	1	0	2.600433	3.967988	-0.754463

O_TS9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.539105	-0.054649	0.174427
2	6	0	-0.687713	0.970189	-0.332739
3	6	0	0.631069	0.760521	-0.060453
4	6	0	1.874572	1.252008	0.037214
5	6	0	3.145808	0.539756	-0.059971
6	6	0	3.254705	-0.795075	-0.489900
7	6	0	4.329189	1.216905	0.282912
8	6	0	4.493288	-1.423961	-0.550796
9	1	0	2.363200	-1.338956	-0.785026
10	6	0	5.565668	0.586650	0.213757
11	1	0	4.268030	2.251595	0.609535
12	6	0	5.657360	-0.741758	-0.199333
13	1	0	4.549723	-2.455491	-0.885503
14	1	0	6.462128	1.135829	0.485216
15	1	0	6.621483	-1.236598	-0.251923
16	6	0	-3.011627	-0.044072	0.037287
17	6	0	-3.684352	1.176307	-0.065822
18	6	0	-3.738505	-1.239677	0.023527
19	6	0	-5.070694	1.202376	-0.184499

20	1	0	-3.122144	2.104627	-0.037532
21	6	0	-5.123149	-1.209564	-0.094526
22	1	0	-3.209489	-2.183994	0.095837
23	6	0	-5.791169	0.010297	-0.199626
24	1	0	-5.587026	2.153340	-0.262318
25	1	0	-5.683019	-2.138775	-0.110307
26	1	0	-6.871977	0.030573	-0.294492
27	7	0	-0.975949	-1.116232	0.690984
28	1	0	-1.017355	1.695812	-1.062178
29	1	0	1.911440	2.323887	0.214297
30	8	0	0.439957	-0.864487	0.594740
31	1	0	0.794923	-0.849869	1.500835

O_TS10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.502295	-0.661663	0.009657
2	6	0	-0.287924	-0.129684	0.582433
3	6	0	0.671478	-1.069012	0.386082
4	6	0	2.046985	-1.379045	0.215970
5	6	0	3.074446	-0.345927	0.083116
6	6	0	4.422934	-0.670350	0.316852
7	6	0	2.785836	0.972101	-0.315379
8	6	0	5.432462	0.272668	0.159647
9	1	0	4.674293	-1.682021	0.625321
10	6	0	3.796979	1.914772	-0.467146
11	1	0	1.757294	1.256987	-0.517893
12	6	0	5.128690	1.575813	-0.231681
13	1	0	6.463439	-0.011722	0.349377
14	1	0	3.540642	2.924426	-0.774885
15	1	0	5.914538	2.314283	-0.350489
16	6	0	-2.826456	-0.009376	0.021696
17	6	0	-2.918037	1.372393	0.208383
18	6	0	-3.988926	-0.766631	-0.161923
19	6	0	-4.163662	1.992373	0.209455
20	1	0	-2.018612	1.966084	0.336849
21	6	0	-5.229991	-0.142602	-0.159964
22	1	0	-3.910606	-1.840621	-0.293599
23	6	0	-5.319278	1.236752	0.026590
24	1	0	-4.230297	3.065593	0.352037
25	1	0	-6.130055	-0.732274	-0.298043

26	1	0	-6.290101	1.721534	0.031187
27	7	0	-1.379910	-1.837312	-0.546857
28	1	0	-0.174052	0.811098	1.095837
29	1	0	2.361152	-2.308001	0.690916
30	1	0	0.961751	-2.205299	-0.833187
31	8	0	0.000069	-2.174295	-0.236018

O_TS11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.260293	1.042131	-0.294130
2	6	0	2.262909	1.223832	-1.264401
3	6	0	1.042920	1.355376	-0.607640
4	6	0	-0.277388	1.503421	-0.964425
5	6	0	-1.430323	1.887042	-0.143593
6	6	0	-2.677729	1.997764	-0.788626
7	6	0	-1.392217	2.160147	1.236718
8	6	0	-3.830654	2.323821	-0.090341
9	1	0	-2.735231	1.790448	-1.853450
10	6	0	-2.552553	2.484285	1.934384
11	1	0	-0.457868	2.153175	1.784289
12	6	0	-3.780277	2.558654	1.283991
13	1	0	-4.777489	2.382678	-0.619350
14	1	0	-2.488574	2.683993	2.999756
15	1	0	-4.682951	2.803000	1.834408
16	6	0	4.700734	0.827961	-0.543513
17	6	0	5.127853	0.383780	-1.797372
18	6	0	5.635311	1.019515	0.479541
19	6	0	6.477413	0.135726	-2.027087
20	1	0	4.402405	0.209909	-2.585601
21	6	0	6.982852	0.768665	0.246751
22	1	0	5.299586	1.364973	1.451694
23	6	0	7.406390	0.326538	-1.006085
24	1	0	6.802925	-0.212133	-3.001716
25	1	0	7.704651	0.919571	1.042520
26	1	0	8.458445	0.131102	-1.186173
27	7	0	2.862095	1.061892	0.965401
28	1	0	2.397845	1.287617	-2.330983
29	1	0	0.916505	0.578243	1.274187
30	1	0	-0.427424	1.517984	-2.041114
31	6	0	-3.242048	-1.068545	-0.212816

32	6	0	-2.585564	-1.158132	1.016896
33	6	0	-1.216701	-1.281333	0.765453
34	6	0	-0.081155	-1.422281	1.517548
35	6	0	1.287274	-1.758594	1.125241
36	6	0	2.251988	-1.858920	2.151266
37	6	0	1.725833	-1.992301	-0.193748
38	6	0	3.580579	-2.142758	1.876216
39	1	0	1.939072	-1.693754	3.179087
40	6	0	3.062901	-2.271360	-0.463289
41	1	0	1.028770	-1.973806	-1.023028
42	6	0	4.002119	-2.338641	0.561007
43	1	0	4.294553	-2.202730	2.692204
44	1	0	3.371351	-2.428620	-1.492928
45	1	0	5.045214	-2.540357	0.338774
46	6	0	-4.699193	-0.939276	-0.420344
47	6	0	-5.520572	-0.547936	0.641121
48	6	0	-5.263730	-1.175795	-1.678080
49	6	0	-6.889757	-0.401629	0.449586
50	1	0	-5.081738	-0.331661	1.609729
51	6	0	-6.633672	-1.024535	-1.867497
52	1	0	-4.626725	-1.482949	-2.500899
53	6	0	-7.449344	-0.639573	-0.805083
54	1	0	-7.519429	-0.096028	1.278537
55	1	0	-7.065644	-1.209115	-2.845600
56	1	0	-8.517800	-0.522921	-0.954864
57	7	0	-2.473884	-1.106216	-1.294423
58	1	0	-3.035882	-1.196463	1.994518
59	1	0	-0.587598	-0.453895	-0.973962
60	1	0	-0.274620	-1.376243	2.585253
61	8	0	-1.121396	-1.264982	-0.677801
62	8	0	1.395551	1.308226	0.795548

O_TS12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.860041	0.103987	-0.105156
2	6	0	1.053205	1.252756	0.006378
3	6	0	-0.262045	0.802240	-0.049728
4	6	0	-1.517290	1.372682	0.146137
5	6	0	-2.801646	0.816755	-0.247431
6	6	0	-2.965228	-0.329113	-1.062588

7	6	0	-3.986353	1.436030	0.216144
8	6	0	-4.232704	-0.829707	-1.360623
9	1	0	-2.094909	-0.817701	-1.487075
10	6	0	-5.241954	0.933935	-0.088840
11	1	0	-3.899353	2.323448	0.838030
12	6	0	-5.382149	-0.214159	-0.872501
13	1	0	-4.314049	-1.710085	-1.992194
14	1	0	-6.123878	1.438962	0.294798
15	1	0	-6.364581	-0.611682	-1.102842
16	6	0	3.337486	0.055476	-0.120022
17	6	0	4.079088	1.110286	0.418651
18	6	0	4.006120	-1.044860	-0.667476
19	6	0	5.470128	1.067779	0.407679
20	1	0	3.566008	1.959072	0.860201
21	6	0	5.395967	-1.086632	-0.674114
22	1	0	3.427322	-1.857740	-1.093516
23	6	0	6.131372	-0.030259	-0.138328
24	1	0	6.037063	1.891090	0.829970
25	1	0	5.906617	-1.942205	-1.104166
26	1	0	7.216015	-0.062816	-0.147193
27	7	0	1.184937	-1.022230	-0.230338
28	1	0	1.373043	2.280005	0.065617
29	1	0	-1.505133	2.407372	0.470609
30	8	0	-0.182601	-0.590556	-0.220410
31	1	0	-0.930630	-1.084919	0.859907
32	7	0	-2.761819	-1.746363	1.791714
33	1	0	-3.073760	-1.785420	0.816572
34	1	0	-2.455890	-2.677801	2.067616
35	8	0	-1.522967	-1.013185	1.755875
36	1	0	-1.745388	-0.042662	1.761236
