Cartesian coordinates of Ru containing optimized structures

1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.556822	0.995067	-0.129436
2	6	0	-0.517082	-1.075124	0.070590
3	6	0	1.765682	-2.093230	0.120618
4	6	0	-0.330441	-3.402083	0.332331
5	6	0	1.759159	-1.730184	2.624092
6	6	0	-1.812086	-3.035263	0.225643
7	6	0	4.555013	-2.132511	0.059973
8	6	0	1.639456	-2.314465	-2.394202
9	6	0	2.474574	-1.957770	1.323288
10	6	0	2.418268	-2.243554	-1.111405
11	6	0	-3.050282	-1.233001	-2.452906
12	6	0	3.813676	-2.257051	-1.116314
13	6	0	3.868008	-1.978590	1.265576
14	6	0	-2.983835	-0.824983	0.063007
15	6	0	6.057436	-2.185823	0.033572
16	6	0	-5.354876	0.649340	-0.091459
17	6	0	-3.580207	-0.610617	-1.192308
18	6	0	-3.110083	-0.804477	2.607754
19	6	0	-3.610430	-0.402896	1.249450
20	6	0	-4.781684	0.345281	1.142968
21	6	0	-4.753205	0.142028	-1.241923
22	6	0	-6.587157	1.505407	-0.178034
23	6	0	2.234475	2.277904	-0.070678
24	6	0	3.576084	2.347276	-0.494865
25	6	0	4.257670	3.555968	-0.501928
26	6	0	3.616175	4.717535	-0.073304
27	6	0	2.293640	4.664468	0.367274
28	6	0	1.606321	3.459250	0.372059
29	1	0	-0.009760	-4.112018	-0.437279
30	1	0	4.150148	5.664087	-0.073284
31	1	0	1.800687	5.567037	0.717319
32	1	0	-3.123519	-0.535964	-3.291552
33	1	0	2.214468	0.142906	-0.308514
34	1	0	-0.069305	-3.824311	1.309978
35	1	0	1.036703	-2.526234	2.840961
36	1	0	1.201623	-0.785149	2.608118
37	1	0	2.470195	-1.692902	3.454353
38	1	0	-2.287622	-3.450319	-0.671482
39	1	0	-2.392796	-3.352829	1.098230
40	1	0	1.069120	-1.391487	-2.560975
41	1	0	0.919551	-3.141980	-2.392321
42	1	0	2.309813	-2.459719	-3.246153
43	1	0	-3.640004	-2.125475	-2.705040
44	1	0	-2.001418	-1.520165	-2.367359
45	1	0	0.591052	3.415033	0.758470
46	1	0	4.333733	-2.363094	-2.066472
47	1	0	4.431759	-1.862814	2.189219
48	1	0	6.494930	-1.544711	0.805770
49	1	0	6.453397	-1.870200	-0.936848
50	1	0	6.416543	-3.206750	0.216555
51	1	0	-2.049592	-1.059011	2.600907
52	1	0	-3.678524	-1.670825	2.974304
53	1	0	-3.242402	0.008083	3.326956
54	1	0	-5.260861	0.695216	2.055374

55	1	0	-5.209476	0.331918	-2.211635
56	1	0	-7.227946	1.376928	0.700424
57	1	0	-7.177355	1.271600	-1.069950
58	1	0	-6.318175	2.567896	-0.233173
59	1	0	4.070634	1.436510	-0.824942
60	1	0	5.290578	3.595354	-0.837005
61	7	0	0.342947	-2.113952	0.146733
62	7	0	-1.772956	-1.578920	0.144758
63	17	0	-0.645220	1.030102	-2.411610
64	17	0	-0.651300	1.371577	2.168967
65	44	0	-0.264587	0.844944	-0.095342

1c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.169345	0.324082	0.302634
2	6	0	-3.618965	0.210627	0.250139
3	6	0	-4.408072	1.225895	0.822147
4	6	0	-5.793643	1.177111	0.746416
5	6	0	-6.417863	0.106150	0.108988
6	6	0	-5.651079	-0.919098	-0.445431
7	6	0	-4.266256	-0.872826	-0.375308
8	1	0	-7.502265	0.064273	0.053076
9	1	0	-6.137797	-1.763561	-0.925176
10	1	0	-1.794396	1.045587	1.038892
11	1	0	-3.674227	-1.696923	-0.767533
12	1	0	-3.918701	2.062115	1.316558
13	1	0	-6.388997	1.971896	1.187493
14	17	0	-1.004365	0.835892	-2.759288
15	17	0	-1.119604	-2.781360	-0.170244
16	44	0	-1.094321	-0.551463	-0.882722
17	15	0	0.877180	0.043177	0.068208
18	6	0	2.059567	-1.324406	-0.384301
19	6	0	2.227189	-1.369161	-1.912850
20	6	0	3.415871	-1.407217	0.330713
21	1	0	1.480360	-2.214787	-0.097764
22	6	0	3.003474	-2.612746	-2.343579
23	1	0	2.760166	-0.471621	-2.257606
24	1	0	1.247615	-1.351871	-2.409057
25	6	0	4.180840	-2.654506	-0.122711
26	1	0	4.022186	-0.516856	0.125405
27	1	0	3.273119	-1.450649	1.415231
28	6	0	4.354497	-2.697598	-1.638369
29	1	0	3.136107	-2.604269	-3.432329
30	1	0	2.408423	-3.505438	-2.104113
31	1	0	5.156818	-2.686246	0.377879
32	1	0	3.630686	-3.548853	0.203866
33	1	0	4.882987	-3.612407	-1.933483
34	1	0	4.985396	-1.854118	-1.956877
35	6	0	1.479719	1.659032	-0.642161
36	6	0	0.591518	2.817430	-0.162207
37	6	0	2.972430	2.005129	-0.534093
38	1	0	1.253304	1.519549	-1.708562
39	6	0	0.922260	4.108297	-0.911338
40	1	0	0.732576	2.982044	0.916584
41	1	0	-0.461821	2.562080	-0.323510
42	6	0	3.272404	3.305290	-1.286343
43	1	0	3.280782	2.117301	0.512217
44	1	0	3.581712	1.199886	-0.956861
45	6	0	2.402616	4.459047	-0.796008

46	1	0	0.301454	4.926972	-0.526379
47	1	0	0.654265	3.979692	-1.969244
48	1	0	4.336412	3.552039	-1.180365
49	1	0	3.090751	3.147654	-2.359303
50	1	0	2.625381	5.370069	-1.365120
51	1	0	2.646243	4.678170	0.254701
52	6	0	0.781330	0.198015	1.927377
53	6	0	0.447252	-1.148430	2.586362
54	6	0	1.961573	0.883998	2.634103
55	1	0	-0.089968	0.854244	2.073680
56	6	0	0.177592	-0.975326	4.080562
57	1	0	1.290000	-1.841378	2.452932
58	1	0	-0.412678	-1.610437	2.092291
59	6	0	1.680178	1.036113	4.131849
60	1	0	2.880876	0.303050	2.497393
61	1	0	2.146148	1.872828	2.203338
62	6	0	1.346983	-0.299494	4.790090
63	1	0	-0.032862	-1.953773	4.529128
64	1	0	-0.730553	-0.368756	4.214778
65	1	0	2.545357	1.502775	4.619424
66	1	0	0.834636	1.726856	4.268469
67	1	0	1.120267	-0.152553	5.853309
68	1	0	2.227741	-0.957339	4.745262

3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.713429	2.778603	-0.264595
2	6	0	-0.531607	3.153870	0.312565
3	6	0	-2.818688	2.144291	0.539442
4	1	0	-2.552039	2.005192	1.588703
5	1	0	-3.117611	1.170620	0.121703
6	6	0	-2.120301	3.234494	-1.644719
7	1	0	-1.258743	3.261137	-2.315509
8	1	0	-2.811804	2.504541	-2.078666
9	6	0	1.448379	0.867734	-0.421133
10	6	0	-0.314840	-1.388212	-0.083434
11	6	0	2.112323	-1.985844	-0.294583
12	6	0	0.286709	-3.654368	-0.243675
13	6	0	2.213379	-1.995511	2.234217
14	6	0	-1.199567	-3.562364	0.085956
15	6	0	4.885068	-1.672801	-0.461432
16	6	0	1.921704	-2.077532	-2.823022
17	6	0	2.868915	-1.909976	0.887710
18	6	0	2.721992	-1.949303	-1.558690
19	6	0	-3.135424	-1.819346	-2.303180
20	6	0	4.107142	-1.782001	-1.613344
21	6	0	4.248025	-1.749194	0.777907
22	6	0	-2.781727	-1.642906	0.206771
23	6	0	6.370094	-1.458304	-0.543987
24	6	0	-5.416753	-0.761964	0.554553
25	6	0	-3.605870	-1.468002	-0.922101
26	6	0	-2.525115	-1.910222	2.730742
27	6	0	-3.293788	-1.499536	1.507147
28	6	0	-4.603669	-1.036257	1.651372
29	6	0	-4.907181	-1.009996	-0.721459
30	6	0	-6.808050	-0.222829	0.736536
31	6	0	2.582515	1.447549	0.286675
32	6	0	3.759708	1.642250	-0.465806
33	6	0	4.888086	2.222215	0.099754

34	6	0	4.868922	2.607953	1.438666
35	6	0	3.715587	2.418197	2.201360
36	6	0	2.581293	1.853061	1.635230
37	1	0	0.470730	-4.070121	-1.241215
38	1	0	5.749434	3.061302	1.887104
39	1	0	3.699842	2.721423	3.244886
40	1	0	-3.935150	-1.653624	-3.031157
41	1	0	1.721855	0.605010	-1.450795
42	1	0	0.851649	-4.247547	0.481939
43	1	0	1.640191	-2.924729	2.347186
44	1	0	1.512397	-1.166767	2.391437
45	1	0	2.963564	-1.969237	3.029970
46	1	0	-1.831148	-4.094581	-0.631813
47	1	0	-1.433395	-3.935231	1.090925
48	1	0	1.074622	-1.381144	-2.840652
49	1	0	1.517957	-3.091238	-2.943655
50	1	0	2.549539	-1.875005	-3.695923
51	1	0	-2.848077	-2.877051	-2.364142
52	1	0	-2.268606	-1.220307	-2.599820
53	1	0	1.680222	1.706762	2.221793
54	1	0	4.589245	-1.740430	-2.588381
55	1	0	4.840359	-1.677663	1.688001
56	1	0	6.624124	-0.421446	-0.289280
57	1	0	6.750886	-1.658105	-1.550348
58	1	0	6.908278	-2.104504	0.158318
59	1	0	-1.446385	-1.888565	2.574507
60	1	0	-2.823919	-2.923314	3.035000
61	1	0	-2.738194	-1.238683	3.566908
62	1	0	-4.998623	-0.900091	2.656462
63	1	0	-5.545517	-0.858340	-1.589775
64	1	0	-7.222740	-0.502590	1.710172
65	1	0	-7.485289	-0.589522	-0.041933
66	1	0	-6.812947	0.873385	0.681561
67	1	0	3.774705	1.329901	-1.506631
68	1	0	5.780047	2.375865	-0.502049
69	7	0	0.714830	-2.252375	-0.196332
70	7	0	-1.447856	-2.122054	0.018352
71	17	0	-0.389574	0.587789	2.368898
72	44	0	-0.350450	0.636275	-0.070292
73	17	0	-0.629439	0.567154	-2.489997
74	6	0	0.488085	4.044310	-0.334285
75	1	0	0.538443	3.909900	-1.418443
76	1	0	0.235365	5.096472	-0.139713
77	1	0	1.484969	3.873066	0.079100
78	6	0	-2.784519	4.614710	-1.593533
79	1	0	-3.671048	4.619027	-0.948571
80	1	0	-2.094883	5.376726	-1.213942
81	1	0	-3.103851	4.920402	-2.595961
82	1	0	-3.716069	2.776028	0.477824
83	1	0	-0.412552	2.977356	1.380482

3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.573346	2.703527	0.226939
2	6	0	-0.378913	3.309529	-0.077613
3	6	0	-2.770706	2.576630	-0.671499
4	1	0	-2.524704	2.676915	-1.729091

5	1	0	-3.279583	1.614732	-0.537834
6	6	0	1.379075	0.812398	-0.419963
7	6	0	-0.499706	-1.402415	-0.063040
8	6	0	1.879165	-2.134360	-0.298686
9	6	0	-0.048792	-3.698724	-0.225650
10	6	0	2.022647	-2.229192	2.222527
11	6	0	-1.519546	-3.509498	0.135933
12	6	0	4.657110	-1.932599	-0.515286
13	6	0	1.630101	-2.134860	-2.822714
14	6	0	2.661101	-2.130264	0.868083
15	6	0	2.462077	-2.077881	-1.573851
16	6	0	-3.298168	-1.739913	-2.317308
17	6	0	3.851844	-1.967592	-1.652668
18	6	0	4.043092	-2.024559	0.735017
19	6	0	-2.975152	-1.473360	0.188146
20	6	0	6.147996	-1.779157	-0.624049
21	6	0	-5.534996	-0.366574	0.440231
22	6	0	-3.766665	-1.292561	-0.963837
23	6	0	-2.789800	-1.645417	2.726882
24	6	0	-3.493087	-1.221620	1.469322
25	6	0	-4.761968	-0.643340	1.564223
26	6	0	-5.030301	-0.726093	-0.811749
27	6	0	-6.880591	0.291296	0.566229
28	6	0	2.591579	1.206616	0.284257
29	6	0	3.710841	1.501686	-0.523124
30	6	0	4.914087	1.915021	0.034603
31	6	0	5.032808	2.019562	1.419201
32	6	0	3.941761	1.718888	2.235802
33	6	0	2.732255	1.325333	1.680256
34	1	0	0.085442	-4.113354	-1.232056
35	1	0	5.973046	2.338533	1.862168
36	1	0	4.033763	1.801864	3.315535
37	1	0	-4.072867	-1.557862	-3.067979
38	1	0	1.578431	0.694047	-1.494302
39	1	0	0.487954	-4.338066	0.481540
40	1	0	1.485032	-3.178480	2.347118
41	1	0	1.295990	-1.423415	2.381255
42	1	0	2.778932	-2.172891	3.010932
43	1	0	-2.199149	-4.017589	-0.554570
44	1	0	-1.750414	-3.845738	1.154928
45	1	0	0.828132	-1.387146	-2.812103
46	1	0	1.161281	-3.119410	-2.949426
47	1	0	2.251354	-1.957079	-3.705666
48	1	0	-3.075856	-2.814741	-2.325854
49	1	0	-2.392648	-1.205214	-2.620466
50	1	0	1.876056	1.103734	2.308341
51	1	0	4.315423	-1.912518	-2.635936
52	1	0	4.656063	-2.005033	1.633922
53	1	0	6.448663	-0.754389	-0.371401
54	1	0	6.501759	-1.989992	-1.638087
55	1	0	6.671680	-2.450114	0.065783
56	1	0	-1.719757	-1.791095	2.580492
57	1	0	-3.231409	-2.581295	3.097012
58	1	0	-2.901939	-0.891875	3.510954
59	1	0	-5.159025	-0.423519	2.553573
60	1	0	-5.641644	-0.570200	-1.698466
61	1	0	-7.314074	0.132532	1.558697
62	1	0	-7.585162	-0.090894	-0.180045
63	1	0	-6.801212	1.375098	0.412543
64	1	0	3.620345	1.403859	-1.602089
65	1	0	5.757956	2.152795	-0.607793

66	7	0	0.472484	-2.329194	-0.172955
67	7	0	-1.678300	-2.058225	0.041464
68	17	0	-0.419992	0.604187	2.397304
69	44	0	-0.420950	0.612168	-0.035411
70	17	0	-0.775875	0.620807	-2.453057
71	6	0	-0.043561	3.823987	-1.454724
72	1	0	-0.472712	3.170790	-2.218916
73	1	0	1.045032	3.794069	-1.591542
74	6	0	-0.536415	5.261871	-1.651157
75	1	0	-1.625120	5.323035	-1.543643
76	1	0	-0.277506	5.618884	-2.653894
77	1	0	-0.088654	5.951298	-0.926618
78	1	0	-3.495645	3.357537	-0.397054
79	6	0	0.512887	3.780312	1.035488
80	1	0	0.329361	4.851715	1.201525
81	1	0	1.573528	3.673131	0.788781
82	1	0	0.308705	3.250675	1.969700
83	1	0	-1.774879	2.558235	1.289031

3c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.931364	-2.576210	-0.698700
2	6	0	3.490242	-1.341109	-0.574765
3	6	0	2.203282	-3.004491	-1.940985
4	1	0	2.165188	-2.219627	-2.698253
5	1	0	1.173551	-3.311620	-1.703832
6	6	0	3.139742	-3.661286	0.324149
7	1	0	3.281072	-3.229482	1.317073
8	1	0	2.239203	-4.284560	0.384508
9	6	0	1.410449	1.051087	0.783284
10	6	0	2.428606	2.072243	0.591284
11	6	0	2.684803	2.941637	1.672335
12	6	0	3.653644	3.931063	1.581804
13	6	0	4.374026	4.087296	0.398402
14	6	0	4.121565	3.249253	-0.688259
15	6	0	3.166067	2.246712	-0.596316
16	1	0	5.129387	4.864945	0.321234
17	1	0	4.675932	3.379044	-1.613680
18	1	0	0.857940	1.207752	1.723934
19	1	0	2.951522	1.603876	-1.444016
20	1	0	2.116781	2.820833	2.592150
21	1	0	3.844853	4.583958	2.428924
22	17	0	1.168468	0.229936	-2.445867
23	44	0	1.007227	-0.479194	-0.150541
24	17	0	1.058216	-1.725183	1.913895
25	6	0	4.374046	-0.919935	0.565762
26	1	0	3.942755	-1.192145	1.534301
27	1	0	5.362037	-1.394825	0.489734
28	1	0	4.531758	0.161376	0.559190
29	6	0	4.346058	-4.537164	-0.037143
30	1	0	4.224169	-5.021103	-1.012777
31	1	0	5.268707	-3.947305	-0.071185
32	1	0	4.479153	-5.326871	0.710168
33	1	0	2.689224	-3.892105	-2.368581
34	1	0	3.442201	-0.684426	-1.442428
35	15	0	-1.277048	0.053879	0.054932
36	6	0	-2.327040	-1.079584	-1.010482
37	6	0	-3.852716	-1.023544	-0.805612
38	6	0	-2.028685	-1.016276	-2.514148

39	1	0	-1.987085	-2.065628	-0.651565
40	6	0	-4.522628	-2.210601	-1.501191
41	1	0	-4.246343	-0.100925	-1.244887
42	1	0	-4.127108	-1.008501	0.252497
43	6	0	-2.710938	-2.173353	-3.247307
44	1	0	-2.394316	-0.059907	-2.915777
45	1	0	-0.953622	-1.033482	-2.705400
46	6	0	-4.215978	-2.214207	-2.996344
47	1	0	-5.606343	-2.172458	-1.332352
48	1	0	-4.166958	-3.147547	-1.047443
49	1	0	-2.503449	-2.098169	-4.321885
50	1	0	-2.261688	-3.119667	-2.909736
51	1	0	-4.662017	-3.093539	-3.477681
52	1	0	-4.683671	-1.332539	-3.459182
53	6	0	-1.848994	-0.255316	1.824167
54	6	0	-2.944894	0.636269	2.427835
55	6	0	-2.178775	-1.732418	2.102802
56	1	0	-0.922201	-0.048158	2.379367
57	6	0	-3.043613	0.394169	3.937426
58	1	0	-3.917986	0.410527	1.970716
59	1	0	-2.747879	1.699201	2.248876
60	6	0	-2.272038	-1.979227	3.608668
61	1	0	-3.139154	-1.998335	1.642930
62	1	0	-1.410636	-2.382411	1.677250
63	6	0	-3.312716	-1.073022	4.261054
64	1	0	-3.830418	1.031928	4.360500
65	1	0	-2.100032	0.703751	4.410190
66	1	0	-2.514058	-3.033262	3.794120
67	1	0	-1.283757	-1.799858	4.053461
68	1	0	-3.328825	-1.224570	5.347667
69	1	0	-4.313690	-1.344369	3.892700
70	6	0	-1.687630	1.863097	-0.246652
71	6	0	-0.843909	2.573136	-1.311807
72	6	0	-3.169837	2.179114	-0.501860
73	1	0	-1.407798	2.308211	0.723570
74	6	0	-1.087429	4.083125	-1.273421
75	1	0	-1.094404	2.178743	-2.304771
76	1	0	0.216751	2.363835	-1.168368
77	6	0	-3.423539	3.686937	-0.440355
78	1	0	-3.431584	1.820754	-1.506461
79	1	0	-3.828866	1.663454	0.200656
80	6	0	-2.560952	4.435706	-1.451448
81	1	0	-0.480879	4.568018	-2.048167
82	1	0	-0.732810	4.478233	-0.309105
83	1	0	-4.487805	3.888813	-0.616266
84	1	0	-3.199929	4.048776	0.574667
85	1	0	-2.713179	5.518379	-1.358634
86	1	0	-2.879073	4.159916	-2.467682

3d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.576870	-2.485291	-0.767091
2	6	0	3.512150	-1.551359	-0.372550
3	6	0	2.245652	-3.752778	-0.029495
4	1	0	2.376593	-3.667731	1.049446
5	1	0	1.214658	-4.071576	-0.213219
6	6	0	1.891535	0.681334	0.420348
7	6	0	2.311521	1.967392	-0.116605
8	6	0	3.138489	2.763293	0.705541

9	6	0	3.590914	4.005271	0.281277
10	6	0	3.218215	4.482462	-0.974200
11	6	0	2.397520	3.712274	-1.799453
12	6	0	1.946771	2.468110	-1.381599
13	1	0	3.566797	5.455668	-1.310161
14	1	0	2.110968	4.085696	-2.778804
15	1	0	2.235965	0.545116	1.458426
16	1	0	1.327418	1.852797	-2.025881
17	1	0	3.420575	2.389783	1.687662
18	1	0	4.229030	4.602142	0.927027
19	17	0	0.946533	-0.423911	-2.610411
20	44	0	0.973950	-0.791071	-0.209218
21	17	0	0.871679	-1.641495	2.076521
22	6	0	4.178447	-1.600818	0.980356
23	1	0	3.465414	-1.927463	1.742936
24	1	0	4.502155	-0.589784	1.258844
25	6	0	5.400368	-2.526587	0.968704
26	1	0	5.116233	-3.555259	0.722097
27	1	0	5.875533	-2.537843	1.955499
28	1	0	6.151596	-2.201172	0.240705
29	1	0	2.897213	-4.555608	-0.405517
30	6	0	4.167177	-0.664709	-1.394812
31	1	0	5.115309	-1.131858	-1.697953
32	1	0	4.411296	0.322356	-0.989175
33	1	0	3.544253	-0.540810	-2.283430
34	1	0	2.328946	-2.485072	-1.829296
35	15	0	-1.241813	0.017829	0.168663
36	6	0	-2.172465	-1.577631	0.431181
37	6	0	-3.706996	-1.558368	0.427426
38	6	0	-1.658191	-2.651393	-0.543265
39	1	0	-1.822222	-1.868403	1.433814
40	6	0	-4.260255	-2.936925	0.798234
41	1	0	-4.072880	-1.291223	-0.572248
42	1	0	-4.097397	-0.803410	1.116709
43	6	0	-2.214981	-4.028995	-0.185885
44	1	0	-1.931067	-2.391876	-1.574021
45	1	0	-0.558182	-2.699820	-0.518367
46	6	0	-3.741638	-4.019356	-0.145621
47	1	0	-5.357213	-2.910631	0.784253
48	1	0	-3.964574	-3.179409	1.829505
49	1	0	-1.856213	-4.773586	-0.907516
50	1	0	-1.823663	-4.324728	0.797991
51	1	0	-4.120365	-5.003437	0.157048
52	1	0	-4.129355	-3.831306	-1.157811
53	6	0	-1.296362	0.955380	1.787979
54	6	0	-0.838655	2.412556	1.631947
55	6	0	-2.570766	0.862920	2.638322
56	1	0	-0.511320	0.422481	2.343234
57	6	0	-0.620619	3.059791	3.000173
58	1	0	-1.588921	2.997853	1.084541
59	1	0	0.083681	2.465852	1.045771
60	6	0	-2.349094	1.531398	3.999255
61	1	0	-3.418511	1.344242	2.133007
62	1	0	-2.843609	-0.185756	2.799012
63	6	0	-1.881047	2.977096	3.856940
64	1	0	-0.310426	4.104309	2.870491
65	1	0	0.204247	2.545786	3.514786
66	1	0	-3.274260	1.482971	4.587439
67	1	0	-1.592194	0.959541	4.554927
68	1	0	-1.702241	3.417350	4.845878
69	1	0	-2.677496	3.574031	3.387399

70	6	0	-2.093875	1.053665	-1.135289
71	6	0	-2.365372	0.284861	-2.438995
72	6	0	-3.380832	1.775374	-0.700220
73	1	0	-1.334511	1.819753	-1.361914
74	6	0	-2.832286	1.238287	-3.539431
75	1	0	-3.152266	-0.461351	-2.263487
76	1	0	-1.466943	-0.246218	-2.760654
77	6	0	-3.859697	2.731348	-1.796528
78	1	0	-4.165851	1.035275	-0.498490
79	1	0	-3.236649	2.337392	0.225793
80	6	0	-4.080362	2.011516	-3.123726
81	1	0	-3.020550	0.672026	-4.459992
82	1	0	-2.019072	1.942326	-3.768532
83	1	0	-4.781780	3.230071	-1.471491
84	1	0	-3.107421	3.522702	-1.932020
85	1	0	-4.368503	2.728860	-3.902496
86	1	0	-4.921259	1.309862	-3.017539

TS4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.405464	2.511703	-0.121496
2	6	0	-0.034680	2.925097	-0.314732
3	6	0	-2.036968	2.811142	1.221722
4	1	0	-1.315757	2.797480	2.037130
5	1	0	-2.830477	2.093731	1.458155
6	6	0	-2.406189	2.571259	-1.266460
7	1	0	-1.908743	2.379064	-2.216227
8	1	0	-3.128443	1.753823	-1.136504
9	6	0	1.360373	1.389656	-0.467837
10	6	0	-0.407529	-1.452128	-0.015605
11	6	0	2.000004	-2.076521	-0.211010
12	6	0	0.130577	-3.727350	-0.004003
13	6	0	2.190033	-2.053856	2.318900
14	6	0	-1.366264	-3.570640	0.272743
15	6	0	4.754593	-1.662906	-0.465698
16	6	0	1.769786	-2.337250	-2.728805
17	6	0	2.786433	-1.945308	0.946235
18	6	0	2.577572	-2.078760	-1.490017
19	6	0	-3.178141	-1.813035	-2.240769
20	6	0	3.952805	-1.856167	-1.588399
21	6	0	4.154309	-1.728385	0.791605
22	6	0	-2.863073	-1.544228	0.264707
23	6	0	6.226499	-1.389950	-0.597707
24	6	0	-5.407182	-0.401002	0.504044
25	6	0	-3.646932	-1.357638	-0.890054
26	6	0	-2.664406	-1.672306	2.803083
27	6	0	-3.376939	-1.271687	1.543252
28	6	0	-4.639697	-0.680404	1.632173
29	6	0	-4.903788	-0.772573	-0.744212
30	6	0	-6.743933	0.275910	0.624015
31	6	0	2.572855	1.754347	0.277081
32	6	0	3.726070	1.965135	-0.502973
33	6	0	4.936605	2.321947	0.080042
34	6	0	5.016919	2.485770	1.460433
35	6	0	3.882221	2.287496	2.247403
36	6	0	2.673692	1.923294	1.668264
37	1	0	0.331586	-4.233707	-0.954676

38	1	0	5.958877	2.770235	1.922532
39	1	0	3.940814	2.414824	3.325177
40	1	0	-3.965857	-1.668074	-2.986005
41	1	0	1.553328	1.417300	-1.546390
42	1	0	0.657192	-4.268372	0.788085
43	1	0	1.668127	-3.009527	2.457991
44	1	0	1.462269	-1.255817	2.503122
45	1	0	2.972445	-1.992596	3.081180
46	1	0	-1.992222	-4.115719	-0.440608
47	1	0	-1.644326	-3.886894	1.285302
48	1	0	0.936813	-1.632422	-2.820191
49	1	0	1.355332	-3.353912	-2.734966
50	1	0	2.397327	-2.239605	-3.619795
51	1	0	-2.920147	-2.879515	-2.233792
52	1	0	-2.291135	-1.258794	-2.564789
53	1	0	1.796728	1.747822	2.281747
54	1	0	4.407141	-1.844092	-2.577327
55	1	0	4.766696	-1.608175	1.683083
56	1	0	6.444513	-0.337617	-0.376405
57	1	0	6.585462	-1.600203	-1.610081
58	1	0	6.811413	-1.996100	0.103207
59	1	0	-1.589568	-1.780492	2.657081
60	1	0	-3.073401	-2.621822	3.176046
61	1	0	-2.805056	-0.921537	3.585470
62	1	0	-5.035221	-0.446997	2.619053
63	1	0	-5.511014	-0.614285	-1.633388
64	1	0	-7.193181	0.107031	1.607811
65	1	0	-7.444470	-0.081649	-0.137924
66	1	0	-6.645341	1.360943	0.491014
67	1	0	3.664751	1.838199	-1.581248
68	1	0	5.812236	2.481555	-0.543855
69	7	0	0.599723	-2.337058	-0.067133
70	7	0	-1.562850	-2.126119	0.128631
71	17	0	-0.230255	0.540181	2.302274
72	44	0	-0.313945	0.603111	-0.130815
73	17	0	-0.479490	0.374159	-2.566879
74	6	0	0.393430	3.651264	-1.572736
75	1	0	0.145037	3.086437	-2.474963
76	1	0	-0.119698	4.620059	-1.619550
77	1	0	1.470273	3.846429	-1.567516
78	6	0	-3.174598	3.896877	-1.348377
79	1	0	-3.855557	4.040489	-0.503574
80	1	0	-2.497838	4.758871	-1.383140
81	1	0	-3.777129	3.914192	-2.263190
82	1	0	-2.493180	3.809922	1.177831
83	1	0	0.426542	3.298265	0.599890

TS4b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.224469	2.484532	-0.031885
2	6	0	0.157103	2.951666	-0.166361
3	6	0	-2.311394	2.722845	-1.046533
4	1	0	-1.951579	2.718942	-2.075236
5	1	0	-3.085978	1.952584	-0.958342
6	6	0	1.419663	1.335061	-0.394720
7	6	0	-0.697394	-1.412577	-0.126245
8	6	0	1.626591	-2.282062	-0.337336

9	6	0	-0.417451	-3.728186	-0.302238
10	6	0	1.684980	-2.337251	2.196035
11	6	0	-1.891860	-3.424234	-0.031043
12	6	0	4.416175	-2.153997	-0.450532
13	6	0	1.490384	-2.441421	-2.870152
14	6	0	2.363219	-2.263823	0.858623
15	6	0	2.260938	-2.306255	-1.588545
16	6	0	-3.503373	-1.202387	-2.324291
17	6	0	3.654705	-2.227497	-1.615175
18	6	0	3.752283	-2.192155	0.775374
19	6	0	-3.156754	-1.270177	0.190408
20	6	0	5.912473	-2.024847	-0.506826
21	6	0	-5.600318	0.028134	0.606636
22	6	0	-3.930300	-0.886023	-0.920704
23	6	0	-2.926064	-1.680388	2.694778
24	6	0	-3.630362	-1.101220	1.501196
25	6	0	-4.843108	-0.432710	1.680743
26	6	0	-5.137077	-0.228776	-0.685141
27	6	0	-6.883861	0.778464	0.828037
28	6	0	2.650106	1.429948	0.400296
29	6	0	3.821269	1.756637	-0.309606
30	6	0	5.047755	1.872273	0.334639
31	6	0	5.130078	1.657641	1.708524
32	6	0	3.981064	1.325416	2.425758
33	6	0	2.754770	1.209219	1.783725
34	1	0	-0.256205	-4.186392	-1.284034
35	1	0	6.085691	1.748044	2.218864
36	1	0	4.041224	1.153838	3.497410
37	1	0	-4.272689	-0.888879	-3.036196
38	1	0	1.637043	1.448232	-1.461534
39	1	0	0.032746	-4.377271	0.455540
40	1	0	1.079710	-3.248294	2.291806
41	1	0	1.016545	-1.484344	2.359703
42	1	0	2.426218	-2.349899	3.000619
43	1	0	-2.558573	-3.817120	-0.805020
44	1	0	-2.231341	-3.804522	0.939522
45	1	0	0.680479	-1.707788	-2.932751
46	1	0	1.054461	-3.444505	-2.970770
47	1	0	2.150623	-2.290434	-3.729341
48	1	0	-3.346313	-2.279989	-2.460314
49	1	0	-2.565285	-0.700221	-2.585167
50	1	0	1.862406	0.942969	2.339876
51	1	0	4.156786	-2.229337	-2.580796
52	1	0	4.330038	-2.159254	1.696797
53	1	0	6.215986	-0.988881	-0.309928
54	1	0	6.304246	-2.306184	-1.489361
55	1	0	6.398400	-2.654243	0.246932
56	1	0	-1.852603	-1.785186	2.533478
57	1	0	-3.348486	-2.664868	2.940984
58	1	0	-3.057082	-1.038083	3.569823
59	1	0	-5.206162	-0.279026	2.695182
60	1	0	-5.737384	0.079615	-1.539058
61	1	0	-7.314599	0.555775	1.809254
62	1	0	-7.628905	0.532629	0.063852
63	1	0	-6.716664	1.862125	0.781518
64	1	0	3.760394	1.918213	-1.383465
65	1	0	5.936450	2.132358	-0.234614
66	7	0	0.202402	-2.398151	-0.260832
67	7	0	-1.921905	-1.958249	-0.030188
68	17	0	-0.486980	0.579982	2.304587
69	44	0	-0.300915	0.609791	-0.118678

70	17	0	-0.441445	0.520330	-2.553527
71	6	0	0.558466	3.660636	-1.458636
72	1	0	0.234089	3.068508	-2.319771
73	1	0	1.653528	3.717803	-1.503573
74	6	0	0.007040	5.084386	-1.556814
75	1	0	-1.086259	5.106956	-1.516779
76	1	0	0.312585	5.532313	-2.508857
77	1	0	0.387919	5.725939	-0.755079
78	1	0	-2.796165	3.687439	-0.832755
79	6	0	0.702598	3.607002	1.089063
80	1	0	0.170186	4.553410	1.245096
81	1	0	1.770080	3.830407	1.004785
82	1	0	0.534949	2.981951	1.969495
83	1	0	-1.587762	2.546127	0.996857

TS4c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.184208	-2.479110	-0.354318
2	6	0	3.074348	-1.516259	0.282823
3	6	0	2.454134	-2.767118	-1.816199
4	1	0	2.778359	-1.885049	-2.365530
5	1	0	1.568318	-3.169963	-2.319397
6	6	0	1.707260	-3.711270	0.404629
7	1	0	1.601443	-3.487384	1.465021
8	1	0	0.695683	-3.961011	0.055174
9	6	0	2.275523	0.223627	0.862502
10	6	0	3.152819	1.346179	0.499302
11	6	0	3.679018	2.091856	1.570981
12	6	0	4.509754	3.183885	1.348388
13	6	0	4.848202	3.540278	0.045769
14	6	0	4.345522	2.803730	-1.027200
15	6	0	3.503311	1.721350	-0.808837
16	1	0	5.502347	4.389326	-0.134573
17	1	0	4.606881	3.080207	-2.045108
18	1	0	2.259465	0.083206	1.949770
19	1	0	3.086722	1.166862	-1.643604
20	1	0	3.423113	1.807768	2.589464
21	1	0	4.898593	3.749665	2.190609
22	17	0	1.119344	-0.030003	-2.289173
23	44	0	0.894140	-0.757991	0.033096
24	17	0	0.332289	-1.529204	2.280966
25	6	0	3.746078	-1.857716	1.599102
26	1	0	3.014047	-2.085506	2.377972
27	1	0	4.386188	-2.736582	1.455793
28	1	0	4.380622	-1.034507	1.941401
29	6	0	2.598708	-4.946708	0.222676
30	1	0	2.572994	-5.336742	-0.799553
31	1	0	3.644673	-4.736169	0.474406
32	1	0	2.254160	-5.745015	0.888965
33	1	0	3.243904	-3.528740	-1.878847
34	1	0	3.730537	-1.033681	-0.441749
35	15	0	-1.339199	0.248856	0.002967
36	6	0	-2.403505	-1.164702	-0.596580
37	6	0	-3.811863	-0.831079	-1.101218
38	6	0	-1.664731	-2.036075	-1.622962
39	1	0	-2.504436	-1.772257	0.313502
40	6	0	-4.604480	-2.110857	-1.371061

41	1	0	-3.733532	-0.267097	-2.039446
42	1	0	-4.346690	-0.192799	-0.387223
43	6	0	-2.459126	-3.306982	-1.929600
44	1	0	-1.476508	-1.467556	-2.542192
45	1	0	-0.670587	-2.321109	-1.245045
46	6	0	-3.882847	-2.994926	-2.385755
47	1	0	-5.609834	-1.857084	-1.729917
48	1	0	-4.736120	-2.663174	-0.428916
49	1	0	-1.933509	-3.894716	-2.692320
50	1	0	-2.498878	-3.929945	-1.023685
51	1	0	-4.441238	-3.924896	-2.549392
52	1	0	-3.848011	-2.474819	-3.354344
53	6	0	-1.413004	1.679606	-1.193134
54	6	0	-2.733185	2.405806	-1.497067
55	6	0	-0.313818	2.705985	-0.866347
56	1	0	-1.085066	1.173890	-2.113317
57	6	0	-2.535445	3.354524	-2.683948
58	1	0	-3.057026	2.994490	-0.632319
59	1	0	-3.541554	1.705550	-1.720358
60	6	0	-0.123590	3.673885	-2.033447
61	1	0	-0.582596	3.273108	0.036453
62	1	0	0.629304	2.192663	-0.659495
63	6	0	-1.428513	4.370227	-2.411046
64	1	0	-3.480279	3.867988	-2.904200
65	1	0	-2.279539	2.767594	-3.578057
66	1	0	0.646386	4.412676	-1.777633
67	1	0	0.257240	3.105312	-2.893273
68	1	0	-1.279867	5.015371	-3.286141
69	1	0	-1.741529	5.027916	-1.586105
70	6	0	-1.988153	0.741053	1.706622
71	6	0	-2.736015	2.077632	1.793368
72	6	0	-2.824980	-0.358779	2.379666
73	1	0	-1.061279	0.827624	2.289805
74	6	0	-3.029595	2.440560	3.251443
75	1	0	-3.685346	2.011239	1.243471
76	1	0	-2.156304	2.884147	1.334953
77	6	0	-3.121678	0.002006	3.835708
78	1	0	-3.774861	-0.483870	1.839232
79	1	0	-2.288882	-1.310692	2.353570
80	6	0	-3.828263	1.348329	3.954935
81	1	0	-3.566372	3.397058	3.289354
82	1	0	-2.077344	2.593561	3.780015
83	1	0	-3.726925	-0.791480	4.291756
84	1	0	-2.172954	0.029718	4.389932
85	1	0	-3.986592	1.608853	5.008951
86	1	0	-4.825810	1.277751	3.495809

TS4d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.911556	2.351092	-1.152232
2	6	0	-3.055455	1.610529	-0.580995
3	6	0	-1.487530	3.733081	-0.729110
4	1	0	-1.631998	3.928030	0.333273
5	1	0	-0.423715	3.880821	-0.951148
6	6	0	-2.422785	0.028030	0.456742
7	6	0	-3.170237	-1.217951	0.235762
8	6	0	-4.075844	-1.585545	1.250296

9	6	0	-4.826967	-2.750961	1.159013
10	6	0	-4.683401	-3.580782	0.049796
11	6	0	-3.783966	-3.237583	-0.959198
12	6	0	-3.032371	-2.072663	-0.871202
13	1	0	-5.265443	-4.495588	-0.025934
14	1	0	-3.663723	-3.886533	-1.822615
15	1	0	-2.599959	0.408707	1.467346
16	1	0	-2.325667	-1.809102	-1.650841
17	1	0	-4.183747	-0.943257	2.121481
18	1	0	-5.520066	-3.012761	1.953881
19	17	0	-0.852812	-0.167435	-2.537015
20	44	0	-0.859298	0.778692	-0.308645
21	17	0	-0.648443	1.926158	1.844818
22	6	0	-3.831391	2.281037	0.555880
23	1	0	-3.133718	2.624101	1.325622
24	1	0	-4.483057	1.533215	1.025314
25	6	0	-4.709572	3.438326	0.077612
26	1	0	-4.127349	4.222151	-0.415899
27	1	0	-5.216159	3.892999	0.935996
28	1	0	-5.483380	3.101867	-0.620017
29	1	0	-2.036708	4.481468	-1.319556
30	6	0	-3.951051	0.983623	-1.637458
31	1	0	-4.434681	1.787549	-2.205078
32	1	0	-4.735291	0.366245	-1.189175
33	1	0	-3.375171	0.379084	-2.341651
34	1	0	-1.824538	2.200053	-2.231031
35	15	0	1.436801	-0.083769	0.044756
36	6	0	1.432200	-0.710734	1.798929
37	6	0	0.430278	-1.870566	1.932517
38	6	0	2.763785	-1.027632	2.492105
39	1	0	0.985767	0.149717	2.318554
40	6	0	0.217697	-2.244448	3.398930
41	1	0	0.789027	-2.754138	1.387039
42	1	0	-0.528382	-1.591731	1.478313
43	6	0	2.523571	-1.418582	3.953942
44	1	0	3.296019	-1.839209	1.981354
45	1	0	3.418539	-0.151129	2.466135
46	6	0	1.539798	-2.577667	4.084428
47	1	0	-0.477032	-3.090987	3.465715
48	1	0	-0.259455	-1.399861	3.915996
49	1	0	3.481563	-1.671125	4.425968
50	1	0	2.126231	-0.547645	4.494895
51	1	0	1.373339	-2.816199	5.142277
52	1	0	1.973279	-3.478490	3.624291
53	6	0	1.893148	-1.457976	-1.145395
54	6	0	2.372454	-0.913346	-2.503388
55	6	0	2.855102	-2.550301	-0.651887
56	1	0	0.916641	-1.928874	-1.330020
57	6	0	2.454324	-2.041266	-3.531035
58	1	0	3.367299	-0.460992	-2.396783
59	1	0	1.690218	-0.139533	-2.864237
60	6	0	2.953007	-3.676518	-1.685438
61	1	0	3.855021	-2.130604	-0.476963
62	1	0	2.521322	-2.971911	0.300853
63	6	0	3.377069	-3.161256	-3.057917
64	1	0	2.801505	-1.639126	-4.490993
65	1	0	1.443151	-2.435678	-3.703087
66	1	0	3.653773	-4.441956	-1.328200
67	1	0	1.971233	-4.165209	-1.769670
68	1	0	3.389471	-3.983597	-3.784210
69	1	0	4.407972	-2.780827	-2.998345

70	6	0	2.721670	1.256553	-0.198527
71	6	0	2.491965	2.499452	0.670851
72	6	0	4.194624	0.821166	-0.104107
73	1	0	2.536151	1.548236	-1.245309
74	6	0	3.428331	3.635267	0.254825
75	1	0	2.667361	2.244387	1.725511
76	1	0	1.450446	2.826038	0.618072
77	6	0	5.117567	1.957514	-0.550637
78	1	0	4.437851	0.560077	0.931860
79	1	0	4.390363	-0.070883	-0.704718
80	6	0	4.894694	3.214220	0.285986
81	1	0	3.263282	4.500633	0.908384
82	1	0	3.166995	3.959552	-0.763904
83	1	0	6.162620	1.629699	-0.482400
84	1	0	4.928215	2.182743	-1.610770
85	1	0	5.536743	4.029799	-0.069328
86	1	0	5.191311	3.010912	1.325624

5a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.460529	2.169718	-0.000465
2	6	0	-0.046913	2.843337	-0.351534
3	6	0	-1.962866	2.589275	1.367392
4	1	0	-1.201812	2.497478	2.139790
5	1	0	-2.821983	1.972622	1.654973
6	6	0	-2.578762	2.224339	-1.042916
7	1	0	-2.167928	2.189552	-2.051275
8	1	0	-3.146928	1.291387	-0.935130
9	6	0	1.184283	1.885456	-0.663649
10	6	0	-0.397869	-1.437949	0.059677
11	6	0	1.997138	-2.135935	-0.084235
12	6	0	0.062195	-3.721259	0.093266
13	6	0	2.185472	-2.318405	2.443605
14	6	0	-1.400851	-3.504450	0.468900
15	6	0	4.767949	-1.827210	-0.306093
16	6	0	1.781093	-2.299019	-2.613827
17	6	0	2.783300	-2.115418	1.081767
18	6	0	2.582617	-2.102144	-1.359731
19	6	0	-3.180892	-2.038075	-2.161262
20	6	0	3.966260	-1.928895	-1.440317
21	6	0	4.158990	-1.945295	0.943141
22	6	0	-2.875220	-1.475981	0.296161
23	6	0	6.249859	-1.604806	-0.416153
24	6	0	-5.458945	-0.408261	0.417640
25	6	0	-3.672673	-1.470125	-0.862283
26	6	0	-2.593586	-1.170477	2.805069
27	6	0	-3.377448	-1.034252	1.531941
28	6	0	-4.663273	-0.489536	1.559358
29	6	0	-4.953318	-0.923937	-0.776110
30	6	0	-6.824390	0.217992	0.468435
31	6	0	2.493812	2.144329	-0.024429
32	6	0	3.631982	1.834888	-0.785684
33	6	0	4.912439	2.092326	-0.309021
34	6	0	5.083239	2.675523	0.943267
35	6	0	3.963092	2.990391	1.711351
36	6	0	2.684346	2.726571	1.237574
37	1	0	0.177512	-4.196495	-0.888285

38	1	0	6.080982	2.888899	1.318003
39	1	0	4.086203	3.443292	2.691579
40	1	0	-3.977297	-2.021551	-2.910992
41	1	0	1.307560	1.789001	-1.745515
42	1	0	0.611559	-4.312754	0.829955
43	1	0	1.730173	-3.313337	2.537859
44	1	0	1.416517	-1.569503	2.653774
45	1	0	2.958164	-2.239728	3.213801
46	1	0	-2.093588	-4.081566	-0.149446
47	1	0	-1.603159	-3.734939	1.522051
48	1	0	0.962379	-1.577402	-2.699564
49	1	0	1.345528	-3.306200	-2.652643
50	1	0	2.421238	-2.191134	-3.494572
51	1	0	-2.849719	-3.078088	-2.052350
52	1	0	-2.332980	-1.458025	-2.542680
53	1	0	1.829319	2.951653	1.864517
54	1	0	4.427275	-1.888539	-2.425386
55	1	0	4.771682	-1.909796	1.841665
56	1	0	6.503990	-0.570930	-0.151200
57	1	0	6.610007	-1.787264	-1.433489
58	1	0	6.805666	-2.259372	0.264444
59	1	0	-1.629383	-0.652184	2.754901
60	1	0	-2.391054	-2.224046	3.036326
61	1	0	-3.158543	-0.756884	3.645713
62	1	0	-5.056531	-0.134774	2.510119
63	1	0	-5.573081	-0.906181	-1.670469
64	1	0	-7.240963	0.191768	1.480277
65	1	0	-7.524365	-0.290586	-0.202796
66	1	0	-6.782943	1.269853	0.157590
67	1	0	3.502566	1.383243	-1.766399
68	1	0	5.775454	1.850834	-0.924336
69	7	0	0.585628	-2.349922	0.045614
70	7	0	-1.573217	-2.067344	0.228818
71	17	0	0.393899	0.638027	2.208773
72	44	0	-0.220792	0.584516	-0.136380
73	17	0	-0.575546	0.300395	-2.538577
74	6	0	-0.140949	3.800570	-1.542369
75	1	0	-0.329764	3.256491	-2.471200
76	1	0	-0.934824	4.538411	-1.394491
77	1	0	0.808407	4.336492	-1.647150
78	6	0	-3.568352	3.389054	-0.921400
79	1	0	-4.154625	3.344488	0.001817
80	1	0	-3.077114	4.368089	-0.957318
81	1	0	-4.272728	3.347333	-1.759866
82	1	0	-2.307635	3.632699	1.328023
83	1	0	0.225340	3.372605	0.563358

5b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.116238	2.329253	-0.237722
2	6	0	0.398225	2.792239	-0.318478
3	6	0	-2.118880	2.617861	-1.323121
4	1	0	-1.723042	2.499593	-2.331785
5	1	0	-2.963260	1.927999	-1.209148
6	6	0	1.467772	1.532890	-0.389343
7	6	0	-0.767990	-1.400301	0.007518
8	6	0	1.518607	-2.340459	-0.222725

9	6	0	-0.548325	-3.711773	0.208463
10	6	0	1.771908	-2.043139	2.288857
11	6	0	-2.032716	-3.352088	0.160466
12	6	0	4.289877	-2.231993	-0.558724
13	6	0	1.201521	-2.926524	-2.672983
14	6	0	2.338150	-2.140802	0.901588
15	6	0	2.063166	-2.573566	-1.495234
16	6	0	-3.385356	-1.156233	-2.264424
17	6	0	3.449592	-2.500534	-1.637145
18	6	0	3.716001	-2.075885	0.702997
19	6	0	-3.233403	-1.150552	0.273808
20	6	0	5.777051	-2.113792	-0.739233
21	6	0	-5.672721	0.206996	0.455432
22	6	0	-3.907210	-0.790040	-0.905482
23	6	0	-3.167351	-1.445056	2.795598
24	6	0	-3.801051	-0.923098	1.538855
25	6	0	-5.009729	-0.229938	1.601413
26	6	0	-5.115499	-0.101163	-0.785129
27	6	0	-6.954487	0.985937	0.552656
28	6	0	2.698164	1.546200	0.439632
29	6	0	3.911481	1.644330	-0.263657
30	6	0	5.133935	1.686107	0.398682
31	6	0	5.172660	1.613758	1.788471
32	6	0	3.980130	1.497797	2.501040
33	6	0	2.757855	1.462925	1.839550
34	1	0	-0.260473	-4.446123	-0.548544
35	1	0	6.124319	1.643554	2.312988
36	1	0	3.999998	1.430626	3.585920
37	1	0	-4.101731	-0.864055	-3.037917
38	1	0	1.750054	1.421847	-1.438504
39	1	0	-0.236858	-4.088643	1.190108
40	1	0	1.298269	-2.986872	2.590876
41	1	0	1.019990	-1.252693	2.378309
42	1	0	2.568018	-1.832733	3.008746
43	1	0	-2.522354	-3.697541	-0.757962
44	1	0	-2.593805	-3.739982	1.014605
45	1	0	0.394754	-2.200287	-2.805770
46	1	0	0.756598	-3.924381	-2.558262
47	1	0	1.796861	-2.941346	-3.590477
48	1	0	-3.226720	-2.238016	-2.356018
49	1	0	-2.427539	-0.670727	-2.482863
50	1	0	1.839040	1.341743	2.401834
51	1	0	3.880657	-2.658767	-2.623680
52	1	0	4.357347	-1.889557	1.561795
53	1	0	6.105986	-1.085123	-0.547656
54	1	0	6.081788	-2.381802	-1.755478
55	1	0	6.318480	-2.761894	-0.040313
56	1	0	-2.108872	-1.177662	2.848169
57	1	0	-3.253965	-2.538413	2.860394
58	1	0	-3.666117	-1.029690	3.675873
59	1	0	-5.447663	-0.035064	2.578291
60	1	0	-5.641261	0.188029	-1.693164
61	1	0	-7.505914	0.740009	1.465853
62	1	0	-7.607967	0.791196	-0.304013
63	1	0	-6.755511	2.065068	0.572297
64	1	0	3.889734	1.690595	-1.350062
65	1	0	6.054717	1.776450	-0.172273
66	7	0	0.098268	-2.421975	-0.056104
67	7	0	-2.006612	-1.884420	0.189191
68	17	0	-0.508251	0.725805	2.276600
69	44	0	-0.220605	0.555728	-0.124726

70	17	0	-0.173240	0.274201	-2.543574
71	6	0	0.715604	3.552636	-1.631448
72	1	0	0.415617	2.929637	-2.479965
73	1	0	1.808039	3.647162	-1.689158
74	6	0	0.129083	4.956442	-1.754510
75	1	0	-0.961482	4.973418	-1.682242
76	1	0	0.398986	5.373165	-2.731497
77	1	0	0.528287	5.632989	-0.991891
78	1	0	-2.527104	3.631167	-1.200951
79	6	0	0.683941	3.652553	0.913905
80	1	0	0.012269	4.516882	0.923710
81	1	0	1.716258	4.018224	0.901684
82	1	0	0.518061	3.091194	1.835476
83	1	0	-1.514700	2.577496	0.750121

5c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.593714	-2.579209	-0.435713
2	6	0	2.898299	-1.790977	0.106702
3	6	0	1.720447	-2.931211	-1.905729
4	1	0	2.027512	-2.083352	-2.515086
5	1	0	0.759180	-3.297279	-2.287134
6	6	0	1.063858	-3.765250	0.374658
7	1	0	1.218914	-3.600163	1.440147
8	1	0	-0.028081	-3.759971	0.246561
9	6	0	2.703491	-0.365496	0.766309
10	6	0	3.561968	0.776472	0.384052
11	6	0	3.720474	1.781742	1.353203
12	6	0	4.511971	2.899166	1.113775
13	6	0	5.187280	3.023203	-0.097292
14	6	0	5.056945	2.024707	-1.061530
15	6	0	4.250107	0.918151	-0.829622
16	1	0	5.816338	3.888624	-0.287965
17	1	0	5.582625	2.112460	-2.008545
18	1	0	2.667029	-0.461558	1.854115
19	1	0	4.138201	0.172985	-1.608510
20	1	0	3.208620	1.676990	2.307853
21	1	0	4.612056	3.664542	1.878815
22	17	0	1.375200	0.223206	-2.070830
23	44	0	0.876742	-0.785408	0.089038
24	17	0	0.460587	-1.417339	2.414071
25	6	0	3.669081	-2.622428	1.137465
26	1	0	3.096905	-2.731906	2.062073
27	1	0	3.907013	-3.614515	0.743828
28	1	0	4.610007	-2.115113	1.374616
29	6	0	1.572570	-5.155156	-0.025625
30	1	0	1.259366	-5.443128	-1.033928
31	1	0	2.664571	-5.231717	0.018094
32	1	0	1.165987	-5.898671	0.668787
33	1	0	2.446836	-3.746776	-2.030860
34	1	0	3.485043	-1.619879	-0.797424
35	15	0	-1.322148	0.283588	-0.030173
36	6	0	-2.420347	-0.610156	-1.254890
37	6	0	-3.896233	-0.173177	-1.267410
38	6	0	-1.863720	-0.614435	-2.684713
39	1	0	-2.390119	-1.646951	-0.881459
40	6	0	-4.722766	-1.091915	-2.170403

41	1	0	-3.973091	0.855879	-1.637653
42	1	0	-4.321490	-0.176014	-0.260938
43	6	0	-2.697515	-1.519370	-3.592350
44	1	0	-1.876816	0.410606	-3.081928
45	1	0	-0.815323	-0.921485	-2.693638
46	6	0	-4.172017	-1.127144	-3.592459
47	1	0	-5.768780	-0.760400	-2.169146
48	1	0	-4.716291	-2.109023	-1.750803
49	1	0	-2.290623	-1.487049	-4.610446
50	1	0	-2.598634	-2.560860	-3.250171
51	1	0	-4.755638	-1.820038	-4.211258
52	1	0	-4.281473	-0.131457	-4.047216
53	6	0	-0.987546	2.028489	-0.575668
54	6	0	-2.151701	2.923220	-1.019734
55	6	0	-0.100929	2.710247	0.480656
56	1	0	-0.348985	1.856436	-1.453698
57	6	0	-1.623899	4.279435	-1.498829
58	1	0	-2.867961	3.082225	-0.205542
59	1	0	-2.701699	2.447008	-1.838586
60	6	0	0.395720	4.066372	-0.017712
61	1	0	-0.658528	2.847882	1.417992
62	1	0	0.760671	2.070318	0.714296
63	6	0	-0.764600	4.963855	-0.438618
64	1	0	-2.468219	4.919832	-1.783955
65	1	0	-1.022257	4.128362	-2.406722
66	1	0	0.995602	4.548940	0.763687
67	1	0	1.065538	3.903629	-0.873340
68	1	0	-0.388044	5.922002	-0.817779
69	1	0	-1.385558	5.196499	0.439779
70	6	0	-2.211849	0.269878	1.612884
71	6	0	-3.233877	1.380161	1.898493
72	6	0	-2.804380	-1.119064	1.909933
73	1	0	-1.378865	0.397537	2.318145
74	6	0	-3.734514	1.279544	3.343046
75	1	0	-4.088364	1.316270	1.212378
76	1	0	-2.784340	2.366891	1.749434
77	6	0	-3.290557	-1.195198	3.356464
78	1	0	-3.650977	-1.324991	1.241345
79	1	0	-2.045583	-1.888643	1.738329
80	6	0	-4.308243	-0.098812	3.658984
81	1	0	-4.483828	2.060481	3.525249
82	1	0	-2.895506	1.484390	4.023815
83	1	0	-3.724031	-2.184848	3.547579
84	1	0	-2.423596	-1.095757	4.023852
85	1	0	-4.622833	-0.145295	4.709076
86	1	0	-5.212685	-0.263434	3.053750

5d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.727424	2.322029	-1.062769
2	6	0	-2.984220	1.540569	-0.516601
3	6	0	-1.352118	3.707341	-0.604247
4	1	0	-1.499368	3.874296	0.462582
5	1	0	-0.289458	3.872558	-0.820446
6	6	0	-2.595816	0.187885	0.381172
7	6	0	-3.325035	-1.087161	0.176718
8	6	0	-4.164458	-1.490663	1.231263

9	6	0	-4.906499	-2.664119	1.159038
10	6	0	-4.815283	-3.472898	0.029739
11	6	0	-3.973846	-3.098495	-1.016559
12	6	0	-3.234323	-1.923555	-0.947499
13	1	0	-5.388244	-4.394485	-0.031382
14	1	0	-3.885677	-3.731611	-1.895663
15	1	0	-2.689379	0.485509	1.427966
16	1	0	-2.558949	-1.654151	-1.752085
17	1	0	-4.234891	-0.866403	2.119401
18	1	0	-5.551116	-2.947770	1.986745
19	17	0	-0.826072	-0.180210	-2.509447
20	44	0	-0.827119	0.730226	-0.272096
21	17	0	-0.644274	1.776314	1.936208
22	6	0	-3.791774	2.371460	0.515157
23	1	0	-3.116724	2.700220	1.310968
24	1	0	-4.514550	1.690232	0.982942
25	6	0	-4.575370	3.550085	-0.056465
26	1	0	-3.943452	4.267175	-0.587152
27	1	0	-5.064478	4.087929	0.763529
28	1	0	-5.361252	3.220851	-0.743624
29	1	0	-1.904131	4.463876	-1.179431
30	6	0	-3.851959	1.128740	-1.707548
31	1	0	-4.157966	2.020583	-2.263562
32	1	0	-4.753645	0.609531	-1.365983
33	1	0	-3.305804	0.478271	-2.392882
34	1	0	-1.696558	2.238466	-2.153104
35	15	0	1.458893	-0.093950	0.052099
36	6	0	1.412483	-0.831450	1.760233
37	6	0	0.370211	-1.963977	1.785529
38	6	0	2.718343	-1.235709	2.455741
39	1	0	0.978549	0.002070	2.330345
40	6	0	0.115525	-2.437349	3.216270
41	1	0	0.709642	-2.814489	1.178444
42	1	0	-0.572716	-1.619664	1.339348
43	6	0	2.429879	-1.718090	3.881046
44	1	0	3.240048	-2.026607	1.904370
45	1	0	3.398719	-0.379846	2.503897
46	6	0	1.412047	-2.855152	3.904297
47	1	0	-0.602348	-3.266703	3.206401
48	1	0	-0.352155	-1.619161	3.781854
49	1	0	3.367810	-2.029954	4.357648
50	1	0	2.041265	-0.875565	4.471080
51	1	0	1.212789	-3.164096	4.937917
52	1	0	1.832846	-3.732713	3.390494
53	6	0	1.940147	-1.396223	-1.206616
54	6	0	2.429652	-0.768772	-2.523906
55	6	0	2.901773	-2.508274	-0.759957
56	1	0	0.970286	-1.863302	-1.429023
57	6	0	2.540692	-1.834952	-3.612717
58	1	0	3.417338	-0.311096	-2.378379
59	1	0	1.740773	0.015682	-2.848448
60	6	0	3.031916	-3.568370	-1.858114
61	1	0	3.893690	-2.094865	-0.533322
62	1	0	2.545496	-2.990509	0.155029
63	6	0	3.473006	-2.966628	-3.189454
64	1	0	2.895651	-1.374337	-4.543023
65	1	0	1.537858	-2.232600	-3.821087
66	1	0	3.735462	-4.345768	-1.533926
67	1	0	2.057824	-4.061620	-1.989775
68	1	0	3.510943	-3.744408	-3.962325
69	1	0	4.496523	-2.575104	-3.088558

70	6	0	2.727934	1.270475	-0.098078
71	6	0	2.465037	2.476195	0.812583
72	6	0	4.198478	0.833495	0.022477
73	1	0	2.569921	1.602650	-1.137274
74	6	0	3.410117	3.629030	0.469811
75	1	0	2.607535	2.181553	1.861637
76	1	0	1.424364	2.799688	0.737063
77	6	0	5.131752	1.989400	-0.345278
78	1	0	4.408160	0.528721	1.054137
79	1	0	4.415060	-0.031514	-0.610135
80	6	0	4.875977	3.210194	0.533851
81	1	0	3.220633	4.468592	1.149749
82	1	0	3.181251	3.990901	-0.544070
83	1	0	6.174756	1.660695	-0.254764
84	1	0	4.977819	2.257493	-1.401118
85	1	0	5.527057	4.040749	0.234197
86	1	0	5.137431	2.965256	1.573884

TS6a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.617716	1.810398	-0.350908
2	6	0	0.161202	2.898380	-0.883065
3	6	0	-2.132438	2.636178	0.795711
4	1	0	-1.408778	2.755099	1.598630
5	1	0	-3.015882	2.123532	1.200993
6	6	0	-2.597178	1.689972	-1.501976
7	1	0	-2.055208	1.637371	-2.448110
8	1	0	-3.027905	0.686361	-1.391369
9	6	0	1.354112	2.105551	-0.920529
10	6	0	-0.392297	-1.290702	0.347896
11	6	0	1.961971	-2.098084	0.109273
12	6	0	0.086518	-3.513116	0.919366
13	6	0	2.560459	-1.514748	2.506832
14	6	0	-1.372764	-3.219505	1.251040
15	6	0	4.666934	-2.075345	-0.612257
16	6	0	1.344104	-2.998022	-2.197745
17	6	0	2.931902	-1.794383	1.081250
18	6	0	2.330203	-2.468036	-1.195920
19	6	0	-2.972607	-2.292641	-1.730730
20	6	0	3.683558	-2.423595	-1.535963
21	6	0	4.270895	-1.783776	0.692881
22	6	0	-2.875262	-1.338128	0.614508
23	6	0	6.114824	-2.014216	-1.012755
24	6	0	-5.532470	-0.480542	0.433176
25	6	0	-3.601697	-1.590769	-0.561787
26	6	0	-2.719847	-0.509801	3.005538
27	6	0	-3.467692	-0.709510	1.719909
28	6	0	-4.791334	-0.278911	1.597074
29	6	0	-4.924036	-1.150688	-0.628995
30	6	0	-6.945889	0.019261	0.318924
31	6	0	2.538665	2.292123	-0.058704
32	6	0	3.687541	1.551508	-0.368248
33	6	0	4.868416	1.728455	0.344830
34	6	0	4.925226	2.656685	1.379739
35	6	0	3.790161	3.403022	1.696020
36	6	0	2.610813	3.223696	0.986865
37	1	0	0.198437	-4.227187	0.093945

38	1	0	5.848085	2.804190	1.934661
39	1	0	3.825334	4.131387	2.501840
40	1	0	-3.717377	-2.490691	-2.507235
41	1	0	1.611362	1.738106	-1.916292
42	1	0	0.655301	-3.886577	1.775836
43	1	0	1.954020	-2.323410	2.933614
44	1	0	1.972449	-0.593857	2.586843
45	1	0	3.458759	-1.410883	3.122402
46	1	0	-2.072102	-3.912667	0.773730
47	1	0	-1.567890	-3.223946	2.329937
48	1	0	0.326665	-2.658162	-2.004251
49	1	0	1.361399	-4.097086	-2.196988
50	1	0	1.601029	-2.664966	-3.206914
51	1	0	-2.529545	-3.253237	-1.441013
52	1	0	-2.170579	-1.684676	-2.169499
53	1	0	1.737552	3.809410	1.253048
54	1	0	3.973080	-2.694284	-2.549866
55	1	0	5.025000	-1.540158	1.438249
56	1	0	6.775069	-2.190966	-0.157534
57	1	0	6.368429	-1.028211	-1.423889
58	1	0	6.350048	-2.754830	-1.784255
59	1	0	-1.766936	0.007775	2.843137
60	1	0	-2.493702	-1.468897	3.489123
61	1	0	-3.317508	0.075770	3.710636
62	1	0	-5.257534	0.216856	2.446616
63	1	0	-5.491745	-1.337498	-1.538676
64	1	0	-7.408274	0.143812	1.303099
65	1	0	-7.567701	-0.666939	-0.265604
66	1	0	-6.977824	0.994093	-0.184668
67	1	0	3.644715	0.821921	-1.174003
68	1	0	5.746249	1.141318	0.087614
69	7	0	0.589416	-2.198471	0.506625
70	7	0	-1.551603	-1.864352	0.716147
71	17	0	0.329174	1.148303	2.090185
72	44	0	-0.096730	0.670471	-0.266208
73	17	0	-0.170495	-0.035167	-2.601555
74	6	0	-0.287851	3.509134	-2.189632
75	1	0	-0.278241	2.764084	-2.990707
76	1	0	-1.278912	3.966026	-2.133522
77	1	0	0.425519	4.299405	-2.457320
78	6	0	-3.750672	2.690992	-1.585108
79	1	0	-4.407385	2.643521	-0.710424
80	1	0	-3.410648	3.727438	-1.692225
81	1	0	-4.359201	2.457103	-2.465686
82	1	0	-2.474696	3.618119	0.441971
83	1	0	0.056463	3.537109	-0.007897

TS6b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.496468	1.893426	-0.107291
2	6	0	0.443996	2.952125	-0.373008
3	6	0	-2.520810	2.147626	-1.157616
4	1	0	-2.147546	2.007765	-2.173053
5	1	0	-3.308786	1.396632	-1.001287
6	6	0	1.466122	1.940634	-0.534098
7	6	0	-0.693458	-1.360936	0.178840
8	6	0	1.600130	-2.280718	-0.084559

9	6	0	-0.410688	-3.671559	0.453708
10	6	0	2.078295	-1.949223	2.388060
11	6	0	-1.874416	-3.312863	0.707979
12	6	0	4.335986	-2.251635	-0.661054
13	6	0	1.073808	-2.910799	-2.495317
14	6	0	2.521814	-2.085231	0.960884
15	6	0	2.027440	-2.533068	-1.398107
16	6	0	-3.230857	-1.678699	-2.121254
17	6	0	3.398235	-2.494360	-1.660934
18	6	0	3.877801	-2.062448	0.643607
19	6	0	-3.179810	-1.216195	0.371044
20	6	0	5.806702	-2.207425	-0.966686
21	6	0	-5.731979	-0.072018	0.260518
22	6	0	-3.851106	-1.148209	-0.861637
23	6	0	-3.138289	-0.969682	2.898774
24	6	0	-3.789094	-0.782984	1.559272
25	6	0	-5.054423	-0.199041	1.472207
26	6	0	-5.120550	-0.568579	-0.891213
27	6	0	-7.081223	0.587704	0.194251
28	6	0	2.728414	1.799197	0.232845
29	6	0	3.874919	1.547023	-0.541892
30	6	0	5.141022	1.493854	0.029054
31	6	0	5.293500	1.667860	1.401839
32	6	0	4.165815	1.891463	2.188452
33	6	0	2.899661	1.959124	1.616939
34	1	0	-0.277651	-4.307718	-0.428791
35	1	0	6.280530	1.626646	1.855291
36	1	0	4.268461	2.014880	3.263567
37	1	0	-3.948505	-1.644550	-2.946305
38	1	0	1.645209	1.726154	-1.588969
39	1	0	0.062625	-4.166265	1.307567
40	1	0	1.487190	-2.817368	2.707063
41	1	0	1.455873	-1.061039	2.538712
42	1	0	2.946147	-1.877805	3.050131
43	1	0	-2.567998	-3.847307	0.050857
44	1	0	-2.178325	-3.493855	1.744931
45	1	0	0.118165	-2.391081	-2.408403
46	1	0	0.892442	-3.995029	-2.492553
47	1	0	1.492508	-2.654145	-3.472406
48	1	0	-2.905586	-2.720160	-2.006404
49	1	0	-2.347661	-1.094176	-2.407810
50	1	0	2.035738	2.089635	2.254925
51	1	0	3.737273	-2.672284	-2.679680
52	1	0	4.596374	-1.893457	1.442785
53	1	0	6.207856	-1.201215	-0.796447
54	1	0	6.009624	-2.480278	-2.006771
55	1	0	6.369176	-2.892045	-0.321094
56	1	0	-2.095146	-0.639942	2.890711
57	1	0	-3.163345	-2.024069	3.205667
58	1	0	-3.669831	-0.398600	3.665686
59	1	0	-5.527572	0.153286	2.386780
60	1	0	-5.644890	-0.508354	-1.843139
61	1	0	-7.625205	0.483980	1.138522
62	1	0	-7.697577	0.160590	-0.603565
63	1	0	-6.983248	1.661729	-0.009711
64	1	0	3.765502	1.402465	-1.614087
65	1	0	6.009085	1.320838	-0.602282
66	7	0	0.203543	-2.360583	0.222250
67	7	0	-1.911926	-1.873530	0.419319
68	17	0	-0.138991	0.806096	2.323772
69	44	0	-0.149622	0.608668	-0.107722

70	17	0	-0.195888	0.263895	-2.521205
71	6	0	0.151660	3.679079	-1.693038
72	1	0	-0.222042	2.953099	-2.422634
73	1	0	1.130941	3.995759	-2.080460
74	6	0	-0.731516	4.920152	-1.632666
75	1	0	-1.700873	4.736044	-1.162183
76	1	0	-0.922524	5.281989	-2.648840
77	1	0	-0.246566	5.733981	-1.083171
78	1	0	-2.993505	3.129983	-1.043285
79	6	0	0.414131	3.802324	0.873260
80	1	0	-0.416615	4.512111	0.852893
81	1	0	1.348870	4.377608	0.934711
82	1	0	0.322731	3.198577	1.776987
83	1	0	-1.724927	2.329040	0.873714

TS6c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.075821	-2.548194	0.520246
2	6	0	-2.843797	-1.984667	-0.150053
3	6	0	-1.333460	-2.899206	1.964357
4	1	0	-1.800059	-2.089644	2.521644
5	1	0	-0.368611	-3.129199	2.437271
6	6	0	-0.410335	-3.675476	-0.261034
7	1	0	-0.668575	-3.602869	-1.318858
8	1	0	0.661666	-3.428389	-0.234598
9	6	0	-2.908510	-0.684699	-0.820185
10	6	0	-3.748643	0.458383	-0.413029
11	6	0	-3.829410	1.536684	-1.308338
12	6	0	-4.619832	2.645955	-1.030077
13	6	0	-5.365599	2.689003	0.144860
14	6	0	-5.311629	1.615764	1.033342
15	6	0	-4.511211	0.514313	0.761341
16	1	0	-5.992559	3.549028	0.364529
17	1	0	-5.895945	1.639217	1.949274
18	1	0	-2.830330	-0.762944	-1.906205
19	1	0	-4.471569	-0.301852	1.474414
20	1	0	-3.259151	1.495470	-2.234475
21	1	0	-4.661973	3.470675	-1.736642
22	17	0	-1.537323	0.277143	1.957558
23	44	0	-0.919207	-0.768774	-0.154793
24	17	0	-0.473758	-1.357327	-2.485853
25	6	0	-3.242940	-3.151894	-1.035028
26	1	0	-2.687556	-3.133399	-1.976781
27	1	0	-3.102512	-4.121002	-0.550520
28	1	0	-4.309100	-3.048851	-1.270623
29	6	0	-0.577794	-5.109830	0.245832
30	1	0	-0.174292	-5.249914	1.253623
31	1	0	-1.623993	-5.433817	0.258355
32	1	0	-0.036466	-5.789133	-0.421555
33	1	0	-1.943027	-3.810047	2.039539
34	1	0	-3.309768	-1.980127	0.834293
35	15	0	1.265434	0.356523	0.023511
36	6	0	2.343563	-0.420903	1.342964
37	6	0	3.819654	0.012738	1.358567
38	6	0	1.746734	-0.292355	2.751408
39	1	0	2.319513	-1.488633	1.068319
40	6	0	4.615353	-0.816556	2.369794

41	1	0	3.892287	1.073506	1.628865
42	1	0	4.275005	-0.089686	0.370588
43	6	0	2.547745	-1.111561	3.763752
44	1	0	1.758685	0.764549	3.054721
45	1	0	0.695560	-0.590831	2.756168
46	6	0	4.022406	-0.719871	3.771990
47	1	0	5.662113	-0.487172	2.369964
48	1	0	4.619141	-1.868606	2.047106
49	1	0	2.110222	-0.986707	4.761896
50	1	0	2.457769	-2.180347	3.515288
51	1	0	4.586554	-1.350869	4.470085
52	1	0	4.119316	0.314260	4.134264
53	6	0	0.868162	2.116945	0.469036
54	6	0	1.985579	3.073363	0.902524
55	6	0	0.000492	2.716376	-0.650476
56	1	0	0.204310	1.969095	1.333656
57	6	0	1.396527	4.431004	1.298600
58	1	0	2.718404	3.219523	0.100599
59	1	0	2.529322	2.654895	1.756198
60	6	0	-0.559617	4.078062	-0.242757
61	1	0	0.589175	2.823793	-1.572828
62	1	0	-0.831833	2.037534	-0.885434
63	6	0	0.554347	5.033518	0.176404
64	1	0	2.207288	5.114548	1.581021
65	1	0	0.767634	4.301871	2.191304
66	1	0	-1.140655	4.501848	-1.071254
67	1	0	-1.258718	3.935920	0.592853
68	1	0	0.132648	5.995302	0.493778
69	1	0	1.200161	5.244402	-0.689458
70	6	0	2.218530	0.291355	-1.581483
71	6	0	3.254471	1.386915	-1.871976
72	6	0	2.807479	-1.112532	-1.805267
73	1	0	1.412110	0.396513	-2.320805
74	6	0	3.821351	1.223738	-3.285838
75	1	0	4.075957	1.358200	-1.144668
76	1	0	2.796479	2.377859	-1.789208
77	6	0	3.365404	-1.246632	-3.221432
78	1	0	3.615045	-1.310077	-1.087479
79	1	0	2.028179	-1.864895	-1.647399
80	6	0	4.404669	-0.167861	-3.513880
81	1	0	4.580646	1.995200	-3.467191
82	1	0	3.015687	1.398465	-4.013673
83	1	0	3.801070	-2.245200	-3.352774
84	1	0	2.534681	-1.168003	-3.935945
85	1	0	4.774636	-0.259442	-4.542744
86	1	0	5.274196	-0.309989	-2.854222

TS6d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.280558	2.323652	1.028499
2	6	0	3.116832	1.590360	0.374202
3	6	0	0.873139	3.680853	0.549842
4	1	0	0.999782	3.819853	-0.525202
5	1	0	-0.202391	3.774910	0.758985
6	6	0	2.899718	0.374525	-0.420230
7	6	0	3.459579	-0.985239	-0.245261
8	6	0	3.645157	-1.709291	-1.438976

9	6	0	4.197930	-2.983935	-1.441347
10	6	0	4.588569	-3.571716	-0.241426
11	6	0	4.408628	-2.873656	0.950768
12	6	0	3.846622	-1.602375	0.955771
13	1	0	5.025295	-4.566842	-0.233629
14	1	0	4.698933	-3.327488	1.894608
15	1	0	2.864112	0.618213	-1.482865
16	1	0	3.671383	-1.109703	1.900900
17	1	0	3.348608	-1.252762	-2.381029
18	1	0	4.328247	-3.513787	-2.381269
19	17	0	1.132416	-0.384306	2.328365
20	44	0	0.905913	0.703535	0.178818
21	17	0	0.679431	1.634219	-2.077016
22	6	0	3.608525	2.735319	-0.533177
23	1	0	2.826705	2.975994	-1.259956
24	1	0	4.431083	2.310186	-1.125320
25	6	0	4.146131	3.991964	0.142729
26	1	0	3.435360	4.453048	0.833773
27	1	0	4.387981	4.737372	-0.622810
28	1	0	5.066526	3.789762	0.700311
29	1	0	1.370764	4.484083	1.105833
30	6	0	3.831394	1.488402	1.704981
31	1	0	3.935080	2.470321	2.173364
32	1	0	4.840601	1.089093	1.534590
33	1	0	3.308982	0.832868	2.402699
34	1	0	1.481716	2.260191	2.104983
35	15	0	-1.418082	-0.093007	0.012603
36	6	0	-1.426954	-0.981476	-1.621084
37	6	0	-0.390108	-2.116783	-1.565029
38	6	0	-2.749923	-1.449762	-2.239749
39	1	0	-1.010400	-0.206877	-2.280992
40	6	0	-0.168949	-2.725055	-2.948941
41	1	0	-0.722294	-2.902130	-0.871578
42	1	0	0.567793	-1.745992	-1.170544
43	6	0	-2.501004	-2.064676	-3.620503
44	1	0	-3.248598	-2.188423	-1.601724
45	1	0	-3.437676	-0.603937	-2.342753
46	6	0	-1.483875	-3.201941	-3.560670
47	1	0	0.548403	-3.551937	-2.877607
48	1	0	0.284027	-1.965623	-3.602141
49	1	0	-3.450600	-2.419430	-4.040775
50	1	0	-2.128315	-1.283537	-4.298636
51	1	0	-1.312052	-3.610666	-4.564145
52	1	0	-1.891133	-4.023532	-2.952402
53	6	0	-1.866135	-1.273819	1.390679
54	6	0	-2.172059	-0.516069	2.694638
55	6	0	-2.922733	-2.352688	1.114224
56	1	0	-0.908967	-1.786421	1.560220
57	6	0	-2.274997	-1.489227	3.869062
58	1	0	-3.120278	0.031165	2.608013
59	1	0	-1.381218	0.214371	2.891763
60	6	0	-3.034403	-3.306676	2.307892
61	1	0	-3.903671	-1.902362	0.915589
62	1	0	-2.656985	-2.932598	0.224683
63	6	0	-3.325485	-2.565436	3.609322
64	1	0	-2.511116	-0.935254	4.786342
65	1	0	-1.292691	-1.955645	4.026053
66	1	0	-3.812056	-4.054816	2.107368
67	1	0	-2.088108	-3.857387	2.411597
68	1	0	-3.366399	-3.272759	4.447101
69	1	0	-4.319333	-2.096800	3.545734

70	6	0	-2.697997	1.275017	0.013222
71	6	0	-2.548072	2.228434	-1.180252
72	6	0	-4.164329	0.824616	0.143430
73	1	0	-2.444411	1.839118	0.925646
74	6	0	-3.488503	3.427171	-1.052544
75	1	0	-2.781665	1.686916	-2.108268
76	1	0	-1.513148	2.561152	-1.283448
77	6	0	-5.096838	2.032252	0.273013
78	1	0	-4.453355	0.242909	-0.740585
79	1	0	-4.304680	0.170146	1.006990
80	6	0	-4.942977	2.994585	-0.899905
81	1	0	-3.368928	4.077972	-1.927402
82	1	0	-3.195025	4.025576	-0.176411
83	1	0	-6.134276	1.684017	0.354465
84	1	0	-4.870640	2.561914	1.210572
85	1	0	-5.594384	3.867232	-0.766192
86	1	0	-5.271582	2.495410	-1.823573

7a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.808331	1.532587	-0.382478
2	6	0	0.365652	3.271809	0.227681
3	6	0	-2.797220	1.852226	0.692024
4	1	0	-2.481753	1.531936	1.681276
5	1	0	-3.772399	1.414149	0.444561
6	6	0	-2.266798	1.891165	-1.779075
7	1	0	-1.434215	2.358427	-2.312904
8	1	0	-2.382943	0.939699	-2.313288
9	6	0	1.358162	2.627827	-0.476626
10	6	0	-0.448298	-1.151750	0.216331
11	6	0	1.946658	-1.913220	-0.024332
12	6	0	0.103009	-3.402688	0.631115
13	6	0	2.389337	-1.440180	2.435489
14	6	0	-1.412210	-3.257941	0.650899
15	6	0	4.695610	-1.948155	-0.546906
16	6	0	1.476041	-2.709339	-2.401787
17	6	0	2.850731	-1.653166	1.022481
18	6	0	2.399189	-2.249601	-1.309285
19	6	0	-2.764640	-1.680276	-2.157763
20	6	0	3.774994	-2.236873	-1.548491
21	6	0	4.212337	-1.667353	0.731814
22	6	0	-2.944697	-1.363504	0.351285
23	6	0	6.173605	-1.954190	-0.819685
24	6	0	-5.653063	-0.700896	0.129129
25	6	0	-3.537662	-1.316261	-0.921250
26	6	0	-3.067956	-1.242996	2.878152
27	6	0	-3.693351	-1.141090	1.516913
28	6	0	-5.041896	-0.809747	1.378757
29	6	0	-4.885024	-0.962248	-1.007101
30	6	0	-7.097926	-0.301957	0.008397
31	6	0	2.651309	2.160983	0.061834
32	6	0	3.657419	1.844569	-0.863805
33	6	0	4.958709	1.597570	-0.445043
34	6	0	5.274421	1.633700	0.910825
35	6	0	4.273106	1.899103	1.844029
36	6	0	2.973823	2.162845	1.428287
37	1	0	0.455681	-4.126482	-0.110287

38	1	0	6.294537	1.452920	1.240692
39	1	0	4.507777	1.916628	2.905257
40	1	0	-3.362100	-1.492120	-3.055079
41	1	0	1.344890	2.728088	-1.560513
42	1	0	0.516298	-3.682613	1.606716
43	1	0	1.988334	-2.369299	2.863587
44	1	0	1.604831	-0.681319	2.512552
45	1	0	3.228119	-1.129101	3.065054
46	1	0	-1.903376	-3.803818	-0.163738
47	1	0	-1.860544	-3.583416	1.594253
48	1	0	0.447831	-2.386807	-2.238541
49	1	0	1.499304	-3.805530	-2.483388
50	1	0	1.789277	-2.300271	-3.366413
51	1	0	-2.506549	-2.747737	-2.160201
52	1	0	-1.824432	-1.123321	-2.248361
53	1	0	2.204575	2.368971	2.165682
54	1	0	4.131038	-2.481055	-2.547818
55	1	0	4.916470	-1.460378	1.534670
56	1	0	6.607502	-0.960961	-0.651879
57	1	0	6.390387	-2.245560	-1.852009
58	1	0	6.699306	-2.650586	-0.155467
59	1	0	-2.123193	-0.689549	2.924818
60	1	0	-2.854462	-2.286101	3.146937
61	1	0	-3.742422	-0.844780	3.642044
62	1	0	-5.628603	-0.624960	2.276673
63	1	0	-5.351467	-0.913002	-1.989376
64	1	0	-7.675749	-0.622165	0.881327
65	1	0	-7.560168	-0.735529	-0.884311
66	1	0	-7.201226	0.788140	-0.068154
67	1	0	3.408249	1.816091	-1.921213
68	1	0	5.728439	1.382253	-1.181505
69	7	0	0.552397	-2.055289	0.269337
70	7	0	-1.598510	-1.814734	0.467011
71	17	0	-0.188465	1.023511	2.424187
72	44	0	-0.094593	0.872850	-0.039008
73	17	0	0.383714	0.415464	-2.394658
74	6	0	-0.511041	4.309284	-0.405781
75	1	0	-0.590197	4.182955	-1.489009
76	1	0	-1.514658	4.346849	0.027668
77	1	0	-0.055955	5.293324	-0.223561
78	6	0	-3.540320	2.720115	-1.941302
79	1	0	-4.422741	2.208660	-1.543221
80	1	0	-3.469121	3.699660	-1.455487
81	1	0	-3.717625	2.898029	-3.007734
82	1	0	-2.956632	2.941265	0.707431
83	1	0	0.413254	3.298484	1.313818

7b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.851036	1.345098	-0.174991
2	6	0	0.777965	3.429533	-0.207910
3	6	0	-2.721680	1.689473	-1.331630
4	1	0	-2.375592	1.267310	-2.274755
5	1	0	-3.752072	1.375395	-1.119436
6	6	0	1.509697	2.408536	-0.763302
7	6	0	-0.698100	-1.223636	0.290449
8	6	0	1.619451	-2.169589	0.190282

9	6	0	-0.382572	-3.502227	0.768742
10	6	0	2.041365	-1.708671	2.649320
11	6	0	-1.847269	-3.147126	0.994074
12	6	0	4.367433	-2.364303	-0.292896
13	6	0	1.135488	-2.921880	-2.200767
14	6	0	2.521423	-1.969580	1.251266
15	6	0	2.068327	-2.526735	-1.091530
16	6	0	-3.049834	-1.986680	-2.087481
17	6	0	3.445628	-2.595646	-1.309227
18	6	0	3.883943	-2.064413	0.981691
19	6	0	-3.207921	-1.199726	0.313037
20	6	0	5.844713	-2.431626	-0.556275
21	6	0	-5.838631	-0.335409	-0.082896
22	6	0	-3.806975	-1.371110	-0.947406
23	6	0	-3.309130	-0.543782	2.759885
24	6	0	-3.915189	-0.642255	1.390060
25	6	0	-5.219566	-0.200354	1.159691
26	6	0	-5.118912	-0.933389	-1.119750
27	6	0	-7.240316	0.160511	-0.306064
28	6	0	2.813603	1.896763	-0.289459
29	6	0	3.793889	1.666001	-1.269278
30	6	0	5.099073	1.347955	-0.916703
31	6	0	5.450265	1.224104	0.426727
32	6	0	4.474397	1.385058	1.405780
33	6	0	3.166637	1.711305	1.056914
34	1	0	-0.235716	-4.179414	-0.082146
35	1	0	6.474097	0.988081	0.706104
36	1	0	4.728243	1.255903	2.454958
37	1	0	-3.693726	-2.094083	-2.965339
38	1	0	1.303554	2.190555	-1.810889
39	1	0	0.090773	-3.949723	1.647674
40	1	0	1.448147	-2.549904	3.031808
41	1	0	1.407688	-0.817045	2.703770
42	1	0	2.891036	-1.573093	3.325336
43	1	0	-2.536169	-3.777572	0.423532
44	1	0	-2.133471	-3.196997	2.051509
45	1	0	0.125045	-2.540258	-2.053783
46	1	0	1.095449	-4.016696	-2.290153
47	1	0	1.485255	-2.523993	-3.157293
48	1	0	-2.665899	-2.982341	-1.832305
49	1	0	-2.185133	-1.370302	-2.367218
50	1	0	2.404655	1.788542	1.826278
51	1	0	3.801886	-2.857332	-2.303959
52	1	0	4.588617	-1.904962	1.795012
53	1	0	6.258519	-1.422828	-0.677475
54	1	0	6.065441	-2.993478	-1.469367
55	1	0	6.379609	-2.905375	0.274227
56	1	0	-2.284374	-0.158145	2.728069
57	1	0	-3.280817	-1.526861	3.248876
58	1	0	-3.904637	0.115772	3.398240
59	1	0	-5.771668	0.245424	1.984901
60	1	0	-5.589630	-1.059663	-2.092913
61	1	0	-7.809214	0.187624	0.628576
62	1	0	-7.780560	-0.474045	-1.016327
63	1	0	-7.237332	1.178158	-0.717126
64	1	0	3.525554	1.770097	-2.317717
65	1	0	5.846031	1.203609	-1.693389
66	7	0	0.217598	-2.199705	0.475142
67	7	0	-1.915596	-1.760847	0.523343
68	17	0	-0.109988	1.135752	2.270877
69	44	0	-0.152640	0.668957	-0.119008

70	17	0	-0.035112	0.210227	-2.511133
71	6	0	-0.242137	4.141779	-1.066607
72	1	0	-0.587323	3.466029	-1.856830
73	1	0	0.302799	4.950739	-1.580674
74	6	0	-1.421448	4.767076	-0.323887
75	1	0	-1.930398	4.038993	0.316590
76	1	0	-2.151067	5.168284	-1.036024
77	1	0	-1.106482	5.596451	0.317153
78	1	0	-2.755762	2.784416	-1.426434
79	6	0	1.090575	4.065501	1.108084
80	1	0	0.893338	5.141728	1.066145
81	1	0	2.134311	3.911013	1.392648
82	1	0	0.468145	3.634330	1.903030
83	1	0	-2.281219	1.620424	0.800817

7c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.183013	-2.685861	0.038564
2	6	0	2.713252	-2.630120	-0.367066
3	6	0	-0.495887	-3.403507	-1.239290
4	1	0	-0.092685	-2.908890	-2.120496
5	1	0	-1.584654	-3.511684	-1.342017
6	6	0	-0.676481	-3.394912	1.282639
7	1	0	0.224764	-3.739352	1.811344
8	1	0	-1.085476	-2.652870	1.974936
9	6	0	3.031448	-1.650147	0.547902
10	6	0	3.596341	-0.320657	0.252707
11	6	0	3.693966	0.608081	1.303064
12	6	0	4.292359	1.846962	1.101921
13	6	0	4.802060	2.179513	-0.150701
14	6	0	4.700835	1.270463	-1.204799
15	6	0	4.103404	0.032997	-1.009024
16	1	0	5.280085	3.143071	-0.307601
17	1	0	5.094411	1.526815	-2.184533
18	1	0	3.052215	-1.930843	1.598978
19	1	0	4.028400	-0.664348	-1.836211
20	1	0	3.282815	0.342784	2.273242
21	1	0	4.364515	2.551051	1.926455
22	17	0	1.026803	-0.790982	-2.371313
23	44	0	0.856698	-1.131126	0.072002
24	17	0	0.812517	-1.030718	2.527821
25	6	0	2.637560	-4.071410	0.036068
26	1	0	2.399388	-4.186350	1.098266
27	1	0	1.918283	-4.641532	-0.558486
28	1	0	3.620041	-4.534524	-0.132868
29	6	0	-1.645003	-4.566482	1.119784
30	1	0	-2.585469	-4.267536	0.642294
31	1	0	-1.222400	-5.390816	0.536167
32	1	0	-1.895510	-4.962263	2.109855
33	1	0	-0.113084	-4.433219	-1.184504
34	1	0	2.797391	-2.427763	-1.432496
35	15	0	-0.953538	0.493378	-0.111016
36	6	0	-0.371330	1.972984	-1.096654
37	6	0	-1.254006	3.231055	-1.057283
38	6	0	1.082479	2.357251	-0.783614
39	1	0	-0.372265	1.572250	-2.121188
40	6	0	-0.756439	4.265872	-2.069651

41	1	0	-1.211839	3.676324	-0.055087
42	1	0	-2.304608	2.999240	-1.252626
43	6	0	1.587765	3.402509	-1.778661
44	1	0	1.156469	2.754437	0.237181
45	1	0	1.726903	1.474971	-0.838104
46	6	0	0.699023	4.642590	-1.807865
47	1	0	-1.397657	5.155979	-2.032515
48	1	0	-0.850550	3.852270	-3.084633
49	1	0	2.619432	3.675081	-1.526768
50	1	0	1.618712	2.947265	-2.779124
51	1	0	1.052699	5.351710	-2.567065
52	1	0	0.766414	5.160311	-0.839249
53	6	0	-2.330219	-0.274323	-1.128744
54	6	0	-3.185862	-1.239479	-0.298018
55	6	0	-3.226346	0.654486	-1.961762
56	1	0	-1.741335	-0.869088	-1.843291
57	6	0	-4.145287	-2.041566	-1.178012
58	1	0	-3.779497	-0.680191	0.435222
59	1	0	-2.548504	-1.913519	0.281966
60	6	0	-4.182501	-0.160255	-2.837538
61	1	0	-3.813540	1.312762	-1.307301
62	1	0	-2.615460	1.297888	-2.603302
63	6	0	-5.032402	-1.120115	-2.010919
64	1	0	-4.756731	-2.703587	-0.551465
65	1	0	-3.571075	-2.689710	-1.856245
66	1	0	-4.821477	0.520583	-3.413749
67	1	0	-3.595206	-0.734312	-3.569048
68	1	0	-5.689722	-1.708229	-2.663137
69	1	0	-5.687882	-0.543699	-1.341138
70	6	0	-1.656603	1.080854	1.516410
71	6	0	-0.659916	1.960084	2.292745
72	6	0	-3.031178	1.769591	1.514661
73	1	0	-1.740575	0.138868	2.080113
74	6	0	-1.135059	2.152336	3.732899
75	1	0	-0.583694	2.942792	1.807863
76	1	0	0.334805	1.507178	2.292980
77	6	0	-3.524339	1.959545	2.952472
78	1	0	-2.957134	2.751080	1.029850
79	1	0	-3.774474	1.199894	0.949695
80	6	0	-2.532402	2.765676	3.787838
81	1	0	-0.421006	2.784037	4.276318
82	1	0	-1.133037	1.174570	4.234433
83	1	0	-4.505938	2.450793	2.944582
84	1	0	-3.671115	0.971578	3.413165
85	1	0	-2.880712	2.837974	4.825928
86	1	0	-2.490841	3.794410	3.399484

7d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.344303	-2.393949	0.613353
2	6	0	3.823617	-1.565711	-0.063560
3	6	0	0.522897	-3.207219	1.847480
4	1	0	1.079404	-2.685515	2.626803
5	1	0	-0.471858	-3.469834	2.241725
6	6	0	3.395509	-0.492214	0.671026
7	6	0	3.490756	0.942091	0.329273
8	6	0	3.693746	1.850117	1.384051

9	6	0	3.837983	3.209106	1.142449
10	6	0	3.767146	3.701832	-0.160698
11	6	0	3.531466	2.822236	-1.212453
12	6	0	3.383721	1.456998	-0.974301
13	1	0	3.883290	4.765637	-0.350794
14	1	0	3.449558	3.197010	-2.229392
15	1	0	3.190237	-0.683485	1.723886
16	1	0	3.141554	0.794416	-1.798187
17	1	0	3.731344	1.472172	2.401456
18	1	0	4.002755	3.888352	1.974649
19	17	0	1.165363	-1.101472	-2.097932
20	44	0	0.939985	-0.707775	0.286864
21	17	0	0.970064	0.009535	2.616131
22	6	0	3.841282	-2.934736	0.563757
23	1	0	3.309144	-2.910071	1.520570
24	1	0	4.892919	-3.166927	0.797959
25	6	0	3.289186	-4.048897	-0.326000
26	1	0	2.266120	-3.824352	-0.645644
27	1	0	3.290597	-5.003112	0.212245
28	1	0	3.890092	-4.180330	-1.231457
29	1	0	1.011044	-4.160661	1.597876
30	6	0	4.435573	-1.475395	-1.423077
31	1	0	5.189909	-2.260087	-1.550222
32	1	0	4.905860	-0.503243	-1.593129
33	1	0	3.666831	-1.618395	-2.194772
34	1	0	-0.202710	-2.917694	-0.188485
35	15	0	-1.285552	0.051262	-0.065153
36	6	0	-1.149359	1.375560	-1.368472
37	6	0	-2.436357	1.878698	-2.036694
38	6	0	-0.292406	2.538143	-0.840285
39	1	0	-0.554008	0.859079	-2.136412
40	6	0	-2.111875	2.895880	-3.133583
41	1	0	-3.104375	2.341243	-1.300456
42	1	0	-2.985528	1.041853	-2.480067
43	6	0	0.005137	3.547744	-1.948188
44	1	0	-0.809598	3.050459	-0.017111
45	1	0	0.651721	2.161087	-0.425261
46	6	0	-1.276866	4.056873	-2.601863
47	1	0	-3.044539	3.263962	-3.579643
48	1	0	-1.556975	2.390453	-3.937446
49	1	0	0.590064	4.379580	-1.537303
50	1	0	0.635419	3.065527	-2.709142
51	1	0	-1.040381	4.757713	-3.412247
52	1	0	-1.865093	4.620357	-1.861956
53	6	0	-1.991611	0.784926	1.501258
54	6	0	-3.101365	1.841927	1.396394
55	6	0	-2.365219	-0.325953	2.497529
56	1	0	-1.108772	1.281167	1.927979
57	6	0	-3.423944	2.410203	2.782057
58	1	0	-4.014931	1.421712	0.958637
59	1	0	-2.789639	2.661966	0.742233
60	6	0	-2.693766	0.264904	3.867892
61	1	0	-3.233481	-0.893100	2.134530
62	1	0	-1.526406	-1.022237	2.594140
63	6	0	-3.798467	1.314005	3.775286
64	1	0	-4.233398	3.146433	2.695990
65	1	0	-2.544240	2.951810	3.158814
66	1	0	-2.983915	-0.538547	4.556767
67	1	0	-1.781692	0.719611	4.277958
68	1	0	-3.997904	1.749142	4.762588
69	1	0	-4.733841	0.833399	3.450010

70	6	0	-2.500449	-1.261754	-0.635186
71	6	0	-3.995123	-0.903948	-0.564343
72	6	0	-2.164818	-1.832854	-2.020571
73	1	0	-2.331031	-2.062081	0.103593
74	6	0	-4.862168	-2.122985	-0.891617
75	1	0	-4.224772	-0.099580	-1.273095
76	1	0	-4.266420	-0.534663	0.427395
77	6	0	-3.038079	-3.044961	-2.344846
78	1	0	-2.330255	-1.058047	-2.782274
79	1	0	-1.105942	-2.092860	-2.089399
80	6	0	-4.524192	-2.713407	-2.256762
81	1	0	-5.921223	-1.839554	-0.844234
82	1	0	-4.709370	-2.889513	-0.117025
83	1	0	-2.784474	-3.419794	-3.344050
84	1	0	-2.805055	-3.857157	-1.639317
85	1	0	-5.132431	-3.606116	-2.448819
86	1	0	-4.779481	-1.984638	-3.040388

8a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.215932	2.097416	-0.456943
2	6	0	-0.597442	3.440428	-0.755698
3	1	0	0.511404	3.353901	-0.788643
4	6	0	-2.687995	1.977468	-0.393290
5	1	0	-3.174167	2.837539	-0.871661
6	1	0	-3.041964	1.055644	-0.858468
7	6	0	0.059296	-0.779212	0.146259
8	6	0	2.518554	-1.123185	0.218716
9	6	0	0.852131	-2.952513	0.593806
10	6	0	2.625087	-0.842515	2.750261
11	6	0	-0.673362	-2.945383	0.686711
12	6	0	5.180027	-0.292593	-0.006233
13	6	0	2.527279	-1.868798	-2.220018
14	6	0	3.216595	-0.727518	1.374133
15	6	0	3.167473	-1.220512	-1.025457
16	6	0	-2.298283	-1.865049	-2.234294
17	6	0	4.487972	-0.780741	-1.113474
18	6	0	4.535915	-0.300112	1.230232
19	6	0	-2.398768	-1.240320	0.214365
20	6	0	6.583780	0.227200	-0.141454
21	6	0	-5.155027	-0.820069	0.069671
22	6	0	-3.057006	-1.449153	-1.006257
23	6	0	-2.360455	-0.591105	2.658221
24	6	0	-3.087260	-0.831947	1.365740
25	6	0	-4.463901	-0.627882	1.267316
26	6	0	-4.434845	-1.228265	-1.054039
27	6	0	-6.634950	-0.566738	-0.012348
28	1	0	1.223771	-3.576202	-0.228436
29	1	0	-2.972106	-1.958502	-3.090912
30	1	0	1.334171	-3.283758	1.519600
31	1	0	2.969632	-1.771451	3.226423
32	1	0	1.534880	-0.837201	2.736237
33	1	0	2.942856	-0.008312	3.381288
34	1	0	-1.147165	-3.656406	0.002217
35	1	0	-1.036618	-3.159248	1.698902
36	1	0	1.438148	-1.859668	-2.167336
37	1	0	2.870073	-2.909760	-2.304871

38	1	0	2.805850	-1.350088	-3.140870
39	1	0	-1.801110	-2.833736	-2.098149
40	1	0	-1.518774	-1.135237	-2.486604
41	1	0	4.989872	-0.830861	-2.077951
42	1	0	5.075581	0.030303	2.115766
43	1	0	6.579776	1.301174	-0.366976
44	1	0	7.121662	-0.274027	-0.952753
45	1	0	7.153652	0.090457	0.783344
46	1	0	-1.568143	0.158675	2.538919
47	1	0	-1.881688	-1.504230	3.033510
48	1	0	-3.052047	-0.242989	3.431123
49	1	0	-5.010883	-0.309839	2.153163
50	1	0	-4.957917	-1.382324	-1.995914
51	1	0	-7.143297	-0.861148	0.911753
52	1	0	-7.090211	-1.117011	-0.841658
53	1	0	-6.843524	0.498803	-0.172331
54	7	0	1.158708	-1.548310	0.336400
55	7	0	-1.018968	-1.571008	0.310044
56	17	0	0.711571	1.722273	1.993346
57	44	0	0.294455	1.129667	-0.275313
58	17	0	0.612254	0.767320	-2.604483
59	1	0	-0.881595	3.719980	-1.781812
60	1	0	-3.004902	1.949520	0.657812
61	6	0	-0.969606	4.524259	0.257538
62	1	0	-0.489589	5.472075	-0.005920
63	1	0	-2.052366	4.688521	0.279755
64	1	0	-0.638160	4.233228	1.258650

8b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.535837	1.912623	-0.176579
2	6	0	1.708581	3.390441	-0.260675
3	1	0	0.758842	3.939038	-0.279034
4	1	0	2.286636	3.742098	0.606331
5	6	0	0.012781	-0.610850	0.072743
6	6	0	-2.446304	-0.982069	0.091059
7	6	0	-0.755413	-2.797997	0.450484
8	6	0	-2.438985	-1.527310	-2.388444
9	6	0	0.758088	-2.828426	0.252837
10	6	0	-5.120689	-0.180034	-0.045200
11	6	0	-2.515577	-0.850124	2.636092
12	6	0	-3.111970	-1.011501	-1.149298
13	6	0	-3.127599	-0.664331	1.276552
14	6	0	2.492545	-0.812808	2.609930
15	6	0	-4.456777	-0.246269	1.176512
16	6	0	-4.439128	-0.594000	-1.191830
17	6	0	2.472341	-1.038695	0.093308
18	6	0	-6.535503	0.319273	-0.132736
19	6	0	5.187569	-0.411725	-0.061407
20	6	0	3.183077	-0.788780	1.276157
21	6	0	2.302673	-1.205364	-2.427388
22	6	0	3.087997	-0.985368	-1.165612
23	6	0	4.446383	-0.669505	-1.215565
24	6	0	4.538646	-0.476570	1.173029
25	6	0	6.643433	-0.045092	-0.146100
26	1	0	-1.048203	-3.032156	1.481993
27	1	0	3.203842	-0.615833	3.417256

28	1	0	-1.288886	-3.478536	-0.219743
29	1	0	-2.074787	-2.553040	-2.247669
30	1	0	-1.587669	-0.901120	-2.670043
31	1	0	-3.141869	-1.538454	-3.226441
32	1	0	1.289023	-3.309425	1.079908
33	1	0	1.050865	-3.330716	-0.677765
34	1	0	-1.425568	-0.819322	2.613438
35	1	0	-2.834426	-1.813132	3.059094
36	1	0	-2.842013	-0.063065	3.320917
37	1	0	2.023752	-1.784328	2.809423
38	1	0	1.699286	-0.056406	2.658446
39	1	0	-4.986082	0.025473	2.087807
40	1	0	-4.957294	-0.597319	-2.148651
41	1	0	-6.556362	1.376842	-0.424711
42	1	0	-7.052325	0.233898	0.828299
43	1	0	-7.111196	-0.235082	-0.881618
44	1	0	1.488953	-0.475397	-2.520909
45	1	0	1.848541	-2.203171	-2.461644
46	1	0	2.948508	-1.107928	-3.304746
47	1	0	4.936448	-0.619741	-2.186009
48	1	0	5.101459	-0.276546	2.082844
49	1	0	7.106054	-0.448366	-1.052343
50	1	0	7.201709	-0.420553	0.717648
51	1	0	6.774125	1.044338	-0.169087
52	7	0	-1.082153	-1.407982	0.141544
53	7	0	1.100173	-1.405420	0.185520
54	17	0	-0.676637	1.435180	-2.393253
55	44	0	-0.163915	1.320933	-0.094770
56	17	0	-0.557068	1.774248	2.183850
57	1	0	2.271146	3.649467	-1.169124
58	1	0	2.444549	1.307832	-0.170809

8c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.767931	0.313023	0.444280
2	6	0	-4.161450	0.211951	-0.128584
3	1	0	-4.111735	-0.175862	-1.160946
4	1	0	-4.565285	1.232317	-0.225221
5	6	0	-2.619520	0.835454	1.829286
6	1	0	-3.132617	0.157390	2.526409
7	1	0	-1.580387	0.922469	2.146134
8	17	0	-1.452907	1.161627	-2.519372
9	44	0	-1.628684	-0.401937	-0.764738
10	17	0	-1.837283	-2.677989	-0.212465
11	15	0	0.455626	0.129222	-0.027572
12	6	0	1.554461	-0.711090	-1.296151
13	6	0	2.955855	-0.134644	-1.547299
14	6	0	1.622007	-2.234963	-1.107063
15	1	0	0.972601	-0.517716	-2.213439
16	6	0	3.604679	-0.817727	-2.754869
17	1	0	3.589809	-0.284557	-0.663202
18	1	0	2.904273	0.943104	-1.734313
19	6	0	2.270404	-2.902980	-2.319636
20	1	0	2.220012	-2.468545	-0.215788
21	1	0	0.624217	-2.651706	-0.936097
22	6	0	3.659568	-2.334394	-2.594369
23	1	0	4.611841	-0.409433	-2.907029

24	1	0	3.026277	-0.568439	-3.656319
25	1	0	2.322089	-3.986448	-2.156916
26	1	0	1.630062	-2.749066	-3.200321
27	1	0	4.094787	-2.794761	-3.489985
28	1	0	4.326361	-2.586736	-1.756207
29	6	0	0.825513	1.966216	-0.169976
30	6	0	-0.334794	2.845103	0.318465
31	6	0	2.127137	2.462592	0.480258
32	1	0	0.892989	2.104434	-1.259016
33	6	0	-0.091890	4.314521	-0.026764
34	1	0	-0.433696	2.747560	1.410123
35	1	0	-1.270434	2.508197	-0.133988
36	6	0	2.383772	3.932330	0.133336
37	1	0	2.046120	2.367509	1.572637
38	1	0	2.990528	1.866605	0.173275
39	6	0	1.221544	4.823435	0.558595
40	1	0	-0.932617	4.920580	0.333588
41	1	0	-0.076490	4.420462	-1.120746
42	1	0	3.316308	4.261999	0.608670
43	1	0	2.536031	4.022480	-0.952188
44	1	0	1.403957	5.861292	0.253562
45	1	0	1.153030	4.826321	1.656860
46	6	0	0.936650	-0.331210	1.725033
47	6	0	0.169313	-1.536095	2.284753
48	6	0	2.442638	-0.519542	1.980409
49	1	0	0.620776	0.559859	2.294840
50	6	0	0.445787	-1.712440	3.778120
51	1	0	0.468827	-2.441575	1.741819
52	1	0	-0.903300	-1.431245	2.103855
53	6	0	2.718668	-0.683255	3.477480
54	1	0	2.787013	-1.420034	1.457114
55	1	0	3.028842	0.316003	1.591038
56	6	0	1.937419	-1.853062	4.068489
57	1	0	-0.101549	-2.587164	4.149945
58	1	0	0.051253	-0.841522	4.324085
59	1	0	3.795676	-0.818252	3.638262
60	1	0	2.438630	0.244843	3.998264
61	1	0	2.114725	-1.924134	5.148785
62	1	0	2.304638	-2.791181	3.627437
63	1	0	-3.102994	1.818652	1.925406
64	6	0	-5.107685	-0.672365	0.688743
65	1	0	-5.292230	-0.255719	1.684415
66	1	0	-6.073126	-0.761345	0.180646
67	1	0	-4.687152	-1.676742	0.802633

8d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.446367	-0.105067	-1.574960
2	6	0	-3.877045	-0.245283	-1.972783
3	1	0	-4.536588	-0.455449	-1.122714
4	1	0	-4.225710	0.680331	-2.453452
5	17	0	-2.002928	-2.574019	0.579119
6	44	0	-2.029042	-0.270574	0.170759
7	17	0	-2.563656	1.810314	1.095945
8	1	0	-3.989417	-1.061588	-2.700692
9	1	0	-1.738380	0.103567	-2.386584
10	15	0	0.209115	0.024157	-0.032999

11	6	0	0.946698	-0.820206	1.454542
12	6	0	2.463692	-1.049977	1.508138
13	6	0	0.445228	-0.142155	2.741374
14	1	0	0.462947	-1.807185	1.402539
15	6	0	2.829199	-1.871519	2.748129
16	1	0	3.001495	-0.094618	1.538178
17	1	0	2.806489	-1.578166	0.612819
18	6	0	0.826132	-0.964337	3.972115
19	1	0	0.881500	0.863380	2.827780
20	1	0	-0.642783	-0.001752	2.708948
21	6	0	2.331045	-1.213606	4.032157
22	1	0	3.916407	-2.014561	2.785299
23	1	0	2.382785	-2.872246	2.657256
24	1	0	0.484580	-0.450025	4.878557
25	1	0	0.295152	-1.926090	3.935542
26	1	0	2.580224	-1.837673	4.898998
27	1	0	2.852692	-0.255418	4.175415
28	6	0	0.622258	1.842200	-0.000770
29	6	0	2.054219	2.275636	0.344596
30	6	0	0.112636	2.533220	-1.276280
31	1	0	-0.028770	2.189286	0.813549
32	6	0	2.134853	3.801775	0.450283
33	1	0	2.768898	1.928987	-0.411170
34	1	0	2.365778	1.837664	1.297956
35	6	0	0.218714	4.052822	-1.154862
36	1	0	0.696186	2.201352	-2.147754
37	1	0	-0.931411	2.252643	-1.452887
38	6	0	1.642232	4.488883	-0.820220
39	1	0	3.167614	4.097577	0.673662
40	1	0	1.521373	4.133674	1.300134
41	1	0	-0.118924	4.521782	-2.087464
42	1	0	-0.466681	4.391484	-0.365619
43	1	0	1.691742	5.578592	-0.705623
44	1	0	2.309724	4.230383	-1.656216
45	6	0	0.914299	-0.740726	-1.586025
46	6	0	2.320277	-0.280216	-2.001405
47	6	0	0.822328	-2.274190	-1.558040
48	1	0	0.225102	-0.391623	-2.369233
49	6	0	2.718351	-0.899785	-3.344131
50	1	0	3.056034	-0.565322	-1.239174
51	1	0	2.359453	0.809508	-2.085324
52	6	0	1.229535	-2.873268	-2.904321
53	1	0	1.490131	-2.667901	-0.779237
54	1	0	-0.189216	-2.591465	-1.286214
55	6	0	2.625929	-2.422345	-3.321471
56	1	0	3.733834	-0.577853	-3.606506
57	1	0	2.054300	-0.508446	-4.129198
58	1	0	1.178002	-3.967271	-2.847520
59	1	0	0.503005	-2.566669	-3.671647
60	1	0	2.886498	-2.833826	-4.304233
61	1	0	3.363684	-2.820335	-2.609038

10a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.870820	2.405448	0.692169
2	6	0	-0.943987	3.343527	0.312298
3	1	0	-1.872764	2.138484	1.749126

4	6	0	-3.103380	2.007751	-0.068000
5	1	0	-3.045936	2.239874	-1.131671
6	1	0	-3.313161	0.936747	0.028109
7	6	0	1.453484	1.475759	-0.274974
8	6	0	0.153042	-1.253373	0.034890
9	6	0	2.632202	-1.488923	-0.156291
10	6	0	1.079080	-3.410194	-0.014243
11	6	0	3.002145	-1.805900	2.327842
12	6	0	-0.395094	-3.515906	0.344178
13	6	0	5.294948	-0.721833	-0.520812
14	6	0	2.219701	-1.433718	-2.657670
15	6	0	3.486638	-1.431040	0.955879
16	6	0	3.098724	-1.233672	-1.455042
17	6	0	-2.175487	-2.370660	-2.423582
18	6	0	4.427435	-0.833868	-1.608046
19	6	0	4.808999	-1.038662	0.749396
20	6	0	-2.272426	-1.899386	0.070540
21	6	0	6.714376	-0.262529	-0.708760
22	6	0	-5.041417	-1.503426	-0.075425
23	6	0	-2.919856	-1.987057	-1.178053
24	6	0	-2.396203	-1.927123	2.615395
25	6	0	-3.009449	-1.748794	1.256789
26	6	0	-4.385733	-1.524793	1.152275
27	6	0	-4.293633	-1.766606	-1.225330
28	6	0	-6.514619	-1.219700	-0.165285
29	6	0	2.615672	1.903648	0.598115
30	1	0	2.818465	2.942685	0.280331
31	1	0	3.464640	1.343167	0.170998
32	6	0	2.712003	1.835779	2.110381
33	1	0	1.297304	-3.792365	-1.020314
34	1	0	-2.863647	-2.444262	-3.270734
35	6	0	1.799835	1.878793	-1.695290
36	1	0	1.731825	-3.922788	0.697226
37	1	0	2.917115	-2.896251	2.433470
38	1	0	2.018828	-1.373642	2.541510
39	1	0	3.705066	-1.463433	3.093101
40	1	0	-0.944633	-4.220003	-0.286572
41	1	0	-0.551749	-3.794299	1.394336
42	1	0	1.220844	-1.004229	-2.526644
43	1	0	2.091609	-2.503251	-2.872273
44	1	0	2.670724	-0.980194	-3.545308
45	1	0	-1.683726	-3.345495	-2.310227
46	1	0	-1.413395	-1.625808	-2.668216
47	1	0	4.796924	-0.619870	-2.609214
48	1	0	5.477324	-0.978993	1.606435
49	1	0	6.809829	0.812603	-0.509973
50	1	0	7.059985	-0.437840	-1.732365
51	1	0	7.396374	-0.779483	-0.025530
52	1	0	-1.350447	-1.618093	2.644910
53	1	0	-2.468512	-2.980573	2.920776
54	1	0	-2.930042	-1.335344	3.364989
55	1	0	-4.958541	-1.383785	2.067023
56	1	0	-4.796043	-1.812652	-2.189460
57	1	0	-7.017657	-1.400588	0.789850
58	1	0	-6.996508	-1.840438	-0.928342
59	1	0	-6.694561	-0.172337	-0.439277
60	7	0	1.302642	-1.961968	0.028954
61	7	0	-0.863582	-2.147303	0.117723
62	17	0	-0.048247	0.510567	2.543149
63	44	0	-0.219569	0.735659	0.124420
64	17	0	-0.970179	0.769524	-2.207350

65	6	0	-0.983311	4.031555	-1.027731
66	1	0	-1.244226	3.314684	-1.813059
67	6	0	-1.972542	5.203193	-1.032585
68	1	0	0.016251	4.419272	-1.265042
69	1	0	-3.962379	2.537987	0.370395
70	6	0	-0.070096	3.983428	1.354615
71	1	0	3.700923	2.214259	2.400721
72	1	0	2.607070	0.819905	2.485664
73	1	0	1.954370	2.441227	2.607595
74	1	0	1.227304	2.778178	-1.953805
75	1	0	1.506276	1.133835	-2.430597
76	1	0	2.866326	2.113430	-1.801199
77	1	0	-1.963250	5.704233	-2.006659
78	1	0	-1.722677	5.950629	-0.271126
79	1	0	-2.994113	4.858143	-0.841621
80	1	0	0.949408	4.155894	0.993271
81	1	0	-0.032196	3.384502	2.267494
82	1	0	-0.485138	4.970319	1.606194

10b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.093675	2.501247	-0.379144
2	6	0	0.990867	3.090255	-0.934388
3	6	0	2.948952	1.528936	-1.146239
4	1	0	2.554477	1.311352	-2.139948
5	1	0	3.064020	0.581052	-0.601877
6	6	0	2.699882	2.982720	0.916319
7	1	0	1.927424	3.346960	1.595937
8	1	0	3.178592	2.138447	1.426350
9	6	0	-1.509815	1.575762	-0.172585
10	6	0	-0.421527	-1.060684	0.280188
11	6	0	-2.921868	-1.006673	0.308640
12	6	0	-1.574941	-2.987036	0.960684
13	6	0	-2.843106	-1.778635	-2.100692
14	6	0	-0.101823	-3.337970	0.768954
15	6	0	-5.519548	-0.027047	-0.028322
16	6	0	-2.942694	-0.358428	2.759792
17	6	0	-3.550083	-1.140412	-0.941526
18	6	0	-3.583727	-0.430093	1.404117
19	6	0	2.224775	-1.496502	2.742638
20	6	0	-4.873674	0.066532	1.203763
21	6	0	-4.844478	-0.643032	-1.084890
22	6	0	1.904227	-1.935795	0.263487
23	6	0	-6.903800	0.527188	-0.221591
24	6	0	4.668567	-1.816068	-0.160230
25	6	0	2.756441	-1.659852	1.349200
26	6	0	1.551218	-2.739438	-2.128407
27	6	0	2.420217	-2.248141	-1.006444
28	6	0	3.801034	-2.163083	-1.194179
29	6	0	4.128145	-1.588682	1.106386
30	6	0	6.146574	-1.687746	-0.402122
31	6	0	-2.354423	2.055451	-1.297352
32	1	0	-2.508812	3.138969	-1.178743
33	1	0	-3.351973	1.602023	-1.204711
34	1	0	-1.939388	1.842000	-2.282163
35	1	0	-1.884490	-3.038923	2.011405
36	1	0	3.045051	-1.328004	3.446706

37	1	0	-1.932426	1.801622	0.817688
38	1	0	-2.247344	-3.621363	0.375053
39	1	0	-2.479728	-2.783926	-1.853744
40	1	0	-1.970668	-1.184401	-2.402836
41	1	0	-3.514230	-1.868648	-2.959964
42	1	0	0.349259	-3.788687	1.658039
43	1	0	0.063357	-4.012899	-0.080234
44	1	0	-1.922210	0.038163	2.709715
45	1	0	-2.891738	-1.351129	3.226612
46	1	0	-3.526172	0.282123	3.427764
47	1	0	1.688578	-2.396939	3.068939
48	1	0	1.529216	-0.653267	2.811213
49	1	0	-5.390745	0.527097	2.043294
50	1	0	-5.337933	-0.739295	-2.050283
51	1	0	-6.872326	1.499009	-0.730399
52	1	0	-7.413643	0.674195	0.735470
53	1	0	-7.518694	-0.138954	-0.836374
54	1	0	0.549102	-2.309864	-2.096193
55	1	0	1.472747	-3.835351	-2.094838
56	1	0	1.982477	-2.470875	-3.096476
57	1	0	4.206104	-2.383295	-2.180016
58	1	0	4.793505	-1.364089	1.937807
59	1	0	6.477629	-2.337903	-1.218276
60	1	0	6.723419	-1.941448	0.493218
61	1	0	6.409036	-0.658355	-0.678307
62	7	0	-1.638712	-1.601028	0.487631
63	7	0	0.496711	-2.030921	0.495394
64	17	0	0.139316	0.313687	-2.572556
65	44	0	0.151295	0.815200	-0.179882
66	17	0	0.254187	1.327687	2.197655
67	6	0	0.272039	4.262707	-0.327006
68	1	0	0.134528	4.147732	0.752283
69	1	0	0.839989	5.188065	-0.496696
70	1	0	-0.710796	4.404152	-0.784032
71	6	0	3.733135	4.087400	0.664679
72	1	0	4.552260	3.746160	0.021752
73	1	0	3.275632	4.959685	0.184547
74	1	0	4.171790	4.418333	1.612317
75	1	0	3.962595	1.943115	-1.241919
76	1	0	0.744545	2.831560	-1.963490

TS11a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.295761	2.277804	0.510796
2	6	0	-0.069464	3.060505	0.174706
3	1	0	-1.460412	2.228437	1.589978
4	6	0	-2.597431	2.349762	-0.245072
5	1	0	-2.478978	2.504444	-1.316988
6	1	0	-3.157576	1.418179	-0.105393
7	6	0	1.464037	1.856258	-0.267167
8	6	0	-0.120230	-1.349123	0.071818
9	6	0	2.318494	-1.797876	-0.148612
10	6	0	0.569526	-3.582244	-0.017645
11	6	0	2.644997	-2.136380	2.343324
12	6	0	-0.921770	-3.532453	0.302619
13	6	0	5.033767	-1.209689	-0.476238
14	6	0	1.948040	-1.681008	-2.659319

15	6	0	3.161854	-1.798744	0.974470
16	6	0	2.820189	-1.574855	-1.441334
17	6	0	-2.606998	-2.209338	-2.359658
18	6	0	4.176713	-1.270235	-1.574762
19	6	0	4.509649	-1.492761	0.785227
20	6	0	-2.594388	-1.671863	0.126049
21	6	0	6.482881	-0.846254	-0.644622
22	6	0	-5.276456	-0.882041	0.001082
23	6	0	-3.261488	-1.690049	-1.111789
24	6	0	-2.645481	-1.550121	2.666732
25	6	0	-3.278143	-1.374102	1.316943
26	6	0	-4.609510	-0.963418	1.222422
27	6	0	-4.591771	-1.274010	-1.148793
28	6	0	-6.695376	-0.391859	-0.074442
29	6	0	2.721764	2.126294	0.566000
30	1	0	2.956271	3.190693	0.400484
31	1	0	3.497447	1.596650	-0.007306
32	6	0	2.972651	1.792875	2.029322
33	1	0	0.776585	-3.998558	-1.011286
34	1	0	-3.195919	-1.939486	-3.240742
35	6	0	1.903104	2.059236	-1.712192
36	1	0	1.145657	-4.149901	0.717965
37	1	0	2.336492	-3.188247	2.407436
38	1	0	1.780367	-1.517356	2.607071
39	1	0	3.423663	-1.981032	3.095944
40	1	0	-1.528975	-4.117767	-0.393123
41	1	0	-1.144088	-3.867515	1.322708
42	1	0	1.145908	-0.932922	-2.659116
43	1	0	1.469727	-2.666053	-2.727222
44	1	0	2.542872	-1.543521	-3.567338
45	1	0	-2.539384	-3.306177	-2.336870
46	1	0	-1.605031	-1.796646	-2.493579
47	1	0	4.574356	-1.090974	-2.572007
48	1	0	5.167615	-1.480230	1.651991
49	1	0	6.642979	0.223655	-0.459463
50	1	0	6.834428	-1.058542	-1.659242
51	1	0	7.118327	-1.394815	0.058499
52	1	0	-1.705129	-0.998382	2.759262
53	1	0	-2.432996	-2.609428	2.863546
54	1	0	-3.323448	-1.204512	3.452791
55	1	0	-5.142352	-0.715780	2.138518
56	1	0	-5.107367	-1.264333	-2.106973
57	1	0	-7.240721	-0.595661	0.852788
58	1	0	-7.238729	-0.861438	-0.900907
59	1	0	-6.725547	0.692753	-0.239577
60	7	0	0.946559	-2.164216	0.018842
61	7	0	-1.228717	-2.103150	0.170831
62	17	0	0.187364	0.488311	2.494869
63	44	0	-0.044911	0.714019	0.085913
64	17	0	-0.780571	0.628259	-2.248733
65	6	0	-0.170306	3.941569	-1.071067
66	1	0	-0.570295	3.351008	-1.900043
67	6	0	-1.027204	5.193081	-0.867991
68	1	0	0.831452	4.270483	-1.368395
69	1	0	-3.213568	3.157539	0.177591
70	6	0	0.431593	3.811332	1.401443
71	1	0	4.009210	2.076894	2.255138
72	1	0	2.863274	0.726843	2.225109
73	1	0	2.321707	2.321912	2.723787
74	1	0	1.092135	2.163366	-2.425074
75	1	0	2.472833	1.167540	-2.001368

76	1	0	2.589516	2.914239	-1.794938
77	1	0	-1.125226	5.727293	-1.819572
78	1	0	-0.576272	5.886099	-0.150146
79	1	0	-2.035685	4.954656	-0.517528
80	1	0	1.381131	4.326021	1.223922
81	1	0	0.534039	3.138731	2.254082
82	1	0	-0.309452	4.573150	1.669902

TS11b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.625357	2.415753	0.459387
2	6	0	-0.418577	3.158250	0.260731
3	6	0	-2.173526	2.304863	1.866174
4	1	0	-1.391089	2.313536	2.623049
5	1	0	-2.763184	1.389381	1.991478
6	6	0	-2.713573	2.386733	-0.602968
7	1	0	-2.279275	2.481556	-1.597417
8	1	0	-3.195902	1.400057	-0.581801
9	6	0	1.321402	1.974025	-0.197448
10	6	0	0.335111	-1.173774	-0.036358
11	6	0	2.826840	-1.178371	-0.133364
12	6	0	1.409115	-3.238114	-0.241533
13	6	0	3.090795	-1.674339	2.341602
14	6	0	-0.072536	-3.476970	0.039136
15	6	0	5.399720	-0.081275	-0.234599
16	6	0	2.568929	-0.906574	-2.643796
17	6	0	3.600575	-1.131216	1.038574
18	6	0	3.342234	-0.750439	-1.367034
19	6	0	-2.041356	-2.201776	-2.538788
20	6	0	4.622146	-0.191693	-1.386601
21	6	0	4.876253	-0.571857	0.962429
22	6	0	-2.033876	-1.887136	-0.020786
23	6	0	6.764248	0.549031	-0.276813
24	6	0	-4.798763	-1.456195	-0.021739
25	6	0	-2.734344	-1.908688	-1.240498
26	6	0	-2.004799	-1.905366	2.523737
27	6	0	-2.707388	-1.750417	1.205589
28	6	0	-4.084580	-1.517107	1.173621
29	6	0	-4.108915	-1.678563	-1.214165
30	6	0	-6.273798	-1.166562	-0.028821
31	6	0	2.424636	2.437537	0.688196
32	1	0	2.677168	3.485130	0.467557
33	1	0	3.310009	1.837990	0.430460
34	1	0	2.217883	2.302362	1.749370
35	1	0	1.695692	-3.526519	-1.260727
36	1	0	-2.760528	-2.206720	-3.362951
37	1	0	1.454875	2.251340	-1.251414
38	1	0	2.066300	-3.759329	0.459363
39	1	0	2.919050	-2.757357	2.289687
40	1	0	2.147186	-1.193917	2.620307
41	1	0	3.817540	-1.497886	3.140039
42	1	0	-0.548893	-4.131557	-0.695930
43	1	0	-0.246665	-3.894570	1.038423
44	1	0	1.622533	-0.354172	-2.622175
45	1	0	2.326834	-1.959074	-2.838691
46	1	0	3.156207	-0.544294	-3.492906
47	1	0	-1.551908	-3.183828	-2.521620

48	1	0	-1.281335	-1.444003	-2.753224
49	1	0	5.025404	0.150998	-2.337641
50	1	0	5.477914	-0.522658	1.868037
51	1	0	6.727727	1.591239	0.065221
52	1	0	7.173279	0.551456	-1.291989
53	1	0	7.469647	0.020711	0.373498
54	1	0	-1.174891	-1.199844	2.639707
55	1	0	-1.599153	-2.919043	2.636854
56	1	0	-2.704976	-1.742407	3.348425
57	1	0	-4.613398	-1.399710	2.117557
58	1	0	-4.655694	-1.680137	-2.155024
59	1	0	-6.740254	-1.434419	0.924501
60	1	0	-6.786097	-1.715218	-0.826148
61	1	0	-6.461622	-0.098475	-0.197642
62	7	0	1.532328	-1.783356	-0.081040
63	7	0	-0.621680	-2.120682	-0.040623
64	17	0	0.426214	0.629180	2.475618
65	44	0	-0.107484	0.826471	0.096081
66	17	0	-0.487422	0.882725	-2.315718
67	6	0	-0.252983	4.105173	-0.907647
68	1	0	-0.426865	3.605192	-1.864004
69	1	0	-0.975585	4.925590	-0.811367
70	1	0	0.747349	4.548876	-0.925279
71	6	0	-3.785421	3.466142	-0.404533
72	1	0	-4.387949	3.298447	0.493718
73	1	0	-3.344323	4.467290	-0.329716
74	1	0	-4.466566	3.468819	-1.262546
75	1	0	-2.847586	3.153880	2.047260
76	1	0	0.053189	3.475997	1.191357

12a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.189705	2.138250	0.567288
2	6	0	0.174393	2.941143	0.222745
3	1	0	-1.329797	2.151381	1.652062
4	6	0	-2.489284	2.389893	-0.151932
5	1	0	-2.381391	2.564585	-1.221905
6	1	0	-3.127144	1.506709	-0.027995
7	6	0	1.463351	1.960373	-0.145774
8	6	0	-0.214698	-1.390716	0.049972
9	6	0	2.202194	-1.938940	-0.126769
10	6	0	0.357473	-3.646911	-0.105431
11	6	0	2.466378	-2.459797	2.344306
12	6	0	-1.128073	-3.527444	0.226025
13	6	0	4.943049	-1.422461	-0.354816
14	6	0	1.909524	-1.676503	-2.640457
15	6	0	3.019089	-2.042198	1.012924
16	6	0	2.744735	-1.660255	-1.392534
17	6	0	-2.778019	-2.075432	-2.394502
18	6	0	4.113093	-1.391430	-1.474330
19	6	0	4.379444	-1.768494	0.873558
20	6	0	-2.701019	-1.572244	0.095328
21	6	0	6.404965	-1.090915	-0.465518
22	6	0	-5.337847	-0.640343	0.027362
23	6	0	-3.391812	-1.549784	-1.128972
24	6	0	-2.669940	-1.405328	2.632105
25	6	0	-3.336688	-1.227382	1.299207

26	6	0	-4.647171	-0.749195	1.233394
27	6	0	-4.699469	-1.066450	-1.137197
28	6	0	-6.731571	-0.079303	-0.018909
29	6	0	2.614779	1.892392	0.861904
30	1	0	3.046718	0.887653	0.761146
31	1	0	2.247678	1.938551	1.884368
32	6	0	3.745023	2.911722	0.667707
33	1	0	0.534864	-4.027241	-1.119170
34	1	0	-3.399634	-1.816603	-3.256275
35	6	0	2.028423	2.086833	-1.549220
36	1	0	0.903297	-4.278704	0.599771
37	1	0	2.129150	-3.504754	2.329186
38	1	0	1.618879	-1.830460	2.632578
39	1	0	3.233777	-2.377951	3.119421
40	1	0	-1.767986	-4.073117	-0.471963
41	1	0	-1.359838	-3.863468	1.243963
42	1	0	1.179790	-0.858418	-2.663329
43	1	0	1.343105	-2.610846	-2.734557
44	1	0	2.547660	-1.588554	-3.524783
45	1	0	-2.696259	-3.170894	-2.370078
46	1	0	-1.784063	-1.652870	-2.561333
47	1	0	4.541481	-1.168763	-2.449762
48	1	0	5.016041	-1.833350	1.753741
49	1	0	6.783690	-1.278235	-1.475282
50	1	0	7.003913	-1.677698	0.238678
51	1	0	6.583015	-0.031692	-0.239622
52	1	0	-1.732409	-0.844217	2.706566
53	1	0	-2.434321	-2.461237	2.818472
54	1	0	-3.333240	-1.073493	3.436400
55	1	0	-5.143808	-0.466983	2.159746
56	1	0	-5.234033	-1.027830	-2.084184
57	1	0	-7.253774	-0.221012	0.932750
58	1	0	-7.327055	-0.548768	-0.808807
59	1	0	-6.711644	0.998666	-0.224119
60	7	0	0.811741	-2.254714	-0.008252
61	7	0	-1.362852	-2.082820	0.113447
62	17	0	0.372265	0.361882	2.481653
63	44	0	-0.020962	0.635988	0.083454
64	17	0	-0.745092	0.671181	-2.242388
65	6	0	-0.043828	3.907458	-0.965433
66	1	0	-0.468454	3.348097	-1.804241
67	6	0	-0.885821	5.149665	-0.678625
68	1	0	0.936759	4.262340	-1.300231
69	1	0	-3.022636	3.231053	0.312618
70	6	0	0.488468	3.705617	1.518802
71	1	0	4.440725	2.842188	1.511582
72	1	0	3.379842	3.944455	0.629854
73	1	0	4.320366	2.729972	-0.245466
74	1	0	1.275607	2.071193	-2.332706
75	1	0	2.712247	1.245888	-1.715521
76	1	0	2.626522	3.003147	-1.646982
77	1	0	-1.037300	5.702504	-1.612751
78	1	0	-0.385755	5.828059	0.020417
79	1	0	-1.873765	4.919517	-0.272240
80	1	0	1.389637	4.318048	1.411562
81	1	0	0.615355	3.024839	2.362531
82	1	0	-0.344248	4.374576	1.756798

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.501088	2.107225	-0.464571
2	6	0	0.266342	3.083161	-0.182853
3	6	0	1.996470	2.203754	-1.894204
4	1	0	1.187857	2.167360	-2.621669
5	1	0	2.690904	1.382550	-2.107062
6	6	0	2.664620	2.082907	0.527785
7	1	0	2.308120	2.269301	1.540137
8	1	0	3.041392	1.051359	0.542201
9	6	0	-1.134801	2.424849	0.232210
10	6	0	-0.295608	-1.175103	0.064263
11	6	0	-2.779644	-1.247469	0.137162
12	6	0	-1.294115	-3.276265	0.212728
13	6	0	-3.043450	-1.849134	-2.321430
14	6	0	0.201946	-3.451235	-0.050472
15	6	0	-5.355684	-0.158294	0.180236
16	6	0	-2.584491	-0.979264	2.656383
17	6	0	-3.537373	-1.229039	-1.045933
18	6	0	-3.322217	-0.817233	1.359360
19	6	0	2.167386	-2.136871	2.516258
20	6	0	-4.603159	-0.262979	1.349446
21	6	0	-4.812582	-0.666328	-0.999379
22	6	0	2.103595	-1.796792	0.002946
23	6	0	-6.716378	0.480724	0.190040
24	6	0	4.859523	-1.327499	-0.053863
25	6	0	2.831138	-1.834056	1.204892
26	6	0	1.993490	-1.700235	-2.533804
27	6	0	2.739704	-1.603628	-1.234393
28	6	0	4.114010	-1.355060	-1.231660
29	6	0	4.202876	-1.588607	1.149293
30	6	0	6.330578	-1.019103	-0.076632
31	6	0	-2.329095	2.806235	-0.596969
32	1	0	-2.618199	3.843068	-0.364501
33	1	0	-3.177186	2.164935	-0.332009
34	1	0	-2.148507	2.707645	-1.667887
35	1	0	-1.590752	-3.620531	1.210981
36	1	0	2.906419	-2.161234	3.322292
37	1	0	-1.307518	2.576131	1.302816
38	1	0	-1.918340	-3.784583	-0.526841
39	1	0	-3.238985	-2.930989	-2.328115
40	1	0	-1.975056	-1.679835	-2.467529
41	1	0	-3.564548	-1.421158	-3.182414
42	1	0	0.695544	-4.088454	0.688419
43	1	0	0.409069	-3.856499	-1.048224
44	1	0	-1.692624	-0.344425	2.706352
45	1	0	-2.251845	-2.014579	2.801346
46	1	0	-3.234856	-0.721345	3.497558
47	1	0	1.662290	-3.110833	2.501888
48	1	0	1.421180	-1.371943	2.757191
49	1	0	-5.027538	0.081490	2.290540
50	1	0	-5.398873	-0.630947	-1.915586
51	1	0	-6.651210	1.544791	-0.070852
52	1	0	-7.183580	0.414843	1.177856
53	1	0	-7.386142	0.009339	-0.536794
54	1	0	1.148093	-1.004403	-2.582529
55	1	0	1.595257	-2.711728	-2.687186
56	1	0	2.660700	-1.483992	-3.373443
57	1	0	4.615542	-1.195548	-2.184295
58	1	0	4.772977	-1.604066	2.076083

59	1	0	6.778802	-1.270672	-1.043071
60	1	0	6.867878	-1.569032	0.703017
61	1	0	6.507613	0.049833	0.098869
62	7	0	-1.468711	-1.822390	0.113022
63	7	0	0.700300	-2.074479	0.042924
64	17	0	-0.709940	0.625989	-2.353328
65	44	0	-0.010650	0.839264	-0.030311
66	17	0	0.379247	0.891867	2.374110
67	6	0	0.579282	4.145643	0.871639
68	1	0	0.689640	3.693517	1.860677
69	1	0	1.494496	4.692587	0.626250
70	1	0	-0.243771	4.867189	0.916458
71	6	0	3.845562	3.007694	0.209616
72	1	0	4.367647	2.718096	-0.707736
73	1	0	3.543558	4.056039	0.104204
74	1	0	4.570355	2.957878	1.030077
75	1	0	2.552215	3.143319	-2.025621
76	1	0	0.057157	3.524476	-1.161638

TS13a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.280518	1.862835	-0.516833
2	6	0	-0.477330	3.011801	-0.175988
3	1	0	1.368750	2.045297	-1.594026
4	6	0	2.484724	2.260099	0.270257
5	1	0	2.279004	2.460977	1.322056
6	1	0	3.173433	1.403949	0.246298
7	6	0	-1.615587	2.124326	0.109288
8	6	0	0.288260	-1.381591	0.038925
9	6	0	-2.108899	-2.014855	0.169806
10	6	0	-0.205061	-3.651445	0.330774
11	6	0	-2.202420	-2.630234	-2.291902
12	6	0	1.284748	-3.495237	0.036688
13	6	0	-4.870106	-1.557726	0.203054
14	6	0	-1.994272	-1.698786	2.692302
15	6	0	-2.848435	-2.174850	-1.016163
16	6	0	-2.741319	-1.720466	1.389984
17	6	0	3.001625	-1.771252	2.463007
18	6	0	-4.117641	-1.480508	1.373681
19	6	0	-4.220042	-1.928072	-0.974706
20	6	0	2.781661	-1.493863	-0.051919
21	6	0	-6.342175	-1.253745	0.207820
22	6	0	5.400965	-0.519771	-0.214433
23	6	0	3.541380	-1.363563	1.123000
24	6	0	2.581524	-1.481043	-2.584272
25	6	0	3.335895	-1.221176	-1.313388
26	6	0	4.638606	-0.721595	-1.364347
27	6	0	4.839805	-0.863765	1.015194
28	6	0	6.788541	0.052921	-0.297230
29	6	0	-2.710165	1.918055	-0.934860
30	1	0	-3.132077	0.914251	-0.794653
31	1	0	-2.298634	1.923171	-1.941520
32	6	0	-3.847718	2.944204	-0.841973
33	1	0	-0.399482	-3.983619	1.357932
34	1	0	3.705333	-1.502656	3.256276
35	6	0	-2.210349	2.126279	1.505599
36	1	0	-0.706538	-4.341230	-0.353491

37	1	0	-1.792381	-3.643951	-2.194931
38	1	0	-1.389707	-1.957102	-2.581629
39	1	0	-2.934425	-2.650957	-3.104401
40	1	0	1.920778	-3.959410	0.795040
41	1	0	1.565691	-3.901220	-0.942801
42	1	0	-1.248935	-0.896117	2.729880
43	1	0	-1.460214	-2.641398	2.863567
44	1	0	-2.689548	-1.559005	3.525364
45	1	0	2.845681	-2.856718	2.520394
46	1	0	2.048586	-1.275138	2.669080
47	1	0	-4.614717	-1.244076	2.312598
48	1	0	-4.796335	-2.035368	-1.891498
49	1	0	-6.524960	-0.205387	-0.060989
50	1	0	-6.783301	-1.419655	1.195808
51	1	0	-6.882216	-1.872823	-0.516115
52	1	0	1.684121	-0.857039	-2.664413
53	1	0	2.253486	-2.526078	-2.649342
54	1	0	3.217483	-1.282506	-3.452148
55	1	0	5.071926	-0.499562	-2.337717
56	1	0	5.429218	-0.746729	1.922472
57	1	0	7.266829	-0.191802	-1.251114
58	1	0	7.425857	-0.321864	0.510291
59	1	0	6.767433	1.147146	-0.213980
60	7	0	-0.703494	-2.284893	0.143120
61	7	0	1.460756	-2.037261	0.039950
62	17	0	-0.430372	0.351513	-2.457045
63	44	0	-0.059438	0.648078	-0.057156
64	17	0	0.553856	0.713205	2.311490
65	6	0	-0.061870	3.916733	0.989811
66	1	0	0.377837	3.307422	1.786229
67	6	0	0.835947	5.107335	0.667878
68	1	0	-0.990200	4.321789	1.416687
69	1	0	3.003830	3.106908	-0.195403
70	6	0	-0.464760	3.681260	-1.541348
71	1	0	-4.532573	2.808449	-1.686495
72	1	0	-3.475396	3.974956	-0.883457
73	1	0	-4.433158	2.838235	0.076821
74	1	0	-1.469027	2.123395	2.300832
75	1	0	-2.853180	1.248114	1.634691
76	1	0	-2.849079	3.014246	1.626593
77	1	0	1.068592	5.642865	1.595022
78	1	0	0.343577	5.818913	-0.003540
79	1	0	1.786779	4.821782	0.210487
80	1	0	-1.284534	4.410231	-1.594429
81	1	0	-0.591730	2.959451	-2.350270
82	1	0	0.467061	4.225450	-1.714494

TS13b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.498280	1.806868	-0.430227
2	6	0	-0.106900	3.235994	-0.216690
3	6	0	1.980247	2.116154	-1.820937
4	1	0	1.198269	2.053878	-2.573820
5	1	0	2.760993	1.384288	-2.071364
6	6	0	2.576503	1.935842	0.628086
7	1	0	2.139688	2.298287	1.560514
8	1	0	2.862553	0.901590	0.862496

9	6	0	-1.345448	2.645870	0.197295
10	6	0	-0.200785	-1.146166	0.097053
11	6	0	-2.675872	-1.339842	0.157864
12	6	0	-1.114887	-3.299076	0.277864
13	6	0	-2.826126	-1.936976	-2.314437
14	6	0	0.401274	-3.412025	0.112493
15	6	0	-5.299687	-0.368622	0.106148
16	6	0	-2.608547	-1.120509	2.690625
17	6	0	-3.386684	-1.342285	-1.054154
18	6	0	-3.291071	-0.956726	1.363482
19	6	0	2.333406	-1.863713	2.547997
20	6	0	-4.593398	-0.459420	1.305766
21	6	0	-4.686881	-0.836254	-1.055187
22	6	0	2.220956	-1.700629	0.021253
23	6	0	-6.684648	0.214406	0.067094
24	6	0	4.971550	-1.217785	-0.125869
25	6	0	2.975496	-1.666635	1.205425
26	6	0	2.029121	-1.666342	-2.506798
27	6	0	2.822067	-1.546072	-1.237386
28	6	0	4.194739	-1.292403	-1.281937
29	6	0	4.345928	-1.422129	1.104512
30	6	0	6.441752	-0.912101	-0.200265
31	6	0	-2.588851	2.665709	-0.649317
32	1	0	-3.176090	3.556384	-0.378047
33	1	0	-3.218615	1.789621	-0.458043
34	1	0	-2.361963	2.694104	-1.715744
35	1	0	-1.465833	-3.673270	1.246562
36	1	0	3.084185	-1.821111	3.342483
37	1	0	-1.534590	2.710101	1.271891
38	1	0	-1.668203	-3.819359	-0.510195
39	1	0	-3.160539	-2.978753	-2.422528
40	1	0	-1.736236	-1.908112	-2.334270
41	1	0	-3.177155	-1.385486	-3.190786
42	1	0	0.881124	-3.949812	0.935928
43	1	0	0.690417	-3.900025	-0.825669
44	1	0	-1.737651	-0.463370	2.789738
45	1	0	-2.258650	-2.150290	2.834358
46	1	0	-3.303525	-0.892114	3.504223
47	1	0	1.828969	-2.834970	2.622700
48	1	0	1.584075	-1.085693	2.737687
49	1	0	-5.073172	-0.149678	2.232175
50	1	0	-5.235379	-0.814738	-1.995026
51	1	0	-6.648620	1.292816	-0.133589
52	1	0	-7.205113	0.077542	1.020522
53	1	0	-7.290485	-0.242858	-0.721981
54	1	0	1.212808	-0.935301	-2.555324
55	1	0	1.575754	-2.661421	-2.601410
56	1	0	2.674720	-1.518656	-3.377784
57	1	0	4.670144	-1.166206	-2.253001
58	1	0	4.938307	-1.387602	2.016884
59	1	0	6.864591	-1.206120	-1.166172
60	1	0	6.999033	-1.429048	0.587873
61	1	0	6.624761	0.163036	-0.075693
62	7	0	-1.340735	-1.853795	0.182769
63	7	0	0.829132	-2.007751	0.100111
64	17	0	-0.766887	0.668934	-2.370361
65	44	0	-0.136589	0.923519	-0.025410
66	17	0	0.145048	1.029168	2.401643
67	6	0	0.562529	4.206907	0.727165
68	1	0	0.583940	3.810760	1.746836
69	1	0	1.578763	4.472170	0.423653

70	1	0	-0.028286	5.132158	0.740770
71	6	0	3.846112	2.715288	0.281111
72	1	0	4.388518	2.273382	-0.560833
73	1	0	3.648525	3.765842	0.038774
74	1	0	4.516864	2.702758	1.147419
75	1	0	2.459462	3.104233	-1.849568
76	1	0	-0.064982	3.495307	-1.274703

14a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.501265	1.355392	-0.493855
2	6	0	-1.170049	3.193475	-0.187331
3	1	0	1.804741	1.235345	-1.544399
4	6	0	2.448583	2.183147	0.296109
5	1	0	2.124128	2.381228	1.316891
6	1	0	3.420504	1.667584	0.318340
7	6	0	-2.160518	2.259558	0.021319
8	6	0	0.493355	-1.285903	0.106538
9	6	0	-1.846527	-2.132164	0.232554
10	6	0	0.187594	-3.559341	0.596828
11	6	0	-1.769037	-2.841369	-2.205582
12	6	0	1.650117	-3.316797	0.243626
13	6	0	-4.637812	-1.929056	0.121895
14	6	0	-1.899383	-1.825600	2.759912
15	6	0	-2.511287	-2.393842	-0.980749
16	6	0	-2.566102	-1.886999	1.416026
17	6	0	3.207203	-1.193038	2.521423
18	6	0	-3.955509	-1.769616	1.326740
19	6	0	-3.899555	-2.268908	-1.012205
20	6	0	2.991344	-1.239565	-0.002714
21	6	0	-6.127645	-1.746473	0.046619
22	6	0	5.566033	-0.186741	-0.297478
23	6	0	3.750366	-0.952764	1.143222
24	6	0	2.740870	-1.454415	-2.518293
25	6	0	3.515211	-1.059269	-1.293988
26	6	0	4.795664	-0.516507	-1.412907
27	6	0	5.030382	-0.424940	0.969194
28	6	0	6.933871	0.416911	-0.456569
29	6	0	-3.044608	1.719363	-1.083621
30	1	0	-3.238924	0.652950	-0.909171
31	1	0	-2.556003	1.777390	-2.054999
32	6	0	-4.384606	2.463765	-1.138232
33	1	0	0.047318	-3.785022	1.661487
34	1	0	3.943480	-0.909467	3.279230
35	6	0	-2.739890	2.050498	1.401443
36	1	0	-0.269594	-4.361260	0.010700
37	1	0	-1.175159	-3.742835	-2.008824
38	1	0	-1.091837	-2.057784	-2.559528
39	1	0	-2.470858	-3.077384	-3.010815
40	1	0	2.342511	-3.688474	1.003693
41	1	0	1.928238	-3.759809	-0.721281
42	1	0	-1.048439	-1.138323	2.773006
43	1	0	-1.542516	-2.819574	3.061118
44	1	0	-2.609421	-1.492923	3.522823
45	1	0	2.958218	-2.249565	2.682834
46	1	0	2.292790	-0.611790	2.688992
47	1	0	-4.517853	-1.565142	2.235870

48	1	0	-4.417747	-2.452907	-1.951171
49	1	0	-6.379195	-0.709937	-0.212602
50	1	0	-6.609128	-1.969668	1.004126
51	1	0	-6.572967	-2.390069	-0.719041
52	1	0	1.758636	-0.969068	-2.561676
53	1	0	2.569994	-2.538255	-2.548449
54	1	0	3.293102	-1.186843	-3.423955
55	1	0	5.206790	-0.363762	-2.408985
56	1	0	5.624329	-0.193955	1.851401
57	1	0	7.425301	0.060053	-1.367492
58	1	0	7.578634	0.178146	0.395244
59	1	0	6.875401	1.510733	-0.525383
60	7	0	-0.422460	-2.269080	0.271338
61	7	0	1.714769	-1.854091	0.159105
62	17	0	-0.452508	0.315982	-2.455744
63	44	0	-0.112803	0.617657	-0.060583
64	17	0	0.241143	0.887944	2.337881
65	6	0	-0.671892	4.010002	0.996715
66	1	0	-0.215037	3.337629	1.733425
67	6	0	0.280753	5.162073	0.695509
68	1	0	-1.557968	4.426457	1.499720
69	1	0	2.624514	3.126201	-0.242254
70	6	0	-0.803637	3.679205	-1.565694
71	1	0	-4.995854	2.078175	-1.961860
72	1	0	-4.235031	3.537115	-1.306005
73	1	0	-4.959549	2.346420	-0.213287
74	1	0	-1.992546	2.084622	2.193715
75	1	0	-3.252033	1.083916	1.463194
76	1	0	-3.489789	2.830390	1.604544
77	1	0	0.516696	5.691342	1.625140
78	1	0	-0.154692	5.891249	0.003204
79	1	0	1.228419	4.820779	0.268502
80	1	0	-1.425001	4.549488	-1.825376
81	1	0	-0.940984	2.914085	-2.330433
82	1	0	0.237406	4.010594	-1.612734

14b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.509491	1.605478	-0.225737
2	6	0	-0.587732	3.443117	-0.451810
3	6	0	2.136444	1.918670	-1.550123
4	1	0	1.467523	1.774150	-2.394406
5	1	0	3.023992	1.281616	-1.671099
6	6	0	2.394355	1.906220	0.963181
7	1	0	1.859801	2.635187	1.584571
8	1	0	2.410789	1.017107	1.597955
9	6	0	-1.626057	2.866692	0.236685
10	6	0	-0.089704	-1.021648	0.100202
11	6	0	-2.562249	-1.414149	0.157331
12	6	0	-0.864784	-3.190381	0.573386
13	6	0	-2.509574	-2.043713	-2.301890
14	6	0	0.627035	-3.251140	0.281319
15	6	0	-5.273514	-0.741547	-0.033679
16	6	0	-2.677716	-1.246636	2.696769
17	6	0	-3.211055	-1.505764	-1.088943
18	6	0	-3.280374	-1.114654	1.328143
19	6	0	2.575737	-1.545516	2.551117

20	6	0	-4.625825	-0.759830	1.199739
21	6	0	-4.554902	-1.144118	-1.160333
22	6	0	2.366730	-1.521627	0.027900
23	6	0	-6.708995	-0.311351	-0.149259
24	6	0	5.127755	-1.183291	-0.259603
25	6	0	3.172373	-1.443095	1.175394
26	6	0	2.060432	-1.603975	-2.485645
27	6	0	2.918289	-1.466306	-1.261025
28	6	0	4.298677	-1.286879	-1.376822
29	6	0	4.545528	-1.267692	1.006312
30	6	0	6.607604	-0.966149	-0.412647
31	6	0	-2.899210	2.355747	-0.373462
32	1	0	-3.702195	3.068200	-0.133478
33	1	0	-3.205913	1.393961	0.056236
34	1	0	-2.824620	2.248358	-1.457030
35	1	0	-1.092065	-3.380550	1.629628
36	1	0	3.323363	-1.306800	3.313427
37	1	0	-1.647177	3.016751	1.316374
38	1	0	-1.453097	-3.881417	-0.036877
39	1	0	-2.157424	-3.069662	-2.131769
40	1	0	-1.649136	-1.424913	-2.571355
41	1	0	-3.191728	-2.066954	-3.156727
42	1	0	1.201001	-3.740849	1.072683
43	1	0	0.852546	-3.754907	-0.667534
44	1	0	-1.647490	-0.885893	2.732391
45	1	0	-2.699587	-2.296167	3.022168
46	1	0	-3.252796	-0.670825	3.427847
47	1	0	2.213661	-2.561214	2.758739
48	1	0	1.723044	-0.866817	2.676177
49	1	0	-5.183008	-0.504862	2.099222
50	1	0	-5.057183	-1.193177	-2.124399
51	1	0	-6.777999	0.744947	-0.439166
52	1	0	-7.240443	-0.425605	0.800856
53	1	0	-7.241320	-0.891009	-0.910826
54	1	0	1.272285	-0.842226	-2.522810
55	1	0	1.562169	-2.581219	-2.520244
56	1	0	2.666732	-1.514089	-3.391902
57	1	0	4.736701	-1.240945	-2.372262
58	1	0	5.177246	-1.199547	1.890039
59	1	0	6.968467	-1.330669	-1.379594
60	1	0	7.170878	-1.476027	0.375876
61	1	0	6.857355	0.101113	-0.351079
62	7	0	-1.187714	-1.802675	0.235488
63	7	0	0.985031	-1.831287	0.188419
64	17	0	-0.741074	0.858196	-2.458124
65	44	0	-0.259591	1.016131	-0.055246
66	17	0	-0.199866	1.097589	2.393330
67	6	0	0.338103	4.428462	0.197245
68	1	0	0.382399	4.280246	1.280804
69	1	0	1.353938	4.403833	-0.209342
70	1	0	-0.049606	5.441055	0.017795
71	6	0	3.822590	2.386918	0.710602
72	1	0	4.407208	1.660316	0.137698
73	1	0	3.860760	3.347009	0.183736
74	1	0	4.325659	2.526287	1.673941
75	1	0	2.513184	2.951903	-1.546523
76	1	0	-0.597827	3.402856	-1.540859

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.481124	1.579800	-0.158415
2	6	0	-2.399412	1.714708	1.018099
3	1	0	-2.097185	1.120163	1.874592
4	1	0	-3.429845	1.473393	0.725786
5	6	0	-2.108205	2.072705	-1.443580
6	1	0	-1.365172	2.140405	-2.237405
7	1	0	-2.792463	1.260871	-1.740530
8	6	0	0.019671	-1.088619	0.109548
9	6	0	2.477076	-1.493972	0.029117
10	6	0	0.783533	-3.314325	0.231587
11	6	0	2.683829	-1.464672	2.561592
12	6	0	-0.737778	-3.301219	0.357828
13	6	0	5.173713	-0.788235	-0.236849
14	6	0	2.351873	-1.992867	-2.469583
15	6	0	3.247643	-1.263813	1.185739
16	6	0	3.067865	-1.496421	-1.246161
17	6	0	-2.276159	-1.611047	-2.391459
18	6	0	4.406996	-1.115025	-1.352280
19	6	0	4.583004	-0.896771	1.023694
20	6	0	-2.442939	-1.523459	0.132916
21	6	0	6.601838	-0.342285	-0.381229
22	6	0	-5.191689	-1.033416	-0.000423
23	6	0	-3.061252	-1.426432	-1.124619
24	6	0	-2.515606	-1.548443	2.665351
25	6	0	-3.177257	-1.416228	1.322474
26	6	0	-4.548218	-1.168512	1.228995
27	6	0	-4.431346	-1.168812	-1.164496
28	6	0	-6.663936	-0.736831	-0.076671
29	1	0	1.127681	-3.815253	-0.681170
30	1	0	-2.928425	-1.521984	-3.265409
31	1	0	1.278992	-3.785068	1.086695
32	1	0	2.354093	-2.501734	2.705811
33	1	0	1.826000	-0.809860	2.743325
34	1	0	3.444200	-1.253855	3.319428
35	1	0	-1.237238	-3.894494	-0.415362
36	1	0	-1.082851	-3.657983	1.334720
37	1	0	1.267729	-1.933922	-2.372912
38	1	0	2.638409	-3.035822	-2.666951
39	1	0	2.624448	-1.400346	-3.346506
40	1	0	-1.808479	-2.603567	-2.429024
41	1	0	-1.468338	-0.874702	-2.487156
42	1	0	4.863094	-1.090911	-2.340189
43	1	0	5.181807	-0.705295	1.912115
44	1	0	6.668217	0.752884	-0.409233
45	1	0	7.048899	-0.719964	-1.306277
46	1	0	7.215251	-0.682978	0.459558
47	1	0	-1.573322	-0.990163	2.710685
48	1	0	-2.291781	-2.596854	2.903703
49	1	0	-3.172596	-1.173892	3.455966
50	1	0	-5.126019	-1.074076	2.146516
51	1	0	-4.920314	-1.087905	-2.133733
52	1	0	-7.172736	-0.989539	0.858686
53	1	0	-7.143322	-1.296793	-0.886837
54	1	0	-6.842279	0.328509	-0.270866
55	7	0	1.109362	-1.888671	0.172933
56	7	0	-1.065752	-1.881025	0.193855
57	44	0	0.264734	0.927745	-0.041887
58	17	0	0.613870	0.754278	-2.455017

59	6	0	-2.915394	3.372310	-1.348898
60	1	0	-3.760063	3.300406	-0.657338
61	1	0	-2.289682	4.213091	-1.028986
62	1	0	-3.316102	3.621904	-2.337170
63	1	0	-2.394674	2.768584	1.335301
64	6	0	0.601097	3.414558	-0.200777
65	6	0	1.787071	2.725362	-0.249220
66	1	0	2.117689	2.400808	-1.235307
67	17	0	0.350618	1.072890	2.399129
68	1	0	0.098945	3.569226	-1.153982
69	6	0	2.819725	2.686741	0.836766
70	1	0	3.604904	3.417707	0.592342
71	1	0	3.303514	1.705640	0.894235
72	1	0	2.411332	2.922332	1.820166
73	6	0	0.134256	4.231765	0.966102
74	1	0	0.710192	5.166260	1.017624
75	1	0	0.264453	3.694271	1.909856
76	1	0	-0.920087	4.506472	0.869967

17b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.478437	1.646162	0.004049
2	6	0	-2.458566	2.084101	-1.021790
3	1	0	-2.144726	1.877106	-2.044543
4	1	0	-3.422067	1.595785	-0.816308
5	6	0	-0.145501	-0.992819	0.152106
6	6	0	2.264068	-1.523407	0.134381
7	6	0	0.442133	-3.255673	0.320172
8	6	0	2.434530	-1.484266	2.665748
9	6	0	-1.058551	-3.107572	0.563653
10	6	0	4.975159	-0.874624	-0.106001
11	6	0	2.128842	-1.965866	-2.371904
12	6	0	3.028947	-1.316075	1.298628
13	6	0	2.858024	-1.514202	-1.138964
14	6	0	-2.663440	-1.765893	-2.263072
15	6	0	4.207188	-1.161995	-1.231490
16	6	0	4.373659	-0.983069	1.150279
17	6	0	-2.625326	-1.195251	0.203845
18	6	0	6.415826	-0.465041	-0.234033
19	6	0	-5.294002	-0.368094	0.115903
20	6	0	-3.326786	-1.271424	-1.010506
21	6	0	-2.502981	-0.717908	2.689728
22	6	0	-3.240181	-0.742871	1.381858
23	6	0	-4.569828	-0.321788	1.306846
24	6	0	-4.657318	-0.854627	-1.028138
25	6	0	-6.719998	0.105727	0.057365
26	1	0	0.665123	-3.752262	-0.633173
27	1	0	-3.379512	-1.801018	-3.089435
28	1	0	0.954407	-3.798444	1.119862
29	1	0	1.972295	-2.472304	2.782763
30	1	0	1.664593	-0.728211	2.852201
31	1	0	3.208103	-1.385711	3.433005
32	1	0	-1.663822	-3.748847	-0.083466
33	1	0	-1.334915	-3.312297	1.605617
34	1	0	1.053383	-1.795796	-2.310974
35	1	0	2.313828	-3.036012	-2.541619
36	1	0	2.483423	-1.425477	-3.253591

37	1	0	-2.252431	-2.775220	-2.137349
38	1	0	-1.832822	-1.109726	-2.552733
39	1	0	4.669739	-1.132633	-2.216218
40	1	0	4.970037	-0.811151	2.044195
41	1	0	6.516424	0.627199	-0.197099
42	1	0	6.846381	-0.801748	-1.182269
43	1	0	7.022199	-0.873520	0.581365
44	1	0	-1.570607	-0.143487	2.625066
45	1	0	-2.239827	-1.731291	3.019215
46	1	0	-3.124341	-0.272423	3.472217
47	1	0	-5.054681	0.038924	2.211948
48	1	0	-5.210148	-0.908453	-1.964200
49	1	0	-7.178884	0.119698	1.050794
50	1	0	-7.327997	-0.535335	-0.589867
51	1	0	-6.780848	1.124109	-0.347158
52	7	0	0.881706	-1.861064	0.274422
53	7	0	-1.290649	-1.693064	0.251897
54	44	0	0.215392	0.967060	-0.156243
55	17	0	0.108751	0.696077	-2.576352
56	6	0	0.561083	3.410954	-0.613129
57	6	0	1.743044	2.717135	-0.656561
58	1	0	1.994273	2.261655	-1.615298
59	17	0	0.492219	1.358365	2.232287
60	1	0	-0.021770	3.422715	-1.532993
61	6	0	2.847852	2.786756	0.353447
62	1	0	3.627508	3.464776	-0.023786
63	1	0	3.315243	1.806487	0.499132
64	1	0	2.507907	3.144008	1.326265
65	6	0	0.159544	4.364585	0.471929
66	1	0	0.649730	5.334279	0.307470
67	1	0	0.444291	3.995255	1.460468
68	1	0	-0.920457	4.541500	0.470790
69	1	0	-1.807829	1.838643	1.036974
70	1	0	-2.636231	3.164223	-0.893816

17c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.398855	1.653414	0.270372
2	6	0	-2.097172	2.069860	1.529897
3	1	0	-1.528609	1.854508	2.431269
4	1	0	-3.066655	1.554690	1.578685
5	6	0	-2.156400	1.985939	-0.994557
6	1	0	-1.527134	2.689736	-1.556012
7	1	0	-2.158623	1.102350	-1.636340
8	6	0	0.001113	-1.087634	0.071377
9	6	0	2.438121	-1.522354	-0.078756
10	6	0	0.706129	-3.329789	-0.059236
11	6	0	2.767806	-1.940089	2.407380
12	6	0	-0.811725	-3.290034	0.103334
13	6	0	5.123737	-0.772238	-0.340468
14	6	0	2.202822	-1.605676	-2.617945
15	6	0	3.257901	-1.478726	1.065727
16	6	0	2.975474	-1.317993	-1.362345
17	6	0	-2.236481	-1.514847	-2.548790
18	6	0	4.311303	-0.924692	-1.462513
19	6	0	4.584581	-1.078826	0.909554
20	6	0	-2.469144	-1.451232	-0.029770

21	6	0	6.543591	-0.297209	-0.473251
22	6	0	-5.201947	-0.900810	-0.229965
23	6	0	-3.056905	-1.343943	-1.300996
24	6	0	-2.596632	-1.469771	2.497965
25	6	0	-3.223395	-1.309017	1.143015
26	6	0	-4.585540	-1.023594	1.014832
27	6	0	-4.420808	-1.066906	-1.375807
28	6	0	-6.665078	-0.572762	-0.341536
29	1	0	1.017370	-3.718686	-1.037070
30	1	0	-2.858024	-1.385653	-3.439763
31	1	0	1.202120	-3.918750	0.718290
32	1	0	2.739800	-3.038310	2.444235
33	1	0	1.770905	-1.556580	2.633246
34	1	0	3.443202	-1.605702	3.200139
35	1	0	-1.343576	-3.819097	-0.693730
36	1	0	-1.142573	-3.701638	1.064360
37	1	0	1.124617	-1.545417	-2.469550
38	1	0	2.456795	-2.609954	-2.986143
39	1	0	2.454956	-0.887602	-3.402000
40	1	0	-1.784682	-2.513573	-2.604052
41	1	0	-1.414429	-0.788145	-2.596072
42	1	0	4.726579	-0.743747	-2.452215
43	1	0	5.218680	-1.024045	1.792328
44	1	0	6.598797	0.795687	-0.388087
45	1	0	6.968693	-0.569983	-1.444518
46	1	0	7.182481	-0.717143	0.310502
47	1	0	-1.679437	-0.877643	2.597704
48	1	0	-2.330474	-2.517313	2.691906
49	1	0	-3.293346	-1.162834	3.283822
50	1	0	-5.181396	-0.907970	1.918400
51	1	0	-4.885303	-0.979196	-2.356252
52	1	0	-7.201425	-0.810527	0.582301
53	1	0	-7.137478	-1.124404	-1.161344
54	1	0	-6.813975	0.495985	-0.543068
55	7	0	1.070005	-1.917468	0.055390
56	7	0	-1.104874	-1.853689	0.047775
57	44	0	0.320694	0.910186	0.253724
58	17	0	0.573631	1.190562	-2.154562
59	6	0	-3.574759	2.540777	-0.871593
60	1	0	-4.248063	1.842826	-0.364147
61	1	0	-3.610617	3.497284	-0.338345
62	1	0	-3.976982	2.713724	-1.875978
63	1	0	-2.332805	3.143816	1.482559
64	6	0	0.740229	3.325473	0.690752
65	6	0	1.910573	2.610237	0.621850
66	1	0	2.242299	2.145021	1.550670
67	17	0	0.503656	0.593311	2.681427
68	1	0	0.249740	3.355168	1.661867
69	6	0	2.937077	2.706077	-0.465363
70	1	0	3.391336	1.731440	-0.671523
71	1	0	3.740127	3.375771	-0.122767
72	1	0	2.531022	3.090511	-1.401553
73	6	0	0.285998	4.310245	-0.343493
74	1	0	0.450931	3.932357	-1.357279
75	1	0	0.849552	5.247301	-0.234769
76	1	0	-0.774412	4.556544	-0.230491

TS18a

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	1.534429	1.823599	-0.065494
2	6	0	-0.052227	3.262345	0.271681
3	6	0	2.144691	2.087756	-1.413989
4	1	0	1.440523	1.987655	-2.236377
5	1	0	2.944272	1.344144	-1.544326
6	6	0	2.510204	2.038183	1.075662
7	1	0	1.975500	2.071789	2.024955
8	1	0	3.105971	1.113242	1.113600
9	6	0	-1.274466	2.632966	0.674267
10	6	0	-0.162039	-1.143429	0.074019
11	6	0	-2.638877	-1.396071	0.072868
12	6	0	-1.021978	-3.300569	0.352697
13	6	0	-2.576586	-1.871055	-2.420529
14	6	0	0.467043	-3.395900	0.037574
15	6	0	-5.282875	-0.501129	-0.122120
16	6	0	-2.771423	-1.325031	2.613057
17	6	0	-3.267436	-1.369780	-1.185623
18	6	0	-3.347108	-1.090413	1.246576
19	6	0	2.580165	-1.990100	2.404903
20	6	0	-4.658181	-0.624516	1.117326
21	6	0	-4.579180	-0.905587	-1.257176
22	6	0	2.265659	-1.670094	-0.090443
23	6	0	-6.678942	0.044437	-0.235766
24	6	0	5.004699	-1.212226	-0.430454
25	6	0	3.111650	-1.704183	1.030400
26	6	0	1.878336	-1.491885	-2.590866
27	6	0	2.770032	-1.459294	-1.383161
28	6	0	4.139517	-1.223060	-1.524028
29	6	0	4.472524	-1.465694	0.834486
30	6	0	6.470607	-0.927672	-0.605272
31	1	0	-1.247231	-3.574844	1.390667
32	1	0	3.380005	-1.918696	3.147896
33	1	0	-1.388534	2.506127	1.750771
34	1	0	-1.643453	-3.909705	-0.309380
35	1	0	-2.263943	-2.917239	-2.308446
36	1	0	-1.691281	-1.269820	-2.646625
37	1	0	-3.249867	-1.818823	-3.281022
38	1	0	1.023862	-3.983508	0.772093
39	1	0	0.662461	-3.814943	-0.957997
40	1	0	-1.744889	-0.959053	2.702093
41	1	0	-2.778404	-2.397203	2.853243
42	1	0	-3.374037	-0.821208	3.374633
43	1	0	2.158970	-3.001351	2.474063
44	1	0	1.787657	-1.282808	2.675036
45	1	0	-5.209086	-0.368526	2.020401
46	1	0	-5.065480	-0.865037	-2.229740
47	1	0	-6.660897	1.118215	-0.461938
48	1	0	-7.238107	-0.084578	0.696404
49	1	0	-7.237157	-0.446296	-1.040027
50	1	0	1.114625	-0.705358	-2.557821
51	1	0	1.349453	-2.449217	-2.676594
52	1	0	2.465478	-1.358568	-3.504371
53	1	0	4.539588	-1.056110	-2.522529
54	1	0	5.134538	-1.484833	1.698228
55	1	0	6.800458	-1.135484	-1.628028
56	1	0	7.079678	-1.528923	0.077976
57	1	0	6.694406	0.126307	-0.396164
58	7	0	-1.290710	-1.874185	0.144816
59	7	0	0.883610	-1.988659	0.078007

60	17	0	-0.776531	1.026194	-2.220396
61	44	0	-0.126998	0.925662	0.130335
62	17	0	0.110218	0.631475	2.554909
63	6	0	3.456643	3.235848	0.956781
64	1	0	4.167442	3.138734	0.130220
65	1	0	2.908685	4.176661	0.820741
66	1	0	4.038217	3.329097	1.880353
67	1	0	2.625910	3.072590	-1.452772
68	6	0	-2.570292	2.791213	-0.072204
69	1	0	-3.244230	1.954362	0.142700
70	1	0	-3.068865	3.707903	0.279338
71	1	0	-2.436447	2.848845	-1.152563
72	6	0	-0.020420	4.153656	-0.943209
73	1	0	0.975403	4.567996	-1.120347
74	1	0	-0.343857	3.619855	-1.841104
75	1	0	-0.706029	4.996385	-0.782814
76	1	0	0.558585	3.588752	1.112524

TS18b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.455031	1.919786	0.024247
2	6	0	0.168498	3.345912	-0.528310
3	6	0	-2.573483	2.160260	-0.926432
4	1	0	-2.326249	1.910833	-1.958029
5	1	0	-3.413583	1.529855	-0.600588
6	6	0	1.417707	2.695628	-0.660280
7	6	0	-0.053332	-1.022351	0.121531
8	6	0	2.379991	-1.471822	0.096303
9	6	0	0.618780	-3.254402	0.373117
10	6	0	2.536652	-1.440731	2.631274
11	6	0	-0.895292	-3.159804	0.567217
12	6	0	5.080062	-0.770799	-0.120925
13	6	0	2.241158	-1.839110	-2.417981
14	6	0	3.129999	-1.250293	1.265895
15	6	0	2.982562	-1.444209	-1.173698
16	6	0	-2.564924	-1.922050	-2.241565
17	6	0	4.326681	-1.074056	-1.253434
18	6	0	4.469197	-0.887175	1.128357
19	6	0	-2.526428	-1.298994	0.214916
20	6	0	6.515072	-0.338771	-0.238799
21	6	0	-5.220897	-0.556566	0.125345
22	6	0	-3.229397	-1.413764	-0.995086
23	6	0	-2.418250	-0.792697	2.697129
24	6	0	-3.153330	-0.856204	1.389845
25	6	0	-4.496253	-0.480083	1.314650
26	6	0	-4.571801	-1.034404	-1.014110
27	6	0	-6.660198	-0.124869	0.066622
28	1	0	0.894660	-3.824217	-0.522088
29	1	0	-3.286020	-1.986094	-3.061752
30	1	0	1.675704	2.410375	-1.680974
31	1	0	1.130576	-3.699354	1.231432
32	1	0	2.261924	-2.489849	2.803072
33	1	0	1.643825	-0.823364	2.766198
34	1	0	3.259724	-1.162661	3.403467
35	1	0	-1.454429	-3.812802	-0.109636
36	1	0	-1.203396	-3.389963	1.594073
37	1	0	1.446208	-1.125236	-2.660377

38	1	0	1.778267	-2.827901	-2.314727
39	1	0	2.927704	-1.884573	-3.268540
40	1	0	-2.137446	-2.922198	-2.098468
41	1	0	-1.749964	-1.256525	-2.549888
42	1	0	4.798592	-1.039505	-2.233367
43	1	0	5.053043	-0.700578	2.027543
44	1	0	6.595490	0.755773	-0.238411
45	1	0	6.967582	-0.699267	-1.168005
46	1	0	7.115071	-0.707926	0.599584
47	1	0	-1.554112	-0.119380	2.645750
48	1	0	-2.041733	-1.779006	2.996394
49	1	0	-3.081449	-0.440454	3.492796
50	1	0	-4.990905	-0.130676	2.218967
51	1	0	-5.124587	-1.116862	-1.948043
52	1	0	-7.132929	-0.169973	1.052815
53	1	0	-7.239011	-0.753865	-0.617863
54	1	0	-6.747577	0.908977	-0.291450
55	7	0	1.004364	-1.849006	0.216837
56	7	0	-1.172631	-1.750526	0.265533
57	17	0	0.482379	1.322802	2.225151
58	44	0	0.139281	0.998787	-0.163669
59	17	0	-0.101092	0.747243	-2.575975
60	6	0	2.586730	2.910032	0.257944
61	1	0	3.224263	2.019643	0.291773
62	1	0	3.198861	3.734967	-0.137161
63	1	0	2.286965	3.145700	1.279208
64	6	0	-0.099798	4.349268	0.563817
65	1	0	-1.144112	4.676134	0.564460
66	1	0	0.139057	3.940316	1.549587
67	1	0	0.525349	5.236717	0.398145
68	1	0	-0.368002	3.485254	-1.466147
69	1	0	-1.649513	2.278137	1.044616
70	1	0	-2.918272	3.202471	-0.851029

TS18c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.521200	1.827367	0.400198
2	6	0	-2.281565	2.015104	1.685685
3	1	0	-1.666261	1.871207	2.570821
4	1	0	-3.089112	1.269691	1.703011
5	6	0	-2.357678	2.089341	-0.838107
6	1	0	-1.719331	2.412096	-1.661585
7	1	0	-2.710505	1.094619	-1.145589
8	6	0	0.180481	-1.158729	0.061600
9	6	0	2.646322	-1.371195	-0.081161
10	6	0	1.068289	-3.317075	-0.140793
11	6	0	2.961152	-1.735270	2.412429
12	6	0	-0.450060	-3.413129	0.004411
13	6	0	5.263871	-0.406896	-0.312249
14	6	0	2.424411	-1.413419	-2.623048
15	6	0	3.447166	-1.269297	1.071535
16	6	0	3.169994	-1.101127	-1.356533
17	6	0	-1.998965	-1.635938	-2.609798
18	6	0	4.471549	-0.601871	-1.441140
19	6	0	4.740419	-0.768712	0.930271
20	6	0	-2.249154	-1.676200	-0.087181
21	6	0	6.646535	0.171752	-0.427503

22	6	0	-4.992255	-1.168635	-0.299360
23	6	0	-2.825498	-1.531297	-1.360533
24	6	0	-2.429208	-1.858294	2.435559
25	6	0	-3.027056	-1.622670	1.079230
26	6	0	-4.391635	-1.354638	0.945124
27	6	0	-4.194734	-1.275147	-1.439611
28	6	0	-6.457485	-0.851600	-0.413451
29	1	0	1.419178	-3.632133	-1.131245
30	1	0	-2.637381	-1.592790	-3.497200
31	1	0	1.606845	-3.896181	0.614970
32	1	0	2.748813	-2.812518	2.402373
33	1	0	2.045407	-1.215338	2.709664
34	1	0	3.723384	-1.558931	3.177126
35	1	0	-0.927579	-3.955102	-0.817734
36	1	0	-0.753071	-3.884484	0.946543
37	1	0	1.343150	-1.423946	-2.483299
38	1	0	2.744021	-2.390196	-3.013072
39	1	0	2.634975	-0.664117	-3.390499
40	1	0	-1.438145	-2.577952	-2.650188
41	1	0	-1.269544	-0.818169	-2.670788
42	1	0	4.875766	-0.370587	-2.424894
43	1	0	5.361058	-0.672838	1.819041
44	1	0	6.626026	1.262117	-0.304005
45	1	0	7.088297	-0.037064	-1.407094
46	1	0	7.314641	-0.229661	0.341579
47	1	0	-1.572006	-1.200487	2.619610
48	1	0	-2.080002	-2.893387	2.543884
49	1	0	-3.173193	-1.683732	3.218567
50	1	0	-5.002292	-1.303657	1.844708
51	1	0	-4.647865	-1.156844	-2.422136
52	1	0	-7.006902	-1.165115	0.479683
53	1	0	-6.907744	-1.344876	-1.281406
54	1	0	-6.616842	0.227481	-0.535683
55	7	0	1.314335	-1.883089	0.039101
56	7	0	-0.860976	-2.003570	-0.004511
57	44	0	0.135718	0.901690	0.262680
58	17	0	0.359257	1.138540	-2.151853
59	6	0	-3.574345	3.006418	-0.698043
60	1	0	-4.323229	2.605848	-0.007363
61	1	0	-3.305965	4.011780	-0.353459
62	1	0	-4.053956	3.114999	-1.677079
63	1	0	-2.762140	3.001946	1.715605
64	6	0	0.087439	3.205159	0.566292
65	6	0	1.368195	2.559165	0.698693
66	1	0	1.677650	2.374376	1.727571
67	17	0	0.298424	0.473090	2.674375
68	1	0	-0.343804	3.480182	1.527461
69	6	0	2.510412	2.790652	-0.251655
70	1	0	3.203823	1.942333	-0.232786
71	1	0	3.072210	3.677218	0.081248
72	1	0	2.186819	2.938738	-1.282068
73	6	0	-0.140975	4.192078	-0.550912
74	1	0	0.046616	3.744060	-1.530677
75	1	0	0.552383	5.034559	-0.427303
76	1	0	-1.156421	4.596009	-0.538948

19a

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

1	6	0	1.522126	2.141489	-0.031960
2	6	0	0.247092	3.103961	0.224858
3	6	0	2.189238	2.249666	-1.389429
4	1	0	1.493536	2.188117	-2.223206
5	1	0	2.914616	1.432700	-1.484694
6	6	0	2.556279	2.216024	1.089218
7	1	0	2.057751	2.156166	2.056785
8	1	0	3.193747	1.325044	1.018286
9	6	0	-1.130247	2.391997	0.606027
10	6	0	-0.243239	-1.174311	0.075761
11	6	0	-2.731602	-1.304185	0.094400
12	6	0	-1.196308	-3.285741	0.315028
13	6	0	-2.730384	-1.772803	-2.401585
14	6	0	0.287665	-3.443092	-0.008808
15	6	0	-5.344317	-0.315669	-0.050089
16	6	0	-2.782146	-1.163940	2.632930
17	6	0	-3.382853	-1.259070	-1.150845
18	6	0	-3.397394	-0.954736	1.280091
19	6	0	2.471562	-2.213140	2.376290
20	6	0	-4.694180	-0.446073	1.175949
21	6	0	-4.679758	-0.750208	-1.196989
22	6	0	2.161385	-1.769784	-0.105279
23	6	0	-6.724830	0.272977	-0.136025
24	6	0	4.906924	-1.320839	-0.410813
25	6	0	3.001446	-1.852074	1.019413
26	6	0	1.816908	-1.562982	-2.618234
27	6	0	2.680681	-1.540248	-1.390263
28	6	0	4.052688	-1.306574	-1.511692
29	6	0	4.363456	-1.612094	0.841021
30	6	0	6.374196	-1.032874	-0.564810
31	1	0	-1.432029	-3.576246	1.345875
32	1	0	3.265366	-2.147743	3.126052
33	1	0	-1.264338	2.406366	1.690222
34	1	0	-1.846538	-3.848122	-0.360119
35	1	0	-2.446784	-2.828785	-2.305541
36	1	0	-1.830420	-1.196866	-2.638752
37	1	0	-3.417127	-1.693586	-3.249243
38	1	0	0.819514	-4.064821	0.715679
39	1	0	0.460184	-3.855876	-1.010866
40	1	0	-1.789433	-0.709397	2.711283
41	1	0	-2.678971	-2.234439	2.855682
42	1	0	-3.417705	-0.732337	3.411868
43	1	0	2.087331	-3.241449	2.397692
44	1	0	1.659764	-1.541296	2.672508
45	1	0	-5.213747	-0.159423	2.088292
46	1	0	-5.184949	-0.697860	-2.159330
47	1	0	-6.678783	1.344420	-0.369228
48	1	0	-7.266435	0.166768	0.809294
49	1	0	-7.316242	-0.204699	-0.924202
50	1	0	1.161744	-0.685419	-2.675516
51	1	0	1.167218	-2.445462	-2.643807
52	1	0	2.438578	-1.583064	-3.518353
53	1	0	4.462878	-1.124182	-2.503182
54	1	0	5.018695	-1.664196	1.708360
55	1	0	6.716948	-1.230480	-1.585369
56	1	0	6.975853	-1.638732	0.120857
57	1	0	6.591872	0.019847	-0.343658
58	7	0	-1.404700	-1.842614	0.145350
59	7	0	0.767754	-2.057447	0.049956
60	17	0	-0.649277	0.976854	-2.248680

61	44	0	-0.010372	0.853736	0.093798
62	17	0	0.284652	0.542655	2.501876
63	6	0	3.437788	3.469817	1.053515
64	1	0	4.109363	3.494574	0.189585
65	1	0	2.836170	4.387734	1.038188
66	1	0	4.060818	3.504925	1.954057
67	1	0	2.752985	3.189363	-1.467706
68	6	0	-2.390777	2.769309	-0.121823
69	1	0	-3.169865	2.041596	0.133182
70	1	0	-2.742226	3.753046	0.225055
71	1	0	-2.281472	2.781194	-1.205883
72	6	0	0.067623	4.136786	-0.880700
73	1	0	0.995935	4.695773	-1.034476
74	1	0	-0.214849	3.668057	-1.826575
75	1	0	-0.713675	4.851935	-0.603705
76	1	0	0.524193	3.571689	1.175104

19b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.333551	2.411933	0.021618
2	6	0	-0.024935	3.222303	-0.412886
3	6	0	-2.543931	2.544659	-0.859481
4	1	0	-2.312020	2.396486	-1.914857
5	1	0	-3.295204	1.804263	-0.562556
6	6	0	1.310732	2.379621	-0.583759
7	6	0	-0.000682	-1.040573	0.119147
8	6	0	2.454298	-1.402865	0.054791
9	6	0	0.748855	-3.239880	0.313131
10	6	0	2.642677	-1.410016	2.586668
11	6	0	-0.757003	-3.197444	0.576528
12	6	0	5.140668	-0.667658	-0.190198
13	6	0	2.252825	-1.652047	-2.466554
14	6	0	3.219466	-1.202738	1.216667
15	6	0	3.026781	-1.316733	-1.224877
16	6	0	-2.474147	-2.032856	-2.236938
17	6	0	4.365784	-0.932683	-1.318244
18	6	0	4.553872	-0.826453	1.065732
19	6	0	-2.460113	-1.375016	0.213949
20	6	0	6.570998	-0.223715	-0.321158
21	6	0	-5.149077	-0.622541	0.077009
22	6	0	-3.144007	-1.490143	-1.008512
23	6	0	-2.429721	-0.954179	2.720843
24	6	0	-3.114763	-0.961338	1.385246
25	6	0	-4.453631	-0.577125	1.284258
26	6	0	-4.481519	-1.098934	-1.051808
27	6	0	-6.580363	-0.170773	-0.009374
28	1	0	1.000539	-3.767026	-0.614975
29	1	0	-3.191120	-2.112052	-3.059238
30	1	0	1.558916	2.305595	-1.645600
31	1	0	1.312030	-3.697492	1.130897
32	1	0	2.338169	-2.453236	2.742244
33	1	0	1.766925	-0.772717	2.746553
34	1	0	3.384815	-1.169738	3.353476
35	1	0	-1.323990	-3.874986	-0.067999
36	1	0	-1.007042	-3.424863	1.619547
37	1	0	1.432726	-0.945299	-2.637215
38	1	0	1.814667	-2.656167	-2.410804

39	1	0	2.909347	-1.628513	-3.341283
40	1	0	-2.056938	-3.032957	-2.064760
41	1	0	-1.656788	-1.377730	-2.557205
42	1	0	4.816436	-0.854641	-2.305680
43	1	0	5.151899	-0.659032	1.959350
44	1	0	6.645916	0.870751	-0.288887
45	1	0	7.008068	-0.553227	-1.269057
46	1	0	7.188377	-0.614916	0.494239
47	1	0	-1.570004	-0.274727	2.736441
48	1	0	-2.063463	-1.952912	2.989919
49	1	0	-3.126677	-0.640708	3.503652
50	1	0	-4.968366	-0.245994	2.184069
51	1	0	-5.016689	-1.175047	-1.996287
52	1	0	-7.075352	-0.216486	0.965808
53	1	0	-7.152912	-0.785171	-0.712193
54	1	0	-6.642762	0.867082	-0.360737
55	7	0	1.090224	-1.817493	0.189685
56	7	0	-1.094151	-1.801544	0.274126
57	17	0	0.330273	1.222810	2.273590
58	44	0	-0.002815	0.975660	-0.119986
59	17	0	-0.333703	0.761011	-2.512801
60	6	0	2.513119	2.684489	0.265591
61	1	0	3.244694	1.877739	0.142293
62	1	0	2.992923	3.610859	-0.084937
63	1	0	2.282351	2.772948	1.326998
64	6	0	0.154730	4.377099	0.570168
65	1	0	-0.744258	5.002504	0.576360
66	1	0	0.319382	3.999975	1.583169
67	1	0	1.004885	5.005377	0.284705
68	1	0	-0.257575	3.555320	-1.429088
69	1	0	-1.553468	2.609584	1.075585
70	1	0	-2.992932	3.540029	-0.718003

19c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.471642	2.140059	0.447637
2	6	0	-2.363154	2.120208	1.672680
3	1	0	-1.810035	1.936564	2.591849
4	1	0	-3.121778	1.335642	1.569056
5	6	0	-2.285377	2.350931	-0.830806
6	1	0	-1.628361	2.597978	-1.664338
7	1	0	-2.725377	1.377080	-1.084107
8	6	0	0.227001	-1.188515	0.004949
9	6	0	2.703739	-1.309974	-0.106845
10	6	0	1.184129	-3.300465	-0.263755
11	6	0	2.917569	-1.636387	2.401548
12	6	0	-0.337014	-3.447613	-0.176919
13	6	0	5.298607	-0.272970	-0.238800
14	6	0	2.564866	-1.333028	-2.653438
15	6	0	3.451899	-1.178219	1.076490
16	6	0	3.264243	-1.019961	-1.361080
17	6	0	-1.938066	-1.431257	-2.679478
18	6	0	4.554380	-0.487212	-1.396595
19	6	0	4.736471	-0.644013	0.983936
20	6	0	-2.185822	-1.738010	-0.169439
21	6	0	6.668991	0.341808	-0.301912
22	6	0	-4.926492	-1.195270	-0.333814

23	6	0	-2.754254	-1.436196	-1.419419
24	6	0	-2.416646	-2.323021	2.295594
25	6	0	-2.978760	-1.853487	0.985158
26	6	0	-4.339322	-1.561652	0.876950
27	6	0	-4.121186	-1.158503	-1.471458
28	6	0	-6.387297	-0.849155	-0.410339
29	1	0	1.580387	-3.579898	-1.246993
30	1	0	-2.590409	-1.362000	-3.555013
31	1	0	1.712849	-3.881391	0.497828
32	1	0	2.686734	-2.709600	2.385968
33	1	0	1.997198	-1.107738	2.671259
34	1	0	3.658182	-1.471142	3.189679
35	1	0	-0.770692	-3.947343	-1.048898
36	1	0	-0.654097	-3.987098	0.722105
37	1	0	1.478830	-1.333257	-2.552692
38	1	0	2.889149	-2.313202	-3.030953
39	1	0	2.811345	-0.588142	-3.414660
40	1	0	-1.343756	-2.347706	-2.779216
41	1	0	-1.238988	-0.586370	-2.705680
42	1	0	4.987725	-0.240561	-2.364030
43	1	0	5.318510	-0.527656	1.896129
44	1	0	6.615230	1.431160	-0.179307
45	1	0	7.152960	0.145929	-1.264066
46	1	0	7.318006	-0.042685	0.491774
47	1	0	-1.477126	-1.818435	2.538354
48	1	0	-2.238321	-3.406871	2.279976
49	1	0	-3.123401	-2.125903	3.106907
50	1	0	-4.958319	-1.635350	1.769048
51	1	0	-4.567663	-0.917962	-2.434375
52	1	0	-6.968636	-1.391770	0.342101
53	1	0	-6.803066	-1.080802	-1.396237
54	1	0	-6.544689	0.222627	-0.233540
55	7	0	1.384894	-1.864486	-0.038711
56	7	0	-0.791213	-2.053750	-0.111032
57	44	0	0.032577	0.824781	0.266518
58	17	0	0.424275	1.181765	-2.102467
59	6	0	-3.429780	3.368340	-0.742834
60	1	0	-4.228403	3.039943	-0.070292
61	1	0	-3.091688	4.353421	-0.401212
62	1	0	-3.870920	3.500417	-1.737151
63	1	0	-2.890900	3.080736	1.759721
64	6	0	-0.150664	3.051614	0.654448
65	6	0	1.235577	2.272431	0.840704
66	1	0	1.462449	2.171502	1.904791
67	17	0	-0.037147	0.242577	2.642803
68	1	0	-0.319966	3.437142	1.664421
69	6	0	2.439492	2.697177	0.046452
70	1	0	3.219860	1.937066	0.168192
71	1	0	2.841753	3.639692	0.448337
72	1	0	2.239966	2.810190	-1.018822
73	6	0	-0.027717	4.174675	-0.366772
74	1	0	0.181756	3.782745	-1.364814
75	1	0	0.788187	4.847865	-0.084117
76	1	0	-0.947427	4.764633	-0.408314

TS20a

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

1	6	0	-1.687424	2.397151	0.000903
2	6	0	-0.503993	3.161596	-0.264882
3	6	0	-2.338520	2.482292	1.363308
4	1	0	-1.624755	2.479914	2.184352
5	1	0	-3.028310	1.642950	1.506948
6	6	0	-2.693928	2.193106	-1.121163
7	1	0	-2.179255	2.187018	-2.082015
8	1	0	-3.162415	1.205700	-1.015924
9	6	0	1.297234	1.976453	-0.510512
10	6	0	0.335333	-1.159299	0.049528
11	6	0	2.829992	-1.193384	-0.040503
12	6	0	1.399871	-3.240739	0.066194
13	6	0	3.006560	-1.352157	2.485146
14	6	0	-0.085794	-3.443769	0.356260
15	6	0	5.420904	-0.147932	-0.202778
16	6	0	2.656099	-1.261219	-2.572876
17	6	0	3.566151	-0.994088	1.139197
18	6	0	3.391190	-0.944955	-1.303412
19	6	0	-2.091983	-2.431964	-2.297275
20	6	0	4.679679	-0.408803	-1.354860
21	6	0	4.851765	-0.462675	1.031542
22	6	0	-2.037796	-1.857755	0.174982
23	6	0	6.794326	0.458228	-0.287188
24	6	0	-4.804038	-1.432470	0.180512
25	6	0	-2.760009	-2.003680	-1.023774
26	6	0	-1.964370	-1.625046	2.706866
27	6	0	-2.690867	-1.601804	1.393339
28	6	0	-4.068847	-1.374068	1.363162
29	6	0	-4.134799	-1.772944	-0.995678
30	6	0	-6.279400	-1.144903	0.171362
31	1	0	1.697529	-3.647835	-0.907810
32	1	0	-2.821945	-2.492923	-3.109624
33	1	0	1.427255	2.146689	-1.587172
34	1	0	2.048232	-3.676201	0.831461
35	1	0	2.801635	-2.427659	2.564690
36	1	0	2.070935	-0.816265	2.676267
37	1	0	3.717864	-1.096291	3.275940
38	1	0	-0.562051	-4.153370	-0.326140
39	1	0	-0.271776	-3.776833	1.384601
40	1	0	1.728600	-0.683880	-2.661929
41	1	0	2.383885	-2.322934	-2.625291
42	1	0	3.283022	-1.040913	-3.442063
43	1	0	-1.630319	-3.422427	-2.194597
44	1	0	-1.313710	-1.720159	-2.589777
45	1	0	5.119252	-0.205233	-2.329479
46	1	0	5.424425	-0.295289	1.941732
47	1	0	6.748746	1.550973	-0.194673
48	1	0	7.274017	0.231929	-1.244776
49	1	0	7.443848	0.092164	0.514726
50	1	0	-1.147699	-0.896411	2.739935
51	1	0	-1.537575	-2.616689	2.904635
52	1	0	-2.653182	-1.397949	3.525864
53	1	0	-4.581159	-1.165017	2.300312
54	1	0	-4.698246	-1.870780	-1.921498
55	1	0	-6.729234	-1.322781	1.153293
56	1	0	-6.804413	-1.765160	-0.562631
57	1	0	-6.471493	-0.097016	-0.092544
58	7	0	1.528168	-1.777838	0.055087
59	7	0	-0.626117	-2.095554	0.158930
60	17	0	0.338296	0.989116	2.330397
61	44	0	-0.112422	0.844277	-0.071652

62	17	0	-0.377069	0.569090	-2.487505
63	6	0	-3.786767	3.268624	-1.138965
64	1	0	-4.436989	3.226079	-0.259109
65	1	0	-3.354923	4.275930	-1.191323
66	1	0	-4.419373	3.133985	-2.023330
67	1	0	-2.932221	3.406617	1.418134
68	6	0	2.430841	2.470774	0.315976
69	1	0	3.260601	1.771878	0.132315
70	1	0	2.771104	3.457346	-0.026997
71	1	0	2.228822	2.474869	1.386501
72	6	0	-0.011033	4.168976	0.744702
73	1	0	-0.792275	4.924852	0.901549
74	1	0	0.204306	3.704293	1.710700
75	1	0	0.886184	4.687563	0.398624
76	1	0	-0.397864	3.444034	-1.313160

TS20b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.443064	2.738393	0.063812
2	6	0	-0.267272	3.372690	-0.409066
3	6	0	-2.685979	2.551398	-0.762876
4	1	0	-2.465476	2.496690	-1.829754
5	1	0	-3.228394	1.643180	-0.475237
6	6	0	1.438165	1.907150	-0.527466
7	6	0	0.048101	-1.005396	0.107329
8	6	0	2.517455	-1.331012	0.028909
9	6	0	0.866303	-3.192336	0.243734
10	6	0	2.686319	-1.338553	2.556599
11	6	0	-0.634288	-3.206903	0.525988
12	6	0	5.217060	-0.641314	-0.206946
13	6	0	2.279459	-1.454484	-2.493370
14	6	0	3.285347	-1.160762	1.191829
15	6	0	3.082134	-1.204680	-1.249847
16	6	0	-2.395791	-2.064447	-2.257792
17	6	0	4.428929	-0.847270	-1.339240
18	6	0	4.629045	-0.812960	1.047153
19	6	0	-2.392226	-1.431391	0.199815
20	6	0	6.658450	-0.231933	-0.332700
21	6	0	-5.098224	-0.734681	0.071347
22	6	0	-3.074118	-1.541386	-1.025650
23	6	0	-2.391882	-1.104249	2.722331
24	6	0	-3.062991	-1.066827	1.379896
25	6	0	-4.408946	-0.706444	1.282500
26	6	0	-4.418676	-1.175687	-1.064927
27	6	0	-6.536717	-0.306140	-0.010547
28	1	0	1.122259	-3.680974	-0.704611
29	1	0	-3.104644	-2.119650	-3.089037
30	1	0	1.606154	2.034061	-1.605765
31	1	0	1.455496	-3.658796	1.038086
32	1	0	2.322355	-2.362368	2.711259
33	1	0	1.838752	-0.659200	2.703341
34	1	0	3.430791	-1.135230	3.331930
35	1	0	-1.186051	-3.892826	-0.123062
36	1	0	-0.862214	-3.461146	1.568184
37	1	0	1.436765	-0.758172	-2.580667
38	1	0	1.863796	-2.469853	-2.508273
39	1	0	2.906959	-1.344319	-3.382761

40	1	0	-1.992765	-3.072744	-2.099459
41	1	0	-1.570541	-1.409977	-2.556864
42	1	0	4.874996	-0.741101	-2.326285
43	1	0	5.231346	-0.673141	1.942789
44	1	0	6.762864	0.859716	-0.287181
45	1	0	7.086754	-0.560996	-1.284777
46	1	0	7.265568	-0.649585	0.477163
47	1	0	-1.519851	-0.442740	2.765100
48	1	0	-2.054531	-2.118945	2.969265
49	1	0	-3.090858	-0.794238	3.504714
50	1	0	-4.934433	-0.410903	2.188456
51	1	0	-4.950388	-1.244917	-2.011837
52	1	0	-7.038318	-0.395932	0.958232
53	1	0	-7.092444	-0.904592	-0.740062
54	1	0	-6.614883	0.742624	-0.324399
55	7	0	1.160682	-1.756229	0.160516
56	7	0	-1.015216	-1.818245	0.251606
57	17	0	0.165489	1.271704	2.316012
58	44	0	-0.137138	1.031659	-0.092110
59	17	0	-0.509003	0.841430	-2.493019
60	6	0	2.596345	2.286191	0.323143
61	1	0	3.336079	1.479861	0.206857
62	1	0	3.076367	3.202929	-0.044799
63	1	0	2.353883	2.369838	1.382660
64	6	0	0.420534	4.383444	0.473315
65	1	0	-0.200661	5.288181	0.504534
66	1	0	0.519098	4.006520	1.495782
67	1	0	1.405308	4.677081	0.102204
68	1	0	-0.218612	3.536082	-1.486366
69	1	0	-3.358849	3.401258	-0.572794
70	1	0	-1.616957	2.846928	1.136901

TS20c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.660949	2.375541	-0.491866
2	6	0	2.580501	2.096607	-1.660296
3	1	0	2.041196	1.995354	-2.600577
4	1	0	3.161779	1.181232	-1.501643
5	6	0	2.408062	2.543691	0.824668
6	1	0	1.710497	2.758454	1.633571
7	1	0	2.882417	1.586700	1.080831
8	6	0	-0.309533	-1.150744	0.139029
9	6	0	-2.807199	-1.194744	0.165460
10	6	0	-1.364890	-3.212166	0.460076
11	6	0	-2.744866	-1.590095	-2.342295
12	6	0	0.131043	-3.378715	0.714408
13	6	0	-5.418735	-0.203684	-0.012476
14	6	0	-2.871760	-1.026809	2.696076
15	6	0	-3.426122	-1.114220	-1.092617
16	6	0	-3.494596	-0.853278	1.341761
17	6	0	2.063000	-1.257600	2.748440
18	6	0	-4.792040	-0.352862	1.224737
19	6	0	-4.723295	-0.600890	-1.154395
20	6	0	2.070699	-1.836204	0.269868
21	6	0	-6.803956	0.372564	-0.112119
22	6	0	4.837798	-1.429397	0.149513
23	6	0	2.756010	-1.424830	1.426915

24	6	0	2.062979	-2.731827	-2.107026
25	6	0	2.761671	-2.143345	-0.916406
26	6	0	4.137449	-1.916971	-0.953932
27	6	0	4.133333	-1.213011	1.332885
28	6	0	6.312777	-1.152482	0.066511
29	1	0	-1.981905	-3.550478	1.297025
30	1	0	2.784749	-0.979510	3.522222
31	1	0	-1.698756	-3.734406	-0.444758
32	1	0	-2.526320	-2.664667	-2.293435
33	1	0	-1.795364	-1.071287	-2.516424
34	1	0	-3.387883	-1.428679	-3.212622
35	1	0	0.358312	-3.576794	1.769053
36	1	0	0.582547	-4.171630	0.111794
37	1	0	-1.960488	-0.425688	2.784770
38	1	0	-2.603872	-2.073434	2.889072
39	1	0	-3.568535	-0.716824	3.480414
40	1	0	1.584754	-2.191703	3.068452
41	1	0	1.287757	-0.484326	2.713742
42	1	0	-5.327960	-0.077421	2.131015
43	1	0	-5.207454	-0.527396	-2.126402
44	1	0	-6.769674	1.465759	-0.204333
45	1	0	-7.399234	0.140554	0.777014
46	1	0	-7.335706	-0.011527	-0.988598
47	1	0	1.294567	-2.050796	-2.486775
48	1	0	1.581108	-3.686215	-1.859263
49	1	0	2.778371	-2.924743	-2.911730
50	1	0	4.676422	-2.139409	-1.872725
51	1	0	4.670002	-0.885163	2.221153
52	1	0	6.807048	-1.820510	-0.646293
53	1	0	6.799288	-1.270840	1.040102
54	1	0	6.498764	-0.123931	-0.268391
55	7	0	-1.498608	-1.761374	0.275845
56	7	0	0.658981	-2.068135	0.323264
57	44	0	0.106548	0.827726	-0.259918
58	17	0	-0.271932	1.290427	2.110793
59	6	0	3.492714	3.628194	0.780785
60	1	0	4.327798	3.359808	0.126135
61	1	0	3.093931	4.589860	0.436821
62	1	0	3.898997	3.780365	1.786752
63	1	0	3.291860	2.929257	-1.752595
64	6	0	0.452259	3.109697	-0.738550
65	6	0	-1.326753	1.875709	-0.814914
66	1	0	-1.481096	1.897802	-1.901491
67	17	0	0.305085	0.207630	-2.615511
68	1	0	0.281803	3.302176	-1.798905
69	6	0	-2.450968	2.463750	-0.037883
70	1	0	-3.275132	1.738240	-0.108430
71	1	0	-2.810649	3.391433	-0.503695
72	1	0	-2.228830	2.616734	1.017685
73	6	0	-0.005891	4.200504	0.198723
74	1	0	-0.154442	3.829683	1.216101
75	1	0	-0.936066	4.660900	-0.142837
76	1	0	0.757240	4.988410	0.230534

21a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.860403	2.694958	0.043649

2	6	0	-0.864142	3.236831	-0.723439
3	6	0	-2.176220	3.208227	1.419586
4	1	0	-1.291982	3.560348	1.951264
5	1	0	-2.644726	2.435313	2.035031
6	6	0	-2.894577	1.773221	-0.563905
7	1	0	-2.585014	1.470927	-1.569158
8	1	0	-2.973133	0.858147	0.044365
9	6	0	1.599623	1.536350	-0.381345
10	6	0	0.373191	-1.075443	-0.008583
11	6	0	2.876701	-1.138380	0.001467
12	6	0	1.446220	-3.163007	-0.022362
13	6	0	2.810228	-1.192679	2.532449
14	6	0	-0.042193	-3.377480	0.231345
15	6	0	5.515267	-0.209047	0.035473
16	6	0	2.893302	-1.229940	-2.534192
17	6	0	3.518867	-0.936923	1.235048
18	6	0	3.546064	-0.929761	-1.215708
19	6	0	-2.089185	-2.274241	-2.379748
20	6	0	4.855805	-0.448336	-1.170121
21	6	0	4.833359	-0.471253	1.225353
22	6	0	-2.001554	-1.832382	0.118120
23	6	0	6.919693	0.327272	0.055221
24	6	0	-4.783969	-1.528330	0.202866
25	6	0	-2.743573	-1.937961	-1.072313
26	6	0	-1.890526	-1.772786	2.660837
27	6	0	-2.640396	-1.685953	1.363087
28	6	0	-4.026246	-1.515027	1.373256
29	6	0	-4.126173	-1.764903	-1.004238
30	6	0	-6.269659	-1.302391	0.241206
31	1	0	1.765763	-3.549702	-0.997755
32	1	0	-2.831864	-2.304682	-3.182370
33	1	0	1.993754	1.434051	-1.403667
34	1	0	2.081573	-3.611031	0.747380
35	1	0	2.419753	-2.216269	2.591023
36	1	0	1.957092	-0.512601	2.649694
37	1	0	3.489389	-1.047157	3.377611
38	1	0	-0.503126	-4.065195	-0.483620
39	1	0	-0.247382	-3.745866	1.243782
40	1	0	1.909711	-0.755226	-2.625786
41	1	0	2.751045	-2.310217	-2.669459
42	1	0	3.519553	-0.880829	-3.360556
43	1	0	-1.606621	-3.259526	-2.340519
44	1	0	-1.327339	-1.534254	-2.644265
45	1	0	5.378890	-0.271808	-2.108055
46	1	0	5.337014	-0.308669	2.176373
47	1	0	6.922071	1.422211	0.131072
48	1	0	7.462697	0.062641	-0.857599
49	1	0	7.483103	-0.058024	0.911379
50	1	0	-1.038100	-1.087800	2.689526
51	1	0	-1.523084	-2.793082	2.833368
52	1	0	-2.548409	-1.520710	3.497673
53	1	0	-4.526357	-1.385273	2.331046
54	1	0	-4.704861	-1.830739	-1.923539
55	1	0	-6.699366	-1.619519	1.196883
56	1	0	-6.778904	-1.847260	-0.560423
57	1	0	-6.506998	-0.238217	0.113928
58	7	0	1.567177	-1.702041	0.001039
59	7	0	-0.585086	-2.027482	0.067175
60	17	0	-0.000207	1.097885	2.281389
61	44	0	-0.093510	0.892151	-0.138779
62	17	0	-0.250504	0.649577	-2.574174

63	6	0	-4.285742	2.413131	-0.628734
64	1	0	-4.674380	2.652747	0.366543
65	1	0	-4.265799	3.336451	-1.219028
66	1	0	-4.988726	1.721916	-1.105887
67	1	0	-2.881129	4.047482	1.329176
68	6	0	2.506902	2.281626	0.527339
69	1	0	3.481875	1.773149	0.540558
70	1	0	2.692544	3.276476	0.094671
71	1	0	2.127328	2.381960	1.543679
72	6	0	0.005341	4.382289	-0.293732
73	1	0	-0.553808	5.326152	-0.363803
74	1	0	0.351004	4.282762	0.739576
75	1	0	0.881033	4.476495	-0.942244
76	1	0	-0.838239	2.973509	-1.779023

21b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.568196	2.933195	-0.221254
2	6	0	0.582381	3.532625	0.511947
3	6	0	2.795793	2.289148	0.355480
4	1	0	2.716361	2.139974	1.435247
5	1	0	3.017341	1.324928	-0.122312
6	6	0	-1.599705	1.564517	0.273396
7	6	0	-0.074237	-0.937849	0.076955
8	6	0	-2.552853	-1.268291	0.069082
9	6	0	-0.923092	-3.120999	0.274119
10	6	0	-2.378944	-1.470713	-2.448534
11	6	0	0.597853	-3.192759	0.151875
12	6	0	-5.275769	-0.658280	-0.108643
13	6	0	-2.645017	-1.178506	2.600970
14	6	0	-3.164570	-1.222277	-1.194675
15	6	0	-3.284707	-1.053140	1.248068
16	6	0	2.605336	-1.639395	2.491720
17	6	0	-4.638801	-0.733919	1.130250
18	6	0	-4.523583	-0.915145	-1.256764
19	6	0	2.365560	-1.441077	-0.031040
20	6	0	-6.731344	-0.294650	-0.207674
21	6	0	5.091194	-0.855722	-0.281703
22	6	0	3.161752	-1.361954	1.125939
23	6	0	2.130543	-1.583730	-2.559013
24	6	0	2.931951	-1.335178	-1.314365
25	6	0	4.289419	-1.024170	-1.409960
26	6	0	4.513314	-1.052237	0.972499
27	6	0	6.539853	-0.476927	-0.412826
28	1	0	-1.287573	-3.491352	1.238930
29	1	0	3.352001	-1.418685	3.260153
30	1	0	-1.979557	1.495758	1.303996
31	1	0	-1.441907	-3.672170	-0.517217
32	1	0	-1.862239	-2.438077	-2.423966
33	1	0	-1.613314	-0.696674	-2.588761
34	1	0	-3.036981	-1.467455	-3.322470
35	1	0	1.069419	-3.677903	1.012026
36	1	0	0.927624	-3.713395	-0.754536
37	1	0	-1.709438	-0.611493	2.667951
38	1	0	-2.411247	-2.226055	2.833344
39	1	0	-3.322014	-0.818112	3.381191
40	1	0	2.330347	-2.697010	2.600374

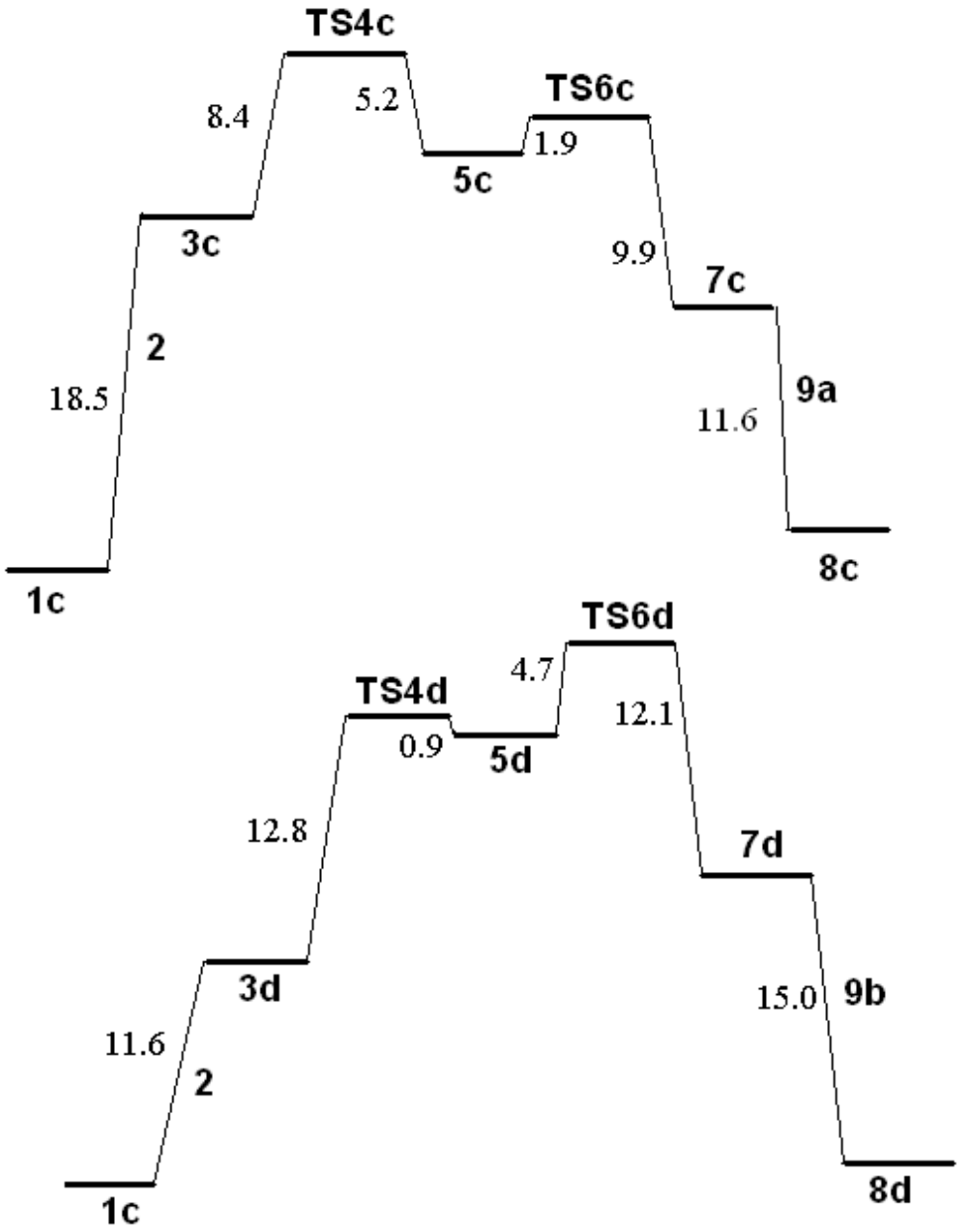
41	1	0	1.718165	-1.031532	2.693640
42	1	0	-5.213273	-0.554483	2.037058
43	1	0	-5.006004	-0.873729	-2.231456
44	1	0	-6.859103	0.788748	-0.328524
45	1	0	-7.280154	-0.588862	0.692598
46	1	0	-7.205991	-0.775314	-1.069250
47	1	0	1.365683	-0.812703	-2.704092
48	1	0	1.623739	-2.555867	-2.524316
49	1	0	2.783868	-1.583583	-3.436531
50	1	0	4.731942	-0.925972	-2.399256
51	1	0	5.132764	-0.972441	1.863659
52	1	0	6.959036	-0.816598	-1.365347
53	1	0	7.141040	-0.902635	0.397208
54	1	0	6.663527	0.612895	-0.371874
55	7	0	-1.192318	-1.685386	0.151619
56	7	0	0.981640	-1.780429	0.091198
57	17	0	0.091255	1.225356	-2.367148
58	44	0	0.156167	1.087932	0.072000
59	17	0	0.342343	0.996078	2.504327
60	6	0	-2.585863	2.123774	-0.684043
61	1	0	-3.482094	1.486551	-0.666315
62	1	0	-2.914038	3.108631	-0.318812
63	1	0	-2.211337	2.208746	-1.703680
64	6	0	-0.375781	4.522802	-0.076025
65	1	0	0.048437	5.531597	0.025682
66	1	0	-0.547209	4.335340	-1.140495
67	1	0	-1.337209	4.530688	0.445188
68	1	0	0.620689	3.456641	1.597810
69	1	0	3.661833	2.933382	0.146449
70	1	0	1.575838	3.100650	-1.297725

21c

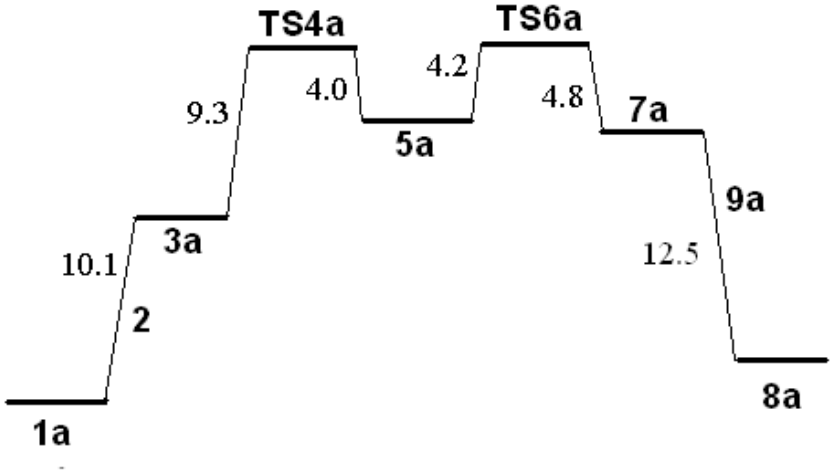
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.948457	2.580873	-0.318382
2	6	0	2.935283	1.583558	-0.868182
3	1	0	2.685418	1.258665	-1.880183
4	1	0	3.016651	0.697390	-0.221814
5	6	0	2.338562	3.205683	0.998496
6	1	0	1.459595	3.593639	1.518106
7	1	0	2.758778	2.437279	1.656490
8	6	0	-0.369153	-1.105118	0.116011
9	6	0	-2.873190	-1.103403	0.178432
10	6	0	-1.487142	-3.135205	0.480349
11	6	0	-2.840136	-1.522445	-2.322407
12	6	0	-0.000550	-3.338420	0.745225
13	6	0	-5.497318	-0.146567	0.037248
14	6	0	-2.855750	-0.835712	2.697284
15	6	0	-3.515384	-1.045751	-1.069107
16	6	0	-3.534289	-0.735461	1.362513
17	6	0	2.076934	-1.478790	2.740920
18	6	0	-4.841497	-0.259832	1.265114
19	6	0	-4.818967	-0.546794	-1.113608
20	6	0	1.988682	-1.917034	0.233990
21	6	0	-6.895580	0.400923	-0.039496
22	6	0	4.776214	-1.714670	0.070933
23	6	0	2.725162	-1.613996	1.393393
24	6	0	1.870508	-2.716871	-2.173345

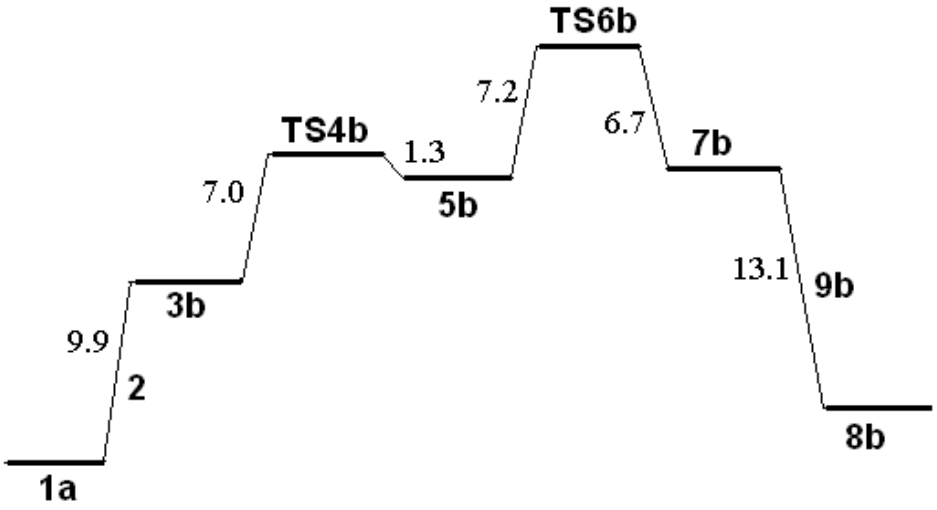
25	6	0	2.633273	-2.225970	-0.978064
26	6	0	4.020820	-2.100598	-1.036560
27	6	0	4.112343	-1.499140	1.277666
28	6	0	6.265561	-1.541549	-0.034537
29	1	0	-2.118896	-3.444215	1.317839
30	1	0	2.772890	-1.030855	3.456293
31	1	0	-1.830424	-3.660956	-0.419505
32	1	0	-2.657924	-2.604444	-2.289262
33	1	0	-1.871398	-1.034022	-2.481941
34	1	0	-3.469077	-1.325591	-3.195604
35	1	0	0.216821	-3.502562	1.807879
36	1	0	0.429071	-4.166133	0.173612
37	1	0	-1.951634	-0.215309	2.725800
38	1	0	-2.551472	-1.865521	2.923786
39	1	0	-3.528069	-0.507833	3.495579
40	1	0	1.796375	-2.464310	3.137027
41	1	0	1.183955	-0.848667	2.708678
42	1	0	-5.361192	0.031156	2.176118
43	1	0	-5.321952	-0.487995	-2.076889
44	1	0	-6.889702	1.498411	-0.040371
45	1	0	-7.497593	0.081648	0.817820
46	1	0	-7.403408	0.075600	-0.952759
47	1	0	1.199557	-1.941474	-2.558429
48	1	0	1.261773	-3.596008	-1.927633
49	1	0	2.559738	-3.004093	-2.972888
50	1	0	4.524673	-2.322892	-1.975118
51	1	0	4.688406	-1.247592	2.166157
52	1	0	6.699009	-2.233545	-0.764024
53	1	0	6.758709	-1.706780	0.928720
54	1	0	6.518364	-0.524707	-0.361434
55	7	0	-1.575751	-1.685898	0.276810
56	7	0	0.568027	-2.062041	0.308020
57	44	0	0.140015	0.814653	-0.276416
58	17	0	0.065185	1.283924	2.111458
59	6	0	3.359273	4.330991	0.792421
60	1	0	4.275981	3.970648	0.311930
61	1	0	2.950776	5.132853	0.167249
62	1	0	3.641363	4.768377	1.756316
63	1	0	3.937173	2.035394	-0.875400
64	6	0	0.937266	3.081469	-1.094234
65	6	0	-1.543127	1.461466	-0.580503
66	1	0	-1.942290	1.262423	-1.586825
67	17	0	0.286698	0.319618	-2.670425
68	1	0	0.868015	2.732007	-2.122469
69	6	0	-2.432764	2.314417	0.247551
70	1	0	-3.422461	1.838632	0.303732
71	1	0	-2.588082	3.267980	-0.279541
72	1	0	-2.051904	2.502691	1.251015
73	6	0	0.100722	4.273025	-0.729061
74	1	0	-0.210041	4.257779	0.319946
75	1	0	-0.795875	4.328568	-1.352858
76	1	0	0.666395	5.200493	-0.894540

The Gas Phase Free Gibbs Energy Profiles

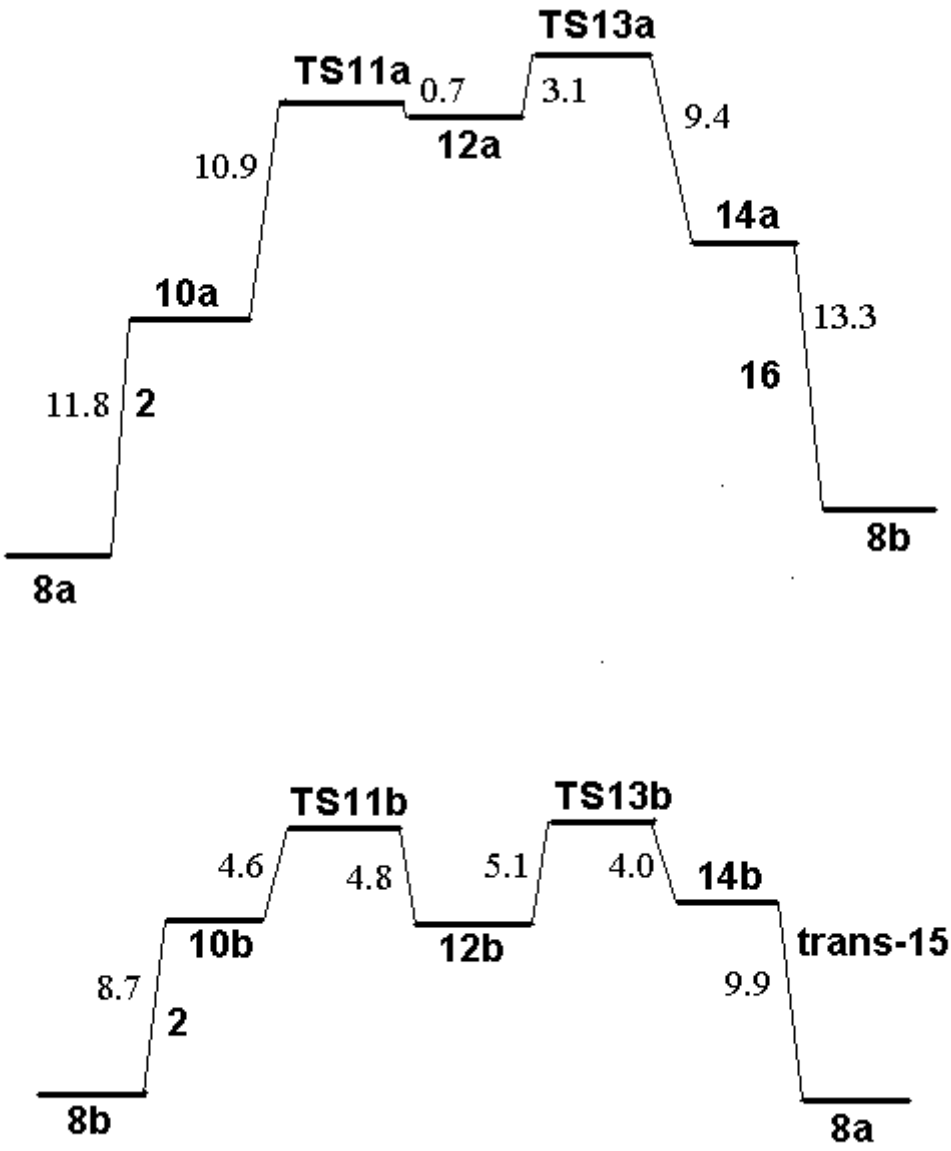


The free Gibbs energy profile (kcal/mol) of **2** metathesis by the first generation Grubbs catalyst.

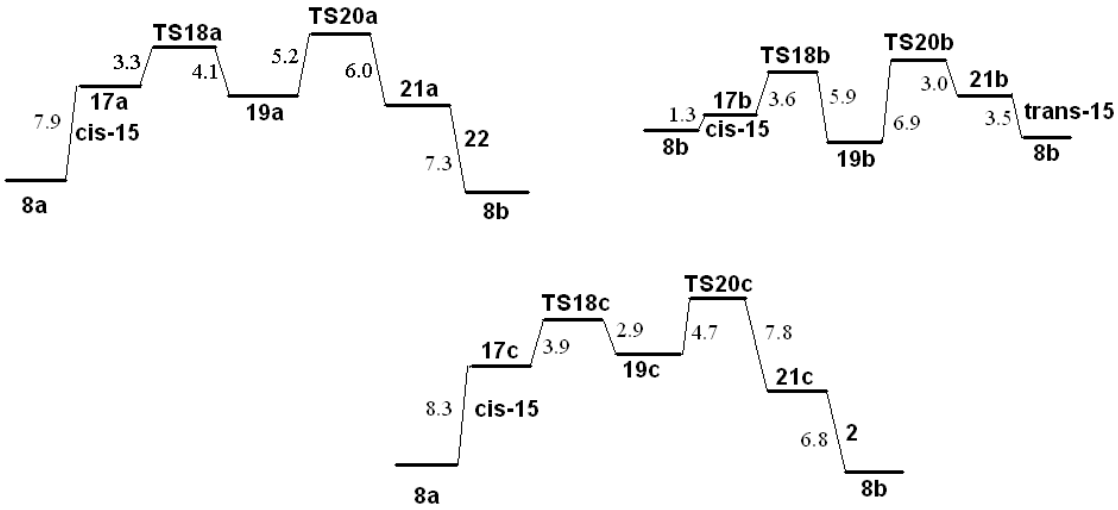




The free Gibbs energy profile (kcal/mol) of **2** metathesis by the second generation Grubbs catalyst.



The free Gibbs energy profiles (kcal/mol) of **2** metathesis by metallacarbenes **8a** and **8b**



The free Gibbs reaction energy profile (kcal/mol) of **cis-15** metathesis mediated by metallacarbenes **8a** and **8b**