

XYZ coordinates of pyrene-benzene complex

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.259284	-1.133271	0.061505
2	6	0	1.071959	-0.599109	2.500709
3	6	0	-0.950285	-1.255635	1.304500
4	6	0	-0.234791	-0.979741	2.519407
5	6	0	1.109010	-0.736046	0.041591
6	6	0	1.790582	-0.456826	1.264538
7	6	0	1.795771	-0.598701	-1.202564
8	6	0	3.135603	-0.179970	-1.198844
9	6	0	3.130565	-0.040993	1.218579
10	6	0	3.792262	0.097658	-0.000699
11	1	0	1.597420	-0.389066	3.429448
12	1	0	3.659232	-0.071211	-2.145717
13	1	0	3.650130	0.175663	2.148994
14	1	0	4.829103	0.422771	-0.017312
15	1	0	-0.765833	-1.077190	3.463467
16	6	0	-0.945168	-1.397427	-1.162029
17	6	0	-2.301658	-1.634096	1.298414
18	6	0	-2.296709	-1.772865	-1.118349
19	1	0	-2.821414	-1.971609	-2.049847
20	6	0	-2.965151	-1.887749	0.099218
21	1	0	-4.012299	-2.178136	0.113748
22	1	0	-2.830329	-1.725169	2.244321
23	6	0	-0.224579	-1.262399	-2.397666
24	6	0	1.082190	-0.881763	-2.417265
25	1	0	-0.751698	-1.467507	-3.326553
26	1	0	1.611506	-0.779421	-3.361799
27	6	0	-2.437283	2.083996	-0.119020
28	6	0	-1.753798	2.276951	1.082815
29	6	0	-0.378224	2.513715	1.073863
30	6	0	0.314939	2.556520	-0.136692
31	6	0	-0.368489	2.366420	-1.338581
32	6	0	-1.743980	2.129459	-1.329820

33	1	0	-3.505383	1.883673	-0.111156
34	1	0	-2.290442	2.228539	2.026804
35	1	0	0.157202	2.642721	2.010324
36	1	0	1.390368	2.710874	-0.141805
37	1	0	0.174486	2.380511	-2.279431
38	1	0	-2.272925	1.965799	-2.265146

XYZ coordinates of each optimised geometry on C₉₆H₂₄

Benzene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.221586	-1.330550	0.000000
2	6	0	-0.221586	-0.618950	1.232527
3	6	0	-0.221586	0.804250	1.232527
4	6	0	-0.221586	1.515850	0.000000
5	6	0	-0.221586	0.804250	-1.232527
6	6	0	-0.221586	-0.618950	-1.232527
7	6	0	-0.221586	-2.749850	0.000000
8	6	0	-0.221586	-1.328600	2.461677
9	6	0	-0.221586	1.513900	2.461677
10	6	0	-0.221586	2.935150	0.000000
11	6	0	-0.221586	1.513900	-2.461677
12	6	0	-0.221586	-1.328600	-2.461677
13	6	0	-0.221586	-3.460742	-1.233398
14	6	0	-0.221586	-3.460742	1.233398
15	6	0	-0.221586	-2.752199	2.460629
16	6	0	-0.221586	-0.615892	3.694026
17	6	0	-0.221586	0.801192	3.694026
18	6	0	-0.221586	2.937500	2.460629
19	6	0	-0.221586	3.646042	1.233398
20	6	0	-0.221586	3.646042	-1.233398
21	6	0	-0.221586	2.937500	-2.460629
22	6	0	-0.221586	0.801192	-3.694026

23	6	0	-0.221586	-0.615892	-3.694026
24	6	0	-0.221586	-2.752199	-2.460629
25	6	0	-0.221586	-4.888141	-1.232765
26	6	0	-0.221586	-4.888141	1.232765
27	6	0	-0.221586	-3.465351	3.697110
28	6	0	-0.221586	-1.330140	4.929875
29	6	0	-0.221586	1.515440	4.929875
30	6	0	-0.221586	3.650652	3.697110
31	6	0	-0.221586	5.073442	1.232765
32	6	0	-0.221586	5.073442	-1.232765
33	6	0	-0.221586	3.650652	-3.697110
34	6	0	-0.221586	1.515440	-4.929875
35	6	0	-0.221586	-1.330140	-4.929875
36	6	0	-0.221586	-3.465351	-3.697110
37	6	0	-0.221586	-5.597750	0.000000
38	6	0	-0.221586	-2.752550	4.928031
39	6	0	-0.221586	2.937850	4.928031
40	6	0	-0.221586	5.783050	0.000000
41	6	0	-0.221586	2.937850	-4.928031
42	6	0	-0.221586	-2.752550	-4.928031
43	6	0	-0.221586	-5.595350	-2.463782
44	6	0	-0.221586	-5.595350	2.463782
45	6	0	-0.221586	-4.885048	3.694062
46	6	0	-0.221586	-0.617652	6.157844
47	6	0	-0.221586	0.802953	6.157844
48	6	0	-0.221586	5.070348	3.694062
49	6	0	-0.221586	5.780651	2.463782
50	6	0	-0.221586	5.780651	-2.463782
51	6	0	-0.221586	5.070348	-3.694062
52	6	0	-0.221586	0.802953	-6.157844
53	6	0	-0.221586	-0.617652	-6.157844
54	6	0	-0.221586	-4.885048	-3.694062
55	6	0	-0.221586	-7.030550	0.000000
56	6	0	-0.221586	-3.468950	6.168872
57	6	0	-0.221586	3.654250	6.168872
58	6	0	-0.221586	7.215850	0.000000
59	6	0	-0.221586	3.654250	-6.168872
60	6	0	-0.221586	-3.468950	-6.168872

61	6	0	-0.221586	-7.033523	-2.454947
62	6	0	-0.221586	-7.033523	2.454947
63	6	0	-0.221586	-5.596483	4.943974
64	6	0	-0.221586	-1.344390	7.398921
65	6	0	-0.221586	1.529691	7.398921
66	6	0	-0.221586	5.781783	4.943974
67	6	0	-0.221586	7.218824	2.454947
68	6	0	-0.221586	7.218824	-2.454947
69	6	0	-0.221586	5.781783	-4.943974
70	6	0	-0.221586	1.529691	-7.398921
71	6	0	-0.221586	-1.344390	-7.398921
72	6	0	-0.221586	-5.596483	-4.943974
73	6	0	-0.221586	-7.711368	-1.241703
74	6	0	-0.221586	-7.711368	1.241703
75	6	0	-0.221586	-4.884705	6.137627
76	6	0	-0.221586	-2.734013	7.379329
77	6	0	-0.221586	2.919313	7.379329
78	6	0	-0.221586	5.070005	6.137627
79	6	0	-0.221586	7.896669	1.241703
80	6	0	-0.221586	7.896669	-1.241703
81	6	0	-0.221586	5.070005	-6.137627
82	6	0	-0.221586	2.919313	-7.379329
83	6	0	-0.221586	-2.734013	-7.379329
84	6	0	-0.221586	-4.884705	-6.137627
85	6	0	-0.221586	-7.718471	-3.725024
86	6	0	-0.221586	-7.718471	3.725024
87	6	0	-0.221586	-7.038875	4.902117
88	6	0	-0.221586	-0.586945	8.627141
89	6	0	-0.221586	0.772245	8.627141
90	6	0	-0.221586	7.224176	4.902117
91	6	0	-0.221586	7.903771	3.725024
92	6	0	-0.221586	7.903771	-3.725024
93	6	0	-0.221586	7.224176	-4.902117
94	6	0	-0.221586	0.772245	-8.627141
95	6	0	-0.221586	-0.586945	-8.627141
96	6	0	-0.221586	-7.038875	-4.902117
97	1	0	-0.221586	-8.799368	-1.240852
98	1	0	-0.221586	-8.799368	1.240852

99	1	0	-0.221586	-5.427968	7.080287
100	1	0	-0.221586	-3.278749	8.321139
101	1	0	-0.221586	3.464050	8.321139
102	1	0	-0.221586	5.613269	7.080287
103	1	0	-0.221586	8.984668	1.240852
104	1	0	-0.221586	8.984668	-1.240852
105	1	0	-0.221586	5.613269	-7.080287
106	1	0	-0.221586	3.464050	-8.321139
107	1	0	-0.221586	-3.278749	-8.321139
108	1	0	-0.221586	-5.427968	-7.080287
109	1	0	-0.221586	-8.805759	-3.719972
110	1	0	-0.221586	-8.805759	3.719972
111	1	0	-0.221586	-7.578145	5.846262
112	1	0	-0.221586	-1.134964	9.566234
113	1	0	-0.221586	1.320264	9.566234
114	1	0	-0.221586	7.763445	5.846262
115	1	0	-0.221586	8.991059	3.719972
116	1	0	-0.221586	8.991059	-3.719972
117	1	0	-0.221586	7.763445	-5.846262
118	1	0	-0.221586	1.320264	-9.566234
119	1	0	-0.221586	-1.134964	-9.566234
120	1	0	-0.221586	-7.578145	-5.846262
121	6	0	3.166963	0.072686	0.000000
122	6	0	3.167093	-0.625646	-1.209157
123	6	0	3.169573	-2.021700	-1.209537
124	6	0	3.171276	-2.719410	0.000000
125	6	0	3.169573	-2.021700	1.209537
126	6	0	3.167093	-0.625646	1.209157
127	1	0	3.145105	1.159130	0.000000
128	1	0	3.143908	-0.081978	-2.149980
129	1	0	3.149220	-2.565405	-2.150146
130	1	0	3.150659	-3.806015	0.000000
131	1	0	3.149220	-2.565405	2.150146
132	1	0	3.143908	-0.081978	2.149980

Naphthalene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.563980	-1.149947	-0.372716
2	6	0	-1.233833	0.105731	-0.380877
3	6	0	-0.481898	1.313611	-0.347427
4	6	0	0.939891	1.265811	-0.305815
5	6	0	1.609744	0.010133	-0.297655
6	6	0	0.857808	-1.197747	-0.331105
7	6	0	-1.313855	-2.354517	-0.406075
8	6	0	-2.651725	0.153400	-0.422374
9	6	0	-1.149915	2.565848	-0.355565
10	6	0	1.689766	2.470381	-0.272456
11	6	0	3.027636	-0.037536	-0.256157
12	6	0	1.525825	-2.449984	-0.322967
13	6	0	-0.642889	-3.610054	-0.397880
14	6	0	-2.736008	-2.305656	-0.447687
15	6	0	-3.402982	-1.055373	-0.455813
16	6	0	-3.320842	1.409924	-0.430505
17	6	0	-2.572137	2.612613	-0.397199
18	6	0	-0.396879	3.773512	-0.322084
19	6	0	1.018800	3.725918	-0.280651
20	6	0	3.111918	2.421520	-0.230844
21	6	0	3.778893	1.171237	-0.222719
22	6	0	3.696752	-1.294060	-0.248026
23	6	0	2.948048	-2.496749	-0.281333
24	6	0	0.772789	-3.657648	-0.356448
25	6	0	-1.397581	-4.821164	-0.431442
26	6	0	-3.489625	-3.517434	-0.481224
27	6	0	-4.828945	-1.006801	-0.497541
28	6	0	-4.746847	1.457232	-0.472246
29	6	0	-3.243409	3.872295	-0.405364
30	6	0	-1.069266	5.032599	-0.330288
31	6	0	1.773491	4.937028	-0.247089
32	6	0	3.865536	3.633298	-0.197308
33	6	0	5.204855	1.122665	-0.180991
34	6	0	5.122757	-1.341368	-0.206286

35	6	0	3.619319	-3.756431	-0.273168
36	6	0	1.445177	-4.916735	-0.348244
37	6	0	-2.818518	-4.771548	-0.473012
38	6	0	-5.496800	0.249049	-0.505641
39	6	0	-2.490327	5.078529	-0.371895
40	6	0	3.194429	4.887412	-0.205520
41	6	0	5.872711	-0.133185	-0.172891
42	6	0	2.866237	-4.962665	-0.306637
43	6	0	-0.726689	-6.072317	-0.423209
44	6	0	-4.907812	-3.466707	-0.522701
45	6	0	-5.576443	-2.213318	-0.530847
46	6	0	-5.412363	2.711254	-0.480294
47	6	0	-4.661799	3.916931	-0.446904
48	6	0	-0.316596	6.235893	-0.296858
49	6	0	1.102600	6.188181	-0.255323
50	6	0	5.283723	3.582571	-0.155830
51	6	0	5.952354	2.329182	-0.147684
52	6	0	5.788274	-2.595390	-0.198238
53	6	0	5.037709	-3.801067	-0.231627
54	6	0	0.692506	-6.120029	-0.381674
55	6	0	-3.575526	-5.987575	-0.506688
56	6	0	-6.928179	0.297170	-0.547533
57	6	0	-3.164698	6.342678	-0.380111
58	6	0	3.951436	6.103439	-0.171844
59	6	0	7.304090	-0.181306	-0.130999
60	6	0	3.540608	-6.226814	-0.298421
61	6	0	-1.494033	-7.288232	-0.457190
62	6	0	-5.660161	-4.691966	-0.556325
63	6	0	-7.012896	-2.156186	-0.572806
64	6	0	-6.849404	2.750726	-0.522433
65	6	0	-5.330908	5.189978	-0.454882
66	6	0	-1.001287	7.500624	-0.305374
67	6	0	1.869943	7.404096	-0.221342
68	6	0	6.036072	4.807830	-0.122206
69	6	0	7.388806	2.272050	-0.105726
70	6	0	7.225314	-2.634862	-0.156098
71	6	0	5.706818	-5.074114	-0.223650
72	6	0	1.377198	-7.384760	-0.373158

73	6	0	-2.881624	-7.221981	-0.497618
74	6	0	-4.988836	-5.908800	-0.547761
75	6	0	-7.649669	-0.920913	-0.580177
76	6	0	-7.566975	1.560985	-0.554699
77	6	0	-4.580089	6.359000	-0.421825
78	6	0	-2.390184	7.527716	-0.346204
79	6	0	3.257535	7.337845	-0.180913
80	6	0	5.364747	6.024664	-0.130771
81	6	0	8.025579	1.036777	-0.098354
82	6	0	7.942886	-1.445121	-0.123833
83	6	0	4.956000	-6.243136	-0.256707
84	6	0	2.766094	-7.411852	-0.332327
85	6	0	-0.778236	-8.541146	-0.447644
86	6	0	-7.099729	-4.601691	-0.598068
87	6	0	-7.739455	-3.402487	-0.605862
88	6	0	-7.491380	4.043037	-0.529430
89	6	0	-6.773264	5.196590	-0.497484
90	6	0	-0.203695	8.702659	-0.270627
91	6	0	1.154147	8.657010	-0.230887
92	6	0	7.475640	4.717555	-0.080463
93	6	0	8.115366	3.518351	-0.072670
94	6	0	7.867290	-3.927173	-0.149102
95	6	0	7.149174	-5.080726	-0.181048
96	6	0	0.579606	-8.586795	-0.407905
97	1	0	-3.457181	-8.144924	-0.523208
98	1	0	-5.562950	-6.832642	-0.573316
99	1	0	-8.736561	-0.883521	-0.611979
100	1	0	-8.653924	1.596676	-0.586519
101	1	0	-5.091424	7.319335	-0.428038
102	1	0	-2.903019	8.487250	-0.352469
103	1	0	3.833092	8.260788	-0.155324
104	1	0	5.938860	6.948506	-0.105216
105	1	0	9.112472	0.999385	-0.066552
106	1	0	9.029835	-1.480812	-0.092013
107	1	0	5.467335	-7.203471	-0.250494
108	1	0	3.278930	-8.371386	-0.326063
109	1	0	-1.356982	-9.461263	-0.473302
110	1	0	-7.669902	-5.527151	-0.623522

111	1	0	-8.825497	-3.360921	-0.637600
112	1	0	-8.577758	4.074505	-0.561271
113	1	0	-7.280559	6.158274	-0.503564
114	1	0	-0.719900	9.659588	-0.277015
115	1	0	1.732893	9.577127	-0.205230
116	1	0	8.045813	5.643015	-0.055010
117	1	0	9.201407	3.476785	-0.040931
118	1	0	8.953668	-3.958641	-0.117260
119	1	0	7.656470	-6.042410	-0.174967
120	1	0	1.095811	-9.543724	-0.401516
121	6	0	0.141091	0.010059	3.056666
122	6	0	-1.355216	-2.360972	2.990834
123	6	0	0.775054	-1.211314	3.050626
124	6	0	0.019829	-2.409071	3.017980
125	6	0	-1.276460	0.094734	3.030268
126	6	0	-2.041424	-1.117343	2.996217
127	6	0	-1.961715	1.338767	3.008032
128	6	0	-3.335935	1.386262	2.955635
129	6	0	-3.458418	-1.032163	2.942371
130	6	0	-4.092232	0.189080	2.923331
131	1	0	0.719589	0.930751	3.061137
132	1	0	-1.937247	-3.278416	2.943369
133	1	0	-1.378573	2.256511	3.012355
134	1	0	-3.846493	2.344516	2.915730
135	1	0	-4.035299	-1.952826	2.894738
136	1	0	-5.175474	0.239987	2.860178
137	1	0	0.532503	-3.366427	2.992391
138	1	0	1.860410	-1.261539	3.047861

Anthracene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.018639	-1.224180	-0.497678
2	6	0	-1.225006	-0.532558	-0.475231

3	6	0	-1.247551	0.889764	-0.430609
4	6	0	-0.026451	1.620463	-0.408434
5	6	0	1.217194	0.928841	-0.430881
6	6	0	1.239739	-0.493481	-0.475503
7	6	0	0.041122	-2.642604	-0.542178
8	6	0	-2.442760	-1.261255	-0.497346
9	6	0	-2.487788	1.579491	-0.408224
10	6	0	-0.048935	3.038887	-0.363935
11	6	0	2.434948	1.657538	-0.408767
12	6	0	2.479976	-1.183208	-0.497889
13	6	0	1.285626	-3.333505	-0.564603
14	6	0	-1.180859	-3.372609	-0.564331
15	6	0	-2.419160	-2.683959	-0.541980
16	6	0	-3.686244	-0.568522	-0.474864
17	6	0	-3.708692	0.847688	-0.430434
18	6	0	-2.509291	3.002229	-0.363590
19	6	0	-1.293439	3.729788	-0.341510
20	6	0	1.173047	3.768893	-0.341782
21	6	0	2.411348	3.080242	-0.364133
22	6	0	3.678432	0.964806	-0.431249
23	6	0	3.700880	-0.451404	-0.475679
24	6	0	2.501479	-2.605945	-0.542523
25	6	0	1.307605	-4.760034	-0.609357
26	6	0	-1.157615	-4.799118	-0.609084
27	6	0	-3.644188	-3.416272	-0.564203
28	6	0	-4.910623	-1.301920	-0.497122
29	6	0	-4.955700	1.541903	-0.407903
30	6	0	-3.756914	3.695339	-0.341094
31	6	0	-1.315417	5.156317	-0.296756
32	6	0	1.149803	5.195402	-0.297028
33	6	0	3.636376	3.812555	-0.341909
34	6	0	4.902810	1.698204	-0.408991
35	6	0	4.947887	-1.145620	-0.498209
36	6	0	3.749102	-3.299056	-0.565019
37	6	0	0.086236	-5.488746	-0.631469
38	6	0	-4.886247	-2.723423	-0.541719
39	6	0	-4.976389	2.963465	-0.363306
40	6	0	-0.094048	5.885030	-0.274644

41	6	0	4.878434	3.119707	-0.364394
42	6	0	4.968577	-2.567181	-0.542806
43	6	0	2.549671	-5.447292	-0.631666
44	6	0	-2.377274	-5.525405	-0.631122
45	6	0	-3.618651	-4.835044	-0.608716
46	6	0	-6.149724	-0.609339	-0.474647
47	6	0	-6.172228	0.810389	-0.430107
48	6	0	-3.776356	5.114208	-0.296582
49	6	0	-2.557483	5.843575	-0.274447
50	6	0	2.369462	5.921689	-0.274991
51	6	0	3.610839	5.231328	-0.297397
52	6	0	6.141912	1.005622	-0.431466
53	6	0	6.164416	-0.414106	-0.476006
54	6	0	3.768544	-4.717925	-0.609531
55	6	0	0.108933	-6.920662	-0.676392
56	6	0	-6.115583	-3.459051	-0.564044
57	6	0	-6.228423	3.659752	-0.340708
58	6	0	-0.116746	7.316945	-0.229721
59	6	0	6.107771	3.855335	-0.342069
60	6	0	6.220611	-3.263469	-0.565405
61	6	0	2.563619	-6.884717	-0.676756
62	6	0	-2.345658	-6.962550	-0.676214
63	6	0	-4.857136	-5.565854	-0.630884
64	6	0	-7.379133	-1.355302	-0.497296
65	6	0	-7.424661	1.517005	-0.407184
66	6	0	-5.037381	5.805390	-0.274138
67	6	0	-2.571431	7.281000	-0.229357
68	6	0	2.337845	7.358834	-0.229899
69	6	0	4.849324	5.962137	-0.275229
70	6	0	7.371320	1.751586	-0.408817
71	6	0	7.416849	-1.120721	-0.498929
72	6	0	5.029569	-5.409106	-0.631975
73	6	0	1.361265	-7.581376	-0.697875
74	6	0	-1.121828	-7.620744	-0.697601
75	6	0	-6.061915	-4.873438	-0.608436
76	6	0	-7.337531	-2.743757	-0.540867
77	6	0	-7.427086	2.906080	-0.363617
78	6	0	-6.219609	5.075129	-0.296323

79	6	0	-1.369077	7.977660	-0.208238
80	6	0	1.114016	8.017028	-0.208512
81	6	0	6.054102	5.269721	-0.297677
82	6	0	7.329718	3.140040	-0.365245
83	6	0	7.419274	-2.509797	-0.542496
84	6	0	6.211796	-4.678846	-0.609790
85	6	0	3.844387	-7.549108	-0.698372
86	6	0	-3.604725	-7.667209	-0.697550
87	6	0	-4.792436	-7.006693	-0.676112
88	6	0	-8.619197	-0.617795	-0.473412
89	6	0	-8.640729	0.740557	-0.430797
90	6	0	-5.018379	7.247556	-0.228919
91	6	0	-3.852199	7.945391	-0.207741
92	6	0	3.596913	8.063492	-0.208563
93	6	0	4.784624	7.402976	-0.230001
94	6	0	8.611385	1.014078	-0.432701
95	6	0	8.632916	-0.344273	-0.475316
96	6	0	5.010566	-6.851272	-0.677194
97	1	0	1.377650	-8.668718	-0.731987
98	1	0	-1.103743	-8.708059	-0.731713
99	1	0	-6.995851	-5.431309	-0.625365
100	1	0	-8.270593	-3.303087	-0.557843
101	1	0	-8.377407	3.435551	-0.346434
102	1	0	-7.170757	5.603114	-0.279186
103	1	0	-1.385462	9.065001	-0.174126
104	1	0	1.095930	9.104342	-0.174400
105	1	0	6.988039	5.827592	-0.280748
106	1	0	8.262781	3.699371	-0.348270
107	1	0	8.369594	-3.039267	-0.559679
108	1	0	7.162944	-5.206830	-0.626927
109	1	0	3.856559	-8.635805	-0.732461
110	1	0	-3.582450	-8.753746	-0.731640
111	1	0	-5.727920	-7.560596	-0.692916
112	1	0	-9.549492	-1.180362	-0.490491
113	1	0	-9.588385	1.273351	-0.413511
114	1	0	-5.970948	7.771525	-0.211907
115	1	0	-3.864372	9.032089	-0.173652
116	1	0	3.574638	9.150029	-0.174473

117	1	0	5.720107	7.956880	-0.213197
118	1	0	9.541679	1.576646	-0.415622
119	1	0	9.580573	-0.877067	-0.492602
120	1	0	5.963135	-7.375242	-0.694206
121	6	0	0.015525	0.137145	2.958469
122	6	0	0.034333	-2.668069	2.866395
123	6	0	1.243010	-0.535267	2.936996
124	6	0	1.253054	-1.979468	2.890389
125	6	0	-1.202783	-0.551690	2.938713
126	6	0	-1.193442	-1.995905	2.891112
127	6	0	2.492655	0.158051	2.934850
128	6	0	3.677611	-0.527128	2.893084
129	6	0	2.512439	-2.653992	2.846710
130	6	0	3.688262	-1.951909	2.850188
131	6	0	-2.461725	0.124718	2.938333
132	6	0	-3.637321	-0.576302	2.896203
133	6	0	-2.443695	-2.687292	2.846817
134	6	0	-3.628818	-2.001108	2.851124
135	1	0	0.008222	1.225067	2.974292
136	1	0	0.041601	-3.754838	2.810903
137	1	0	2.482318	1.245140	2.946777
138	1	0	4.619626	0.013605	2.868735
139	1	0	2.516827	-3.739923	2.790801
140	1	0	4.637682	-2.476708	2.795512
141	1	0	-2.466088	1.211832	2.952035
142	1	0	-4.586565	-0.048290	2.873381
143	1	0	-2.433473	-3.773095	2.789386
144	1	0	-4.571097	-2.538542	2.795731

Phenanthrene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.680537	-1.153485	-0.476784
2	6	0	-1.336818	0.109367	-0.476084

3	6	0	-0.571418	1.309075	-0.457104
4	6	0	0.850264	1.245932	-0.438823
5	6	0	1.506544	-0.016919	-0.439523
6	6	0	0.741144	-1.216628	-0.458503
7	6	0	-1.443841	-2.349906	-0.495713
8	6	0	-2.754603	0.172337	-0.494315
9	6	0	-1.225899	2.568465	-0.456405
10	6	0	1.613567	2.442353	-0.419895
11	6	0	2.924330	-0.079889	-0.421292
12	6	0	1.395626	-2.476018	-0.459201
13	6	0	-0.786445	-3.612628	-0.496397
14	6	0	-2.865874	-2.285697	-0.513990
15	6	0	-3.519334	-1.028273	-0.513293
16	6	0	-3.410138	1.436027	-0.493599
17	6	0	-2.648026	2.630579	-0.474700
18	6	0	-0.459400	3.767947	-0.437412
19	6	0	0.956172	3.705075	-0.419210
20	6	0	3.035601	2.378144	-0.401617
21	6	0	3.689061	1.120720	-0.402314
22	6	0	3.579864	-1.343579	-0.422009
23	6	0	2.817753	-2.538132	-0.440907
24	6	0	0.629127	-3.675500	-0.478194
25	6	0	-1.554638	-4.815536	-0.515437
26	6	0	-3.633000	-3.489287	-0.533022
27	6	0	-4.945183	-0.964311	-0.531622
28	6	0	-4.836042	1.498723	-0.511939
29	6	0	-3.305682	3.897449	-0.473989
30	6	0	-1.118179	5.034233	-0.436720
31	6	0	1.724364	4.907984	-0.400169
32	6	0	3.802727	3.581734	-0.382585
33	6	0	5.114910	1.056758	-0.383984
34	6	0	5.005768	-1.406276	-0.403669
35	6	0	3.475408	-3.805002	-0.441619
36	6	0	1.287906	-4.941786	-0.478887
37	6	0	-2.975448	-4.750587	-0.533693
38	6	0	-5.599464	0.298689	-0.530895
39	6	0	-2.539152	5.095499	-0.455005
40	6	0	3.145175	4.843034	-0.381913

41	6	0	5.769190	-0.206242	-0.384712
42	6	0	2.708879	-5.003052	-0.460602
43	6	0	-0.897269	-6.073874	-0.516090
44	6	0	-5.051046	-3.423254	-0.551233
45	6	0	-5.706131	-2.162706	-0.550534
46	6	0	-5.488003	2.759871	-0.511194
47	6	0	-4.723998	3.957392	-0.492248
48	6	0	-0.352093	6.229349	-0.417765
49	6	0	1.066996	6.166321	-0.399518
50	6	0	5.220773	3.515701	-0.364374
51	6	0	5.875857	2.255153	-0.365072
52	6	0	5.657729	-2.667424	-0.404412
53	6	0	4.893725	-3.864944	-0.423358
54	6	0	0.521820	-6.136901	-0.497843
55	6	0	-3.746012	-5.958388	-0.552803
56	6	0	-7.030734	0.362258	-0.549300
57	6	0	-3.199859	6.366869	-0.454301
58	6	0	3.915738	6.050835	-0.362805
59	6	0	7.200461	-0.269811	-0.366308
60	6	0	3.369586	-6.274422	-0.461307
61	6	0	-1.678170	-7.281451	-0.535333
62	6	0	-5.817052	-4.640337	-0.570351
63	6	0	-7.142377	-2.090071	-0.568937
64	6	0	-6.925032	2.814852	-0.529738
65	6	0	-5.379344	5.237603	-0.491408
66	6	0	-1.023117	7.501413	-0.417191
67	6	0	1.847896	7.373898	-0.380274
68	6	0	5.986778	4.732784	-0.345257
69	6	0	7.312103	2.182519	-0.346671
70	6	0	7.094759	-2.722405	-0.385870
71	6	0	5.549071	-5.145156	-0.424200
72	6	0	1.192844	-7.408965	-0.498417
73	6	0	-3.065442	-7.200226	-0.553026
74	6	0	-5.158873	-5.864361	-0.570737
75	6	0	-7.765792	-0.847982	-0.567958
76	6	0	-7.655860	1.632910	-0.548131
77	6	0	-4.615487	6.398469	-0.472735
78	6	0	-2.412124	7.543494	-0.435197

79	6	0	3.235168	7.292674	-0.362581
80	6	0	5.328599	5.956808	-0.344869
81	6	0	7.935519	0.940429	-0.347650
82	6	0	7.825587	-1.540463	-0.367476
83	6	0	4.785214	-6.306021	-0.442872
84	6	0	2.581851	-7.451047	-0.480411
85	6	0	-0.975902	-8.542034	-0.535409
86	6	0	-7.256052	-4.534528	-0.588544
87	6	0	-7.882816	-3.328475	-0.587875
88	6	0	-7.553026	4.114033	-0.528396
89	6	0	-6.822050	5.259783	-0.510269
90	6	0	-0.212111	8.694784	-0.397656
91	6	0	1.145629	8.634481	-0.380197
92	6	0	7.425778	4.626975	-0.327064
93	6	0	8.052542	3.420922	-0.327732
94	6	0	7.722753	-4.021585	-0.387211
95	6	0	6.991777	-5.167335	-0.405338
96	6	0	0.381838	-8.602336	-0.517951
97	1	0	-3.651288	-8.116915	-0.567542
98	1	0	-5.743284	-6.781964	-0.585242
99	1	0	-8.852593	-0.798860	-0.581926
100	1	0	-8.742736	1.680331	-0.562113
101	1	0	-5.116442	7.364278	-0.472188
102	1	0	-2.914588	8.508519	-0.434674
103	1	0	3.821015	8.209362	-0.348065
104	1	0	5.913011	6.874411	-0.330365
105	1	0	9.022319	0.891308	-0.333681
106	1	0	8.912462	-1.587884	-0.353495
107	1	0	5.286168	-7.271830	-0.443420
108	1	0	3.084315	-8.416072	-0.480932
109	1	0	-1.564907	-9.455863	-0.549947
110	1	0	-7.836540	-5.453792	-0.603008
111	1	0	-8.968719	-3.275188	-0.601800
112	1	0	-8.639378	4.157226	-0.542402
113	1	0	-7.318950	6.226898	-0.509659
114	1	0	-0.717975	9.657241	-0.397198
115	1	0	1.734634	9.548310	-0.365661
116	1	0	8.006266	5.546239	-0.312599

117	1	0	9.138446	3.367635	-0.313806
118	1	0	8.809104	-4.064779	-0.373205
119	1	0	7.488677	-6.134451	-0.405949
120	1	0	0.887701	-9.564794	-0.518409
121	6	0	0.204417	0.049268	2.959103
122	6	0	-1.323943	-2.351403	2.901274
123	6	0	0.835500	-1.230818	2.952726
124	6	0	0.033203	-2.419579	2.921814
125	6	0	-1.250601	0.122075	2.940042
126	6	0	-2.005360	-1.089019	2.913066
127	6	0	-1.961842	1.344311	2.925539
128	6	0	-3.343634	1.374692	2.886829
129	6	0	-3.417405	-1.031703	2.873595
130	6	0	-4.082296	0.177842	2.861695
131	1	0	-1.921273	-3.258760	2.856356
132	1	0	-1.422232	2.284839	2.926130
133	1	0	-3.859696	2.330214	2.854439
134	1	0	-3.974619	-1.964596	2.831859
135	1	0	-5.166724	0.207254	2.809465
136	1	0	0.538129	-3.381867	2.894277
137	6	0	1.033948	1.194746	2.961838
138	6	0	2.246811	-1.314254	2.950261
139	6	0	2.412513	1.088518	2.959758
140	1	0	3.021675	1.987686	2.941154
141	6	0	3.027951	-0.176386	2.953949
142	1	0	4.111149	-0.255183	2.928510
143	1	0	2.709785	-2.297685	2.924337
144	1	0	0.590256	2.184193	2.946660

Pyrene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.651498	1.232505	-0.516045
2	6	0	1.363056	-0.000029	-0.522706

3	6	0	0.651476	-1.232550	-0.516044
4	6	0	-0.771661	-1.232537	-0.502720
5	6	0	-1.483219	-0.000004	-0.496059
6	6	0	-0.771640	1.232517	-0.502721
7	6	0	1.361128	2.461648	-0.522689
8	6	0	2.782294	-0.000041	-0.535993
9	6	0	1.361084	-2.461706	-0.522687
10	6	0	-1.481291	-2.461681	-0.496076
11	6	0	-2.902457	0.000009	-0.482772
12	6	0	-1.481248	2.461673	-0.496078
13	6	0	0.648462	3.694004	-0.516017
14	6	0	2.784665	2.460587	-0.536016
15	6	0	3.493165	1.233350	-0.542649
16	6	0	3.493144	-1.233445	-0.542648
17	6	0	2.784622	-2.460670	-0.536014
18	6	0	0.648397	-3.694049	-0.516014
19	6	0	-0.768625	-3.694036	-0.502748
20	6	0	-2.904828	-2.460620	-0.482749
21	6	0	-3.613328	-1.233383	-0.476116
22	6	0	-3.613307	1.233413	-0.476117
23	6	0	-2.904785	2.460637	-0.482751
24	6	0	-0.768560	3.694016	-0.502751
25	6	0	1.362689	4.929846	-0.522704
26	6	0	3.497796	3.697062	-0.542692
27	6	0	4.920503	1.232705	-0.556011
28	6	0	4.920481	-1.232825	-0.556011
29	6	0	3.497732	-3.697157	-0.542690
30	6	0	1.362603	-4.929903	-0.522700
31	6	0	-1.482853	-4.929878	-0.496061
32	6	0	-3.617960	-3.697095	-0.476072
33	6	0	-5.040666	-1.232737	-0.462754
34	6	0	-5.040644	1.232792	-0.462754
35	6	0	-3.617895	3.697125	-0.476075
36	6	0	-1.482766	4.929871	-0.496064
37	6	0	2.785037	4.927990	-0.536020
38	6	0	5.630069	-0.000066	-0.562654
39	6	0	2.784950	-4.928072	-0.536017
40	6	0	-2.905200	-4.928022	-0.482745

41	6	0	-5.750232	0.000034	-0.456111
42	6	0	-2.905114	4.928040	-0.482748
43	6	0	0.650244	6.157822	-0.516034
44	6	0	4.917431	3.694002	-0.555983
45	6	0	5.627691	2.463716	-0.562632
46	6	0	5.627648	-2.463848	-0.562631
47	6	0	4.917366	-3.694122	-0.555981
48	6	0	0.650135	-6.157867	-0.516030
49	6	0	-0.770407	-6.157854	-0.502731
50	6	0	-5.037594	-3.694034	-0.462782
51	6	0	-5.747855	-2.463748	-0.456132
52	6	0	-5.747811	2.463816	-0.456134
53	6	0	-5.037529	3.694089	-0.462784
54	6	0	-0.770299	6.157834	-0.502735
55	6	0	3.501416	6.168825	-0.542727
56	6	0	7.062806	-0.000079	-0.576067
57	6	0	3.501308	-6.168920	-0.542723
58	6	0	-3.621580	-6.168857	-0.476038
59	6	0	-7.182969	0.000046	-0.442697
60	6	0	-3.621471	6.168887	-0.476042
61	6	0	1.376961	7.398892	-0.522838
62	6	0	5.628845	4.943908	-0.562644
63	6	0	7.065801	2.454868	-0.576096
64	6	0	7.065758	-2.455025	-0.576094
65	6	0	5.628758	-4.944040	-0.562641
66	6	0	1.376831	-7.398949	-0.522833
67	6	0	-1.497124	-7.398924	-0.495927
68	6	0	-5.749009	-4.943940	-0.456121
69	6	0	-7.185964	-2.454900	-0.442669
70	6	0	-7.185921	2.454993	-0.442670
71	6	0	-5.748922	4.944008	-0.456124
72	6	0	-1.496994	7.398917	-0.495932
73	6	0	2.766522	7.379288	-0.535847
74	6	0	4.917109	6.137567	-0.555981
75	6	0	7.743606	1.241618	-0.582441
76	6	0	7.743584	-1.241787	-0.582441
77	6	0	4.917002	-6.137687	-0.555977
78	6	0	2.766393	-7.379371	-0.535842

79	6	0	-2.886686	-7.379321	-0.482918
80	6	0	-5.037273	-6.137599	-0.462784
81	6	0	-7.863769	-1.241650	-0.436323
82	6	0	-7.863747	1.241755	-0.436324
83	6	0	-5.037165	6.137654	-0.462788
84	6	0	-2.886556	7.379338	-0.482923
85	6	0	0.619559	8.627119	-0.515747
86	6	0	7.071175	4.902038	-0.576147
87	6	0	7.750730	3.724939	-0.582509
88	6	0	7.750664	-3.725109	-0.582506
89	6	0	7.071088	-4.902196	-0.576144
90	6	0	0.619408	-8.627163	-0.515742
91	6	0	-0.739723	-8.627151	-0.503017
92	6	0	-7.191338	-4.902071	-0.442618
93	6	0	-7.870893	-3.724971	-0.436256
94	6	0	-7.870827	3.725076	-0.436259
95	6	0	-7.191252	4.902163	-0.442621
96	6	0	-0.739571	8.627131	-0.503023
97	1	0	3.311243	8.321094	-0.540947
98	1	0	5.460357	7.080223	-0.561067
99	1	0	8.831558	1.240758	-0.592627
100	1	0	8.831536	-1.240946	-0.592626
101	1	0	5.460233	-7.080352	-0.561062
102	1	0	3.311097	-8.321185	-0.540942
103	1	0	-3.431407	-8.321126	-0.477818
104	1	0	-5.580520	-7.080255	-0.457698
105	1	0	-8.951721	-1.240790	-0.426138
106	1	0	-8.951699	1.240914	-0.426139
107	1	0	-5.580396	7.080320	-0.457703
108	1	0	-3.431260	8.321153	-0.477823
109	1	0	1.167563	9.566207	-0.520878
110	1	0	7.610428	5.846179	-0.581196
111	1	0	8.837970	3.719878	-0.592688
112	1	0	8.837905	-3.720067	-0.592685
113	1	0	7.610326	-5.846346	-0.581192
114	1	0	1.167395	-9.566261	-0.520872
115	1	0	-1.287726	-9.566240	-0.497887
116	1	0	-7.730592	-5.846211	-0.437569

117	1	0	-8.958133	-3.719910	-0.426077
118	1	0	-8.958068	3.720034	-0.426080
119	1	0	-7.730489	5.846313	-0.437573
120	1	0	-1.287558	9.566229	-0.497893
121	6	0	-0.372755	0.000109	2.918272
122	6	0	1.020356	2.463019	2.873260
123	6	0	-1.088169	1.236196	2.913026
124	6	0	-0.340601	2.463356	2.887633
125	6	0	1.053465	0.000080	2.904104
126	6	0	1.768682	1.236068	2.884690
127	6	0	1.768641	-1.235914	2.884905
128	6	0	3.171643	-1.210073	2.851354
129	6	0	3.171671	1.210168	2.851149
130	6	0	3.862234	0.000031	2.837569
131	1	0	1.569561	3.400483	2.833399
132	1	0	3.717345	-2.149641	2.815762
133	1	0	3.717429	2.149699	2.815427
134	1	0	4.947460	0.000028	2.789922
135	1	0	-0.890303	3.400801	2.859857
136	6	0	-1.088193	-1.235964	2.913304
137	6	0	-2.491554	1.210630	2.905975
138	6	0	-2.491576	-1.210363	2.906222
139	1	0	-3.038077	-2.149664	2.881850
140	6	0	-3.181456	0.000136	2.903644
141	1	0	-4.267562	0.000155	2.874449
142	1	0	-3.038045	2.149932	2.881439
143	6	0	-0.340667	-2.463147	2.888198
144	6	0	1.020294	-2.462851	2.873781
145	1	0	-0.890393	-3.400585	2.860671
146	1	0	1.569471	-3.400342	2.834178

Tetracene

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

1	6	0	-0.000378	-1.296264	-0.590867
2	6	0	-1.232633	-0.584339	-0.576530
3	6	0	-1.232090	0.838572	-0.547816
4	6	0	0.000708	1.549556	-0.533438
5	6	0	1.232964	0.837630	-0.547775
6	6	0	1.232421	-0.585280	-0.576489
7	6	0	-0.000919	-2.715275	-0.619502
8	6	0	-2.462054	-1.293375	-0.590869
9	6	0	-2.460969	1.548547	-0.533519
10	6	0	0.001250	2.968567	-0.504803
11	6	0	2.462385	1.546666	-0.533436
12	6	0	2.461300	-1.295255	-0.590786
13	6	0	1.232207	-3.426494	-0.633824
14	6	0	-1.234588	-3.425551	-0.633866
15	6	0	-2.461549	-2.716685	-0.619591
16	6	0	-3.694131	-0.580341	-0.576510
17	6	0	-3.693590	0.836455	-0.547919
18	6	0	-2.459378	2.971856	-0.504797
19	6	0	-1.231877	3.679785	-0.490481
20	6	0	1.234919	3.678843	-0.490439
21	6	0	2.461879	2.969976	-0.504714
22	6	0	3.694462	0.833633	-0.547795
23	6	0	3.693921	-0.583163	-0.576386
24	6	0	2.459708	-2.718564	-0.619508
25	6	0	1.231030	-4.853602	-0.662623
26	6	0	-1.234500	-4.852661	-0.662665
27	6	0	-3.698302	-3.429219	-0.634000
28	6	0	-4.930252	-1.293972	-0.590941
29	6	0	-4.929166	1.551029	-0.533529
30	6	0	-3.695586	3.685335	-0.490429
31	6	0	-1.230699	5.106894	-0.461682
32	6	0	1.234831	5.105952	-0.461640
33	6	0	3.698632	3.682511	-0.490305
34	6	0	4.930582	1.547263	-0.533364
35	6	0	4.929497	-1.297738	-0.590776
36	6	0	3.695917	-3.432043	-0.633876
37	6	0	-0.002006	-5.562596	-0.676961
38	6	0	-4.928951	-2.716093	-0.619640

39	6	0	-4.926780	2.973149	-0.504831
40	6	0	0.002336	5.815887	-0.447344
41	6	0	4.929281	2.969384	-0.504665
42	6	0	4.927110	-2.719857	-0.619474
43	6	0	2.461777	-5.561138	-0.676871
44	6	0	-2.465787	-5.559255	-0.676954
45	6	0	-3.695796	-4.848628	-0.662644
46	6	0	-6.157949	-0.581160	-0.576587
47	6	0	-6.157407	0.839156	-0.547925
48	6	0	-3.691997	5.104741	-0.461785
49	6	0	-2.461446	5.814429	-0.447434
50	6	0	2.466118	5.812547	-0.447351
51	6	0	3.696126	5.101919	-0.461661
52	6	0	6.158280	0.834451	-0.547718
53	6	0	6.157738	-0.585864	-0.576380
54	6	0	3.692328	-4.851450	-0.662520
55	6	0	-0.002553	-6.995104	-0.705869
56	6	0	-6.170065	-3.431873	-0.634115
57	6	0	-6.167347	3.689877	-0.490398
58	6	0	0.002883	7.248395	-0.418436
59	6	0	6.170396	3.685164	-0.490190
60	6	0	6.167678	-3.436585	-0.633907
61	6	0	2.452393	-6.999014	-0.705888
62	6	0	-2.457500	-6.997139	-0.705970
63	6	0	-4.945979	-5.559440	-0.677019
64	6	0	-7.399303	-1.307276	-0.591271
65	6	0	-7.398206	1.566220	-0.533284
66	6	0	-4.941638	5.816509	-0.447453
67	6	0	-2.452062	7.252306	-0.418417
68	6	0	2.457831	7.250430	-0.418335
69	6	0	4.946310	5.812732	-0.447286
70	6	0	7.399634	1.560568	-0.533034
71	6	0	7.398537	-1.312928	-0.591021
72	6	0	4.941968	-5.563217	-0.676852
73	6	0	1.238890	-7.676258	-0.719584
74	6	0	-1.244515	-7.675309	-0.719626
75	6	0	-6.139360	-4.847352	-0.662678
76	6	0	-7.380242	-2.696623	-0.619307

77	6	0	-7.378085	2.955552	-0.505246
78	6	0	-6.135562	5.105332	-0.461833
79	6	0	-1.238560	7.929549	-0.404721
80	6	0	1.244846	7.928601	-0.404679
81	6	0	6.139691	5.100643	-0.461627
82	6	0	7.380573	2.949915	-0.504998
83	6	0	7.378416	-2.702260	-0.619059
84	6	0	6.135893	-4.852040	-0.662472
85	6	0	3.722209	-7.684307	-0.719686
86	6	0	-3.727839	-7.681462	-0.719811
87	6	0	-4.904672	-7.001555	-0.706120
88	6	0	-8.627234	-0.549516	-0.576009
89	6	0	-8.626716	0.809398	-0.548586
90	6	0	-4.899230	7.258592	-0.418350
91	6	0	-3.721878	7.937599	-0.404619
92	6	0	3.728169	7.934753	-0.404494
93	6	0	4.905003	7.254847	-0.418185
94	6	0	8.627565	0.802807	-0.548296
95	6	0	8.627046	-0.556106	-0.575719
96	6	0	4.899561	-7.005300	-0.705955
97	1	0	1.237625	-8.764036	-0.741536
98	1	0	-1.244079	-8.763088	-0.741577
99	1	0	-7.082228	-5.390144	-0.673655
100	1	0	-8.322260	-3.240889	-0.630313
101	1	0	-8.319687	3.500537	-0.494272
102	1	0	-7.078015	5.648844	-0.450889
103	1	0	-1.237294	9.017327	-0.382769
104	1	0	1.244410	9.016379	-0.382728
105	1	0	7.082559	5.643436	-0.450650
106	1	0	8.322591	3.494181	-0.493992
107	1	0	8.320018	-3.247246	-0.630033
108	1	0	7.078346	-5.395553	-0.673416
109	1	0	3.716742	-8.771372	-0.741623
110	1	0	-3.723202	-8.768530	-0.741748
111	1	0	-5.849023	-7.540354	-0.717016
112	1	0	-9.566537	-1.097064	-0.587082
113	1	0	-9.565600	1.357664	-0.537545
114	1	0	-5.843170	7.798112	-0.407486

115	1	0	-3.716411	9.024664	-0.382682
116	1	0	3.723532	9.021822	-0.382557
117	1	0	5.849354	7.793646	-0.407289
118	1	0	9.566867	1.350356	-0.537223
119	1	0	9.565931	-1.104372	-0.586760
120	1	0	5.843500	-7.544820	-0.716819
121	6	0	-1.235389	0.773000	2.849124
122	6	0	-1.234949	-2.039231	2.803225
123	6	0	-0.000768	0.092830	2.846560
124	6	0	-0.000862	-1.359179	2.822876
125	6	0	-2.449912	0.092415	2.839366
126	6	0	-2.449238	-1.358827	2.814912
127	6	0	1.233890	0.772873	2.849418
128	6	0	2.448378	0.092080	2.839628
129	6	0	1.233089	-2.039391	2.803182
130	6	0	2.447508	-1.359077	2.814896
131	6	0	-3.709666	0.775515	2.830045
132	6	0	-4.886807	0.081869	2.801643
133	6	0	-3.708273	-2.041831	2.780178
134	6	0	-4.885332	-1.347599	2.774581
135	1	0	-1.235242	1.861070	2.846832
136	1	0	-1.234695	-3.126470	2.765357
137	1	0	1.233881	1.860933	2.847466
138	1	0	1.232696	-3.126619	2.765265
139	1	0	-3.707234	1.862855	2.826755
140	1	0	-5.833591	0.613371	2.774001
141	1	0	-3.705515	-3.128144	2.737623
142	1	0	-5.831735	-1.878635	2.724358
143	6	0	3.706408	-2.042268	2.780023
144	6	0	3.708189	0.775012	2.830527
145	6	0	4.883607	-1.348216	2.774555
146	1	0	5.829956	-1.879344	2.724237
147	6	0	4.885277	0.081219	2.802004
148	1	0	5.832155	0.612571	2.774521
149	1	0	3.705842	1.862356	2.827460
150	1	0	3.703411	-3.128572	2.737173

Triphenylene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.175482	0.037347	-0.609618
2	6	0	-0.432334	1.250789	-0.581576
3	6	0	0.989366	1.213468	-0.527974
4	6	0	1.667919	-0.037296	-0.502416
5	6	0	0.924772	-1.250739	-0.530458
6	6	0	-0.496929	-1.213417	-0.584059
7	6	0	-2.593286	0.074566	-0.663072
8	6	0	-1.109026	2.498126	-0.607065
9	6	0	1.730478	2.423585	-0.500010
10	6	0	3.085724	-0.074515	-0.448961
11	6	0	1.601465	-2.498076	-0.504970
12	6	0	-1.238041	-2.423535	-0.612025
13	6	0	-3.335749	-1.139765	-0.691089
14	6	0	-3.271108	1.326182	-0.688604
15	6	0	-2.531154	2.534410	-0.660682
16	6	0	-0.364777	3.711362	-0.578980
17	6	0	1.050814	3.674201	-0.525610
18	6	0	3.152550	2.385205	-0.446394
19	6	0	3.828187	1.139815	-0.420945
20	6	0	3.763547	-1.326131	-0.423430
21	6	0	3.023592	-2.534360	-0.451353
22	6	0	0.857215	-3.711311	-0.533053
23	6	0	-0.558376	-3.674151	-0.586424
24	6	0	-2.660113	-2.385155	-0.665640
25	6	0	-4.761628	-1.101701	-0.744847
26	6	0	-4.697021	1.362981	-0.742364
27	6	0	-3.211153	3.789167	-0.686295
28	6	0	-1.045888	4.965516	-0.604636
29	6	0	1.796694	4.890893	-0.497465
30	6	0	3.897353	3.602560	-0.418290
31	6	0	5.254067	1.101752	-0.367187
32	6	0	5.189458	-1.362931	-0.369671

33	6	0	3.703592	-3.789117	-0.425739
34	6	0	1.538326	-4.965464	-0.507398
35	6	0	-1.304256	-4.890843	-0.614569
36	6	0	-3.404914	-3.602509	-0.693745
37	6	0	-5.438185	0.149249	-0.770331
38	6	0	-2.466847	5.000974	-0.658209
39	6	0	3.217557	4.851750	-0.443895
40	6	0	5.930624	-0.149198	-0.341703
41	6	0	2.959286	-5.000922	-0.453825
42	6	0	-2.725119	-4.851699	-0.668139
43	6	0	-5.500350	-2.313749	-0.772722
44	6	0	-5.371227	2.612121	-0.767758
45	6	0	-4.629435	3.823350	-0.739767
46	6	0	-0.301973	6.174379	-0.576565
47	6	0	1.117135	6.137125	-0.523061
48	6	0	5.315473	3.562283	-0.364824
49	6	0	5.992789	2.313799	-0.339312
50	6	0	5.863665	-2.612071	-0.344276
51	6	0	5.121872	-3.823300	-0.372267
52	6	0	0.794410	-6.174328	-0.535469
53	6	0	-0.624698	-6.137074	-0.588972
54	6	0	-4.823035	-3.562233	-0.747211
55	6	0	-6.869476	0.186822	-0.824294
56	6	0	-3.149977	6.260175	-0.683941
57	6	0	3.965717	6.073378	-0.415664
58	6	0	7.361913	-0.186772	-0.287741
59	6	0	3.642415	-6.260123	-0.428094
60	6	0	-3.473280	-6.073327	-0.696371
61	6	0	-6.936777	-2.267202	-0.826878
62	6	0	-6.808116	2.641002	-0.821932
63	6	0	-5.307366	5.091489	-0.765303
64	6	0	-0.995424	7.434086	-0.602686
65	6	0	1.875629	7.358716	-0.494441
66	6	0	6.058911	4.793109	-0.336770
67	6	0	7.429214	2.267252	-0.285155
68	6	0	7.300553	-2.640952	-0.290102
69	6	0	5.799804	-5.091439	-0.346732
70	6	0	1.487861	-7.434036	-0.509349

71	6	0	-1.383192	-7.358666	-0.617593
72	6	0	-5.566473	-4.793058	-0.775264
73	6	0	-7.582115	-1.036600	-0.851185
74	6	0	-7.517039	1.445952	-0.848684
75	6	0	-4.565060	6.266066	-0.737292
76	6	0	-2.384095	7.450942	-0.655042
77	6	0	3.263275	7.302691	-0.442124
78	6	0	5.379163	6.005017	-0.362375
79	6	0	8.074553	1.036651	-0.260848
80	6	0	8.009476	-1.445901	-0.263351
81	6	0	5.057497	-6.266015	-0.374742
82	6	0	2.876533	-7.450892	-0.456993
83	6	0	-2.770837	-7.302641	-0.669911
84	6	0	-4.886725	-6.004967	-0.749660
85	6	0	-7.654284	-3.518881	-0.853955
86	6	0	-7.459059	3.928605	-0.846449
87	6	0	-6.749336	5.087472	-0.819668
88	6	0	-0.206591	8.642020	-0.572921
89	6	0	1.151167	8.606377	-0.521731
90	6	0	7.498687	4.713441	-0.282488
91	6	0	8.146721	3.518932	-0.258080
92	6	0	7.951498	-3.928554	-0.265585
93	6	0	7.241774	-5.087421	-0.292366
94	6	0	0.699029	-8.641970	-0.539114
95	6	0	-0.658729	-8.606327	-0.590303
96	6	0	-7.006250	-4.713391	-0.829545
97	1	0	-8.668946	-1.007218	-0.892161
98	1	0	-8.603914	1.473632	-0.889662
99	1	0	-5.083049	7.222649	-0.756804
100	1	0	-2.903578	8.406714	-0.674609
101	1	0	3.832117	8.229893	-0.420659
102	1	0	5.946555	6.933107	-0.340965
103	1	0	9.161383	1.007268	-0.219873
104	1	0	9.096352	-1.473582	-0.222373
105	1	0	5.575486	-7.222598	-0.355231
106	1	0	3.396016	-8.406663	-0.437426
107	1	0	-3.339679	-8.229842	-0.691375
108	1	0	-5.454117	-6.933057	-0.771069

109	1	0	-8.740295	-3.485318	-0.894899
110	1	0	-8.545335	3.952068	-0.887405
111	1	0	-7.263296	6.045433	-0.839027
112	1	0	-0.729424	9.595162	-0.592614
113	1	0	1.723217	9.530777	-0.500145
114	1	0	8.062129	5.643120	-0.261227
115	1	0	9.232732	3.485369	-0.217135
116	1	0	9.037773	-3.952017	-0.224630
117	1	0	7.755734	-6.045383	-0.273007
118	1	0	1.221863	-9.595112	-0.519419
119	1	0	-1.230779	-9.530727	-0.611890
120	1	0	-7.569692	-5.643070	-0.850807
121	6	0	0.209063	-0.070913	2.858914
122	6	0	-2.674143	0.044921	2.751540
123	6	0	-0.549993	-1.272489	2.832265
124	6	0	-2.013897	-1.213637	2.777932
125	6	0	-0.472002	1.227217	2.833007
126	6	0	-1.891352	1.284220	2.780907
127	6	0	0.250133	2.441511	2.837274
128	6	0	-0.383575	3.669492	2.792688
129	6	0	-2.512322	2.552508	2.737293
130	6	0	-1.781633	3.726215	2.743220
131	1	0	1.332909	2.427565	2.856744
132	1	0	0.204976	4.582348	2.773733
133	1	0	-3.591497	2.624872	2.678739
134	1	0	-2.292127	4.683129	2.686480
135	6	0	-2.799880	-2.386506	2.728065
136	6	0	-4.084666	0.062912	2.675092
137	6	0	-4.179702	-2.340786	2.654122
138	1	0	-4.750293	-3.262935	2.594663
139	6	0	-4.829323	-1.100925	2.626106
140	1	0	-5.911111	-1.048552	2.542921
141	1	0	-2.321930	-3.358581	2.727424
142	1	0	-4.612533	1.007592	2.631800
143	6	0	1.618308	-0.166353	2.888883
144	6	0	0.140941	-2.504779	2.837476
145	6	0	2.269839	-1.385842	2.893062
146	1	0	3.355351	-1.420740	2.895085

147	6	0	1.521706	-2.568983	2.866728
148	1	0	2.019637	-3.534257	2.846510
149	1	0	2.221706	0.733222	2.890239
150	1	0	-0.411471	-3.435510	2.798470

Perylene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.840862	-0.785302	-0.658986
2	6	0	-0.517518	-1.208850	-0.628819
3	6	0	-1.562472	-0.244438	-0.569839
4	6	0	-1.249046	1.143522	-0.541027
5	6	0	0.109333	1.567069	-0.571194
6	6	0	1.154287	0.602658	-0.630174
7	6	0	1.882952	-1.747071	-0.717805
8	6	0	-0.830084	-2.593006	-0.657552
9	6	0	-2.917129	-0.666824	-0.539754
10	6	0	-2.291137	2.105292	-0.482209
11	6	0	0.421900	2.951226	-0.542461
12	6	0	2.508945	1.025045	-0.660259
13	6	0	3.241403	-1.322404	-0.747943
14	6	0	1.568416	-3.135190	-0.746587
15	6	0	0.215874	-3.556918	-0.716549
16	6	0	-2.189157	-3.015672	-0.627339
17	6	0	-3.229621	-2.055405	-0.568613
18	6	0	-3.961666	0.298629	-0.480758
19	6	0	-3.649586	1.680624	-0.452070
20	6	0	-1.976601	3.493411	-0.453426
21	6	0	-0.624058	3.915139	-0.483464
22	6	0	1.780973	3.373893	-0.572674
23	6	0	2.821437	2.413624	-0.631401
24	6	0	3.553482	0.059592	-0.719254
25	6	0	4.289011	-2.290127	-0.807097
26	6	0	2.616883	-4.101983	-0.805741

27	6	0	-0.099093	-4.948836	-0.745423
28	6	0	-2.502890	-4.407867	-0.656259
29	6	0	-4.592197	-2.479598	-0.538333
30	6	0	-5.323866	-0.126772	-0.450525
31	6	0	-4.697195	2.648348	-0.392917
32	6	0	-3.025067	4.460204	-0.394272
33	6	0	-0.309091	5.307055	-0.454590
34	6	0	2.094706	4.766087	-0.543754
35	6	0	4.184013	2.837819	-0.661679
36	6	0	4.915681	0.484993	-0.749488
37	6	0	3.973962	-3.676912	-0.835826
38	6	0	-1.457267	-5.370389	-0.715208
39	6	0	-5.635320	-1.514366	-0.479388
40	6	0	-4.382146	4.035133	-0.364188
41	6	0	1.049082	5.728608	-0.484806
42	6	0	5.227136	1.872587	-0.720626
43	6	0	5.643142	-1.864714	-0.837081
44	6	0	2.301258	-5.485858	-0.834372
45	6	0	0.945355	-5.908634	-0.804260
46	6	0	-3.858832	-4.827463	-0.626057
47	6	0	-4.901880	-3.864810	-0.567185
48	6	0	-6.364181	0.837506	-0.391692
49	6	0	-6.051327	2.222934	-0.362932
50	6	0	-2.709442	5.844079	-0.365641
51	6	0	-1.353540	6.266854	-0.395753
52	6	0	3.450647	5.185684	-0.573956
53	6	0	4.493696	4.223031	-0.632828
54	6	0	5.955996	-0.479285	-0.808321
55	6	0	5.025965	-4.647829	-0.895203
56	6	0	-1.772806	-6.767711	-0.744214
57	6	0	-7.002863	-1.940771	-0.449017
58	6	0	-5.434149	5.006050	-0.304810
59	6	0	1.364622	7.125931	-0.455800
60	6	0	6.594678	2.298992	-0.750996
61	6	0	6.693098	-2.845765	-0.896676
62	6	0	3.363198	-6.453924	-0.893977
63	6	0	0.620018	-7.309257	-0.833055
64	6	0	-4.166940	-6.231964	-0.655492

65	6	0	-6.277173	-4.284381	-0.536386
66	6	0	-7.734230	0.401070	-0.361522
67	6	0	-7.101282	3.203985	-0.303337
68	6	0	-3.771381	6.812144	-0.306036
69	6	0	-1.028202	7.667477	-0.366958
70	6	0	3.758755	6.590184	-0.544521
71	6	0	5.868988	4.642602	-0.663628
72	6	0	7.326045	-0.042849	-0.838492
73	6	0	6.367966	-4.196681	-0.924100
74	6	0	4.683715	-6.021673	-0.922735
75	6	0	-0.712127	-7.704116	-0.802902
76	6	0	-3.133353	-7.159226	-0.713091
77	6	0	-7.284186	-3.328326	-0.478809
78	6	0	-8.021160	-0.958443	-0.390363
79	6	0	-6.776151	4.554900	-0.275913
80	6	0	-5.091899	6.379894	-0.277278
81	6	0	0.303944	8.062337	-0.397111
82	6	0	2.725168	7.517446	-0.486921
83	6	0	6.876001	3.686547	-0.721205
84	6	0	7.612975	1.316662	-0.809651
85	6	0	8.057374	-2.376562	-0.925760
86	6	0	3.004736	-7.851417	-0.921664
87	6	0	1.707451	-8.255916	-0.892854
88	6	0	-5.556059	-6.621280	-0.623428
89	6	0	-6.554015	-5.700243	-0.567101
90	6	0	-8.764888	1.409247	-0.301769
91	6	0	-8.465559	2.734782	-0.274253
92	6	0	-3.412921	8.209637	-0.278348
93	6	0	-2.115635	8.614135	-0.307159
94	6	0	5.147875	6.979500	-0.576586
95	6	0	6.145832	6.058463	-0.632913
96	6	0	8.356704	-1.051027	-0.898243
97	1	0	7.166229	-4.934573	-0.969189
98	1	0	5.483133	-6.758316	-0.967824
99	1	0	-0.952563	-8.764989	-0.824897
100	1	0	-3.372129	-8.220472	-0.735149
101	1	0	-8.322885	-3.651305	-0.455716
102	1	0	-9.059353	-1.283045	-0.367331

103	1	0	-7.574414	5.292794	-0.230825
104	1	0	-5.891317	7.116537	-0.232189
105	1	0	0.544379	9.123210	-0.375115
106	1	0	2.963945	8.578692	-0.464865
107	1	0	7.914700	4.009526	-0.744297
108	1	0	8.651170	1.641266	-0.832683
109	1	0	8.852267	-3.117060	-0.970816
110	1	0	3.806481	-8.584491	-0.966726
111	1	0	1.463077	-9.315173	-0.914682
112	1	0	-5.790584	-7.682754	-0.645622
113	1	0	-7.593282	-6.019002	-0.543873
114	1	0	-9.801157	1.080847	-0.278902
115	1	0	-9.260451	3.475281	-0.229197
116	1	0	-4.214665	8.942711	-0.233287
117	1	0	-1.871261	9.673392	-0.285330
118	1	0	5.382400	8.040974	-0.554391
119	1	0	7.185098	6.377222	-0.656140
120	1	0	9.392972	-0.722627	-0.921111
121	6	0	-0.154509	0.149012	2.814289
122	6	0	2.011783	-1.779016	2.695398
123	6	0	2.297668	-0.375208	2.727732
124	6	0	-0.440298	-1.254658	2.785769
125	6	0	0.607607	-2.229816	2.725125
126	6	0	-1.806653	-1.692737	2.794519
127	6	0	-2.098422	-3.078730	2.741149
128	6	0	0.259829	-3.576032	2.674354
129	6	0	-1.080043	-4.000646	2.682932
130	1	0	-3.137935	-3.395709	2.725178
131	1	0	1.029360	-4.336215	2.607009
132	1	0	-1.302193	-5.061866	2.619231
133	6	0	3.662845	0.063969	2.679800
134	6	0	3.075523	-2.672347	2.616151
135	6	0	4.704558	-0.893530	2.598442
136	1	0	5.732640	-0.546648	2.539070
137	6	0	4.410768	-2.236258	2.565954
138	1	0	5.206536	-2.970560	2.478640
139	1	0	2.890706	-3.739095	2.570172
140	6	0	1.249565	0.600260	2.783680

141	6	0	3.953405	1.451107	2.686178
142	6	0	1.595308	1.948122	2.787044
143	6	0	-2.849676	-0.733759	2.829552
144	6	0	-1.220064	1.043048	2.848417
145	6	0	2.934279	2.372585	2.737760
146	1	0	3.154144	3.436298	2.718001
147	6	0	-2.557033	0.609480	2.856608
148	1	0	-3.355226	1.346046	2.862242
149	1	0	-1.036259	2.111153	2.850448
150	1	0	0.824778	2.709714	2.809240
151	1	0	4.990370	1.770447	2.626525
152	1	0	-3.880242	-1.078735	2.813089

Coronene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.112935	0.001394	-0.753608
2	6	0	-0.400892	1.233224	-0.720638
3	6	0	1.020785	1.231831	-0.654806
4	6	0	1.730416	-0.001393	-0.621945
5	6	0	1.018373	-1.233223	-0.654914
6	6	0	-0.403304	-1.231829	-0.720747
7	6	0	-2.530715	0.002784	-0.819260
8	6	0	-1.108579	2.463069	-0.753409
9	6	0	1.730877	2.460285	-0.621927
10	6	0	3.148196	-0.002783	-0.556293
11	6	0	1.726061	-2.463067	-0.622143
12	6	0	-1.113396	-2.460284	-0.753626
13	6	0	-3.242053	-1.229917	-0.852197
14	6	0	-3.239639	1.236877	-0.852089
15	6	0	-2.530655	2.463414	-0.819260
16	6	0	-0.395429	3.694719	-0.720388
17	6	0	1.020138	3.693332	-0.654840
18	6	0	3.152951	2.457842	-0.556076

19	6	0	3.859534	1.229918	-0.523356
20	6	0	3.857120	-1.236877	-0.523464
21	6	0	3.148136	-2.463413	-0.556293
22	6	0	1.012910	-3.694718	-0.655165
23	6	0	-0.402657	-3.693330	-0.720713
24	6	0	-2.535470	-2.457841	-0.819477
25	6	0	-4.667923	-1.227887	-0.918224
26	6	0	-4.665511	1.237642	-0.918115
27	6	0	-3.241835	3.700593	-0.852193
28	6	0	-1.107704	4.931266	-0.753372
29	6	0	1.734829	4.928480	-0.621746
30	6	0	3.866548	3.693624	-0.523033
31	6	0	5.285404	1.227887	-0.457329
32	6	0	5.282992	-1.237641	-0.457438
33	6	0	3.859315	-3.700591	-0.523359
34	6	0	1.725184	-4.931265	-0.622181
35	6	0	-1.117348	-4.928478	-0.753807
36	6	0	-3.249067	-3.693623	-0.852519
37	6	0	-5.375566	0.005572	-0.950992
38	6	0	-2.528592	4.930815	-0.819167
39	6	0	3.155715	4.925243	-0.555951
40	6	0	5.993047	-0.005572	-0.424560
41	6	0	3.146073	-4.930814	-0.556385
42	6	0	-2.538234	-4.925242	-0.819602
43	6	0	-5.375579	-2.458211	-0.950990
44	6	0	-5.370759	2.469351	-0.950773
45	6	0	-4.660013	3.698934	-0.917864
46	6	0	-0.394777	6.158537	-0.720361
47	6	0	1.024305	6.157146	-0.654649
48	6	0	5.284722	3.689186	-0.457364
49	6	0	5.993060	2.458211	-0.424563
50	6	0	5.988240	-2.469350	-0.424779
51	6	0	5.277494	-3.698934	-0.457689
52	6	0	1.012258	-6.158536	-0.655192
53	6	0	-0.406825	-6.157145	-0.720904
54	6	0	-4.667241	-3.689186	-0.918189
55	6	0	-6.806831	0.006976	-1.017269
56	6	0	-3.243011	6.172357	-0.852251

57	6	0	3.872561	6.165382	-0.522758
58	6	0	7.424312	-0.006975	-0.358284
59	6	0	3.860492	-6.172357	-0.523302
60	6	0	-3.255080	-6.165381	-0.852795
61	6	0	-6.812203	-2.447967	-1.017514
62	6	0	-6.807400	2.461924	-1.017298
63	6	0	-5.369464	4.949542	-0.950717
64	6	0	-1.119523	7.400324	-0.753923
65	6	0	1.751480	7.397510	-0.620979
66	6	0	5.996617	4.938401	-0.424400
67	6	0	7.429684	2.447967	-0.358038
68	6	0	7.424881	-2.461923	-0.358254
69	6	0	5.986945	-4.949542	-0.424836
70	6	0	1.737004	-7.400324	-0.621630
71	6	0	-1.133999	-7.397509	-0.754574
72	6	0	-5.379136	-4.938400	-0.951152
73	6	0	-7.488136	-1.234060	-1.048816
74	6	0	-7.485706	1.249344	-1.048706
75	6	0	-4.657280	6.142498	-0.917740
76	6	0	-2.507677	7.382094	-0.818202
77	6	0	3.139595	7.376558	-0.556700
78	6	0	5.286769	6.132750	-0.457272
79	6	0	8.105617	1.234061	-0.326737
80	6	0	8.103187	-1.249344	-0.326847
81	6	0	5.274761	-6.142498	-0.457813
82	6	0	3.125158	-7.382094	-0.557350
83	6	0	-2.522114	-7.376558	-0.818852
84	6	0	-4.669288	-6.132750	-0.918281
85	6	0	-7.497659	-3.717372	-1.049253
86	6	0	-7.490372	3.732672	-1.048925
87	6	0	-6.810352	4.909098	-1.017438
88	6	0	-0.361687	8.627803	-0.718833
89	6	0	0.996048	8.626472	-0.655961
90	6	0	7.437424	4.895132	-0.357683
91	6	0	8.115140	3.717374	-0.326300
92	6	0	8.107853	-3.732670	-0.326627
93	6	0	7.427834	-4.909098	-0.358114
94	6	0	0.979168	-8.627802	-0.656720

95	6	0	-0.378567	-8.626471	-0.719591
96	6	0	-6.819943	-4.895131	-1.017870
97	1	0	-8.574969	-1.232144	-1.099142
98	1	0	-8.572541	1.249559	-1.099033
99	1	0	-5.199040	7.085691	-0.942828
100	1	0	-3.050909	8.324437	-0.843358
101	1	0	3.684669	8.317835	-0.531462
102	1	0	5.830373	7.074879	-0.432101
103	1	0	9.192450	1.232145	-0.276410
104	1	0	9.190022	-1.249558	-0.276520
105	1	0	5.816521	-7.085689	-0.432725
106	1	0	3.668390	-8.324436	-0.532194
107	1	0	-3.067189	-8.317833	-0.844091
108	1	0	-5.212892	-7.074877	-0.943451
109	1	0	-8.583778	-3.711257	-1.099547
110	1	0	-8.576500	3.728684	-1.099220
111	1	0	-7.348121	5.853771	-1.042341
112	1	0	-0.908201	9.567432	-0.744140
113	1	0	1.544398	9.565028	-0.630570
114	1	0	7.977040	5.838748	-0.332696
115	1	0	9.201259	3.711257	-0.276006
116	1	0	9.193982	-3.728684	-0.276333
117	1	0	7.965602	-5.853770	-0.333211
118	1	0	1.525682	-9.567432	-0.631412
119	1	0	-0.926917	-9.565027	-0.744983
120	1	0	-7.359559	-5.838748	-1.042856
121	6	0	0.236436	-0.001571	2.745575
122	6	0	-0.477800	-1.236538	2.712588
123	6	0	-1.903257	-1.235125	2.648450
124	6	0	-2.614455	0.001565	2.615138
125	6	0	-1.900555	1.236688	2.648780
126	6	0	-0.475099	1.234965	2.712863
127	6	0	1.656989	-0.003132	2.786532
128	6	0	0.231731	-2.467910	2.720462
129	6	0	-2.613269	-2.464979	2.592782
130	6	0	-4.032662	0.003129	2.525269
131	6	0	-2.607868	2.468104	2.593261
132	6	0	0.237135	2.464777	2.720827

133	6	0	2.343837	1.243675	2.792808
134	6	0	2.341102	-1.251437	2.792602
135	6	0	1.654301	-2.438332	2.759754
136	6	0	-0.506013	-3.683750	2.662062
137	6	0	-1.876393	-3.682734	2.601888
138	6	0	-4.033444	-2.432859	2.502586
139	6	0	-4.716566	-1.243939	2.468439
140	6	0	-4.713831	1.251700	2.468598
141	6	0	-4.028103	2.439114	2.502928
142	6	0	-1.868317	3.684238	2.602371
143	6	0	-0.497933	3.682241	2.662499
144	6	0	1.659643	2.432075	2.760081
145	1	0	3.430758	1.239179	2.801896
146	1	0	3.428029	-1.249326	2.801695
147	1	0	2.194828	-3.381456	2.741618
148	1	0	0.040552	-4.623379	2.643755
149	1	0	-2.420944	-4.621135	2.536205
150	1	0	-4.572100	-3.374616	2.436612
151	1	0	-5.799611	-1.239154	2.374503
152	1	0	-5.796878	1.249300	2.374600
153	1	0	-4.564688	3.382063	2.437067
154	1	0	-2.410809	4.623837	2.536755
155	1	0	0.050695	4.620667	2.644199
156	1	0	2.202236	3.374014	2.742062

Ovalene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.232407	-0.514482	-0.884452
2	6	0	-0.000045	-1.225913	-0.905194
3	6	0	-1.232649	-0.514748	-0.884394
4	6	0	-1.232799	0.907846	-0.842853
5	6	0	-0.000349	1.619275	-0.822111
6	6	0	1.232256	0.908111	-0.842912

7	6	0	2.461633	-1.223698	-0.905196
8	6	0	0.000106	-2.644608	-0.946621
9	6	0	-2.461722	-1.224227	-0.905080
10	6	0	-2.462024	1.617061	-0.822109
11	6	0	-0.000501	3.037971	-0.780684
12	6	0	2.461329	1.617591	-0.822226
13	6	0	3.693906	-0.511162	-0.884422
14	6	0	2.460736	-2.646691	-0.946748
15	6	0	1.233580	-3.355063	-0.967401
16	6	0	-1.233215	-3.355328	-0.967342
17	6	0	-2.460521	-2.647221	-0.946632
18	6	0	-3.694147	-0.511956	-0.884247
19	6	0	-3.694299	0.904524	-0.842884
20	6	0	-2.461128	3.040054	-0.780557
21	6	0	-1.233973	3.748427	-0.759904
22	6	0	1.232822	3.748692	-0.759963
23	6	0	2.460129	3.040582	-0.780673
24	6	0	3.693754	0.905319	-0.843059
25	6	0	4.929830	-1.224972	-0.905298
26	6	0	3.697293	-3.359407	-0.967594
27	6	0	1.233101	-4.781856	-1.009064
28	6	0	-1.232429	-4.782121	-1.009006
29	6	0	-3.696926	-3.360203	-0.967419
30	6	0	-4.929919	-1.226034	-0.905065
31	6	0	-4.930222	1.618335	-0.822007
32	6	0	-3.697685	3.752769	-0.759711
33	6	0	-1.233493	5.175218	-0.718241
34	6	0	1.232036	5.175484	-0.718299
35	6	0	3.696532	3.753564	-0.759887
36	6	0	4.929525	1.619395	-0.822240
37	6	0	4.928139	-2.646776	-0.946817
38	6	0	0.000411	-5.491293	-1.029748
39	6	0	-4.927924	-2.647836	-0.946584
40	6	0	-4.928531	3.040140	-0.780488
41	6	0	-0.000804	5.884657	-0.697558
42	6	0	4.927531	3.041199	-0.780721
43	6	0	6.157724	-0.512656	-0.884530
44	6	0	3.694398	-4.778498	-1.009032

45	6	0	2.464194	-5.488630	-1.029737
46	6	0	-2.463371	-5.489159	-1.029620
47	6	0	-3.693726	-4.779293	-1.008857
48	6	0	-6.157964	-0.513980	-0.884240
49	6	0	-6.158117	0.906020	-0.842775
50	6	0	-3.694789	5.171862	-0.718273
51	6	0	-2.464586	5.881993	-0.697568
52	6	0	2.462978	5.882524	-0.697686
53	6	0	3.693335	5.172656	-0.718448
54	6	0	6.157572	0.907343	-0.843066
55	6	0	6.169055	-3.362738	-0.967758
56	6	0	0.000564	-6.923483	-1.071569
57	6	0	-6.168687	-3.364065	-0.967464
58	6	0	-6.169448	3.756100	-0.759548
59	6	0	-0.000957	7.316846	-0.655736
60	6	0	6.168296	3.757427	-0.759841
61	6	0	7.398878	-1.238951	-0.905773
62	6	0	4.944385	-5.489496	-1.029828
63	6	0	2.455512	-6.926192	-1.071714
64	6	0	-2.454382	-6.926719	-1.071598
65	6	0	-4.943563	-5.490558	-1.029594
66	6	0	-7.398963	-1.240543	-0.905422
67	6	0	-7.399269	1.632314	-0.821533
68	6	0	-4.944778	5.882859	-0.697476
69	6	0	-2.455904	7.319555	-0.655591
70	6	0	2.453989	7.320082	-0.655707
71	6	0	4.943169	5.883923	-0.697712
72	6	0	7.398571	1.633906	-0.821882
73	6	0	7.379436	-2.627984	-0.946334
74	6	0	6.137962	-4.777893	-1.009080
75	6	0	1.242339	-7.603878	-1.091470
76	6	0	-1.241065	-7.604145	-1.091411
77	6	0	-6.137291	-4.779213	-1.008789
78	6	0	-7.379223	-2.629571	-0.945985
79	6	0	-7.379828	3.021346	-0.780971
80	6	0	-6.138354	5.171257	-0.718225
81	6	0	-1.242731	7.997241	-0.635835
82	6	0	1.240673	7.997508	-0.635893

83	6	0	6.136899	5.172576	-0.718515
84	6	0	7.378832	3.022934	-0.781321
85	6	0	8.627017	-0.481697	-0.883693
86	6	0	4.902683	-6.931279	-1.071927
87	6	0	3.725661	-7.610710	-1.091738
88	6	0	-3.724386	-7.611511	-1.091561
89	6	0	-4.901551	-6.932333	-1.071696
90	6	0	-8.627265	-0.483552	-0.883285
91	6	0	-8.627409	0.875059	-0.843612
92	6	0	-4.903075	7.324641	-0.655377
93	6	0	-3.726054	8.004074	-0.635568
94	6	0	3.723994	8.004874	-0.635744
95	6	0	4.901160	7.325696	-0.655608
96	6	0	8.626872	0.876914	-0.844020
97	1	0	8.321303	-3.172387	-0.962256
98	1	0	7.080680	-5.320824	-1.024960
99	1	0	1.241605	-8.691415	-1.123228
100	1	0	-1.240099	-8.691681	-1.123169
101	1	0	-7.079895	-5.322346	-1.024625
102	1	0	-8.320976	-3.174177	-0.961862
103	1	0	-8.321696	3.565749	-0.765048
104	1	0	-7.081074	5.714186	-0.702345
105	1	0	-1.241998	9.084778	-0.604078
106	1	0	1.239706	9.085044	-0.604135
107	1	0	7.079501	5.715709	-0.702681
108	1	0	8.320584	3.567539	-0.765442
109	1	0	9.566169	-1.029381	-0.899711
110	1	0	5.846885	-7.470216	-1.087692
111	1	0	3.720726	-8.697536	-1.123473
112	1	0	-3.719218	-8.698337	-1.123297
113	1	0	-5.845639	-7.471474	-1.087415
114	1	0	-9.566300	-1.031438	-0.899259
115	1	0	-9.566561	1.422744	-0.827594
116	1	0	-5.847278	7.863580	-0.639614
117	1	0	-3.721118	9.090898	-0.603832
118	1	0	3.718825	9.091699	-0.604008
119	1	0	5.845247	7.864836	-0.639890
120	1	0	9.565907	1.424801	-0.828047

121	6	0	0.000491	0.142882	2.583007
122	6	0	1.227955	0.851579	2.592583
123	6	0	2.463885	0.139392	2.567489
124	6	0	2.463725	-1.286086	2.526036
125	6	0	1.228207	-1.999117	2.512866
126	6	0	0.000657	-1.291139	2.542236
127	6	0	-1.227140	0.851289	2.592695
128	6	0	1.224269	2.283241	2.607648
129	6	0	3.695897	0.849497	2.560405
130	6	0	3.695677	-1.994485	2.476263
131	6	0	1.224550	-3.429358	2.448457
132	6	0	-1.226727	-1.999409	2.513022
133	6	0	-2.462905	0.138812	2.567733
134	6	0	-1.223797	2.282953	2.607779
135	6	0	0.000157	2.963794	2.611362
136	6	0	2.484935	2.966761	2.594876
137	6	0	3.664499	2.281388	2.574884
138	6	0	4.905347	0.117951	2.511882
139	6	0	4.904682	-1.260811	2.469529
140	6	0	3.663639	-3.424733	2.407788
141	6	0	2.484746	-4.111332	2.395117
142	6	0	0.000984	-4.109785	2.416371
143	6	0	-1.222740	-3.429647	2.448548
144	6	0	-2.462411	-1.286668	2.526243
145	1	0	0.000028	4.051583	2.600231
146	1	0	2.481971	4.053732	2.580707
147	1	0	4.608835	2.818787	2.545209
148	1	0	5.845624	0.662357	2.483768
149	1	0	5.844950	-1.802740	2.406528
150	1	0	4.608137	-3.959104	2.342534
151	1	0	2.481878	-5.195611	2.321011
152	1	0	0.001110	-5.195129	2.345912
153	6	0	-2.482778	-4.111912	2.395236
154	6	0	-3.694202	-1.995349	2.476446
155	6	0	-3.695084	0.848631	2.560688
156	6	0	-2.484622	2.966180	2.595149
157	6	0	-3.661831	-3.425589	2.407934
158	1	0	-4.606204	-3.960179	2.342657

159	6	0	-4.903379	-1.261955	2.469733
160	1	0	-5.843521	-1.804102	2.406715
161	6	0	-4.904366	0.116805	2.512151
162	1	0	-5.844771	0.660992	2.484058
163	6	0	-3.664028	2.280530	2.575243
164	1	0	-4.608496	2.817704	2.545688
165	1	0	-2.481912	4.053153	2.581046
166	1	0	-2.479660	-5.196186	2.321067

Circumpyrene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.910451	-1.232813	-1.029045
2	6	0	-1.621748	-0.000254	-1.010285
3	6	0	-0.910343	1.232242	-1.029157
4	6	0	0.512359	1.232177	-1.066788
5	6	0	1.223656	-0.000382	-1.085548
6	6	0	0.512252	-1.232877	-1.066676
7	6	0	-1.619907	-2.461931	-1.010225
8	6	0	-3.040552	-0.000190	-0.972757
9	6	0	-1.619691	2.461423	-1.010449
10	6	0	1.221815	2.461295	-1.085607
11	6	0	2.642460	-0.000446	-1.123076
12	6	0	1.221600	-2.462059	-1.085384
13	6	0	-0.907502	-3.694313	-1.029014
14	6	0	-3.043009	-2.460818	-0.972583
15	6	0	-3.751249	-1.233556	-0.953905
16	6	0	-3.751142	1.233239	-0.954016
17	6	0	-3.042794	2.460439	-0.972806
18	6	0	-0.907179	3.693740	-1.029349
19	6	0	0.509410	3.693676	-1.066819
20	6	0	2.644916	2.460183	-1.123249
21	6	0	3.353157	1.232920	-1.141928
22	6	0	3.353050	-1.233876	-1.141816

23	6	0	2.644701	-2.461074	-1.123026
24	6	0	0.509086	-3.694376	-1.066484
25	6	0	-1.621554	-4.930129	-1.010072
26	6	0	-3.755965	-3.697268	-0.953670
27	6	0	-5.178151	-1.232859	-0.916162
28	6	0	-5.178042	1.232671	-0.916274
29	6	0	-3.755642	3.696951	-0.954006
30	6	0	-1.621123	4.929620	-1.010519
31	6	0	1.223463	4.929492	-1.085761
32	6	0	3.357874	3.696632	-1.142162
33	6	0	4.780058	1.232223	-1.179671
34	6	0	4.779950	-1.233306	-1.179559
35	6	0	3.357550	-3.697588	-1.141827
36	6	0	1.223031	-4.930257	-1.085312
37	6	0	-3.043467	-4.928221	-0.972462
38	6	0	-5.887456	-0.000062	-0.897455
39	6	0	-3.043035	4.927841	-0.972910
40	6	0	2.645375	4.927585	-1.123371
41	6	0	5.489364	-0.000574	-1.198378
42	6	0	2.644944	-4.928477	-1.122923
43	6	0	-0.909370	-6.158130	-1.028855
44	6	0	-5.175166	-3.694156	-0.916132
45	6	0	-5.885165	-2.463845	-0.897406
46	6	0	-5.884950	2.463719	-0.897630
47	6	0	-5.174842	3.693968	-0.916468
48	6	0	-0.908830	6.157559	-1.029415
49	6	0	0.511277	6.157494	-1.066978
50	6	0	4.777073	3.693520	-1.179701
51	6	0	5.487074	2.463208	-1.198426
52	6	0	5.486858	-2.464356	-1.198202
53	6	0	4.776750	-3.694603	-1.179365
54	6	0	0.510739	-6.158194	-1.066418
55	6	0	-3.759670	-6.169030	-0.953463
56	6	0	-7.319755	0.000002	-0.859569
57	6	0	-3.759131	6.168715	-0.954023
58	6	0	3.361579	6.168394	-1.142370
59	6	0	6.921663	-0.000638	-1.236262
60	6	0	3.361038	-6.169350	-1.141809

61	6	0	-1.635908	-7.399174	-1.009583
62	6	0	-5.886406	-4.944036	-0.897264
63	6	0	-7.322835	-2.454945	-0.859380
64	6	0	-7.322620	2.454948	-0.859602
65	6	0	-5.885973	4.943912	-0.897713
66	6	0	-1.635260	7.398667	-1.010255
67	6	0	1.237816	7.398538	-1.086250
68	6	0	5.488314	4.943400	-1.198569
69	6	0	6.924743	2.454308	-1.236453
70	6	0	6.924528	-2.455585	-1.236230
71	6	0	5.487882	-4.944548	-1.198119
72	6	0	1.237168	-7.399303	-1.085578
73	6	0	-3.025043	-7.379520	-0.972841
74	6	0	-5.174929	-6.137721	-0.916030
75	6	0	-8.000390	-1.241670	-0.841511
76	6	0	-8.000282	1.241735	-0.841625
77	6	0	-5.174393	6.137533	-0.916588
78	6	0	-3.024398	7.379139	-0.973511
79	6	0	2.626952	7.378885	-1.122992
80	6	0	4.776838	6.137085	-1.179803
81	6	0	7.602298	1.241034	-1.254321
82	6	0	7.602189	-1.242371	-1.254208
83	6	0	4.776301	-6.138168	-1.179245
84	6	0	2.626306	-7.379774	-1.122322
85	6	0	-0.878780	-8.627429	-1.029555
86	6	0	-7.328293	-4.902114	-0.859127
87	6	0	-8.007599	-3.724991	-0.841211
88	6	0	-8.007273	3.725057	-0.841549
89	6	0	-7.327863	4.902120	-0.859573
90	6	0	-0.878026	8.626853	-1.030339
91	6	0	0.480689	8.626792	-1.066277
92	6	0	6.930201	4.901479	-1.236706
93	6	0	7.609507	3.724354	-1.254621
94	6	0	7.609180	-3.725693	-1.254284
95	6	0	6.929772	-4.902755	-1.236260
96	6	0	0.479934	-8.627490	-1.065494
97	1	0	-3.569631	-8.321306	-0.958394
98	1	0	-5.718044	-7.080358	-0.901623

99	1	0	-9.088010	-1.240771	-0.812744
100	1	0	-9.087901	1.240933	-0.812856
101	1	0	-5.717425	7.080217	-0.902265
102	1	0	-3.568903	8.320973	-0.959151
103	1	0	3.171539	8.320670	-1.137439
104	1	0	5.319952	7.079721	-1.194210
105	1	0	8.689917	1.240134	-1.283089
106	1	0	8.689809	-1.241570	-1.282977
107	1	0	5.319332	-7.080854	-1.193567
108	1	0	3.170810	-8.321609	-1.136682
109	1	0	-1.426650	-9.566497	-1.015022
110	1	0	-7.867414	-5.846236	-0.844825
111	1	0	-9.094506	-3.719890	-0.812463
112	1	0	-9.094181	3.720055	-0.812800
113	1	0	-7.866903	5.846289	-0.845356
114	1	0	-1.425813	9.565971	-1.015891
115	1	0	1.028557	9.565861	-1.080811
116	1	0	7.469323	5.845600	-1.251007
117	1	0	8.696414	3.719254	-1.283370
118	1	0	8.696089	-3.720690	-1.283033
119	1	0	7.468811	-5.846924	-1.250477
120	1	0	1.027720	-9.566608	-1.079942
121	6	0	-0.258422	0.000810	2.415720
122	6	0	1.156297	-2.464835	2.356596
123	6	0	-0.972918	-1.235954	2.425852
124	6	0	-0.264208	-2.464873	2.394917
125	6	0	1.152545	0.000644	2.378082
126	6	0	1.866343	-1.236287	2.352710
127	6	0	1.866664	1.237387	2.352593
128	6	0	3.286571	1.236214	2.305510
129	6	0	3.286240	-1.235458	2.305446
130	6	0	3.999718	0.000284	2.287606
131	6	0	-0.972651	1.237735	2.425491
132	6	0	-2.393463	-1.234883	2.451026
133	6	0	-2.393181	1.236989	2.450878
134	6	0	-3.106345	0.001132	2.464404
135	6	0	-0.263617	2.466471	2.394376
136	6	0	1.156904	2.466090	2.356153

137	6	0	-3.104425	2.474973	2.442136
138	6	0	1.879480	3.705462	2.304433
139	6	0	3.996093	-2.473463	2.260361
140	6	0	-0.988918	-3.704078	2.382914
141	6	0	-2.379815	-3.681715	2.406338
142	6	0	1.878590	-3.704370	2.304783
143	6	0	3.268858	-3.681889	2.255432
144	6	0	3.269756	3.682649	2.255265
145	6	0	-0.988034	3.705837	2.382384
146	6	0	-2.378942	3.683802	2.405888
147	6	0	5.421308	-2.436893	2.200292
148	6	0	-0.235954	-4.931304	2.322918
149	1	0	-0.785697	-5.868141	2.286480
150	6	0	-4.530925	2.438904	2.446010
151	1	0	-5.073871	3.379802	2.414972
152	6	0	1.123442	4.932279	2.283607
153	1	0	1.670396	5.869168	2.214836
154	6	0	5.418555	0.000107	2.230712
155	6	0	6.103034	-1.248410	2.190804
156	6	0	6.103342	1.248458	2.190817
157	6	0	-5.211736	1.249902	2.459332
158	1	0	-6.298631	1.244563	2.436580
159	6	0	-0.234784	4.932885	2.322392
160	1	0	-0.784302	5.869853	2.285925
161	6	0	3.996712	2.474050	2.260320
162	6	0	5.421922	2.437120	2.200286
163	1	0	5.962873	3.378115	2.142485
164	6	0	1.122267	-4.931017	2.284040
165	1	0	1.668996	-5.868035	2.215266
166	6	0	-4.526417	0.001298	2.470167
167	6	0	-3.105005	-2.472697	2.442436
168	6	0	-4.531492	-2.436303	2.446303
169	1	0	-5.074647	-3.377084	2.415392
170	6	0	-5.212033	-1.247140	2.459491
171	1	0	-6.298926	-1.241550	2.436762
172	1	0	-2.926975	-4.621214	2.377140
173	1	0	3.813450	-4.621559	2.194721
174	1	0	3.814583	4.622186	2.194552

175	1	0	-2.925874	4.623435	2.376678
176	1	0	7.187876	-1.243227	2.126076
177	1	0	5.962012	-3.378031	2.142518
178	1	0	7.188184	1.243000	2.126111

Methane

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.065903	-1.265573	-0.524598
2	6	0	-1.153749	-0.532215	-0.521871
3	6	0	-1.128653	0.889863	-0.484663
4	6	0	0.116239	1.579108	-0.449687
5	6	0	1.335143	0.845211	-0.452967
6	6	0	1.311564	-0.576923	-0.489618
7	6	0	0.041014	-2.684451	-0.561787
8	6	0	-2.395004	-1.219748	-0.556462
9	6	0	-2.344851	1.621567	-0.481688
10	6	0	0.141100	2.997714	-0.412746
11	6	0	2.577083	1.533124	-0.417677
12	6	0	2.527111	-1.308125	-0.492412
13	6	0	1.261577	-3.417140	-0.564384
14	6	0	-1.204612	-3.372835	-0.596435
15	6	0	-2.419061	-2.642605	-0.593795
16	6	0	-3.614524	-0.485212	-0.553782
17	6	0	-3.589562	0.931166	-0.516685
18	6	0	-2.318837	3.044252	-0.444522
19	6	0	-1.079428	3.730398	-0.409929
20	6	0	1.386762	3.686094	-0.377922
21	6	0	2.601211	2.955864	-0.380570
22	6	0	3.796675	0.798473	-0.420671
23	6	0	3.771713	-0.617905	-0.457770
24	6	0	2.500987	-2.730993	-0.529848
25	6	0	1.235801	-4.843815	-0.601845
26	6	0	-1.229123	-4.799533	-0.633887

27	6	0	-3.667800	-3.333193	-0.628584
28	6	0	-4.862650	-1.176907	-0.588584
29	6	0	-4.812526	1.667252	-0.513926
30	6	0	-3.542452	3.779256	-0.441884
31	6	0	-1.053651	5.157075	-0.372529
32	6	0	1.411273	5.112793	-0.340487
33	6	0	3.849950	3.646452	-0.345790
34	6	0	5.044800	1.490166	-0.385790
35	6	0	4.994676	-1.353993	-0.460448
36	6	0	3.724602	-3.465997	-0.532490
37	6	0	-0.009161	-5.530928	-0.636484
38	6	0	-4.885863	-2.598640	-0.625879
39	6	0	-4.785627	3.088918	-0.476583
40	6	0	0.191311	5.844188	-0.337890
41	6	0	5.068013	2.911899	-0.348495
42	6	0	4.967777	-2.775659	-0.497791
43	6	0	2.454058	-5.572781	-0.604402
44	6	0	-2.472295	-5.484279	-0.668440
45	6	0	-3.689760	-4.752235	-0.665793
46	6	0	-6.077768	-0.442720	-0.585849
47	6	0	-6.052744	0.977175	-0.548578
48	6	0	-3.514398	5.198189	-0.404597
49	6	0	-2.271908	5.886040	-0.369972
50	6	0	2.654445	5.797539	-0.305934
51	6	0	3.871910	5.065495	-0.308581
52	6	0	6.259918	0.755979	-0.388525
53	6	0	6.234894	-0.663916	-0.425796
54	6	0	3.696548	-4.884930	-0.569777
55	6	0	-0.034399	-6.963013	-0.674076
56	6	0	-6.139018	-3.292396	-0.660801
57	6	0	-6.013544	3.827247	-0.473913
58	6	0	0.216549	7.276272	-0.300298
59	6	0	6.321168	3.605655	-0.313573
60	6	0	6.195694	-3.513987	-0.500461
61	6	0	2.419892	-7.010077	-0.642249
62	6	0	-2.488795	-6.921893	-0.706058
63	6	0	-4.951897	-5.440866	-0.700702
64	6	0	-7.331340	-1.146805	-0.621046

65	6	0	-7.280714	1.725841	-0.545639
66	6	0	-4.751471	5.931717	-0.402175
67	6	0	-2.237742	7.323336	-0.332124
68	6	0	2.670945	7.235152	-0.268316
69	6	0	5.134047	5.754125	-0.273672
70	6	0	7.513490	1.460064	-0.353328
71	6	0	7.462864	-1.412581	-0.428735
72	6	0	4.933621	-5.618458	-0.572199
73	6	0	1.195006	-7.665793	-0.675801
74	6	0	-1.287789	-7.621189	-0.708075
75	6	0	-6.132719	-4.708005	-0.697540
76	6	0	-7.336232	-2.536086	-0.657250
77	6	0	-7.236650	3.114417	-0.508926
78	6	0	-5.957368	5.241734	-0.436362
79	6	0	-1.012856	7.979052	-0.298573
80	6	0	1.469939	7.934449	-0.266299
81	6	0	6.314869	5.021264	-0.276834
82	6	0	7.518382	2.849345	-0.317124
83	6	0	7.418800	-2.801158	-0.465448
84	6	0	6.139518	-4.928474	-0.538012
85	6	0	3.677592	-7.717493	-0.643714
86	6	0	-3.770625	-7.583687	-0.740534
87	6	0	-4.935458	-6.883290	-0.738001
88	6	0	-8.545917	-0.367679	-0.617134
89	6	0	-8.521975	0.990833	-0.581474
90	6	0	-4.684217	7.372638	-0.363787
91	6	0	-3.495442	8.030752	-0.330660
92	6	0	3.952775	7.896946	-0.233840
93	6	0	5.117608	7.196549	-0.236373
94	6	0	8.728067	0.680938	-0.357239
95	6	0	8.704125	-0.677574	-0.392900
96	6	0	4.866367	-7.059378	-0.610587
97	1	0	1.174990	-8.753234	-0.704358
98	1	0	-1.306104	-8.708661	-0.736609
99	1	0	-7.084717	-5.234066	-0.724044
100	1	0	-8.287406	-3.063635	-0.683782
101	1	0	-8.168633	3.675797	-0.506873
102	1	0	-6.890227	5.801656	-0.434359

103	1	0	-0.992840	9.066493	-0.270016
104	1	0	1.488254	9.021920	-0.237765
105	1	0	7.266867	5.547325	-0.250330
106	1	0	8.469556	3.376894	-0.290592
107	1	0	8.350783	-3.362538	-0.467501
108	1	0	7.072378	-5.488397	-0.540015
109	1	0	3.653389	-8.804148	-0.672307
110	1	0	-3.784727	-8.670523	-0.768995
111	1	0	-5.888870	-7.405333	-0.764420
112	1	0	-9.494433	-0.898557	-0.643717
113	1	0	-9.451184	1.555445	-0.579300
114	1	0	-5.618630	7.928595	-0.361909
115	1	0	-3.471239	9.117407	-0.302067
116	1	0	3.966877	8.983782	-0.205379
117	1	0	6.071020	7.718592	-0.209954
118	1	0	9.676583	1.211817	-0.330657
119	1	0	9.633334	-1.242185	-0.395074
120	1	0	5.800780	-7.615336	-0.612465
121	6	0	0.049011	-0.892884	2.846377
122	1	0	0.035424	-0.782352	3.934068
123	1	0	0.001497	0.091603	2.374488
124	1	0	0.969502	-1.394792	2.537877
125	1	0	-0.810304	-1.486845	2.525077

Ethane

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.065804	-1.265833	-0.524530
2	6	0	-1.153739	-0.532367	-0.521842
3	6	0	-1.128592	0.889603	-0.484629
4	6	0	0.116122	1.579140	-0.449845
5	6	0	1.335979	0.845930	-0.452411
6	6	0	1.310663	-0.576717	-0.489880
7	6	0	0.041085	-2.684452	-0.561762

8	6	0	-2.395002	-1.219752	-0.556463
9	6	0	-2.344889	1.621504	-0.481869
10	6	0	0.141150	2.997710	-0.412621
11	6	0	2.577207	1.532912	-0.417910
12	6	0	2.527112	-1.308123	-0.492491
13	6	0	1.261577	-3.417140	-0.564383
14	6	0	-1.204612	-3.372835	-0.596446
15	6	0	-2.419061	-2.642605	-0.593798
16	6	0	-3.614524	-0.485212	-0.553791
17	6	0	-3.589563	0.931164	-0.516603
18	6	0	-2.318837	3.044252	-0.444509
19	6	0	-1.079427	3.730399	-0.409990
20	6	0	1.386762	3.686094	-0.377927
21	6	0	2.601211	2.955864	-0.380574
22	6	0	3.796674	0.798471	-0.420593
23	6	0	3.771713	-0.617905	-0.457770
24	6	0	2.500987	-2.730993	-0.529848
25	6	0	1.235801	-4.843815	-0.601845
26	6	0	-1.229123	-4.799533	-0.633887
27	6	0	-3.667800	-3.333193	-0.628584
28	6	0	-4.862650	-1.176907	-0.588584
29	6	0	-4.812526	1.667252	-0.513926
30	6	0	-3.542452	3.779256	-0.441884
31	6	0	-1.053651	5.157075	-0.372529
32	6	0	1.411273	5.112793	-0.340487
33	6	0	3.849950	3.646452	-0.345790
34	6	0	5.044800	1.490166	-0.385790
35	6	0	4.994676	-1.353993	-0.460448
36	6	0	3.724602	-3.465997	-0.532490
37	6	0	-0.009161	-5.530928	-0.636484
38	6	0	-4.885863	-2.598640	-0.625879
39	6	0	-4.785627	3.088918	-0.476583
40	6	0	0.191311	5.844188	-0.337890
41	6	0	5.068013	2.911899	-0.348495
42	6	0	4.967777	-2.775659	-0.497791
43	6	0	2.454058	-5.572781	-0.604402
44	6	0	-2.472295	-5.484279	-0.668440
45	6	0	-3.689760	-4.752235	-0.665793

46	6	0	-6.077768	-0.442720	-0.585849
47	6	0	-6.052744	0.977175	-0.548578
48	6	0	-3.514398	5.198189	-0.404597
49	6	0	-2.271908	5.886040	-0.369972
50	6	0	2.654445	5.797539	-0.305934
51	6	0	3.871910	5.065495	-0.308581
52	6	0	6.259918	0.755979	-0.388525
53	6	0	6.234894	-0.663916	-0.425796
54	6	0	3.696548	-4.884930	-0.569777
55	6	0	-0.034399	-6.963013	-0.674076
56	6	0	-6.139018	-3.292396	-0.660801
57	6	0	-6.013544	3.827247	-0.473913
58	6	0	0.216549	7.276272	-0.300298
59	6	0	6.321168	3.605655	-0.313573
60	6	0	6.195694	-3.513987	-0.500461
61	6	0	2.419892	-7.010077	-0.642249
62	6	0	-2.488795	-6.921893	-0.706058
63	6	0	-4.951897	-5.440866	-0.700702
64	6	0	-7.331340	-1.146805	-0.621046
65	6	0	-7.280714	1.725841	-0.545639
66	6	0	-4.751471	5.931717	-0.402175
67	6	0	-2.237742	7.323336	-0.332124
68	6	0	2.670945	7.235152	-0.268316
69	6	0	5.134047	5.754125	-0.273672
70	6	0	7.513490	1.460064	-0.353328
71	6	0	7.462864	-1.412581	-0.428735
72	6	0	4.933621	-5.618458	-0.572199
73	6	0	1.195006	-7.665793	-0.675801
74	6	0	-1.287789	-7.621189	-0.708075
75	6	0	-6.132719	-4.708005	-0.697540
76	6	0	-7.336232	-2.536086	-0.657250
77	6	0	-7.236650	3.114417	-0.508926
78	6	0	-5.957368	5.241734	-0.436362
79	6	0	-1.012856	7.979052	-0.298573
80	6	0	1.469939	7.934449	-0.266299
81	6	0	6.314869	5.021264	-0.276834
82	6	0	7.518382	2.849345	-0.317124
83	6	0	7.418800	-2.801158	-0.465448

84	6	0	6.139518	-4.928474	-0.538012
85	6	0	3.677592	-7.717493	-0.643714
86	6	0	-3.770625	-7.583687	-0.740534
87	6	0	-4.935458	-6.883290	-0.738001
88	6	0	-8.545917	-0.367679	-0.617134
89	6	0	-8.521975	0.990833	-0.581474
90	6	0	-4.684217	7.372638	-0.363787
91	6	0	-3.495442	8.030752	-0.330660
92	6	0	3.952775	7.896946	-0.233840
93	6	0	5.117608	7.196549	-0.236373
94	6	0	8.728067	0.680938	-0.357239
95	6	0	8.704125	-0.677574	-0.392900
96	6	0	4.866367	-7.059378	-0.610587
97	1	0	1.174990	-8.753234	-0.704358
98	1	0	-1.306104	-8.708661	-0.736609
99	1	0	-7.084717	-5.234066	-0.724044
100	1	0	-8.287406	-3.063635	-0.683782
101	1	0	-8.168633	3.675797	-0.506873
102	1	0	-6.890227	5.801656	-0.434359
103	1	0	-0.992840	9.066493	-0.270016
104	1	0	1.488254	9.021920	-0.237765
105	1	0	7.266867	5.547325	-0.250330
106	1	0	8.469556	3.376894	-0.290592
107	1	0	8.350783	-3.362538	-0.467501
108	1	0	7.072378	-5.488397	-0.540015
109	1	0	3.653389	-8.804148	-0.672307
110	1	0	-3.784727	-8.670523	-0.768995
111	1	0	-5.888870	-7.405333	-0.764420
112	1	0	-9.494433	-0.898557	-0.643717
113	1	0	-9.451184	1.555445	-0.579300
114	1	0	-5.618630	7.928595	-0.361909
115	1	0	-3.471239	9.117407	-0.302067
116	1	0	3.966877	8.983782	-0.205379
117	1	0	6.071020	7.718592	-0.209954
118	1	0	9.676583	1.211817	-0.330657
119	1	0	9.633334	-1.242185	-0.395074
120	1	0	5.800780	-7.615336	-0.612465
121	6	0	-0.172314	-0.356394	3.052432

122	6	0	-1.342205	-1.325583	2.866679
123	1	0	-0.403102	0.408783	3.802970
124	1	0	0.068048	0.159173	2.117776
125	1	0	-1.103443	-2.098900	2.129336
126	1	0	-1.597376	-1.828310	3.806975
127	1	0	-2.238432	-0.804019	2.512734
128	1	0	0.732065	-0.881957	3.380910

Propane

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.371714	-0.036415	-0.156720
2	6	0	0.628005	-1.249807	-0.150610
3	6	0	-0.794620	-1.212392	-0.138536
4	6	0	-1.473576	0.038377	-0.132545
5	6	0	-0.729833	1.251724	-0.138685
6	6	0	0.692786	1.214369	-0.150756
7	6	0	2.790494	-0.073713	-0.168769
8	6	0	1.305103	-2.497195	-0.156563
9	6	0	-1.536319	-2.422503	-0.132434
10	6	0	-2.892338	0.075669	-0.120505
11	6	0	-1.406953	2.499144	-0.132718
12	6	0	1.434471	2.424458	-0.156843
13	6	0	3.533524	1.140578	-0.174876
14	6	0	3.468705	-1.325365	-0.174736
15	6	0	2.728185	-2.533555	-0.168650
16	6	0	0.560283	-3.710392	-0.150442
17	6	0	-0.856261	-3.673157	-0.138412
18	6	0	-2.959344	-2.384051	-0.120347
19	6	0	-3.635369	-1.138626	-0.114404
20	6	0	-3.570549	1.327318	-0.114544
21	6	0	-2.830030	2.535507	-0.120631
22	6	0	-0.662127	3.712345	-0.138836
23	6	0	0.754417	3.675109	-0.150868

24	6	0	2.857500	2.386003	-0.168932
25	6	0	4.960363	1.102439	-0.186995
26	6	0	4.895577	-1.362240	-0.186853
27	6	0	3.408575	-3.788348	-0.174632
28	6	0	1.241784	-4.964582	-0.156435
29	6	0	-1.602711	-4.889810	-0.132278
30	6	0	-3.704715	-3.601366	-0.114222
31	6	0	-5.062207	-1.100486	-0.102286
32	6	0	-4.997421	1.364192	-0.102427
33	6	0	-3.510419	3.790300	-0.114648
34	6	0	-1.343629	4.966534	-0.132845
35	6	0	1.500866	4.891763	-0.157002
36	6	0	3.602871	3.603318	-0.175058
37	6	0	5.637308	-0.148546	-0.192948
38	6	0	2.663700	-5.000114	-0.168510
39	6	0	-3.024530	-4.850592	-0.120203
40	6	0	-5.739152	0.150499	-0.096332
41	6	0	-2.765545	5.002067	-0.120770
42	6	0	2.922685	4.852544	-0.169077
43	6	0	5.699650	2.314448	-0.193069
44	6	0	5.570169	-2.611415	-0.192786
45	6	0	4.827810	-3.822605	-0.186685
46	6	0	0.497301	-6.173406	-0.150316
47	6	0	-0.922762	-6.136077	-0.138256
48	6	0	-5.123790	-3.561015	-0.102170
49	6	0	-5.801494	-2.312496	-0.096211
50	6	0	-5.672014	2.613367	-0.096495
51	6	0	-4.929654	3.824558	-0.102595
52	6	0	-0.599146	6.175358	-0.138964
53	6	0	0.820917	6.138030	-0.151024
54	6	0	5.021946	3.562967	-0.187110
55	6	0	7.069562	-0.186195	-0.205111
56	6	0	3.347222	-6.259351	-0.174521
57	6	0	-3.773262	-6.072180	-0.114050
58	6	0	-7.171406	0.188147	-0.084169
59	6	0	-3.449066	6.261304	-0.114759
60	6	0	3.671417	6.074133	-0.175231
61	6	0	7.137042	2.267826	-0.205278

62	6	0	7.008026	-2.640372	-0.204995
63	6	0	5.506130	-5.090780	-0.192653
64	6	0	1.191151	-7.433149	-0.156414
65	6	0	-1.681834	-7.357629	-0.132015
66	6	0	-5.867797	-4.791801	-0.096059
67	6	0	-7.238886	-2.265873	-0.084002
68	6	0	-7.109870	2.642324	-0.084285
69	6	0	-5.607974	5.092732	-0.096628
70	6	0	-1.292995	7.435102	-0.132866
71	6	0	1.579990	7.359582	-0.157265
72	6	0	5.765953	4.793754	-0.193221
73	6	0	7.782748	1.037190	-0.210962
74	6	0	7.717492	-1.445358	-0.210819
75	6	0	4.763258	-6.265317	-0.186541
76	6	0	2.580758	-7.450079	-0.168212
77	6	0	-3.070412	-7.301531	-0.120219
78	6	0	-5.187656	-6.003745	-0.102033
79	6	0	-7.884592	-1.035237	-0.078318
80	6	0	-7.819337	1.447311	-0.078461
81	6	0	-4.865103	6.267270	-0.102739
82	6	0	-2.682603	7.452032	-0.121068
83	6	0	2.968568	7.303484	-0.169061
84	6	0	5.085812	6.005697	-0.187248
85	6	0	7.855101	3.519467	-0.211166
86	6	0	7.659339	-3.928008	-0.210737
87	6	0	6.949072	-5.086838	-0.204900
88	6	0	0.401721	-8.641043	-0.149913
89	6	0	-0.956951	-8.605329	-0.138374
90	6	0	-7.308540	-4.712058	-0.083816
91	6	0	-7.956946	-3.517514	-0.078115
92	6	0	-7.761183	3.929961	-0.078543
93	6	0	-7.050917	5.088791	-0.084380
94	6	0	-0.503565	8.642996	-0.139367
95	6	0	0.855107	8.607281	-0.150906
96	6	0	7.206696	4.714011	-0.205464
97	1	0	8.870311	1.007751	-0.220199
98	1	0	8.805100	-1.473096	-0.220056
99	1	0	5.281544	-7.221928	-0.191099

100	1	0	3.100540	-8.405878	-0.172782
101	1	0	-3.639688	-8.228702	-0.115540
102	1	0	-5.755482	-6.931805	-0.097366
103	1	0	-8.972155	-1.005798	-0.069081
104	1	0	-8.906944	1.475049	-0.069224
105	1	0	-5.383389	7.223880	-0.098181
106	1	0	-3.202384	8.407830	-0.116498
107	1	0	3.537844	8.230655	-0.173740
108	1	0	5.653638	6.933758	-0.191914
109	1	0	8.941842	3.485847	-0.220396
110	1	0	8.746345	-3.951528	-0.219968
111	1	0	7.463327	-6.044827	-0.209424
112	1	0	0.924855	-9.594212	-0.154511
113	1	0	-1.529437	-9.529698	-0.133668
114	1	0	-7.872413	-5.641707	-0.079184
115	1	0	-9.043687	-3.483894	-0.068885
116	1	0	-8.848189	3.953481	-0.069313
117	1	0	-7.565171	6.046780	-0.079857
118	1	0	-1.026699	9.596165	-0.134769
119	1	0	1.427593	9.531650	-0.155612
120	1	0	7.770568	5.643660	-0.210096
121	6	0	0.586493	-0.007505	3.325148
122	6	0	1.469818	1.244328	3.342581
123	6	0	1.401513	-1.302975	3.345479
124	1	0	-0.096226	0.014118	4.185923
125	1	0	-0.050533	0.010232	2.432954
126	1	0	0.870773	2.160705	3.291779
127	1	0	2.075806	1.286565	4.256337
128	1	0	2.157033	1.249397	2.489284
129	1	0	0.756202	-2.188402	3.297382
130	1	0	2.005463	-1.374623	4.258969
131	1	0	2.087830	-1.346851	2.492163

Butane

Center	Atomic	Atomic	Coordinates (Angstroms)
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Number	Number	Type	X	Y	Z
1	6	0	0.066006	-1.265860	-0.524527
2	6	0	-1.153684	-0.532478	-0.521875
3	6	0	-1.128615	0.890011	-0.484535
4	6	0	0.116144	1.579119	-0.449847
5	6	0	1.335834	0.845737	-0.452499
6	6	0	1.310765	-0.576752	-0.489839
7	6	0	0.041005	-2.684451	-0.561765
8	6	0	-2.395032	-1.219698	-0.556467
9	6	0	-2.344962	1.621383	-0.481890
10	6	0	0.141145	2.997710	-0.412609
11	6	0	2.577182	1.532957	-0.417907
12	6	0	2.527112	-1.308123	-0.492484
13	6	0	1.261577	-3.417140	-0.564387
14	6	0	-1.204612	-3.372835	-0.596445
15	6	0	-2.419061	-2.642605	-0.593804
16	6	0	-3.614524	-0.485212	-0.553784
17	6	0	-3.589563	0.931164	-0.516604
18	6	0	-2.318837	3.044252	-0.444526
19	6	0	-1.079427	3.730399	-0.409987
20	6	0	1.386762	3.686094	-0.377929
21	6	0	2.601211	2.955864	-0.380570
22	6	0	3.796674	0.798471	-0.420590
23	6	0	3.771713	-0.617905	-0.457770
24	6	0	2.500987	-2.730993	-0.529848
25	6	0	1.235801	-4.843815	-0.601845
26	6	0	-1.229123	-4.799533	-0.633887
27	6	0	-3.667800	-3.333193	-0.628584
28	6	0	-4.862650	-1.176907	-0.588584
29	6	0	-4.812526	1.667252	-0.513926
30	6	0	-3.542452	3.779256	-0.441884
31	6	0	-1.053651	5.157075	-0.372529
32	6	0	1.411273	5.112793	-0.340487
33	6	0	3.849950	3.646452	-0.345790
34	6	0	5.044800	1.490166	-0.385790
35	6	0	4.994676	-1.353993	-0.460448
36	6	0	3.724602	-3.465997	-0.532490

37	6	0	-0.009161	-5.530928	-0.636484
38	6	0	-4.885863	-2.598640	-0.625879
39	6	0	-4.785627	3.088918	-0.476583
40	6	0	0.191311	5.844188	-0.337890
41	6	0	5.068013	2.911899	-0.348495
42	6	0	4.967777	-2.775659	-0.497791
43	6	0	2.454058	-5.572781	-0.604402
44	6	0	-2.472295	-5.484279	-0.668440
45	6	0	-3.689760	-4.752235	-0.665793
46	6	0	-6.077768	-0.442720	-0.585849
47	6	0	-6.052744	0.977175	-0.548578
48	6	0	-3.514398	5.198189	-0.404597
49	6	0	-2.271908	5.886040	-0.369972
50	6	0	2.654445	5.797539	-0.305934
51	6	0	3.871910	5.065495	-0.308581
52	6	0	6.259918	0.755979	-0.388525
53	6	0	6.234894	-0.663916	-0.425796
54	6	0	3.696548	-4.884930	-0.569777
55	6	0	-0.034399	-6.963013	-0.674076
56	6	0	-6.139018	-3.292396	-0.660801
57	6	0	-6.013544	3.827247	-0.473913
58	6	0	0.216549	7.276272	-0.300298
59	6	0	6.321168	3.605655	-0.313573
60	6	0	6.195694	-3.513987	-0.500461
61	6	0	2.419892	-7.010077	-0.642249
62	6	0	-2.488795	-6.921893	-0.706058
63	6	0	-4.951897	-5.440866	-0.700702
64	6	0	-7.331340	-1.146805	-0.621046
65	6	0	-7.280714	1.725841	-0.545639
66	6	0	-4.751471	5.931717	-0.402175
67	6	0	-2.237742	7.323336	-0.332124
68	6	0	2.670945	7.235152	-0.268316
69	6	0	5.134047	5.754125	-0.273672
70	6	0	7.513490	1.460064	-0.353328
71	6	0	7.462864	-1.412581	-0.428735
72	6	0	4.933621	-5.618458	-0.572199
73	6	0	1.195006	-7.665793	-0.675801
74	6	0	-1.287789	-7.621189	-0.708075

75	6	0	-6.132719	-4.708005	-0.697540
76	6	0	-7.336232	-2.536086	-0.657250
77	6	0	-7.236650	3.114417	-0.508926
78	6	0	-5.957368	5.241734	-0.436362
79	6	0	-1.012856	7.979052	-0.298573
80	6	0	1.469939	7.934449	-0.266299
81	6	0	6.314869	5.021264	-0.276834
82	6	0	7.518382	2.849345	-0.317124
83	6	0	7.418800	-2.801158	-0.465448
84	6	0	6.139518	-4.928474	-0.538012
85	6	0	3.677592	-7.717493	-0.643714
86	6	0	-3.770625	-7.583687	-0.740534
87	6	0	-4.935458	-6.883290	-0.738001
88	6	0	-8.545917	-0.367679	-0.617134
89	6	0	-8.521975	0.990833	-0.581474
90	6	0	-4.684217	7.372638	-0.363787
91	6	0	-3.495442	8.030752	-0.330660
92	6	0	3.952775	7.896946	-0.233840
93	6	0	5.117608	7.196549	-0.236373
94	6	0	8.728067	0.680938	-0.357239
95	6	0	8.704125	-0.677574	-0.392900
96	6	0	4.866367	-7.059378	-0.610587
97	1	0	1.174990	-8.753234	-0.704358
98	1	0	-1.306104	-8.708661	-0.736609
99	1	0	-7.084717	-5.234066	-0.724044
100	1	0	-8.287406	-3.063635	-0.683782
101	1	0	-8.168633	3.675797	-0.506873
102	1	0	-6.890227	5.801656	-0.434359
103	1	0	-0.992840	9.066493	-0.270016
104	1	0	1.488254	9.021920	-0.237765
105	1	0	7.266867	5.547325	-0.250330
106	1	0	8.469556	3.376894	-0.290592
107	1	0	8.350783	-3.362538	-0.467501
108	1	0	7.072378	-5.488397	-0.540015
109	1	0	3.653389	-8.804148	-0.672307
110	1	0	-3.784727	-8.670523	-0.768995
111	1	0	-5.888870	-7.405333	-0.764420
112	1	0	-9.494433	-0.898557	-0.643717

113	1	0	-9.451184	1.555445	-0.579300
114	1	0	-5.618630	7.928595	-0.361909
115	1	0	-3.471239	9.117407	-0.302067
116	1	0	3.966877	8.983782	-0.205379
117	1	0	6.071020	7.718592	-0.209954
118	1	0	9.676583	1.211817	-0.330657
119	1	0	9.633334	-1.242185	-0.395074
120	1	0	5.800780	-7.615336	-0.612465
121	6	0	0.077763	-0.597563	2.995607
122	6	0	1.306845	-1.510911	2.986385
123	6	0	-1.244399	-1.373099	2.958450
124	6	0	-2.473308	-0.459453	2.964816
125	1	0	0.098256	0.043165	3.889098
126	1	0	0.118282	0.081356	2.134213
127	1	0	1.325248	-2.156117	3.873678
128	1	0	1.305374	-2.161085	2.105027
129	1	0	-1.262489	-2.006393	2.062247
130	1	0	-1.287461	-2.059082	3.816868
131	1	0	-2.449816	0.234730	2.118004
132	1	0	-2.514552	0.139759	3.883056
133	1	0	-3.403955	-1.034238	2.895534
134	1	0	2.238467	-0.933768	2.970268

Pentane

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.229180	-1.359899	0.000000
2	6	0	-0.229180	-0.648299	1.232527
3	6	0	-0.229180	0.774901	1.232527
4	6	0	-0.229180	1.486501	0.000000
5	6	0	-0.229180	0.774901	-1.232527
6	6	0	-0.229180	-0.648299	-1.232527
7	6	0	-0.229180	-2.779199	0.000000
8	6	0	-0.229180	-1.357949	2.461677

9	6	0	-0.229180	1.484551	2.461677
10	6	0	-0.229180	2.905801	0.000000
11	6	0	-0.229180	1.484551	-2.461677
12	6	0	-0.229180	-1.357949	-2.461677
13	6	0	-0.229180	-3.490091	-1.233398
14	6	0	-0.229180	-3.490091	1.233398
15	6	0	-0.229180	-2.781548	2.460629
16	6	0	-0.229180	-0.645241	3.694026
17	6	0	-0.229180	0.771843	3.694026
18	6	0	-0.229180	2.908151	2.460629
19	6	0	-0.229180	3.616693	1.233398
20	6	0	-0.229180	3.616693	-1.233398
21	6	0	-0.229180	2.908151	-2.460629
22	6	0	-0.229180	0.771843	-3.694026
23	6	0	-0.229180	-0.645241	-3.694026
24	6	0	-0.229180	-2.781548	-2.460629
25	6	0	-0.229180	-4.917490	-1.232765
26	6	0	-0.229180	-4.917490	1.232765
27	6	0	-0.229180	-3.494700	3.697110
28	6	0	-0.229180	-1.359489	4.929875
29	6	0	-0.229180	1.486091	4.929875
30	6	0	-0.229180	3.621303	3.697110
31	6	0	-0.229180	5.044093	1.232765
32	6	0	-0.229180	5.044093	-1.232765
33	6	0	-0.229180	3.621303	-3.697110
34	6	0	-0.229180	1.486091	-4.929875
35	6	0	-0.229180	-1.359489	-4.929875
36	6	0	-0.229180	-3.494700	-3.697110
37	6	0	-0.229180	-5.627099	0.000000
38	6	0	-0.229180	-2.781899	4.928031
39	6	0	-0.229180	2.908501	4.928031
40	6	0	-0.229180	5.753701	0.000000
41	6	0	-0.229180	2.908501	-4.928031
42	6	0	-0.229180	-2.781899	-4.928031
43	6	0	-0.229180	-5.624699	-2.463782
44	6	0	-0.229180	-5.624699	2.463782
45	6	0	-0.229180	-4.914397	3.694062
46	6	0	-0.229180	-0.647001	6.157844

47	6	0	-0.229180	0.773604	6.157844
48	6	0	-0.229180	5.040999	3.694062
49	6	0	-0.229180	5.751302	2.463782
50	6	0	-0.229180	5.751302	-2.463782
51	6	0	-0.229180	5.040999	-3.694062
52	6	0	-0.229180	0.773604	-6.157844
53	6	0	-0.229180	-0.647001	-6.157844
54	6	0	-0.229180	-4.914397	-3.694062
55	6	0	-0.229180	-7.059899	0.000000
56	6	0	-0.229180	-3.498299	6.168872
57	6	0	-0.229180	3.624901	6.168872
58	6	0	-0.229180	7.186501	0.000000
59	6	0	-0.229180	3.624901	-6.168872
60	6	0	-0.229180	-3.498299	-6.168872
61	6	0	-0.229180	-7.062872	-2.454947
62	6	0	-0.229180	-7.062872	2.454947
63	6	0	-0.229180	-5.625832	4.943974
64	6	0	-0.229180	-1.373739	7.398921
65	6	0	-0.229180	1.500342	7.398921
66	6	0	-0.229180	5.752434	4.943974
67	6	0	-0.229180	7.189475	2.454947
68	6	0	-0.229180	7.189475	-2.454947
69	6	0	-0.229180	5.752434	-4.943974
70	6	0	-0.229180	1.500342	-7.398921
71	6	0	-0.229180	-1.373739	-7.398921
72	6	0	-0.229180	-5.625832	-4.943974
73	6	0	-0.229180	-7.740717	-1.241703
74	6	0	-0.229180	-7.740717	1.241703
75	6	0	-0.229180	-4.914054	6.137627
76	6	0	-0.229180	-2.763362	7.379329
77	6	0	-0.229180	2.889964	7.379329
78	6	0	-0.229180	5.040656	6.137627
79	6	0	-0.229180	7.867320	1.241703
80	6	0	-0.229180	7.867320	-1.241703
81	6	0	-0.229180	5.040656	-6.137627
82	6	0	-0.229180	2.889964	-7.379329
83	6	0	-0.229180	-2.763362	-7.379329
84	6	0	-0.229180	-4.914054	-6.137627

85	6	0	-0.229180	-7.747820	-3.725024
86	6	0	-0.229180	-7.747820	3.725024
87	6	0	-0.229180	-7.068224	4.902117
88	6	0	-0.229180	-0.616294	8.627141
89	6	0	-0.229180	0.742896	8.627141
90	6	0	-0.229180	7.194827	4.902117
91	6	0	-0.229180	7.874422	3.725024
92	6	0	-0.229180	7.874422	-3.725024
93	6	0	-0.229180	7.194827	-4.902117
94	6	0	-0.229180	0.742896	-8.627141
95	6	0	-0.229180	-0.616294	-8.627141
96	6	0	-0.229180	-7.068224	-4.902117
97	1	0	-0.229180	-8.828717	-1.240852
98	1	0	-0.229180	-8.828717	1.240852
99	1	0	-0.229180	-5.457317	7.080287
100	1	0	-0.229180	-3.308098	8.321139
101	1	0	-0.229180	3.434701	8.321139
102	1	0	-0.229180	5.583920	7.080287
103	1	0	-0.229180	8.955319	1.240852
104	1	0	-0.229180	8.955319	-1.240852
105	1	0	-0.229180	5.583920	-7.080287
106	1	0	-0.229180	3.434701	-8.321139
107	1	0	-0.229180	-3.308098	-8.321139
108	1	0	-0.229180	-5.457317	-7.080287
109	1	0	-0.229180	-8.835108	-3.719972
110	1	0	-0.229180	-8.835108	3.719972
111	1	0	-0.229180	-7.607494	5.846262
112	1	0	-0.229180	-1.164313	9.566234
113	1	0	-0.229180	1.290915	9.566234
114	1	0	-0.229180	7.734096	5.846262
115	1	0	-0.229180	8.961710	3.719972
116	1	0	-0.229180	8.961710	-3.719972
117	1	0	-0.229180	7.734096	-5.846262
118	1	0	-0.229180	1.290915	-9.566234
119	1	0	-0.229180	-1.164313	-9.566234
120	1	0	-0.229180	-7.607494	-5.846262
121	6	0	3.293168	-0.590422	0.000000
122	6	0	3.267250	-1.430493	-1.281808

123	6	0	3.267250	-1.430493	1.281808
124	6	0	3.272577	-0.577498	-2.553685
125	6	0	3.272577	-0.577498	2.553685
126	1	0	4.188433	0.049806	0.000000
127	1	0	2.432559	0.092776	0.000000
128	1	0	4.130631	-2.111322	-1.288350
129	1	0	2.375926	-2.070360	-1.273646
130	1	0	2.375926	-2.070360	1.273646
131	1	0	4.130631	-2.111322	1.288350
132	1	0	4.186589	0.025802	-2.620275
133	1	0	2.420559	0.110720	-2.567112
134	1	0	3.211251	-1.197277	-3.455605
135	1	0	2.420559	0.110720	2.567112
136	1	0	4.186589	0.025802	2.620275
137	1	0	3.211251	-1.197277	3.455605

Hexane

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.066006	-1.265860	-0.524527
2	6	0	-1.153684	-0.532478	-0.521875
3	6	0	-1.128615	0.890011	-0.484535
4	6	0	0.116144	1.579119	-0.449847
5	6	0	1.335834	0.845737	-0.452499
6	6	0	1.310765	-0.576752	-0.489839
7	6	0	0.041005	-2.684451	-0.561765
8	6	0	-2.395032	-1.219698	-0.556467
9	6	0	-2.344962	1.621383	-0.481890
10	6	0	0.141145	2.997710	-0.412609
11	6	0	2.577182	1.532957	-0.417907
12	6	0	2.527112	-1.308123	-0.492484
13	6	0	1.261577	-3.417140	-0.564387
14	6	0	-1.204612	-3.372835	-0.596445
15	6	0	-2.419061	-2.642605	-0.593804

16	6	0	-3.614524	-0.485212	-0.553784
17	6	0	-3.589563	0.931164	-0.516604
18	6	0	-2.318837	3.044252	-0.444526
19	6	0	-1.079427	3.730399	-0.409987
20	6	0	1.386762	3.686094	-0.377929
21	6	0	2.601211	2.955864	-0.380570
22	6	0	3.796674	0.798471	-0.420590
23	6	0	3.771713	-0.617905	-0.457770
24	6	0	2.500987	-2.730993	-0.529848
25	6	0	1.235801	-4.843815	-0.601845
26	6	0	-1.229123	-4.799533	-0.633887
27	6	0	-3.667800	-3.333193	-0.628584
28	6	0	-4.862650	-1.176907	-0.588584
29	6	0	-4.812526	1.667252	-0.513926
30	6	0	-3.542452	3.779256	-0.441884
31	6	0	-1.053651	5.157075	-0.372529
32	6	0	1.411273	5.112793	-0.340487
33	6	0	3.849950	3.646452	-0.345790
34	6	0	5.044800	1.490166	-0.385790
35	6	0	4.994676	-1.353993	-0.460448
36	6	0	3.724602	-3.465997	-0.532490
37	6	0	-0.009161	-5.530928	-0.636484
38	6	0	-4.885863	-2.598640	-0.625879
39	6	0	-4.785627	3.088918	-0.476583
40	6	0	0.191311	5.844188	-0.337890
41	6	0	5.068013	2.911899	-0.348495
42	6	0	4.967777	-2.775659	-0.497791
43	6	0	2.454058	-5.572781	-0.604402
44	6	0	-2.472295	-5.484279	-0.668440
45	6	0	-3.689760	-4.752235	-0.665793
46	6	0	-6.077768	-0.442720	-0.585849
47	6	0	-6.052744	0.977175	-0.548578
48	6	0	-3.514398	5.198189	-0.404597
49	6	0	-2.271908	5.886040	-0.369972
50	6	0	2.654445	5.797539	-0.305934
51	6	0	3.871910	5.065495	-0.308581
52	6	0	6.259918	0.755979	-0.388525
53	6	0	6.234894	-0.663916	-0.425796

54	6	0	3.696548	-4.884930	-0.569777
55	6	0	-0.034399	-6.963013	-0.674076
56	6	0	-6.139018	-3.292396	-0.660801
57	6	0	-6.013544	3.827247	-0.473913
58	6	0	0.216549	7.276272	-0.300298
59	6	0	6.321168	3.605655	-0.313573
60	6	0	6.195694	-3.513987	-0.500461
61	6	0	2.419892	-7.010077	-0.642249
62	6	0	-2.488795	-6.921893	-0.706058
63	6	0	-4.951897	-5.440866	-0.700702
64	6	0	-7.331340	-1.146805	-0.621046
65	6	0	-7.280714	1.725841	-0.545639
66	6	0	-4.751471	5.931717	-0.402175
67	6	0	-2.237742	7.323336	-0.332124
68	6	0	2.670945	7.235152	-0.268316
69	6	0	5.134047	5.754125	-0.273672
70	6	0	7.513490	1.460064	-0.353328
71	6	0	7.462864	-1.412581	-0.428735
72	6	0	4.933621	-5.618458	-0.572199
73	6	0	1.195006	-7.665793	-0.675801
74	6	0	-1.287789	-7.621189	-0.708075
75	6	0	-6.132719	-4.708005	-0.697540
76	6	0	-7.336232	-2.536086	-0.657250
77	6	0	-7.236650	3.114417	-0.508926
78	6	0	-5.957368	5.241734	-0.436362
79	6	0	-1.012856	7.979052	-0.298573
80	6	0	1.469939	7.934449	-0.266299
81	6	0	6.314869	5.021264	-0.276834
82	6	0	7.518382	2.849345	-0.317124
83	6	0	7.418800	-2.801158	-0.465448
84	6	0	6.139518	-4.928474	-0.538012
85	6	0	3.677592	-7.717493	-0.643714
86	6	0	-3.770625	-7.583687	-0.740534
87	6	0	-4.935458	-6.883290	-0.738001
88	6	0	-8.545917	-0.367679	-0.617134
89	6	0	-8.521975	0.990833	-0.581474
90	6	0	-4.684217	7.372638	-0.363787
91	6	0	-3.495442	8.030752	-0.330660

92	6	0	3.952775	7.896946	-0.233840
93	6	0	5.117608	7.196549	-0.236373
94	6	0	8.728067	0.680938	-0.357239
95	6	0	8.704125	-0.677574	-0.392900
96	6	0	4.866367	-7.059378	-0.610587
97	1	0	1.174990	-8.753234	-0.704358
98	1	0	-1.306104	-8.708661	-0.736609
99	1	0	-7.084717	-5.234066	-0.724044
100	1	0	-8.287406	-3.063635	-0.683782
101	1	0	-8.168633	3.675797	-0.506873
102	1	0	-6.890227	5.801656	-0.434359
103	1	0	-0.992840	9.066493	-0.270016
104	1	0	1.488254	9.021920	-0.237765
105	1	0	7.266867	5.547325	-0.250330
106	1	0	8.469556	3.376894	-0.290592
107	1	0	8.350783	-3.362538	-0.467501
108	1	0	7.072378	-5.488397	-0.540015
109	1	0	3.653389	-8.804148	-0.672307
110	1	0	-3.784727	-8.670523	-0.768995
111	1	0	-5.888870	-7.405333	-0.764420
112	1	0	-9.494433	-0.898557	-0.643717
113	1	0	-9.451184	1.555445	-0.579300
114	1	0	-5.618630	7.928595	-0.361909
115	1	0	-3.471239	9.117407	-0.302067
116	1	0	3.966877	8.983782	-0.205379
117	1	0	6.071020	7.718592	-0.209954
118	1	0	9.676583	1.211817	-0.330657
119	1	0	9.633334	-1.242185	-0.395074
120	1	0	5.800780	-7.615336	-0.612465
121	6	0	0.059132	-0.568112	3.015967
122	6	0	1.331845	-1.422107	2.992121
123	6	0	-1.230061	-1.395140	2.978638
124	6	0	2.612893	-0.583745	3.026316
125	6	0	-2.501987	-0.539860	2.963057
126	1	0	0.061349	0.066115	3.915321
127	1	0	0.072476	0.120374	2.159997
128	1	0	1.320380	-2.116358	3.844674
129	1	0	1.326972	-2.047858	2.090686

130	1	0	-1.220410	-2.041040	2.090011
131	1	0	-1.255616	-2.072412	3.845701
132	1	0	2.676183	0.001871	3.951992
133	1	0	2.642972	0.119893	2.187585
134	1	0	-2.473702	0.129074	2.093683
135	1	0	-2.513192	0.112022	3.848433
136	6	0	-3.783300	-1.377487	2.922535
137	1	0	-3.870614	-2.007639	3.816513
138	1	0	-3.791479	-2.039151	2.049809
139	1	0	-4.677056	-0.745493	2.866675
140	1	0	3.508596	-1.212296	2.963082

Heptane

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.309359	-1.324755	0.000000
2	6	0	-0.309359	-0.613155	1.232527
3	6	0	-0.309359	0.810045	1.232527
4	6	0	-0.309359	1.521645	0.000000
5	6	0	-0.309359	0.810045	-1.232527
6	6	0	-0.309359	-0.613155	-1.232527
7	6	0	-0.309359	-2.744055	0.000000
8	6	0	-0.309359	-1.322805	2.461677
9	6	0	-0.309359	1.519695	2.461677
10	6	0	-0.309359	2.940945	0.000000
11	6	0	-0.309359	1.519695	-2.461677
12	6	0	-0.309359	-1.322805	-2.461677
13	6	0	-0.309359	-3.454947	-1.233398
14	6	0	-0.309359	-3.454947	1.233398
15	6	0	-0.309359	-2.746405	2.460629
16	6	0	-0.309359	-0.610097	3.694026
17	6	0	-0.309359	0.806987	3.694026
18	6	0	-0.309359	2.943295	2.460629
19	6	0	-0.309359	3.651837	1.233398

20	6	0	-0.309359	3.651837	-1.233398
21	6	0	-0.309359	2.943295	-2.460629
22	6	0	-0.309359	0.806987	-3.694026
23	6	0	-0.309359	-0.610097	-3.694026
24	6	0	-0.309359	-2.746405	-2.460629
25	6	0	-0.309359	-4.882347	-1.232765
26	6	0	-0.309359	-4.882347	1.232765
27	6	0	-0.309359	-3.459557	3.697110
28	6	0	-0.309359	-1.324345	4.929875
29	6	0	-0.309359	1.521235	4.929875
30	6	0	-0.309359	3.656446	3.697110
31	6	0	-0.309359	5.079237	1.232765
32	6	0	-0.309359	5.079237	-1.232765
33	6	0	-0.309359	3.656446	-3.697110
34	6	0	-0.309359	1.521235	-4.929875
35	6	0	-0.309359	-1.324345	-4.929875
36	6	0	-0.309359	-3.459557	-3.697110
37	6	0	-0.309359	-5.591955	0.000000
38	6	0	-0.309359	-2.746755	4.928031
39	6	0	-0.309359	2.943645	4.928031
40	6	0	-0.309359	5.788845	0.000000
41	6	0	-0.309359	2.943645	-4.928031
42	6	0	-0.309359	-2.746755	-4.928031
43	6	0	-0.309359	-5.589556	-2.463782
44	6	0	-0.309359	-5.589556	2.463782
45	6	0	-0.309359	-4.879253	3.694062
46	6	0	-0.309359	-0.611857	6.157844
47	6	0	-0.309359	0.808747	6.157844
48	6	0	-0.309359	5.076143	3.694062
49	6	0	-0.309359	5.786445	2.463782
50	6	0	-0.309359	5.786445	-2.463782
51	6	0	-0.309359	5.076143	-3.694062
52	6	0	-0.309359	0.808747	-6.157844
53	6	0	-0.309359	-0.611857	-6.157844
54	6	0	-0.309359	-4.879253	-3.694062
55	6	0	-0.309359	-7.024755	0.000000
56	6	0	-0.309359	-3.463155	6.168872
57	6	0	-0.309359	3.660045	6.168872

58	6	0	-0.309359	7.221645	0.000000
59	6	0	-0.309359	3.660045	-6.168872
60	6	0	-0.309359	-3.463155	-6.168872
61	6	0	-0.309359	-7.027729	-2.454947
62	6	0	-0.309359	-7.027729	2.454947
63	6	0	-0.309359	-5.590688	4.943974
64	6	0	-0.309359	-1.338596	7.398921
65	6	0	-0.309359	1.535485	7.398921
66	6	0	-0.309359	5.787578	4.943974
67	6	0	-0.309359	7.224618	2.454947
68	6	0	-0.309359	7.224618	-2.454947
69	6	0	-0.309359	5.787578	-4.943974
70	6	0	-0.309359	1.535485	-7.398921
71	6	0	-0.309359	-1.338596	-7.398921
72	6	0	-0.309359	-5.590688	-4.943974
73	6	0	-0.309359	-7.705573	-1.241703
74	6	0	-0.309359	-7.705573	1.241703
75	6	0	-0.309359	-4.878910	6.137627
76	6	0	-0.309359	-2.728218	7.379329
77	6	0	-0.309359	2.925108	7.379329
78	6	0	-0.309359	5.075800	6.137627
79	6	0	-0.309359	7.902463	1.241703
80	6	0	-0.309359	7.902463	-1.241703
81	6	0	-0.309359	5.075800	-6.137627
82	6	0	-0.309359	2.925108	-7.379329
83	6	0	-0.309359	-2.728218	-7.379329
84	6	0	-0.309359	-4.878910	-6.137627
85	6	0	-0.309359	-7.712676	-3.725024
86	6	0	-0.309359	-7.712676	3.725024
87	6	0	-0.309359	-7.033081	4.902117
88	6	0	-0.309359	-0.581150	8.627141
89	6	0	-0.309359	0.778040	8.627141
90	6	0	-0.309359	7.229971	4.902117
91	6	0	-0.309359	7.909566	3.725024
92	6	0	-0.309359	7.909566	-3.725024
93	6	0	-0.309359	7.229971	-4.902117
94	6	0	-0.309359	0.778040	-8.627141
95	6	0	-0.309359	-0.581150	-8.627141

96	6	0	-0.309359	-7.033081	-4.902117
97	1	0	-0.309359	-8.793573	-1.240852
98	1	0	-0.309359	-8.793573	1.240852
99	1	0	-0.309359	-5.422173	7.080287
100	1	0	-0.309359	-3.272955	8.321139
101	1	0	-0.309359	3.469845	8.321139
102	1	0	-0.309359	5.619063	7.080287
103	1	0	-0.309359	8.990463	1.240852
104	1	0	-0.309359	8.990463	-1.240852
105	1	0	-0.309359	5.619063	-7.080287
106	1	0	-0.309359	3.469845	-8.321139
107	1	0	-0.309359	-3.272955	-8.321139
108	1	0	-0.309359	-5.422173	-7.080287
109	1	0	-0.309359	-8.799964	-3.719972
110	1	0	-0.309359	-8.799964	3.719972
111	1	0	-0.309359	-7.572350	5.846262
112	1	0	-0.309359	-1.129169	9.566234
113	1	0	-0.309359	1.326059	9.566234
114	1	0	-0.309359	7.769240	5.846262
115	1	0	-0.309359	8.996854	3.719972
116	1	0	-0.309359	8.996854	-3.719972
117	1	0	-0.309359	7.769240	-5.846262
118	1	0	-0.309359	1.326059	-9.566234
119	1	0	-0.309359	-1.129169	-9.566234
120	1	0	-0.309359	-7.572350	-5.846262
121	6	0	3.212599	-0.518682	0.000000
122	6	0	3.219501	-1.360872	-1.280009
123	6	0	3.219501	-1.360872	1.280009
124	6	0	3.188457	-0.521842	-2.562227
125	6	0	3.188457	-0.521842	2.562227
126	6	0	3.189515	-1.375921	-3.833276
127	6	0	3.189515	-1.375921	3.833276
128	1	0	4.083586	0.153774	0.000000
129	1	0	2.327827	0.132142	0.000000
130	1	0	4.110193	-2.007200	-1.287756
131	1	0	2.354175	-2.037818	-1.272272
132	1	0	2.354175	-2.037818	1.272272
133	1	0	4.110193	-2.007200	1.287756

134	1	0	4.051541	0.159283	-2.572651
135	1	0	2.297064	0.117773	-2.550964
136	1	0	2.297064	0.117773	2.550964
137	1	0	4.051541	0.159283	2.572651
138	1	0	3.120630	-0.757327	-4.735469
139	1	0	2.340304	-2.067516	-3.841339
140	1	0	4.105543	-1.975769	-3.904180
141	1	0	3.120630	-0.757327	4.735469
142	1	0	4.105543	-1.975769	3.904180
143	1	0	2.340304	-2.067516	3.841339

Octane

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.066006	-1.265860	-0.524527
2	6	0	-1.153684	-0.532478	-0.521875
3	6	0	-1.128615	0.890011	-0.484535
4	6	0	0.116144	1.579119	-0.449847
5	6	0	1.335834	0.845737	-0.452499
6	6	0	1.310765	-0.576752	-0.489839
7	6	0	0.041005	-2.684451	-0.561765
8	6	0	-2.395032	-1.219698	-0.556467
9	6	0	-2.344962	1.621383	-0.481890
10	6	0	0.141145	2.997710	-0.412609
11	6	0	2.577182	1.532957	-0.417907
12	6	0	2.527112	-1.308123	-0.492484
13	6	0	1.261577	-3.417140	-0.564387
14	6	0	-1.204612	-3.372835	-0.596445
15	6	0	-2.419061	-2.642605	-0.593804
16	6	0	-3.614524	-0.485212	-0.553784
17	6	0	-3.589563	0.931164	-0.516604
18	6	0	-2.318837	3.044252	-0.444526
19	6	0	-1.079427	3.730399	-0.409987
20	6	0	1.386762	3.686094	-0.377929

21	6	0	2.601211	2.955864	-0.380570
22	6	0	3.796674	0.798471	-0.420590
23	6	0	3.771713	-0.617905	-0.457770
24	6	0	2.500987	-2.730993	-0.529848
25	6	0	1.235801	-4.843815	-0.601845
26	6	0	-1.229123	-4.799533	-0.633887
27	6	0	-3.667800	-3.333193	-0.628584
28	6	0	-4.862650	-1.176907	-0.588584
29	6	0	-4.812526	1.667252	-0.513926
30	6	0	-3.542452	3.779256	-0.441884
31	6	0	-1.053651	5.157075	-0.372529
32	6	0	1.411273	5.112793	-0.340487
33	6	0	3.849950	3.646452	-0.345790
34	6	0	5.044800	1.490166	-0.385790
35	6	0	4.994676	-1.353993	-0.460448
36	6	0	3.724602	-3.465997	-0.532490
37	6	0	-0.009161	-5.530928	-0.636484
38	6	0	-4.885863	-2.598640	-0.625879
39	6	0	-4.785627	3.088918	-0.476583
40	6	0	0.191311	5.844188	-0.337890
41	6	0	5.068013	2.911899	-0.348495
42	6	0	4.967777	-2.775659	-0.497791
43	6	0	2.454058	-5.572781	-0.604402
44	6	0	-2.472295	-5.484279	-0.668440
45	6	0	-3.689760	-4.752235	-0.665793
46	6	0	-6.077768	-0.442720	-0.585849
47	6	0	-6.052744	0.977175	-0.548578
48	6	0	-3.514398	5.198189	-0.404597
49	6	0	-2.271908	5.886040	-0.369972
50	6	0	2.654445	5.797539	-0.305934
51	6	0	3.871910	5.065495	-0.308581
52	6	0	6.259918	0.755979	-0.388525
53	6	0	6.234894	-0.663916	-0.425796
54	6	0	3.696548	-4.884930	-0.569777
55	6	0	-0.034399	-6.963013	-0.674076
56	6	0	-6.139018	-3.292396	-0.660801
57	6	0	-6.013544	3.827247	-0.473913
58	6	0	0.216549	7.276272	-0.300298

59	6	0	6.321168	3.605655	-0.313573
60	6	0	6.195694	-3.513987	-0.500461
61	6	0	2.419892	-7.010077	-0.642249
62	6	0	-2.488795	-6.921893	-0.706058
63	6	0	-4.951897	-5.440866	-0.700702
64	6	0	-7.331340	-1.146805	-0.621046
65	6	0	-7.280714	1.725841	-0.545639
66	6	0	-4.751471	5.931717	-0.402175
67	6	0	-2.237742	7.323336	-0.332124
68	6	0	2.670945	7.235152	-0.268316
69	6	0	5.134047	5.754125	-0.273672
70	6	0	7.513490	1.460064	-0.353328
71	6	0	7.462864	-1.412581	-0.428735
72	6	0	4.933621	-5.618458	-0.572199
73	6	0	1.195006	-7.665793	-0.675801
74	6	0	-1.287789	-7.621189	-0.708075
75	6	0	-6.132719	-4.708005	-0.697540
76	6	0	-7.336232	-2.536086	-0.657250
77	6	0	-7.236650	3.114417	-0.508926
78	6	0	-5.957368	5.241734	-0.436362
79	6	0	-1.012856	7.979052	-0.298573
80	6	0	1.469939	7.934449	-0.266299
81	6	0	6.314869	5.021264	-0.276834
82	6	0	7.518382	2.849345	-0.317124
83	6	0	7.418800	-2.801158	-0.465448
84	6	0	6.139518	-4.928474	-0.538012
85	6	0	3.677592	-7.717493	-0.643714
86	6	0	-3.770625	-7.583687	-0.740534
87	6	0	-4.935458	-6.883290	-0.738001
88	6	0	-8.545917	-0.367679	-0.617134
89	6	0	-8.521975	0.990833	-0.581474
90	6	0	-4.684217	7.372638	-0.363787
91	6	0	-3.495442	8.030752	-0.330660
92	6	0	3.952775	7.896946	-0.233840
93	6	0	5.117608	7.196549	-0.236373
94	6	0	8.728067	0.680938	-0.357239
95	6	0	8.704125	-0.677574	-0.392900
96	6	0	4.866367	-7.059378	-0.610587

97	1	0	1.174990	-8.753234	-0.704358
98	1	0	-1.306104	-8.708661	-0.736609
99	1	0	-7.084717	-5.234066	-0.724044
100	1	0	-8.287406	-3.063635	-0.683782
101	1	0	-8.168633	3.675797	-0.506873
102	1	0	-6.890227	5.801656	-0.434359
103	1	0	-0.992840	9.066493	-0.270016
104	1	0	1.488254	9.021920	-0.237765
105	1	0	7.266867	5.547325	-0.250330
106	1	0	8.469556	3.376894	-0.290592
107	1	0	8.350783	-3.362538	-0.467501
108	1	0	7.072378	-5.488397	-0.540015
109	1	0	3.653389	-8.804148	-0.672307
110	1	0	-3.784727	-8.670523	-0.768995
111	1	0	-5.888870	-7.405333	-0.764420
112	1	0	-9.494433	-0.898557	-0.643717
113	1	0	-9.451184	1.555445	-0.579300
114	1	0	-5.618630	7.928595	-0.361909
115	1	0	-3.471239	9.117407	-0.302067
116	1	0	3.966877	8.983782	-0.205379
117	1	0	6.071020	7.718592	-0.209954
118	1	0	9.676583	1.211817	-0.330657
119	1	0	9.633334	-1.242185	-0.395074
120	1	0	5.800780	-7.615336	-0.612465
121	6	0	0.071686	-0.571264	3.021792
122	6	0	1.334576	-1.438545	3.017657
123	6	0	-1.225297	-1.386282	2.985298
124	6	0	2.632600	-0.623664	3.028419
125	6	0	-2.487429	-0.517896	2.988592
126	1	0	0.073694	0.072695	3.914015
127	1	0	0.096012	0.107264	2.158370
128	1	0	1.318650	-2.111915	3.887969
129	1	0	1.324859	-2.088301	2.131784
130	1	0	-1.226565	-2.023731	2.090689
131	1	0	-1.250908	-2.071201	3.846144
132	1	0	2.643708	0.031390	3.911457
133	1	0	2.645356	0.042127	2.156366
134	1	0	-2.454215	0.172623	2.134768

135	1	0	-2.493945	0.114032	3.889568
136	6	0	3.887388	-1.501404	3.021024
137	1	0	3.934856	-2.128293	3.920294
138	1	0	3.893724	-2.168604	2.152536
139	6	0	-3.786026	-1.329528	2.927332
140	1	0	-3.820189	-2.025967	3.777547
141	1	0	-3.777708	-1.952804	2.024303
142	6	0	-5.038942	-0.449087	2.930270
143	1	0	-5.107154	0.135746	3.856173
144	1	0	-5.023245	0.257235	2.093465
145	1	0	-5.952988	-1.047283	2.840666
146	1	0	4.801834	-0.898420	2.981402

Nonane

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.066006	-1.265860	-0.524527
2	6	0	-1.153684	-0.532478	-0.521875
3	6	0	-1.128615	0.890011	-0.484535
4	6	0	0.116144	1.579119	-0.449847
5	6	0	1.335834	0.845737	-0.452499
6	6	0	1.310765	-0.576752	-0.489839
7	6	0	0.041005	-2.684451	-0.561765
8	6	0	-2.395032	-1.219698	-0.556467
9	6	0	-2.344962	1.621383	-0.481890
10	6	0	0.141145	2.997710	-0.412609
11	6	0	2.577182	1.532957	-0.417907
12	6	0	2.527112	-1.308123	-0.492484
13	6	0	1.261577	-3.417140	-0.564387
14	6	0	-1.204612	-3.372835	-0.596445
15	6	0	-2.419061	-2.642605	-0.593804
16	6	0	-3.614524	-0.485212	-0.553784
17	6	0	-3.589563	0.931164	-0.516604
18	6	0	-2.318837	3.044252	-0.444526

19	6	0	-1.079427	3.730399	-0.409987
20	6	0	1.386762	3.686094	-0.377929
21	6	0	2.601211	2.955864	-0.380570
22	6	0	3.796674	0.798471	-0.420590
23	6	0	3.771713	-0.617905	-0.457770
24	6	0	2.500987	-2.730993	-0.529848
25	6	0	1.235801	-4.843815	-0.601845
26	6	0	-1.229123	-4.799533	-0.633887
27	6	0	-3.667800	-3.333193	-0.628584
28	6	0	-4.862650	-1.176907	-0.588584
29	6	0	-4.812526	1.667252	-0.513926
30	6	0	-3.542452	3.779256	-0.441884
31	6	0	-1.053651	5.157075	-0.372529
32	6	0	1.411273	5.112793	-0.340487
33	6	0	3.849950	3.646452	-0.345790
34	6	0	5.044800	1.490166	-0.385790
35	6	0	4.994676	-1.353993	-0.460448
36	6	0	3.724602	-3.465997	-0.532490
37	6	0	-0.009161	-5.530928	-0.636484
38	6	0	-4.885863	-2.598640	-0.625879
39	6	0	-4.785627	3.088918	-0.476583
40	6	0	0.191311	5.844188	-0.337890
41	6	0	5.068013	2.911899	-0.348495
42	6	0	4.967777	-2.775659	-0.497791
43	6	0	2.454058	-5.572781	-0.604402
44	6	0	-2.472295	-5.484279	-0.668440
45	6	0	-3.689760	-4.752235	-0.665793
46	6	0	-6.077768	-0.442720	-0.585849
47	6	0	-6.052744	0.977175	-0.548578
48	6	0	-3.514398	5.198189	-0.404597
49	6	0	-2.271908	5.886040	-0.369972
50	6	0	2.654445	5.797539	-0.305934
51	6	0	3.871910	5.065495	-0.308581
52	6	0	6.259918	0.755979	-0.388525
53	6	0	6.234894	-0.663916	-0.425796
54	6	0	3.696548	-4.884930	-0.569777
55	6	0	-0.034399	-6.963013	-0.674076
56	6	0	-6.139018	-3.292396	-0.660801

57	6	0	-6.013544	3.827247	-0.473913
58	6	0	0.216549	7.276272	-0.300298
59	6	0	6.321168	3.605655	-0.313573
60	6	0	6.195694	-3.513987	-0.500461
61	6	0	2.419892	-7.010077	-0.642249
62	6	0	-2.488795	-6.921893	-0.706058
63	6	0	-4.951897	-5.440866	-0.700702
64	6	0	-7.331340	-1.146805	-0.621046
65	6	0	-7.280714	1.725841	-0.545639
66	6	0	-4.751471	5.931717	-0.402175
67	6	0	-2.237742	7.323336	-0.332124
68	6	0	2.670945	7.235152	-0.268316
69	6	0	5.134047	5.754125	-0.273672
70	6	0	7.513490	1.460064	-0.353328
71	6	0	7.462864	-1.412581	-0.428735
72	6	0	4.933621	-5.618458	-0.572199
73	6	0	1.195006	-7.665793	-0.675801
74	6	0	-1.287789	-7.621189	-0.708075
75	6	0	-6.132719	-4.708005	-0.697540
76	6	0	-7.336232	-2.536086	-0.657250
77	6	0	-7.236650	3.114417	-0.508926
78	6	0	-5.957368	5.241734	-0.436362
79	6	0	-1.012856	7.979052	-0.298573
80	6	0	1.469939	7.934449	-0.266299
81	6	0	6.314869	5.021264	-0.276834
82	6	0	7.518382	2.849345	-0.317124
83	6	0	7.418800	-2.801158	-0.465448
84	6	0	6.139518	-4.928474	-0.538012
85	6	0	3.677592	-7.717493	-0.643714
86	6	0	-3.770625	-7.583687	-0.740534
87	6	0	-4.935458	-6.883290	-0.738001
88	6	0	-8.545917	-0.367679	-0.617134
89	6	0	-8.521975	0.990833	-0.581474
90	6	0	-4.684217	7.372638	-0.363787
91	6	0	-3.495442	8.030752	-0.330660
92	6	0	3.952775	7.896946	-0.233840
93	6	0	5.117608	7.196549	-0.236373
94	6	0	8.728067	0.680938	-0.357239

95	6	0	8.704125	-0.677574	-0.392900
96	6	0	4.866367	-7.059378	-0.610587
97	1	0	1.174990	-8.753234	-0.704358
98	1	0	-1.306104	-8.708661	-0.736609
99	1	0	-7.084717	-5.234066	-0.724044
100	1	0	-8.287406	-3.063635	-0.683782
101	1	0	-8.168633	3.675797	-0.506873
102	1	0	-6.890227	5.801656	-0.434359
103	1	0	-0.992840	9.066493	-0.270016
104	1	0	1.488254	9.021920	-0.237765
105	1	0	7.266867	5.547325	-0.250330
106	1	0	8.469556	3.376894	-0.290592
107	1	0	8.350783	-3.362538	-0.467501
108	1	0	7.072378	-5.488397	-0.540015
109	1	0	3.653389	-8.804148	-0.672307
110	1	0	-3.784727	-8.670523	-0.768995
111	1	0	-5.888870	-7.405333	-0.764420
112	1	0	-9.494433	-0.898557	-0.643717
113	1	0	-9.451184	1.555445	-0.579300
114	1	0	-5.618630	7.928595	-0.361909
115	1	0	-3.471239	9.117407	-0.302067
116	1	0	3.966877	8.983782	-0.205379
117	1	0	6.071020	7.718592	-0.209954
118	1	0	9.676583	1.211817	-0.330657
119	1	0	9.633334	-1.242185	-0.395074
120	1	0	5.800780	-7.615336	-0.612465
121	6	0	0.031843	-0.583274	3.025048
122	6	0	1.297517	-1.446316	3.014761
123	6	0	-1.263167	-1.400653	2.981660
124	6	0	2.590117	-0.625064	3.055401
125	6	0	-2.526126	-0.533547	2.989021
126	1	0	0.031559	0.053172	3.922673
127	1	0	0.054871	0.102870	2.167503
128	1	0	1.276038	-2.136422	3.871567
129	1	0	1.297574	-2.078422	2.116464
130	1	0	-1.262567	-2.032855	2.083424
131	1	0	-1.288628	-2.090571	3.838504
132	1	0	2.595586	0.003043	3.959062

133	1	0	2.604856	0.069250	2.204096
134	1	0	-2.493752	0.160536	2.138006
135	1	0	-2.532553	0.094692	3.892584
136	6	0	3.859327	-1.483329	3.025112
137	1	0	3.846037	-2.182592	3.873579
138	1	0	3.851947	-2.103659	2.120141
139	6	0	-3.824157	-1.345611	2.925212
140	1	0	-3.858076	-2.044698	3.773250
141	1	0	-3.815610	-1.966026	2.020306
142	6	0	5.142773	-0.648967	3.063648
143	1	0	5.208404	-0.070083	3.993470
144	1	0	5.173998	0.060300	2.229763
145	6	0	-5.077310	-0.465580	2.930990
146	1	0	-5.146093	0.115659	3.859111
147	1	0	-5.061405	0.244009	2.096953
148	1	0	6.036662	-1.279495	2.994696
149	1	0	-5.991235	-1.063549	2.838596

Decane

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.066006	-1.265860	-0.524527
2	6	0	-1.153684	-0.532478	-0.521875
3	6	0	-1.128615	0.890011	-0.484535
4	6	0	0.116144	1.579119	-0.449847
5	6	0	1.335834	0.845737	-0.452499
6	6	0	1.310765	-0.576752	-0.489839
7	6	0	0.041005	-2.684451	-0.561765
8	6	0	-2.395032	-1.219698	-0.556467
9	6	0	-2.344962	1.621383	-0.481890
10	6	0	0.141145	2.997710	-0.412609
11	6	0	2.577182	1.532957	-0.417907
12	6	0	2.527112	-1.308123	-0.492484
13	6	0	1.261577	-3.417140	-0.564387

14	6	0	-1.204612	-3.372835	-0.596445
15	6	0	-2.419061	-2.642605	-0.593804
16	6	0	-3.614524	-0.485212	-0.553784
17	6	0	-3.589563	0.931164	-0.516604
18	6	0	-2.318837	3.044252	-0.444526
19	6	0	-1.079427	3.730399	-0.409987
20	6	0	1.386762	3.686094	-0.377929
21	6	0	2.601211	2.955864	-0.380570
22	6	0	3.796674	0.798471	-0.420590
23	6	0	3.771713	-0.617905	-0.457770
24	6	0	2.500987	-2.730993	-0.529848
25	6	0	1.235801	-4.843815	-0.601845
26	6	0	-1.229123	-4.799533	-0.633887
27	6	0	-3.667800	-3.333193	-0.628584
28	6	0	-4.862650	-1.176907	-0.588584
29	6	0	-4.812526	1.667252	-0.513926
30	6	0	-3.542452	3.779256	-0.441884
31	6	0	-1.053651	5.157075	-0.372529
32	6	0	1.411273	5.112793	-0.340487
33	6	0	3.849950	3.646452	-0.345790
34	6	0	5.044800	1.490166	-0.385790
35	6	0	4.994676	-1.353993	-0.460448
36	6	0	3.724602	-3.465997	-0.532490
37	6	0	-0.009161	-5.530928	-0.636484
38	6	0	-4.885863	-2.598640	-0.625879
39	6	0	-4.785627	3.088918	-0.476583
40	6	0	0.191311	5.844188	-0.337890
41	6	0	5.068013	2.911899	-0.348495
42	6	0	4.967777	-2.775659	-0.497791
43	6	0	2.454058	-5.572781	-0.604402
44	6	0	-2.472295	-5.484279	-0.668440
45	6	0	-3.689760	-4.752235	-0.665793
46	6	0	-6.077768	-0.442720	-0.585849
47	6	0	-6.052744	0.977175	-0.548578
48	6	0	-3.514398	5.198189	-0.404597
49	6	0	-2.271908	5.886040	-0.369972
50	6	0	2.654445	5.797539	-0.305934
51	6	0	3.871910	5.065495	-0.308581

52	6	0	6.259918	0.755979	-0.388525
53	6	0	6.234894	-0.663916	-0.425796
54	6	0	3.696548	-4.884930	-0.569777
55	6	0	-0.034399	-6.963013	-0.674076
56	6	0	-6.139018	-3.292396	-0.660801
57	6	0	-6.013544	3.827247	-0.473913
58	6	0	0.216549	7.276272	-0.300298
59	6	0	6.321168	3.605655	-0.313573
60	6	0	6.195694	-3.513987	-0.500461
61	6	0	2.419892	-7.010077	-0.642249
62	6	0	-2.488795	-6.921893	-0.706058
63	6	0	-4.951897	-5.440866	-0.700702
64	6	0	-7.331340	-1.146805	-0.621046
65	6	0	-7.280714	1.725841	-0.545639
66	6	0	-4.751471	5.931717	-0.402175
67	6	0	-2.237742	7.323336	-0.332124
68	6	0	2.670945	7.235152	-0.268316
69	6	0	5.134047	5.754125	-0.273672
70	6	0	7.513490	1.460064	-0.353328
71	6	0	7.462864	-1.412581	-0.428735
72	6	0	4.933621	-5.618458	-0.572199
73	6	0	1.195006	-7.665793	-0.675801
74	6	0	-1.287789	-7.621189	-0.708075
75	6	0	-6.132719	-4.708005	-0.697540
76	6	0	-7.336232	-2.536086	-0.657250
77	6	0	-7.236650	3.114417	-0.508926
78	6	0	-5.957368	5.241734	-0.436362
79	6	0	-1.012856	7.979052	-0.298573
80	6	0	1.469939	7.934449	-0.266299
81	6	0	6.314869	5.021264	-0.276834
82	6	0	7.518382	2.849345	-0.317124
83	6	0	7.418800	-2.801158	-0.465448
84	6	0	6.139518	-4.928474	-0.538012
85	6	0	3.677592	-7.717493	-0.643714
86	6	0	-3.770625	-7.583687	-0.740534
87	6	0	-4.935458	-6.883290	-0.738001
88	6	0	-8.545917	-0.367679	-0.617134
89	6	0	-8.521975	0.990833	-0.581474

90	6	0	-4.684217	7.372638	-0.363787
91	6	0	-3.495442	8.030752	-0.330660
92	6	0	3.952775	7.896946	-0.233840
93	6	0	5.117608	7.196549	-0.236373
94	6	0	8.728067	0.680938	-0.357239
95	6	0	8.704125	-0.677574	-0.392900
96	6	0	4.866367	-7.059378	-0.610587
97	1	0	1.174990	-8.753234	-0.704358
98	1	0	-1.306104	-8.708661	-0.736609
99	1	0	-7.084717	-5.234066	-0.724044
100	1	0	-8.287406	-3.063635	-0.683782
101	1	0	-8.168633	3.675797	-0.506873
102	1	0	-6.890227	5.801656	-0.434359
103	1	0	-0.992840	9.066493	-0.270016
104	1	0	1.488254	9.021920	-0.237765
105	1	0	7.266867	5.547325	-0.250330
106	1	0	8.469556	3.376894	-0.290592
107	1	0	8.350783	-3.362538	-0.467501
108	1	0	7.072378	-5.488397	-0.540015
109	1	0	3.653389	-8.804148	-0.672307
110	1	0	-3.784727	-8.670523	-0.768995
111	1	0	-5.888870	-7.405333	-0.764420
112	1	0	-9.494433	-0.898557	-0.643717
113	1	0	-9.451184	1.555445	-0.579300
114	1	0	-5.618630	7.928595	-0.361909
115	1	0	-3.471239	9.117407	-0.302067
116	1	0	3.966877	8.983782	-0.205379
117	1	0	6.071020	7.718592	-0.209954
118	1	0	9.676583	1.211817	-0.330657
119	1	0	9.633334	-1.242185	-0.395074
120	1	0	5.800780	-7.615336	-0.612465
121	6	0	0.085550	-0.564812	3.024876
122	6	0	1.345996	-1.435226	3.018100
123	6	0	-1.213796	-1.375087	2.988437
124	6	0	2.642991	-0.621171	3.058572
125	6	0	-2.471634	-0.500880	2.988051
126	1	0	0.089943	0.076614	3.918930
127	1	0	0.111536	0.116392	2.163578

128	1	0	1.319479	-2.123146	3.876525
129	1	0	1.343381	-2.069459	2.121273
130	1	0	-1.217227	-2.015707	2.096074
131	1	0	-1.243017	-2.056791	3.851710
132	1	0	2.651455	0.007537	3.961792
133	1	0	2.661866	0.072479	2.206827
134	1	0	-2.443502	0.173188	2.121293
135	1	0	-2.465174	0.147720	3.876955
136	6	0	3.907419	-1.486356	3.029386
137	1	0	3.889469	-2.185715	3.877691
138	1	0	3.897438	-2.106428	2.124264
139	6	0	-3.772887	-1.308216	2.958325
140	1	0	-3.807071	-1.978392	3.830630
141	1	0	-3.775157	-1.960877	2.074526
142	6	0	5.195286	-0.658886	3.069408
143	1	0	5.263782	-0.081836	4.000194
144	1	0	5.230327	0.051542	2.236644
145	6	0	-5.030324	-0.432631	2.939791
146	1	0	-5.026702	0.227243	3.819351
147	1	0	-4.995284	0.227539	2.064146
148	6	0	-6.324693	-1.249973	2.912621
149	1	0	-6.415819	-1.872904	3.811482
150	1	0	-6.348884	-1.915668	2.043218
151	1	0	-7.208399	-0.603589	2.858792
152	1	0	6.085905	-1.293990	2.999558

Undecane

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.066006	-1.265860	-0.524527
2	6	0	-1.153684	-0.532478	-0.521875
3	6	0	-1.128615	0.890011	-0.484535
4	6	0	0.116144	1.579119	-0.449847
5	6	0	1.335834	0.845737	-0.452499

6	6	0	1.310765	-0.576752	-0.489839
7	6	0	0.041005	-2.684451	-0.561765
8	6	0	-2.395032	-1.219698	-0.556467
9	6	0	-2.344962	1.621383	-0.481890
10	6	0	0.141145	2.997710	-0.412609
11	6	0	2.577182	1.532957	-0.417907
12	6	0	2.527112	-1.308123	-0.492484
13	6	0	1.261577	-3.417140	-0.564387
14	6	0	-1.204612	-3.372835	-0.596445
15	6	0	-2.419061	-2.642605	-0.593804
16	6	0	-3.614524	-0.485212	-0.553784
17	6	0	-3.589563	0.931164	-0.516604
18	6	0	-2.318837	3.044252	-0.444526
19	6	0	-1.079427	3.730399	-0.409987
20	6	0	1.386762	3.686094	-0.377929
21	6	0	2.601211	2.955864	-0.380570
22	6	0	3.796674	0.798471	-0.420590
23	6	0	3.771713	-0.617905	-0.457770
24	6	0	2.500987	-2.730993	-0.529848
25	6	0	1.235801	-4.843815	-0.601845
26	6	0	-1.229123	-4.799533	-0.633887
27	6	0	-3.667800	-3.333193	-0.628584
28	6	0	-4.862650	-1.176907	-0.588584
29	6	0	-4.812526	1.667252	-0.513926
30	6	0	-3.542452	3.779256	-0.441884
31	6	0	-1.053651	5.157075	-0.372529
32	6	0	1.411273	5.112793	-0.340487
33	6	0	3.849950	3.646452	-0.345790
34	6	0	5.044800	1.490166	-0.385790
35	6	0	4.994676	-1.353993	-0.460448
36	6	0	3.724602	-3.465997	-0.532490
37	6	0	-0.009161	-5.530928	-0.636484
38	6	0	-4.885863	-2.598640	-0.625879
39	6	0	-4.785627	3.088918	-0.476583
40	6	0	0.191311	5.844188	-0.337890
41	6	0	5.068013	2.911899	-0.348495
42	6	0	4.967777	-2.775659	-0.497791
43	6	0	2.454058	-5.572781	-0.604402

44	6	0	-2.472295	-5.484279	-0.668440
45	6	0	-3.689760	-4.752235	-0.665793
46	6	0	-6.077768	-0.442720	-0.585849
47	6	0	-6.052744	0.977175	-0.548578
48	6	0	-3.514398	5.198189	-0.404597
49	6	0	-2.271908	5.886040	-0.369972
50	6	0	2.654445	5.797539	-0.305934
51	6	0	3.871910	5.065495	-0.308581
52	6	0	6.259918	0.755979	-0.388525
53	6	0	6.234894	-0.663916	-0.425796
54	6	0	3.696548	-4.884930	-0.569777
55	6	0	-0.034399	-6.963013	-0.674076
56	6	0	-6.139018	-3.292396	-0.660801
57	6	0	-6.013544	3.827247	-0.473913
58	6	0	0.216549	7.276272	-0.300298
59	6	0	6.321168	3.605655	-0.313573
60	6	0	6.195694	-3.513987	-0.500461
61	6	0	2.419892	-7.010077	-0.642249
62	6	0	-2.488795	-6.921893	-0.706058
63	6	0	-4.951897	-5.440866	-0.700702
64	6	0	-7.331340	-1.146805	-0.621046
65	6	0	-7.280714	1.725841	-0.545639
66	6	0	-4.751471	5.931717	-0.402175
67	6	0	-2.237742	7.323336	-0.332124
68	6	0	2.670945	7.235152	-0.268316
69	6	0	5.134047	5.754125	-0.273672
70	6	0	7.513490	1.460064	-0.353328
71	6	0	7.462864	-1.412581	-0.428735
72	6	0	4.933621	-5.618458	-0.572199
73	6	0	1.195006	-7.665793	-0.675801
74	6	0	-1.287789	-7.621189	-0.708075
75	6	0	-6.132719	-4.708005	-0.697540
76	6	0	-7.336232	-2.536086	-0.657250
77	6	0	-7.236650	3.114417	-0.508926
78	6	0	-5.957368	5.241734	-0.436362
79	6	0	-1.012856	7.979052	-0.298573
80	6	0	1.469939	7.934449	-0.266299
81	6	0	6.314869	5.021264	-0.276834

82	6	0	7.518382	2.849345	-0.317124
83	6	0	7.418800	-2.801158	-0.465448
84	6	0	6.139518	-4.928474	-0.538012
85	6	0	3.677592	-7.717493	-0.643714
86	6	0	-3.770625	-7.583687	-0.740534
87	6	0	-4.935458	-6.883290	-0.738001
88	6	0	-8.545917	-0.367679	-0.617134
89	6	0	-8.521975	0.990833	-0.581474
90	6	0	-4.684217	7.372638	-0.363787
91	6	0	-3.495442	8.030752	-0.330660
92	6	0	3.952775	7.896946	-0.233840
93	6	0	5.117608	7.196549	-0.236373
94	6	0	8.728067	0.680938	-0.357239
95	6	0	8.704125	-0.677574	-0.392900
96	6	0	4.866367	-7.059378	-0.610587
97	1	0	1.174990	-8.753234	-0.704358
98	1	0	-1.306104	-8.708661	-0.736609
99	1	0	-7.084717	-5.234066	-0.724044
100	1	0	-8.287406	-3.063635	-0.683782
101	1	0	-8.168633	3.675797	-0.506873
102	1	0	-6.890227	5.801656	-0.434359
103	1	0	-0.992840	9.066493	-0.270016
104	1	0	1.488254	9.021920	-0.237765
105	1	0	7.266867	5.547325	-0.250330
106	1	0	8.469556	3.376894	-0.290592
107	1	0	8.350783	-3.362538	-0.467501
108	1	0	7.072378	-5.488397	-0.540015
109	1	0	3.653389	-8.804148	-0.672307
110	1	0	-3.784727	-8.670523	-0.768995
111	1	0	-5.888870	-7.405333	-0.764420
112	1	0	-9.494433	-0.898557	-0.643717
113	1	0	-9.451184	1.555445	-0.579300
114	1	0	-5.618630	7.928595	-0.361909
115	1	0	-3.471239	9.117407	-0.302067
116	1	0	3.966877	8.983782	-0.205379
117	1	0	6.071020	7.718592	-0.209954
118	1	0	9.676583	1.211817	-0.330657
119	1	0	9.633334	-1.242185	-0.395074

120	1	0	5.800780	-7.615336	-0.612465
121	6	0	0.033243	-0.542451	3.019158
122	6	0	1.298217	-1.405663	3.021830
123	6	0	-1.261601	-1.359663	2.988577
124	6	0	2.589751	-0.582986	3.054077
125	6	0	-2.523091	-0.491011	2.987586
126	1	0	0.033340	0.106433	3.907849
127	1	0	0.056580	0.131797	2.152438
128	1	0	1.275395	-2.083927	3.887998
129	1	0	1.300238	-2.049990	2.132114
130	1	0	-1.263673	-2.003951	2.098835
131	1	0	-1.285695	-2.037850	3.854768
132	1	0	2.585143	0.067758	3.941424
133	1	0	2.612184	0.089370	2.185865
134	1	0	-2.498725	0.181295	2.119388
135	1	0	-2.518099	0.159575	3.875049
136	6	0	3.857814	-1.441730	3.061123
137	1	0	3.841054	-2.111163	3.934507
138	1	0	3.858559	-2.095486	2.178135
139	6	0	-3.821044	-1.303473	2.961319
140	1	0	-3.851117	-1.972630	3.834556
141	1	0	-3.822467	-1.957221	2.078323
142	6	0	5.148903	-0.616623	3.076976
143	1	0	5.147594	0.043251	3.956551
144	1	0	5.163437	0.044047	2.201133
145	6	0	-5.081503	-0.432311	2.944000
146	1	0	-5.079196	0.227604	3.823534
147	1	0	-5.049487	0.227925	2.068298
148	6	0	-6.373030	-1.254042	2.918141
149	1	0	-6.461224	-1.877089	3.817181
150	1	0	-6.395668	-1.919923	2.048884
151	6	0	6.410199	-1.484449	3.084143
152	1	0	7.319886	-0.873554	3.054256
153	1	0	6.452505	-2.109878	3.984856
154	1	0	6.431262	-2.151065	2.215400
155	1	0	-7.259022	-0.610767	2.864981

Dodecane

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.066006	-1.265860	-0.524527
2	6	0	-1.153684	-0.532478	-0.521875
3	6	0	-1.128615	0.890011	-0.484535
4	6	0	0.116144	1.579119	-0.449847
5	6	0	1.335834	0.845737	-0.452499
6	6	0	1.310765	-0.576752	-0.489839
7	6	0	0.041005	-2.684451	-0.561765
8	6	0	-2.395032	-1.219698	-0.556467
9	6	0	-2.344962	1.621383	-0.481890
10	6	0	0.141145	2.997710	-0.412609
11	6	0	2.577182	1.532957	-0.417907
12	6	0	2.527112	-1.308123	-0.492484
13	6	0	1.261577	-3.417140	-0.564387
14	6	0	-1.204612	-3.372835	-0.596445
15	6	0	-2.419061	-2.642605	-0.593804
16	6	0	-3.614524	-0.485212	-0.553784
17	6	0	-3.589563	0.931164	-0.516604
18	6	0	-2.318837	3.044252	-0.444526
19	6	0	-1.079427	3.730399	-0.409987
20	6	0	1.386762	3.686094	-0.377929
21	6	0	2.601211	2.955864	-0.380570
22	6	0	3.796674	0.798471	-0.420590
23	6	0	3.771713	-0.617905	-0.457770
24	6	0	2.500987	-2.730993	-0.529848
25	6	0	1.235801	-4.843815	-0.601845
26	6	0	-1.229123	-4.799533	-0.633887
27	6	0	-3.667800	-3.333193	-0.628584
28	6	0	-4.862650	-1.176907	-0.588584
29	6	0	-4.812526	1.667252	-0.513926
30	6	0	-3.542452	3.779256	-0.441884
31	6	0	-1.053651	5.157075	-0.372529
32	6	0	1.411273	5.112793	-0.340487
33	6	0	3.849950	3.646452	-0.345790

34	6	0	5.044800	1.490166	-0.385790
35	6	0	4.994676	-1.353993	-0.460448
36	6	0	3.724602	-3.465997	-0.532490
37	6	0	-0.009161	-5.530928	-0.636484
38	6	0	-4.885863	-2.598640	-0.625879
39	6	0	-4.785627	3.088918	-0.476583
40	6	0	0.191311	5.844188	-0.337890
41	6	0	5.068013	2.911899	-0.348495
42	6	0	4.967777	-2.775659	-0.497791
43	6	0	2.454058	-5.572781	-0.604402
44	6	0	-2.472295	-5.484279	-0.668440
45	6	0	-3.689760	-4.752235	-0.665793
46	6	0	-6.077768	-0.442720	-0.585849
47	6	0	-6.052744	0.977175	-0.548578
48	6	0	-3.514398	5.198189	-0.404597
49	6	0	-2.271908	5.886040	-0.369972
50	6	0	2.654445	5.797539	-0.305934
51	6	0	3.871910	5.065495	-0.308581
52	6	0	6.259918	0.755979	-0.388525
53	6	0	6.234894	-0.663916	-0.425796
54	6	0	3.696548	-4.884930	-0.569777
55	6	0	-0.034399	-6.963013	-0.674076
56	6	0	-6.139018	-3.292396	-0.660801
57	6	0	-6.013544	3.827247	-0.473913
58	6	0	0.216549	7.276272	-0.300298
59	6	0	6.321168	3.605655	-0.313573
60	6	0	6.195694	-3.513987	-0.500461
61	6	0	2.419892	-7.010077	-0.642249
62	6	0	-2.488795	-6.921893	-0.706058
63	6	0	-4.951897	-5.440866	-0.700702
64	6	0	-7.331340	-1.146805	-0.621046
65	6	0	-7.280714	1.725841	-0.545639
66	6	0	-4.751471	5.931717	-0.402175
67	6	0	-2.237742	7.323336	-0.332124
68	6	0	2.670945	7.235152	-0.268316
69	6	0	5.134047	5.754125	-0.273672
70	6	0	7.513490	1.460064	-0.353328
71	6	0	7.462864	-1.412581	-0.428735

72	6	0	4.933621	-5.618458	-0.572199
73	6	0	1.195006	-7.665793	-0.675801
74	6	0	-1.287789	-7.621189	-0.708075
75	6	0	-6.132719	-4.708005	-0.697540
76	6	0	-7.336232	-2.536086	-0.657250
77	6	0	-7.236650	3.114417	-0.508926
78	6	0	-5.957368	5.241734	-0.436362
79	6	0	-1.012856	7.979052	-0.298573
80	6	0	1.469939	7.934449	-0.266299
81	6	0	6.314869	5.021264	-0.276834
82	6	0	7.518382	2.849345	-0.317124
83	6	0	7.418800	-2.801158	-0.465448
84	6	0	6.139518	-4.928474	-0.538012
85	6	0	3.677592	-7.717493	-0.643714
86	6	0	-3.770625	-7.583687	-0.740534
87	6	0	-4.935458	-6.883290	-0.738001
88	6	0	-8.545917	-0.367679	-0.617134
89	6	0	-8.521975	0.990833	-0.581474
90	6	0	-4.684217	7.372638	-0.363787
91	6	0	-3.495442	8.030752	-0.330660
92	6	0	3.952775	7.896946	-0.233840
93	6	0	5.117608	7.196549	-0.236373
94	6	0	8.728067	0.680938	-0.357239
95	6	0	8.704125	-0.677574	-0.392900
96	6	0	4.866367	-7.059378	-0.610587
97	1	0	1.174990	-8.753234	-0.704358
98	1	0	-1.306104	-8.708661	-0.736609
99	1	0	-7.084717	-5.234066	-0.724044
100	1	0	-8.287406	-3.063635	-0.683782
101	1	0	-8.168633	3.675797	-0.506873
102	1	0	-6.890227	5.801656	-0.434359
103	1	0	-0.992840	9.066493	-0.270016
104	1	0	1.488254	9.021920	-0.237765
105	1	0	7.266867	5.547325	-0.250330
106	1	0	8.469556	3.376894	-0.290592
107	1	0	8.350783	-3.362538	-0.467501
108	1	0	7.072378	-5.488397	-0.540015
109	1	0	3.653389	-8.804148	-0.672307

110	1	0	-3.784727	-8.670523	-0.768995
111	1	0	-5.888870	-7.405333	-0.764420
112	1	0	-9.494433	-0.898557	-0.643717
113	1	0	-9.451184	1.555445	-0.579300
114	1	0	-5.618630	7.928595	-0.361909
115	1	0	-3.471239	9.117407	-0.302067
116	1	0	3.966877	8.983782	-0.205379
117	1	0	6.071020	7.718592	-0.209954
118	1	0	9.676583	1.211817	-0.330657
119	1	0	9.633334	-1.242185	-0.395074
120	1	0	5.800780	-7.615336	-0.612465
121	6	0	0.088148	-0.558553	3.017264
122	6	0	1.357708	-1.414600	3.021918
123	6	0	-1.201326	-1.383470	2.981266
124	6	0	2.644386	-0.584828	3.057911
125	6	0	-2.467584	-0.522538	2.987161
126	1	0	0.081863	0.088173	3.907508
127	1	0	0.109675	0.117852	2.152173
128	1	0	1.336521	-2.093687	3.887483
129	1	0	1.365307	-2.058202	2.131756
130	1	0	-1.199710	-2.022211	2.087648
131	1	0	-1.221223	-2.067228	3.843184
132	1	0	2.633772	0.065634	3.945414
133	1	0	2.665387	0.087854	2.189924
134	1	0	-2.448085	0.157772	2.125029
135	1	0	-2.466247	0.120007	3.880473
136	6	0	3.916907	-1.436750	3.068212
137	1	0	3.902128	-2.105195	3.942392
138	1	0	3.922684	-2.091559	2.186018
139	6	0	-3.760098	-1.342901	2.955004
140	1	0	-3.775782	-2.031928	3.812882
141	1	0	-3.766551	-1.976035	2.057486
142	6	0	5.203445	-0.604715	3.085154
143	1	0	5.197024	0.056435	3.963749
144	1	0	5.215882	0.054679	2.208331
145	6	0	-5.024166	-0.478721	2.974970
146	1	0	-5.017010	0.156347	3.873830
147	1	0	-5.008208	0.208418	2.117941

148	6	0	-6.319584	-1.295861	2.941194
149	1	0	-6.330602	-1.993021	3.791576
150	1	0	-6.330091	-1.916389	2.036165
151	6	0	6.469359	-1.465755	3.095829
152	1	0	7.375828	-0.850064	3.066010
153	1	0	6.513729	-2.089162	3.997839
154	1	0	6.495173	-2.133893	2.228360
155	6	0	-7.574632	-0.419588	2.975761
156	1	0	-8.489350	-1.022455	2.930567
157	1	0	-7.611694	0.178438	3.895156
158	1	0	-7.592218	0.272302	2.127042

Tridecane

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.066006	-1.265860	-0.524527
2	6	0	-1.153684	-0.532478	-0.521875
3	6	0	-1.128615	0.890011	-0.484535
4	6	0	0.116144	1.579119	-0.449847
5	6	0	1.335834	0.845737	-0.452499
6	6	0	1.310765	-0.576752	-0.489839
7	6	0	0.041005	-2.684451	-0.561765
8	6	0	-2.395032	-1.219698	-0.556467
9	6	0	-2.344962	1.621383	-0.481890
10	6	0	0.141145	2.997710	-0.412609
11	6	0	2.577182	1.532957	-0.417907
12	6	0	2.527112	-1.308123	-0.492484
13	6	0	1.261577	-3.417140	-0.564387
14	6	0	-1.204612	-3.372835	-0.596445
15	6	0	-2.419061	-2.642605	-0.593804
16	6	0	-3.614524	-0.485212	-0.553784
17	6	0	-3.589563	0.931164	-0.516604
18	6	0	-2.318837	3.044252	-0.444526
19	6	0	-1.079427	3.730399	-0.409987

20	6	0	1.386762	3.686094	-0.377929
21	6	0	2.601211	2.955864	-0.380570
22	6	0	3.796674	0.798471	-0.420590
23	6	0	3.771713	-0.617905	-0.457770
24	6	0	2.500987	-2.730993	-0.529848
25	6	0	1.235801	-4.843815	-0.601845
26	6	0	-1.229123	-4.799533	-0.633887
27	6	0	-3.667800	-3.333193	-0.628584
28	6	0	-4.862650	-1.176907	-0.588584
29	6	0	-4.812526	1.667252	-0.513926
30	6	0	-3.542452	3.779256	-0.441884
31	6	0	-1.053651	5.157075	-0.372529
32	6	0	1.411273	5.112793	-0.340487
33	6	0	3.849950	3.646452	-0.345790
34	6	0	5.044800	1.490166	-0.385790
35	6	0	4.994676	-1.353993	-0.460448
36	6	0	3.724602	-3.465997	-0.532490
37	6	0	-0.009161	-5.530928	-0.636484
38	6	0	-4.885863	-2.598640	-0.625879
39	6	0	-4.785627	3.088918	-0.476583
40	6	0	0.191311	5.844188	-0.337890
41	6	0	5.068013	2.911899	-0.348495
42	6	0	4.967777	-2.775659	-0.497791
43	6	0	2.454058	-5.572781	-0.604402
44	6	0	-2.472295	-5.484279	-0.668440
45	6	0	-3.689760	-4.752235	-0.665793
46	6	0	-6.077768	-0.442720	-0.585849
47	6	0	-6.052744	0.977175	-0.548578
48	6	0	-3.514398	5.198189	-0.404597
49	6	0	-2.271908	5.886040	-0.369972
50	6	0	2.654445	5.797539	-0.305934
51	6	0	3.871910	5.065495	-0.308581
52	6	0	6.259918	0.755979	-0.388525
53	6	0	6.234894	-0.663916	-0.425796
54	6	0	3.696548	-4.884930	-0.569777
55	6	0	-0.034399	-6.963013	-0.674076
56	6	0	-6.139018	-3.292396	-0.660801
57	6	0	-6.013544	3.827247	-0.473913

58	6	0	0.216549	7.276272	-0.300298
59	6	0	6.321168	3.605655	-0.313573
60	6	0	6.195694	-3.513987	-0.500461
61	6	0	2.419892	-7.010077	-0.642249
62	6	0	-2.488795	-6.921893	-0.706058
63	6	0	-4.951897	-5.440866	-0.700702
64	6	0	-7.331340	-1.146805	-0.621046
65	6	0	-7.280714	1.725841	-0.545639
66	6	0	-4.751471	5.931717	-0.402175
67	6	0	-2.237742	7.323336	-0.332124
68	6	0	2.670945	7.235152	-0.268316
69	6	0	5.134047	5.754125	-0.273672
70	6	0	7.513490	1.460064	-0.353328
71	6	0	7.462864	-1.412581	-0.428735
72	6	0	4.933621	-5.618458	-0.572199
73	6	0	1.195006	-7.665793	-0.675801
74	6	0	-1.287789	-7.621189	-0.708075
75	6	0	-6.132719	-4.708005	-0.697540
76	6	0	-7.336232	-2.536086	-0.657250
77	6	0	-7.236650	3.114417	-0.508926
78	6	0	-5.957368	5.241734	-0.436362
79	6	0	-1.012856	7.979052	-0.298573
80	6	0	1.469939	7.934449	-0.266299
81	6	0	6.314869	5.021264	-0.276834
82	6	0	7.518382	2.849345	-0.317124
83	6	0	7.418800	-2.801158	-0.465448
84	6	0	6.139518	-4.928474	-0.538012
85	6	0	3.677592	-7.717493	-0.643714
86	6	0	-3.770625	-7.583687	-0.740534
87	6	0	-4.935458	-6.883290	-0.738001
88	6	0	-8.545917	-0.367679	-0.617134
89	6	0	-8.521975	0.990833	-0.581474
90	6	0	-4.684217	7.372638	-0.363787
91	6	0	-3.495442	8.030752	-0.330660
92	6	0	3.952775	7.896946	-0.233840
93	6	0	5.117608	7.196549	-0.236373
94	6	0	8.728067	0.680938	-0.357239
95	6	0	8.704125	-0.677574	-0.392900

96	6	0	4.866367	-7.059378	-0.610587
97	1	0	1.174990	-8.753234	-0.704358
98	1	0	-1.306104	-8.708661	-0.736609
99	1	0	-7.084717	-5.234066	-0.724044
100	1	0	-8.287406	-3.063635	-0.683782
101	1	0	-8.168633	3.675797	-0.506873
102	1	0	-6.890227	5.801656	-0.434359
103	1	0	-0.992840	9.066493	-0.270016
104	1	0	1.488254	9.021920	-0.237765
105	1	0	7.266867	5.547325	-0.250330
106	1	0	8.469556	3.376894	-0.290592
107	1	0	8.350783	-3.362538	-0.467501
108	1	0	7.072378	-5.488397	-0.540015
109	1	0	3.653389	-8.804148	-0.672307
110	1	0	-3.784727	-8.670523	-0.768995
111	1	0	-5.888870	-7.405333	-0.764420
112	1	0	-9.494433	-0.898557	-0.643717
113	1	0	-9.451184	1.555445	-0.579300
114	1	0	-5.618630	7.928595	-0.361909
115	1	0	-3.471239	9.117407	-0.302067
116	1	0	3.966877	8.983782	-0.205379
117	1	0	6.071020	7.718592	-0.209954
118	1	0	9.676583	1.211817	-0.330657
119	1	0	9.633334	-1.242185	-0.395074
120	1	0	5.800780	-7.615336	-0.612465
121	6	0	0.033555	-0.572361	3.013696
122	6	0	1.296952	-1.436925	3.010284
123	6	0	-1.260269	-1.389876	2.976938
124	6	0	2.589140	-0.617019	3.054567
125	6	0	-2.522107	-0.522943	2.987906
126	1	0	0.033699	0.069039	3.907815
127	1	0	0.057311	0.109176	2.152650
128	1	0	1.271053	-2.123278	3.869993
129	1	0	1.300079	-2.073045	2.114863
130	1	0	-1.263458	-2.025858	2.081421
131	1	0	-1.282048	-2.076330	3.836679
132	1	0	2.582502	0.024517	3.948578
133	1	0	2.616777	0.064150	2.193342

134	1	0	-2.502039	0.158531	2.126709
135	1	0	-2.515297	0.118175	3.882215
136	6	0	3.854239	-1.479446	3.058963
137	1	0	3.822682	-2.167678	3.917057
138	1	0	3.865010	-2.113575	2.162171
139	6	0	-3.817822	-1.338131	2.958436
140	1	0	-3.834123	-2.027153	3.816314
141	1	0	-3.828542	-1.971218	2.060926
142	6	0	5.145298	-0.657973	3.114662
143	1	0	5.133763	-0.021676	4.012598
144	1	0	5.177082	0.027837	2.257042
145	6	0	-5.078662	-0.469511	2.981171
146	1	0	-5.066993	0.166080	3.879615
147	1	0	-5.062616	0.216956	2.123608
148	6	0	-6.376730	-1.282563	2.951399
149	1	0	-6.387901	-1.978578	3.802720
150	1	0	-6.391184	-1.904151	2.047126
151	6	0	6.412761	-1.518478	3.118443
152	1	0	6.375995	-2.214072	3.969380
153	1	0	6.427878	-2.140506	2.214478
154	6	0	-7.629020	-0.402389	2.987784
155	1	0	-8.545724	-1.002536	2.945996
156	1	0	-7.661901	0.197132	3.906367
157	1	0	-7.646621	0.288152	2.137965
158	6	0	7.695387	-0.685164	3.188025
159	1	0	7.726346	-0.086868	4.107472
160	1	0	8.590028	-1.318860	3.169958
161	1	0	7.760749	0.003858	2.339302

XYZ coordinates of benzene on C₅₄H₁₈ for the calculation of E_{int} associated with horizontal displacement

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.419200	0.000000	1.000000
2	6	0	2.848000	0.000000	1.000000
3	6	0	3.556875	-1.230405	1.000000
4	6	0	3.556875	1.230405	1.000000
5	6	0	4.987265	-1.224985	1.000000
6	6	0	4.987265	1.224985	1.000000
7	6	0	5.667400	0.000000	1.000000
8	6	0	5.672661	-2.488111	1.000000
9	6	0	5.672661	2.488111	1.000000
10	1	0	6.755500	0.000000	1.000000
11	1	0	6.759952	-2.483557	1.000000
12	1	0	6.759952	2.483557	1.000000
13	6	0	0.709600	1.229063	1.000000
14	6	0	1.424000	2.466440	1.000000
15	6	0	2.843999	2.465142	1.000000
16	6	0	0.712876	3.695547	1.000000
17	6	0	3.554500	3.706605	1.000000
18	6	0	1.432764	4.931590	1.000000
19	6	0	2.833700	4.908112	1.000000
20	6	0	4.991098	3.668613	1.000000
21	6	0	0.681563	6.156724	1.000000
22	1	0	3.377750	5.850435	1.000000
23	1	0	5.530799	4.612511	1.000000
24	1	0	1.229152	7.096068	1.000000
25	6	0	-0.709600	1.229063	1.000000
26	6	0	-1.424000	2.466440	1.000000
27	6	0	-0.712876	3.695547	1.000000
28	6	0	-2.843999	2.465142	1.000000
29	6	0	-1.432764	4.931590	1.000000
30	6	0	-3.554500	3.706605	1.000000
31	6	0	-2.833700	4.908112	1.000000
32	6	0	-0.681563	6.156724	1.000000
33	6	0	-4.991098	3.668613	1.000000

34	1	0	-3.377750	5.850435	1.000000
35	1	0	-1.229152	7.096068	1.000000
36	1	0	-5.530799	4.612511	1.000000
37	6	0	-1.419200	0.000000	1.000000
38	6	0	-2.848000	0.000000	1.000000
39	6	0	-3.556875	1.230405	1.000000
40	6	0	-3.556875	-1.230405	1.000000
41	6	0	-4.987265	1.224985	1.000000
42	6	0	-4.987265	-1.224985	1.000000
43	6	0	-5.667400	0.000000	1.000000
44	6	0	-5.672661	2.488111	1.000000
45	6	0	-5.672661	-2.488111	1.000000
46	1	0	-6.755500	0.000000	1.000000
47	1	0	-6.759952	2.483557	1.000000
48	1	0	-6.759952	-2.483557	1.000000
49	6	0	-0.709600	-1.229063	1.000000
50	6	0	-1.424000	-2.466440	1.000000
51	6	0	-2.843999	-2.465142	1.000000
52	6	0	-0.712876	-3.695547	1.000000
53	6	0	-3.554500	-3.706605	1.000000
54	6	0	-1.432764	-4.931590	1.000000
55	6	0	-2.833700	-4.908112	1.000000
56	6	0	-4.991098	-3.668613	1.000000
57	6	0	-0.681563	-6.156724	1.000000
58	1	0	-3.377750	-5.850435	1.000000
59	1	0	-5.530799	-4.612511	1.000000
60	1	0	-1.229152	-7.096068	1.000000
61	6	0	0.709600	-1.229063	1.000000
62	6	0	1.424000	-2.466440	1.000000
63	6	0	0.712876	-3.695547	1.000000
64	6	0	2.843999	-2.465142	1.000000
65	6	0	1.432764	-4.931590	1.000000
66	6	0	3.554500	-3.706605	1.000000
67	6	0	2.833700	-4.908112	1.000000
68	6	0	0.681563	-6.156724	1.000000
69	6	0	4.991098	-3.668613	1.000000
70	1	0	3.377750	-5.850435	1.000000
71	1	0	1.229152	-7.096068	1.000000

72	1	0	5.530799	-4.612511	1.000000
73	6	0	0.022300	0.000000	-2.400000
74	6	0	0.720750	-1.209751	-2.400000
75	6	0	2.117650	-1.209751	-2.400000
76	6	0	2.816100	0.000000	-2.400000
77	6	0	2.117650	1.209751	-2.400000
78	6	0	0.720750	1.209751	-2.400000
79	1	0	-1.064700	0.000000	-2.400000
80	1	0	0.177250	-2.151121	-2.400000
81	1	0	2.661150	-2.151121	-2.400000
82	1	0	3.903100	0.000000	-2.400000
83	1	0	2.661150	2.151121	-2.400000
84	1	0	0.177250	2.151121	-2.400000

XYZ coordinates of benzene on C₉₆H₂₄ for the calculation of E_{int} associated with horizontal displacement

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.423200	0.000000	1.000000
2	6	0	0.711600	1.232527	1.000000
3	6	0	-0.711600	1.232527	1.000000
4	6	0	-1.423200	0.000000	1.000000
5	6	0	-0.711600	-1.232527	1.000000
6	6	0	0.711600	-1.232527	1.000000
7	6	0	2.842500	0.000000	1.000000
8	6	0	1.421250	2.461677	1.000000
9	6	0	-1.421250	2.461677	1.000000
10	6	0	-2.842500	0.000000	1.000000
11	6	0	-1.421250	-2.461677	1.000000
12	6	0	1.421250	-2.461677	1.000000
13	6	0	3.553392	-1.233398	1.000000
14	6	0	3.553392	1.233398	1.000000
15	6	0	2.844850	2.460629	1.000000
16	6	0	0.708542	3.694026	1.000000
17	6	0	-0.708542	3.694026	1.000000

18	6	0	-2.844850	2.460629	1.000000
19	6	0	-3.553392	1.233398	1.000000
20	6	0	-3.553392	-1.233398	1.000000
21	6	0	-2.844850	-2.460629	1.000000
22	6	0	-0.708542	-3.694026	1.000000
23	6	0	0.708542	-3.694026	1.000000
24	6	0	2.844850	-2.460629	1.000000
25	6	0	4.980792	-1.232765	1.000000
26	6	0	4.980792	1.232765	1.000000
27	6	0	3.558002	3.697110	1.000000
28	6	0	1.422790	4.929875	1.000000
29	6	0	-1.422790	4.929875	1.000000
30	6	0	-3.558002	3.697110	1.000000
31	6	0	-4.980792	1.232765	1.000000
32	6	0	-4.980792	-1.232765	1.000000
33	6	0	-3.558002	-3.697110	1.000000
34	6	0	-1.422790	-4.929875	1.000000
35	6	0	1.422790	-4.929875	1.000000
36	6	0	3.558002	-3.697110	1.000000
37	6	0	5.690400	0.000000	1.000000
38	6	0	2.845200	4.928031	1.000000
39	6	0	-2.845200	4.928031	1.000000
40	6	0	-5.690400	0.000000	1.000000
41	6	0	-2.845200	-4.928031	1.000000
42	6	0	2.845200	-4.928031	1.000000
43	6	0	5.688001	-2.463782	1.000000
44	6	0	5.688001	2.463782	1.000000
45	6	0	4.977698	3.694062	1.000000
46	6	0	0.710302	6.157844	1.000000
47	6	0	-0.710302	6.157844	1.000000
48	6	0	-4.977698	3.694062	1.000000
49	6	0	-5.688001	2.463782	1.000000
50	6	0	-5.688001	-2.463782	1.000000
51	6	0	-4.977698	-3.694062	1.000000
52	6	0	-0.710302	-6.157844	1.000000
53	6	0	0.710302	-6.157844	1.000000
54	6	0	4.977698	-3.694062	1.000000
55	6	0	7.123200	0.000000	1.000000

56	6	0	3.561600	6.168872	1.000000
57	6	0	-3.561600	6.168872	1.000000
58	6	0	-7.123200	0.000000	1.000000
59	6	0	-3.561600	-6.168872	1.000000
60	6	0	3.561600	-6.168872	1.000000
61	6	0	7.126173	-2.454947	1.000000
62	6	0	7.126173	2.454947	1.000000
63	6	0	5.689133	4.943974	1.000000
64	6	0	1.437041	7.398921	1.000000
65	6	0	-1.437041	7.398921	1.000000
66	6	0	-5.689133	4.943974	1.000000
67	6	0	-7.126173	2.454947	1.000000
68	6	0	-7.126173	-2.454947	1.000000
69	6	0	-5.689133	-4.943974	1.000000
70	6	0	-1.437041	-7.398921	1.000000
71	6	0	1.437041	-7.398921	1.000000
72	6	0	5.689133	-4.943974	1.000000
73	6	0	7.804018	-1.241703	1.000000
74	6	0	7.804018	1.241703	1.000000
75	6	0	4.977355	6.137627	1.000000
76	6	0	2.826663	7.379329	1.000000
77	6	0	-2.826663	7.379329	1.000000
78	6	0	-4.977355	6.137627	1.000000
79	6	0	-7.804018	1.241703	1.000000
80	6	0	-7.804018	-1.241703	1.000000
81	6	0	-4.977355	-6.137627	1.000000
82	6	0	-2.826663	-7.379329	1.000000
83	6	0	2.826663	-7.379329	1.000000
84	6	0	4.977355	-6.137627	1.000000
85	6	0	7.811121	-3.725024	1.000000
86	6	0	7.811121	3.725024	1.000000
87	6	0	7.131526	4.902117	1.000000
88	6	0	0.679595	8.627141	1.000000
89	6	0	-0.679595	8.627141	1.000000
90	6	0	-7.131526	4.902117	1.000000
91	6	0	-7.811121	3.725024	1.000000
92	6	0	-7.811121	-3.725024	1.000000
93	6	0	-7.131526	-4.902117	1.000000

94	6	0	-0.679595	-8.627141	1.000000
95	6	0	0.679595	-8.627141	1.000000
96	6	0	7.131526	-4.902117	1.000000
97	1	0	8.892018	-1.240852	1.000000
98	1	0	8.892018	1.240852	1.000000
99	1	0	5.520618	7.080287	1.000000
100	1	0	3.371400	8.321139	1.000000
101	1	0	-3.371400	8.321139	1.000000
102	1	0	-5.520618	7.080287	1.000000
103	1	0	-8.892018	1.240852	1.000000
104	1	0	-8.892018	-1.240852	1.000000
105	1	0	-5.520618	-7.080287	1.000000
106	1	0	-3.371400	-8.321139	1.000000
107	1	0	3.371400	-8.321139	1.000000
108	1	0	5.520618	-7.080287	1.000000
109	1	0	8.898409	-3.719972	1.000000
110	1	0	8.898409	3.719972	1.000000
111	1	0	7.670795	5.846262	1.000000
112	1	0	1.227614	9.566234	1.000000
113	1	0	-1.227614	9.566234	1.000000
114	1	0	-7.670795	5.846262	1.000000
115	1	0	-8.898409	3.719972	1.000000
116	1	0	-8.898409	-3.719972	1.000000
117	1	0	-7.670795	-5.846262	1.000000
118	1	0	-1.227614	-9.566234	1.000000
119	1	0	1.227614	-9.566234	1.000000
120	1	0	7.670795	-5.846262	1.000000
121	6	0	0.026300	0.000000	-2.400000
122	6	0	0.724750	-1.209751	-2.400000
123	6	0	2.121650	-1.209751	-2.400000
124	6	0	2.820100	0.000000	-2.400000
125	6	0	2.121650	1.209751	-2.400000
126	6	0	0.724750	1.209751	-2.400000
127	1	0	-1.060700	0.000000	-2.400000
128	1	0	0.181250	-2.151121	-2.400000
129	1	0	2.665150	-2.151121	-2.400000
130	1	0	3.907100	0.000000	-2.400000
131	1	0	2.665150	2.151121	-2.400000

132	1	0	0.181250	2.151121	-2.400000
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XYZ coordinates of naphthalene on C₉₆H₂₄ for the calculation of E_{int} associated with horizontal displacement

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

1	6	0	1.423200	0.000000	1.000000
2	6	0	0.711600	1.232527	1.000000
3	6	0	-0.711600	1.232527	1.000000
4	6	0	-1.423200	0.000000	1.000000
5	6	0	-0.711600	-1.232527	1.000000
6	6	0	0.711600	-1.232527	1.000000
7	6	0	2.842500	0.000000	1.000000
8	6	0	1.421250	2.461677	1.000000
9	6	0	-1.421250	2.461677	1.000000
10	6	0	-2.842500	0.000000	1.000000
11	6	0	-1.421250	-2.461677	1.000000
12	6	0	1.421250	-2.461677	1.000000
13	6	0	3.553392	-1.233398	1.000000
14	6	0	3.553392	1.233398	1.000000
15	6	0	2.844850	2.460629	1.000000
16	6	0	0.708542	3.694026	1.000000
17	6	0	-0.708542	3.694026	1.000000
18	6	0	-2.844850	2.460629	1.000000
19	6	0	-3.553392	1.233398	1.000000
20	6	0	-3.553392	-1.233398	1.000000
21	6	0	-2.844850	-2.460629	1.000000
22	6	0	-0.708542	-3.694026	1.000000
23	6	0	0.708542	-3.694026	1.000000
24	6	0	2.844850	-2.460629	1.000000
25	6	0	4.980792	-1.232765	1.000000
26	6	0	4.980792	1.232765	1.000000
27	6	0	3.558002	3.697110	1.000000
28	6	0	1.422790	4.929875	1.000000
29	6	0	-1.422790	4.929875	1.000000

30	6	0	-3.558002	3.697110	1.000000
31	6	0	-4.980792	1.232765	1.000000
32	6	0	-4.980792	-1.232765	1.000000
33	6	0	-3.558002	-3.697110	1.000000
34	6	0	-1.422790	-4.929875	1.000000
35	6	0	1.422790	-4.929875	1.000000
36	6	0	3.558002	-3.697110	1.000000
37	6	0	5.690400	0.000000	1.000000
38	6	0	2.845200	4.928031	1.000000
39	6	0	-2.845200	4.928031	1.000000
40	6	0	-5.690400	0.000000	1.000000
41	6	0	-2.845200	-4.928031	1.000000
42	6	0	2.845200	-4.928031	1.000000
43	6	0	5.688001	-2.463782	1.000000
44	6	0	5.688001	2.463782	1.000000
45	6	0	4.977698	3.694062	1.000000
46	6	0	0.710302	6.157844	1.000000
47	6	0	-0.710302	6.157844	1.000000
48	6	0	-4.977698	3.694062	1.000000
49	6	0	-5.688001	2.463782	1.000000
50	6	0	-5.688001	-2.463782	1.000000
51	6	0	-4.977698	-3.694062	1.000000
52	6	0	-0.710302	-6.157844	1.000000
53	6	0	0.710302	-6.157844	1.000000
54	6	0	4.977698	-3.694062	1.000000
55	6	0	7.123200	0.000000	1.000000
56	6	0	3.561600	6.168872	1.000000
57	6	0	-3.561600	6.168872	1.000000
58	6	0	-7.123200	0.000000	1.000000
59	6	0	-3.561600	-6.168872	1.000000
60	6	0	3.561600	-6.168872	1.000000
61	6	0	7.126173	-2.454947	1.000000
62	6	0	7.126173	2.454947	1.000000
63	6	0	5.689133	4.943974	1.000000
64	6	0	1.437041	7.398921	1.000000
65	6	0	-1.437041	7.398921	1.000000
66	6	0	-5.689133	4.943974	1.000000
67	6	0	-7.126173	2.454947	1.000000

68	6	0	-7.126173	-2.454947	1.000000
69	6	0	-5.689133	-4.943974	1.000000
70	6	0	-1.437041	-7.398921	1.000000
71	6	0	1.437041	-7.398921	1.000000
72	6	0	5.689133	-4.943974	1.000000
73	6	0	7.804018	-1.241703	1.000000
74	6	0	7.804018	1.241703	1.000000
75	6	0	4.977355	6.137627	1.000000
76	6	0	2.826663	7.379329	1.000000
77	6	0	-2.826663	7.379329	1.000000
78	6	0	-4.977355	6.137627	1.000000
79	6	0	-7.804018	1.241703	1.000000
80	6	0	-7.804018	-1.241703	1.000000
81	6	0	-4.977355	-6.137627	1.000000
82	6	0	-2.826663	-7.379329	1.000000
83	6	0	2.826663	-7.379329	1.000000
84	6	0	4.977355	-6.137627	1.000000
85	6	0	7.811121	-3.725024	1.000000
86	6	0	7.811121	3.725024	1.000000
87	6	0	7.131526	4.902117	1.000000
88	6	0	0.679595	8.627141	1.000000
89	6	0	-0.679595	8.627141	1.000000
90	6	0	-7.131526	4.902117	1.000000
91	6	0	-7.811121	3.725024	1.000000
92	6	0	-7.811121	-3.725024	1.000000
93	6	0	-7.131526	-4.902117	1.000000
94	6	0	-0.679595	-8.627141	1.000000
95	6	0	0.679595	-8.627141	1.000000
96	6	0	7.131526	-4.902117	1.000000
97	1	0	8.892018	-1.240852	1.000000
98	1	0	8.892018	1.240852	1.000000
99	1	0	5.520618	7.080287	1.000000
100	1	0	3.371400	8.321139	1.000000
101	1	0	-3.371400	8.321139	1.000000
102	1	0	-5.520618	7.080287	1.000000
103	1	0	-8.892018	1.240852	1.000000
104	1	0	-8.892018	-1.240852	1.000000
105	1	0	-5.520618	-7.080287	1.000000

106	1	0	-3.371400	-8.321139	1.000000
107	1	0	3.371400	-8.321139	1.000000
108	1	0	5.520618	-7.080287	1.000000
109	1	0	8.898409	-3.719972	1.000000
110	1	0	8.898409	3.719972	1.000000
111	1	0	7.670795	5.846262	1.000000
112	1	0	1.227614	9.566234	1.000000
113	1	0	-1.227614	9.566234	1.000000
114	1	0	-7.670795	5.846262	1.000000
115	1	0	-8.898409	3.719972	1.000000
116	1	0	-8.898409	-3.719972	1.000000
117	1	0	-7.670795	-5.846262	1.000000
118	1	0	-1.227614	-9.566234	1.000000
119	1	0	1.227614	-9.566234	1.000000
120	1	0	7.670795	-5.846262	1.000000
121	6	0	-0.713554	1.225464	-2.400000
122	6	0	0.003188	2.467494	-2.400000
123	6	0	0.021529	0.009483	-2.400000
124	6	0	1.398211	0.016524	-2.400000
125	6	0	1.423811	2.439476	-2.400000
126	6	0	2.106553	1.243998	-2.400000
127	6	0	-2.134177	1.253482	-2.400000
128	6	0	-2.816919	2.448960	-2.400000
129	6	0	-0.731895	3.683475	-2.400000
130	6	0	-2.108577	3.676434	-2.400000
131	1	0	-0.524622	-0.931160	-2.400000
132	1	0	1.948080	-0.920792	-2.400000
133	1	0	1.964964	3.383004	-2.400000
134	1	0	3.193230	1.236910	-2.400000
135	1	0	-2.675330	0.309954	-2.400000
136	1	0	-3.903596	2.456049	-2.400000
137	1	0	-0.185744	4.624119	-2.400000
138	1	0	-2.658446	4.613750	-2.400000

XYZ coordinates of anthracene on C₉₆H₂₄ for the calculation of E_{int} associated with horizontal displacement

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

1	6	0	1.423200	0.000000	1.000000
2	6	0	0.711600	1.232527	1.000000
3	6	0	-0.711600	1.232527	1.000000
4	6	0	-1.423200	0.000000	1.000000
5	6	0	-0.711600	-1.232527	1.000000
6	6	0	0.711600	-1.232527	1.000000
7	6	0	2.842500	0.000000	1.000000
8	6	0	1.421250	2.461677	1.000000
9	6	0	-1.421250	2.461677	1.000000
10	6	0	-2.842500	0.000000	1.000000
11	6	0	-1.421250	-2.461677	1.000000
12	6	0	1.421250	-2.461677	1.000000
13	6	0	3.553392	-1.233398	1.000000
14	6	0	3.553392	1.233398	1.000000
15	6	0	2.844850	2.460629	1.000000
16	6	0	0.708542	3.694026	1.000000
17	6	0	-0.708542	3.694026	1.000000
18	6	0	-2.844850	2.460629	1.000000
19	6	0	-3.553392	1.233398	1.000000
20	6	0	-3.553392	-1.233398	1.000000
21	6	0	-2.844850	-2.460629	1.000000
22	6	0	-0.708542	-3.694026	1.000000
23	6	0	0.708542	-3.694026	1.000000
24	6	0	2.844850	-2.460629	1.000000
25	6	0	4.980792	-1.232765	1.000000
26	6	0	4.980792	1.232765	1.000000
27	6	0	3.558002	3.697110	1.000000
28	6	0	1.422790	4.929875	1.000000
29	6	0	-1.422790	4.929875	1.000000
30	6	0	-3.558002	3.697110	1.000000
31	6	0	-4.980792	1.232765	1.000000
32	6	0	-4.980792	-1.232765	1.000000
33	6	0	-3.558002	-3.697110	1.000000
34	6	0	-1.422790	-4.929875	1.000000
35	6	0	1.422790	-4.929875	1.000000

36	6	0	3.558002	-3.697110	1.000000
37	6	0	5.690400	0.000000	1.000000
38	6	0	2.845200	4.928031	1.000000
39	6	0	-2.845200	4.928031	1.000000
40	6	0	-5.690400	0.000000	1.000000
41	6	0	-2.845200	-4.928031	1.000000
42	6	0	2.845200	-4.928031	1.000000
43	6	0	5.688001	-2.463782	1.000000
44	6	0	5.688001	2.463782	1.000000
45	6	0	4.977698	3.694062	1.000000
46	6	0	0.710302	6.157844	1.000000
47	6	0	-0.710302	6.157844	1.000000
48	6	0	-4.977698	3.694062	1.000000
49	6	0	-5.688001	2.463782	1.000000
50	6	0	-5.688001	-2.463782	1.000000
51	6	0	-4.977698	-3.694062	1.000000
52	6	0	-0.710302	-6.157844	1.000000
53	6	0	0.710302	-6.157844	1.000000
54	6	0	4.977698	-3.694062	1.000000
55	6	0	7.123200	0.000000	1.000000
56	6	0	3.561600	6.168872	1.000000
57	6	0	-3.561600	6.168872	1.000000
58	6	0	-7.123200	0.000000	1.000000
59	6	0	-3.561600	-6.168872	1.000000
60	6	0	3.561600	-6.168872	1.000000
61	6	0	7.126173	-2.454947	1.000000
62	6	0	7.126173	2.454947	1.000000
63	6	0	5.689133	4.943974	1.000000
64	6	0	1.437041	7.398921	1.000000
65	6	0	-1.437041	7.398921	1.000000
66	6	0	-5.689133	4.943974	1.000000
67	6	0	-7.126173	2.454947	1.000000
68	6	0	-7.126173	-2.454947	1.000000
69	6	0	-5.689133	-4.943974	1.000000
70	6	0	-1.437041	-7.398921	1.000000
71	6	0	1.437041	-7.398921	1.000000
72	6	0	5.689133	-4.943974	1.000000
73	6	0	7.804018	-1.241703	1.000000

74	6	0	7.804018	1.241703	1.000000
75	6	0	4.977355	6.137627	1.000000
76	6	0	2.826663	7.379329	1.000000
77	6	0	-2.826663	7.379329	1.000000
78	6	0	-4.977355	6.137627	1.000000
79	6	0	-7.804018	1.241703	1.000000
80	6	0	-7.804018	-1.241703	1.000000
81	6	0	-4.977355	-6.137627	1.000000
82	6	0	-2.826663	-7.379329	1.000000
83	6	0	2.826663	-7.379329	1.000000
84	6	0	4.977355	-6.137627	1.000000
85	6	0	7.811121	-3.725024	1.000000
86	6	0	7.811121	3.725024	1.000000
87	6	0	7.131526	4.902117	1.000000
88	6	0	0.679595	8.627141	1.000000
89	6	0	-0.679595	8.627141	1.000000
90	6	0	-7.131526	4.902117	1.000000
91	6	0	-7.811121	3.725024	1.000000
92	6	0	-7.811121	-3.725024	1.000000
93	6	0	-7.131526	-4.902117	1.000000
94	6	0	-0.679595	-8.627141	1.000000
95	6	0	0.679595	-8.627141	1.000000
96	6	0	7.131526	-4.902117	1.000000
97	1	0	8.892018	-1.240852	1.000000
98	1	0	8.892018	1.240852	1.000000
99	1	0	5.520618	7.080287	1.000000
100	1	0	3.371400	8.321139	1.000000
101	1	0	-3.371400	8.321139	1.000000
102	1	0	-5.520618	7.080287	1.000000
103	1	0	-8.892018	1.240852	1.000000
104	1	0	-8.892018	-1.240852	1.000000
105	1	0	-5.520618	-7.080287	1.000000
106	1	0	-3.371400	-8.321139	1.000000
107	1	0	3.371400	-8.321139	1.000000
108	1	0	5.520618	-7.080287	1.000000
109	1	0	8.898409	-3.719972	1.000000
110	1	0	8.898409	3.719972	1.000000
111	1	0	7.670795	5.846262	1.000000

112	1	0	1.227614	9.566234	1.000000
113	1	0	-1.227614	9.566234	1.000000
114	1	0	-7.670795	5.846262	1.000000
115	1	0	-8.898409	3.719972	1.000000
116	1	0	-8.898409	-3.719972	1.000000
117	1	0	-7.670795	-5.846262	1.000000
118	1	0	-1.227614	-9.566234	1.000000
119	1	0	1.227614	-9.566234	1.000000
120	1	0	7.670795	-5.846262	1.000000
121	6	0	0.019500	0.000000	-2.400000
122	6	0	2.826900	0.000000	-2.400000
123	6	0	0.700493	-1.223493	-2.400000
124	6	0	2.145907	-1.223493	-2.400000
125	6	0	0.700493	1.223493	-2.400000
126	6	0	2.145907	1.223493	-2.400000
127	6	0	0.015835	-2.478711	-2.400000
128	6	0	0.709852	-3.659914	-2.400000
129	6	0	2.830565	-2.478711	-2.400000
130	6	0	2.136548	-3.659914	-2.400000
131	6	0	0.015835	2.478711	-2.400000
132	6	0	0.709852	3.659914	-2.400000
133	6	0	2.830565	2.478711	-2.400000
134	6	0	2.136548	3.659914	-2.400000
135	1	0	-1.068900	0.000000	-2.400000
136	1	0	3.915300	0.000000	-2.400000
137	1	0	-1.071761	-2.475913	-2.400000
138	1	0	0.176386	-4.606547	-2.400000
139	1	0	3.918161	-2.475913	-2.400000
140	1	0	2.670014	-4.606547	-2.400000
141	1	0	-1.071761	2.475913	-2.400000
142	1	0	0.176386	4.606547	-2.400000
143	1	0	3.918161	2.475913	-2.400000
144	1	0	2.670014	4.606547	-2.400000
