

XYZ coordinates of each optimised geometry on coronene

Thiophene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.060363	0.001228	0.996346
2	6	0	0.360202	1.236605	0.853900
3	6	0	-1.038341	1.236309	0.570754
4	6	0	-1.737386	0.000070	0.429907
5	6	0	-1.037657	-1.235557	0.571978
6	6	0	0.360995	-1.234987	0.855177
7	6	0	2.453170	0.001572	1.278086
8	6	0	1.056704	2.467944	0.994334
9	6	0	-1.735256	2.466944	0.429157
10	6	0	-3.130522	-0.000455	0.147860
11	6	0	-1.733898	-2.466802	0.431632
12	6	0	1.057976	-2.465752	0.996761
13	6	0	3.124759	1.249934	1.413503
14	6	0	3.125321	-1.246154	1.414617
15	6	0	0.332885	3.685406	0.847286
16	6	0	2.451890	2.438180	1.276825
17	6	0	-3.130537	2.436077	0.146792
18	6	0	-1.012209	3.684899	0.575032
19	6	0	-3.802062	-1.248732	0.012475
20	6	0	-3.802753	1.247316	0.011244
21	6	0	-1.010168	-3.684212	0.578667
22	6	0	-3.129187	-2.436986	0.149196
23	6	0	2.453324	-2.434935	1.279270
24	6	0	0.334925	-3.683705	0.850925
25	1	0	4.190565	1.247105	1.629186
26	1	0	4.191249	-1.242375	1.630436
27	1	0	0.868247	4.625708	0.955257
28	1	0	2.981794	3.381703	1.383619
29	1	0	-3.660953	3.379200	0.039014
30	1	0	-1.548095	4.624798	0.466148
31	1	0	-4.867843	-1.245911	-0.203259

32	1	0	-4.868532	1.243692	-0.204487
33	1	0	-1.545533	-4.624514	0.470711
34	1	0	-3.659081	-3.380509	0.042349
35	1	0	2.983676	-3.378006	1.386906
36	1	0	0.870808	-4.623604	0.959820
37	16	0	0.027358	-0.009385	-2.778218
38	6	0	1.220364	-1.244908	-2.527907
39	6	0	1.205258	1.240906	-2.528894
40	6	0	2.450343	-0.709158	-2.266492
41	6	0	2.441654	0.720352	-2.267024
42	1	0	0.936260	-2.288029	-2.559902
43	1	0	0.908599	2.280480	-2.562220
44	1	0	3.327979	-1.309230	-2.054220
45	1	0	3.312170	1.331244	-2.056312

Furan

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.086895	-0.009168	-0.867824
2	6	0	-0.393516	1.230897	-0.732029
3	6	0	1.006702	1.240293	-0.457881
4	6	0	1.714574	0.008810	-0.319191
5	6	0	1.021892	-1.231605	-0.454331
6	6	0	-0.378458	-1.240365	-0.728514
7	6	0	-2.481211	-0.018084	-1.140311
8	6	0	-1.098882	2.457609	-0.870301
9	6	0	1.696598	2.475617	-0.323179
10	6	0	3.109463	0.017773	-0.046093
11	6	0	1.726916	-2.458032	-0.316097
12	6	0	-1.068483	-2.476003	-0.863182
13	6	0	-3.161783	1.225496	-1.273893
14	6	0	-3.146210	-1.270531	-1.270151
15	6	0	-0.381967	3.679966	-0.730358
16	6	0	-2.495622	2.418334	-1.143889
17	6	0	3.093834	2.454253	-0.049740

18	6	0	0.964822	3.688620	-0.466757
19	6	0	3.789863	-1.225902	0.087384
20	6	0	3.774528	1.270096	0.083781
21	6	0	1.010092	-3.680345	-0.456119
22	6	0	3.123770	-2.418714	-0.042705
23	6	0	-2.465770	-2.454685	-1.136892
24	6	0	-0.336695	-3.689000	-0.719724
25	1	0	-4.228851	1.215444	-1.482680
26	1	0	-4.213554	-1.273988	-1.479099
27	1	0	-0.924041	4.616601	-0.836696
28	1	0	-3.032261	3.358229	-1.249043
29	1	0	3.618862	3.400969	0.052798
30	1	0	1.495348	4.632148	-0.363143
31	1	0	4.856967	-1.215822	0.296251
32	1	0	4.841672	1.273731	0.292657
33	1	0	1.552169	-4.616981	-0.349790
34	1	0	3.660389	-3.358607	0.062556
35	1	0	-2.990744	-3.401347	-1.239237
36	1	0	-0.867220	-4.632528	-0.823344
37	6	0	-1.021229	-1.097121	2.561704
38	6	0	-1.006061	1.094025	2.567708
39	6	0	-2.325158	-0.710648	2.592353
40	6	0	-2.315225	0.725464	2.596265
41	1	0	-0.525924	-2.054910	2.520183
42	1	0	-0.497494	2.045102	2.532115
43	1	0	-3.188462	-1.361019	2.592913
44	1	0	-3.169472	1.387679	2.600183
45	8	0	-0.200840	-0.007125	2.549146

Pyrrole

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.684558	-1.241726	0.000000
2	6	0	-0.684701	-0.527161	1.235825
3	6	0	-0.684721	0.899509	1.235903

4	6	0	-0.684668	1.613059	0.000000
5	6	0	-0.684721	0.899509	-1.235903
6	6	0	-0.684701	-0.527161	-1.235825
7	6	0	-0.684691	-2.662507	0.000000
8	6	0	-0.684674	-1.238413	2.466803
9	6	0	-0.684672	1.610209	2.466873
10	6	0	-0.684681	3.034459	0.000000
11	6	0	-0.684672	1.610209	-2.466873
12	6	0	-0.684674	-1.238413	-2.466803
13	6	0	-0.684695	-3.348093	1.248002
14	6	0	-0.684695	-3.348093	-1.248002
15	6	0	-0.684696	-0.500226	3.684556
16	6	0	-0.684663	-2.661867	2.436532
17	6	0	-0.684681	3.033786	2.436532
18	6	0	-0.684681	0.872144	3.684556
19	6	0	-0.684681	3.719971	-1.248024
20	6	0	-0.684681	3.719971	1.248024
21	6	0	-0.684681	0.872144	-3.684556
22	6	0	-0.684681	3.033786	-2.436532
23	6	0	-0.684663	-2.661867	-2.436532
24	6	0	-0.684696	-0.500226	-3.684556
25	1	0	-0.684683	-4.435447	1.244802
26	1	0	-0.684683	-4.435447	-1.244802
27	1	0	-0.684681	-1.046714	4.624657
28	1	0	-0.684681	-3.202774	3.379855
29	1	0	-0.684681	3.574693	3.379855
30	1	0	-0.684681	1.418633	4.624657
31	1	0	-0.684681	4.807366	-1.244802
32	1	0	-0.684681	4.807366	1.244802
33	1	0	-0.684681	1.418633	-4.624657
34	1	0	-0.684681	3.574693	-3.379855
35	1	0	-0.684681	-3.202774	-3.379855
36	1	0	-0.684681	-1.046714	-4.624657
37	7	0	2.440370	0.183920	0.000000
38	6	0	2.808117	-0.514104	-1.124479
39	6	0	2.808117	-0.514104	1.124479
40	6	0	3.441127	-1.667638	-0.713216
41	6	0	3.441127	-1.667638	0.713216

42	1	0	2.573663	-0.140673	-2.110570
43	1	0	2.573663	-0.140673	2.110570
44	1	0	3.856387	-2.427270	-1.362026
45	1	0	3.856387	-2.427270	1.362026
46	1	0	1.876527	1.019780	0.000000

Pyridine

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.733583	-1.263279	0.000000
2	6	0	-0.733583	-0.549729	1.235905
3	6	0	-0.733583	0.877371	1.235905
4	6	0	-0.733583	1.590921	0.000000
5	6	0	-0.733583	0.877371	-1.235905
6	6	0	-0.733583	-0.549729	-1.235905
7	6	0	-0.733583	-2.684679	0.000000
8	6	0	-0.733583	-1.260429	2.466873
9	6	0	-0.733583	1.588071	2.466873
10	6	0	-0.733583	3.012321	0.000000
11	6	0	-0.733583	1.588071	-2.466873
12	6	0	-0.733583	-1.260429	-2.466873
13	6	0	-0.733583	-3.370191	1.248024
14	6	0	-0.733583	-3.370191	-1.248024
15	6	0	-0.733583	-0.522364	3.684556
16	6	0	-0.733583	-2.684006	2.436532
17	6	0	-0.733583	3.011648	2.436532
18	6	0	-0.733583	0.850006	3.684556
19	6	0	-0.733583	3.697833	-1.248024
20	6	0	-0.733583	3.697833	1.248024
21	6	0	-0.733583	0.850006	-3.684556
22	6	0	-0.733583	3.011648	-2.436532
23	6	0	-0.733583	-2.684006	-2.436532
24	6	0	-0.733583	-0.522364	-3.684556
25	1	0	-0.733583	-4.457586	1.244802
26	1	0	-0.733583	-4.457586	-1.244802

27	1	0	-0.733583	-1.068852	4.624657
28	1	0	-0.733583	-3.224913	3.379855
29	1	0	-0.733583	3.552554	3.379855
30	1	0	-0.733583	1.396494	4.624657
31	1	0	-0.733583	4.785228	-1.244802
32	1	0	-0.733583	4.785228	1.244802
33	1	0	-0.733583	1.396494	-4.624657
34	1	0	-0.733583	3.552554	-3.379855
35	1	0	-0.733583	-3.224913	-3.379855
36	1	0	-0.733583	-1.068852	-4.624657
37	6	0	2.729948	0.113049	-1.141572
38	6	0	2.723816	-1.281456	-1.197917
39	6	0	2.720659	-1.993748	0.000000
40	6	0	2.723816	-1.281456	1.197917
41	6	0	2.729948	0.113049	1.141572
42	1	0	2.713366	0.698817	-2.059216
43	1	0	2.698416	-1.790313	-2.156518
44	1	0	2.696181	-3.079760	0.000000
45	1	0	2.698416	-1.790313	2.156518
46	1	0	2.713366	0.698817	2.059216
47	7	0	2.735717	0.812869	0.000000

XYZ coordinates of each optimised geometry on C₉₆H₂₄

Flat-on thiophene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.233041	-1.331474	0.000000
2	6	0	-0.233041	-0.619874	1.232527
3	6	0	-0.233041	0.803326	1.232527
4	6	0	-0.233041	1.514926	0.000000
5	6	0	-0.233041	0.803326	-1.232527
6	6	0	-0.233041	-0.619874	-1.232527
7	6	0	-0.233041	-2.750774	0.000000

8	6	0	-0.233041	-1.329524	2.461677
9	6	0	-0.233041	1.512976	2.461677
10	6	0	-0.233041	2.934226	0.000000
11	6	0	-0.233041	1.512976	-2.461677
12	6	0	-0.233041	-1.329524	-2.461677
13	6	0	-0.233041	-3.461666	-1.233398
14	6	0	-0.233041	-3.461666	1.233398
15	6	0	-0.233041	-2.753124	2.460629
16	6	0	-0.233041	-0.616816	3.694026
17	6	0	-0.233041	0.800268	3.694026
18	6	0	-0.233041	2.936575	2.460629
19	6	0	-0.233041	3.645117	1.233398
20	6	0	-0.233041	3.645117	-1.233398
21	6	0	-0.233041	2.936575	-2.460629
22	6	0	-0.233041	0.800268	-3.694026
23	6	0	-0.233041	-0.616816	-3.694026
24	6	0	-0.233041	-2.753124	-2.460629
25	6	0	-0.233041	-4.889066	-1.232765
26	6	0	-0.233041	-4.889066	1.232765
27	6	0	-0.233041	-3.466276	3.697110
28	6	0	-0.233041	-1.331064	4.929875
29	6	0	-0.233041	1.514516	4.929875
30	6	0	-0.233041	3.649727	3.697110
31	6	0	-0.233041	5.072517	1.232765
32	6	0	-0.233041	5.072517	-1.232765
33	6	0	-0.233041	3.649727	-3.697110
34	6	0	-0.233041	1.514516	-4.929875
35	6	0	-0.233041	-1.331064	-4.929875
36	6	0	-0.233041	-3.466276	-3.697110
37	6	0	-0.233041	-5.598674	0.000000
38	6	0	-0.233041	-2.753474	4.928031
39	6	0	-0.233041	2.936926	4.928031
40	6	0	-0.233041	5.782126	0.000000
41	6	0	-0.233041	2.936926	-4.928031
42	6	0	-0.233041	-2.753474	-4.928031
43	6	0	-0.233041	-5.596275	-2.463782
44	6	0	-0.233041	-5.596275	2.463782
45	6	0	-0.233041	-4.885973	3.694062

46	6	0	-0.233041	-0.618577	6.157844
47	6	0	-0.233041	0.802028	6.157844
48	6	0	-0.233041	5.069424	3.694062
49	6	0	-0.233041	5.779726	2.463782
50	6	0	-0.233041	5.779726	-2.463782
51	6	0	-0.233041	5.069424	-3.694062
52	6	0	-0.233041	0.802028	-6.157844
53	6	0	-0.233041	-0.618577	-6.157844
54	6	0	-0.233041	-4.885973	-3.694062
55	6	0	-0.233041	-7.031474	0.000000
56	6	0	-0.233041	-3.469874	6.168872
57	6	0	-0.233041	3.653326	6.168872
58	6	0	-0.233041	7.214926	0.000000
59	6	0	-0.233041	3.653326	-6.168872
60	6	0	-0.233041	-3.469874	-6.168872
61	6	0	-0.233041	-7.034448	-2.454947
62	6	0	-0.233041	-7.034448	2.454947
63	6	0	-0.233041	-5.597407	4.943974
64	6	0	-0.233041	-1.345315	7.398921
65	6	0	-0.233041	1.528766	7.398921
66	6	0	-0.233041	5.780859	4.943974
67	6	0	-0.233041	7.217899	2.454947
68	6	0	-0.233041	7.217899	-2.454947
69	6	0	-0.233041	5.780859	-4.943974
70	6	0	-0.233041	1.528766	-7.398921
71	6	0	-0.233041	-1.345315	-7.398921
72	6	0	-0.233041	-5.597407	-4.943974
73	6	0	-0.233041	-7.712293	-1.241703
74	6	0	-0.233041	-7.712293	1.241703
75	6	0	-0.233041	-4.885630	6.137627
76	6	0	-0.233041	-2.734937	7.379329
77	6	0	-0.233041	2.918389	7.379329
78	6	0	-0.233041	5.069081	6.137627
79	6	0	-0.233041	7.895744	1.241703
80	6	0	-0.233041	7.895744	-1.241703
81	6	0	-0.233041	5.069081	-6.137627
82	6	0	-0.233041	2.918389	-7.379329
83	6	0	-0.233041	-2.734937	-7.379329

84	6	0	-0.233041	-4.885630	-6.137627
85	6	0	-0.233041	-7.719395	-3.725024
86	6	0	-0.233041	-7.719395	3.725024
87	6	0	-0.233041	-7.039800	4.902117
88	6	0	-0.233041	-0.587869	8.627141
89	6	0	-0.233041	0.771321	8.627141
90	6	0	-0.233041	7.223251	4.902117
91	6	0	-0.233041	7.902847	3.725024
92	6	0	-0.233041	7.902847	-3.725024
93	6	0	-0.233041	7.223251	-4.902117
94	6	0	-0.233041	0.771321	-8.627141
95	6	0	-0.233041	-0.587869	-8.627141
96	6	0	-0.233041	-7.039800	-4.902117
97	1	0	-0.233041	-8.800292	-1.240852
98	1	0	-0.233041	-8.800292	1.240852
99	1	0	-0.233041	-5.428893	7.080287
100	1	0	-0.233041	-3.279674	8.321139
101	1	0	-0.233041	3.463125	8.321139
102	1	0	-0.233041	5.612344	7.080287
103	1	0	-0.233041	8.983744	1.240852
104	1	0	-0.233041	8.983744	-1.240852
105	1	0	-0.233041	5.612344	-7.080287
106	1	0	-0.233041	3.463125	-8.321139
107	1	0	-0.233041	-3.279674	-8.321139
108	1	0	-0.233041	-5.428893	-7.080287
109	1	0	-0.233041	-8.806683	-3.719972
110	1	0	-0.233041	-8.806683	3.719972
111	1	0	-0.233041	-7.579069	5.846262
112	1	0	-0.233041	-1.135888	9.566234
113	1	0	-0.233041	1.319340	9.566234
114	1	0	-0.233041	7.762521	5.846262
115	1	0	-0.233041	8.990135	3.719972
116	1	0	-0.233041	8.990135	-3.719972
117	1	0	-0.233041	7.762521	-5.846262
118	1	0	-0.233041	1.319340	-9.566234
119	1	0	-0.233041	-1.135888	-9.566234
120	1	0	-0.233041	-7.579069	-5.846262
121	16	0	3.235343	-0.051555	0.000000

122	6	0	3.179418	-1.263135	-1.243255
123	6	0	3.179418	-1.263135	1.243255
124	6	0	3.120823	-2.522358	-0.715237
125	6	0	3.120823	-2.522358	0.715237
126	1	0	3.172037	-0.972259	-2.285074
127	1	0	3.172037	-0.972259	2.285074
128	1	0	3.056156	-3.419943	-1.320064
129	1	0	3.056156	-3.419943	1.320064

Flat-on furan

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.190076	-1.331567	0.000000
2	6	0	-0.189576	-0.619931	1.232548
3	6	0	-0.189130	0.803233	1.232527
4	6	0	-0.189373	1.514833	0.000000
5	6	0	-0.189130	0.803233	-1.232527
6	6	0	-0.189576	-0.619931	-1.232548
7	6	0	-0.190436	-2.750850	0.000000
8	6	0	-0.188815	-1.329669	2.461082
9	6	0	-0.189373	1.512883	2.461677
10	6	0	-0.189373	2.934133	0.000000
11	6	0	-0.189373	1.512883	-2.461677
12	6	0	-0.188815	-1.329669	-2.461082
13	6	0	-0.189449	-3.461639	-1.233330
14	6	0	-0.189449	-3.461639	1.233330
15	6	0	-0.189577	-2.753217	2.460827
16	6	0	-0.189058	-0.616951	3.694051
17	6	0	-0.189540	0.800175	3.694026
18	6	0	-0.189373	2.936482	2.460629
19	6	0	-0.189373	3.645024	1.233398
20	6	0	-0.189373	3.645024	-1.233398
21	6	0	-0.189373	2.936482	-2.460629
22	6	0	-0.189540	0.800175	-3.694026
23	6	0	-0.189058	-0.616951	-3.694051

24	6	0	-0.189577	-2.753217	-2.460827
25	6	0	-0.188957	-4.889159	-1.232779
26	6	0	-0.188957	-4.889159	1.232779
27	6	0	-0.189106	-3.466369	3.697110
28	6	0	-0.189381	-1.331157	4.929875
29	6	0	-0.189373	1.514423	4.929875
30	6	0	-0.189373	3.649634	3.697110
31	6	0	-0.189373	5.072424	1.232765
32	6	0	-0.189373	5.072424	-1.232765
33	6	0	-0.189373	3.649634	-3.697110
34	6	0	-0.189373	1.514423	-4.929875
35	6	0	-0.189381	-1.331157	-4.929875
36	6	0	-0.189106	-3.466369	-3.697110
37	6	0	-0.189410	-5.598767	0.000000
38	6	0	-0.189373	-2.753567	4.928031
39	6	0	-0.189373	2.936833	4.928031
40	6	0	-0.189373	5.782033	0.000000
41	6	0	-0.189373	2.936833	-4.928031
42	6	0	-0.189373	-2.753567	-4.928031
43	6	0	-0.189441	-5.596368	-2.463782
44	6	0	-0.189441	-5.596368	2.463782
45	6	0	-0.189373	-4.886066	3.694062
46	6	0	-0.189373	-0.618670	6.157844
47	6	0	-0.189373	0.801935	6.157844
48	6	0	-0.189373	5.069331	3.694062
49	6	0	-0.189373	5.779633	2.463782
50	6	0	-0.189373	5.779633	-2.463782
51	6	0	-0.189373	5.069331	-3.694062
52	6	0	-0.189373	0.801935	-6.157844
53	6	0	-0.189373	-0.618670	-6.157844
54	6	0	-0.189373	-4.886066	-3.694062
55	6	0	-0.189373	-7.031567	0.000000
56	6	0	-0.189373	-3.469967	6.168872
57	6	0	-0.189373	3.653233	6.168872
58	6	0	-0.189373	7.214833	0.000000
59	6	0	-0.189373	3.653233	-6.168872
60	6	0	-0.189373	-3.469967	-6.168872
61	6	0	-0.189373	-7.034541	-2.454947

62	6	0	-0.189373	-7.034541	2.454947
63	6	0	-0.189373	-5.597500	4.943974
64	6	0	-0.189373	-1.345408	7.398921
65	6	0	-0.189373	1.528673	7.398921
66	6	0	-0.189373	5.780766	4.943974
67	6	0	-0.189373	7.217806	2.454947
68	6	0	-0.189373	7.217806	-2.454947
69	6	0	-0.189373	5.780766	-4.943974
70	6	0	-0.189373	1.528673	-7.398921
71	6	0	-0.189373	-1.345408	-7.398921
72	6	0	-0.189373	-5.597500	-4.943974
73	6	0	-0.189373	-7.712386	-1.241703
74	6	0	-0.189373	-7.712386	1.241703
75	6	0	-0.189373	-4.885723	6.137627
76	6	0	-0.189373	-2.735030	7.379329
77	6	0	-0.189373	2.918296	7.379329
78	6	0	-0.189373	5.068988	6.137627
79	6	0	-0.189373	7.895651	1.241703
80	6	0	-0.189373	7.895651	-1.241703
81	6	0	-0.189373	5.068988	-6.137627
82	6	0	-0.189373	2.918296	-7.379329
83	6	0	-0.189373	-2.735030	-7.379329
84	6	0	-0.189373	-4.885723	-6.137627
85	6	0	-0.189373	-7.719488	-3.725024
86	6	0	-0.189373	-7.719488	3.725024
87	6	0	-0.189373	-7.039893	4.902117
88	6	0	-0.189373	-0.587962	8.627141
89	6	0	-0.189373	0.771228	8.627141
90	6	0	-0.189373	7.223158	4.902117
91	6	0	-0.189373	7.902754	3.725024
92	6	0	-0.189373	7.902754	-3.725024
93	6	0	-0.189373	7.223158	-4.902117
94	6	0	-0.189373	0.771228	-8.627141
95	6	0	-0.189373	-0.587962	-8.627141
96	6	0	-0.189373	-7.039893	-4.902117
97	1	0	-0.189373	-8.800385	-1.240852
98	1	0	-0.189373	-8.800385	1.240852
99	1	0	-0.189373	-5.428986	7.080287

100	1	0	-0.189373	-3.279767	8.321139
101	1	0	-0.189373	3.463032	8.321139
102	1	0	-0.189373	5.612251	7.080287
103	1	0	-0.189373	8.983651	1.240852
104	1	0	-0.189373	8.983651	-1.240852
105	1	0	-0.189373	5.612251	-7.080287
106	1	0	-0.189373	3.463032	-8.321139
107	1	0	-0.189373	-3.279767	-8.321139
108	1	0	-0.189373	-5.428986	-7.080287
109	1	0	-0.189373	-8.806776	-3.719972
110	1	0	-0.189373	-8.806776	3.719972
111	1	0	-0.189373	-7.579162	5.846262
112	1	0	-0.189373	-1.135981	9.566234
113	1	0	-0.189373	1.319247	9.566234
114	1	0	-0.189373	7.762428	5.846262
115	1	0	-0.189373	8.990042	3.719972
116	1	0	-0.189373	8.990042	-3.719972
117	1	0	-0.189373	7.762428	-5.846262
118	1	0	-0.189373	1.319247	-9.566234
119	1	0	-0.189373	-1.135981	-9.566234
120	1	0	-0.189373	-7.579162	-5.846262
121	6	0	3.135328	-1.180729	-1.095936
122	6	0	3.135328	-1.180729	1.095936
123	6	0	3.220609	-2.484751	-0.718107
124	6	0	3.220609	-2.484751	0.718107
125	1	0	3.082039	-0.681716	-2.051260
126	1	0	3.082039	-0.681716	2.051260
127	1	0	3.257517	-3.343370	-1.373555
128	1	0	3.257517	-3.343370	1.373555
129	8	0	3.083896	-0.368094	0.000000

Flat-on pyrrole

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.342659	-0.006636	0.208700

2	6	0	0.636844	1.229205	0.199282
3	6	0	-0.786189	1.235817	0.180157
4	6	0	-1.503455	0.006616	0.170571
5	6	0	-0.797663	-1.229210	0.179977
6	6	0	0.625375	-1.235846	0.199104
7	6	0	2.761802	-0.013246	0.228066
8	6	0	1.352182	2.454920	0.208632
9	6	0	-1.490047	2.468257	0.170764
10	6	0	-2.922612	0.013223	0.151576
11	6	0	-1.512963	-2.455043	0.170431
12	6	0	1.329295	-2.468181	0.208355
13	6	0	3.466876	-1.249906	0.237071
14	6	0	3.478403	1.216820	0.237260
15	6	0	2.775620	2.447381	0.227886
16	6	0	0.645269	3.690679	0.199316
17	6	0	-0.771674	3.697275	0.180422
18	6	0	-2.913508	2.473837	0.151711
19	6	0	-3.627691	1.249917	0.142145
20	6	0	-3.639173	-1.216852	0.141978
21	6	0	-2.936415	-2.447368	0.151378
22	6	0	-0.806063	-3.690697	0.179909
23	6	0	0.610889	-3.697299	0.198809
24	6	0	2.752695	-2.473862	0.227574
25	6	0	4.894157	-1.255968	0.256082
26	6	0	4.905633	1.209556	0.256327
27	6	0	3.494457	3.680498	0.237447
28	6	0	1.365197	4.923189	0.208989
29	6	0	-1.480098	4.936436	0.170911
30	6	0	-3.620833	3.713624	0.142250
31	6	0	-5.054950	1.255929	0.123041
32	6	0	-5.066427	-1.209574	0.122874
33	6	0	-3.655250	-3.680516	0.141749
34	6	0	-1.525992	-4.923207	0.170243
35	6	0	1.319302	-4.936454	0.208330
36	6	0	3.460039	-3.713642	0.236933
37	6	0	5.609431	-0.026499	0.265794
38	6	0	2.787455	4.914724	0.228032
39	6	0	-2.902374	4.941213	0.151874

40	6	0	-5.770226	0.026481	0.113461
41	6	0	-2.948251	-4.914742	0.151206
42	6	0	2.741578	-4.941232	0.227364
43	6	0	5.595564	-2.490243	0.265593
44	6	0	5.618500	2.437268	0.265912
45	6	0	4.913996	3.670841	0.256489
46	6	0	0.658497	6.154462	0.199543
47	6	0	-0.761966	6.161075	0.180530
48	6	0	-5.040401	3.717185	0.123250
49	6	0	-5.756358	2.490225	0.113660
50	6	0	-5.779295	-2.437286	0.113326
51	6	0	-5.074791	-3.670859	0.122749
52	6	0	-0.819291	-6.154480	0.179695
53	6	0	0.601171	-6.161093	0.198708
54	6	0	4.879607	-3.717203	0.255988
55	6	0	7.042087	-0.033169	0.284953
56	6	0	3.509559	6.152216	0.237704
57	6	0	-3.612926	6.185376	0.142370
58	6	0	-7.202883	0.033151	0.094285
59	6	0	-3.670354	-6.152234	0.141534
60	6	0	3.452130	-6.185394	0.236868
61	6	0	7.033634	-2.488103	0.284827
62	6	0	7.056488	2.421738	0.285160
63	6	0	5.631177	4.917427	0.266095
64	6	0	1.390939	7.392142	0.209353
65	6	0	-1.482854	7.405521	0.170888
66	6	0	-5.745947	4.970395	0.113813
67	6	0	-7.194428	2.488085	0.094411
68	6	0	-7.217282	-2.421756	0.094078
69	6	0	-5.791972	-4.917446	0.113143
70	6	0	-1.551733	-7.392160	0.169885
71	6	0	1.322059	-7.405540	0.208350
72	6	0	5.585151	-4.970413	0.265425
73	6	0	7.717058	-1.278028	0.293981
74	6	0	7.728617	1.205351	0.294149
75	6	0	4.925027	6.114381	0.256650
76	6	0	2.780330	7.366081	0.227950
77	6	0	-2.872428	7.392399	0.152288

78	6	0	-5.028684	6.160722	0.123420
79	6	0	-7.877852	1.278010	0.085257
80	6	0	-7.889412	-1.205369	0.085089
81	6	0	-5.085822	-6.114399	0.122588
82	6	0	-2.941125	-7.366099	0.151288
83	6	0	2.711633	-7.392417	0.226950
84	6	0	4.867890	-6.160740	0.255818
85	6	0	7.712600	-3.761355	0.293908
86	6	0	7.747278	3.688612	0.294413
87	6	0	7.073230	4.868856	0.285397
88	6	0	0.639286	8.623875	0.199299
89	6	0	-0.719768	8.630202	0.181108
90	6	0	-7.188389	4.935253	0.094505
91	6	0	-7.873396	3.761337	0.085330
92	6	0	-7.908073	-3.688631	0.084825
93	6	0	-7.234025	-4.868874	0.093841
94	6	0	-0.800081	-8.623893	0.179939
95	6	0	0.558972	-8.630220	0.198130
96	6	0	7.027594	-4.935272	0.284733
97	1	0	8.804952	-1.282242	0.308542
98	1	0	8.816503	1.199435	0.308711
99	1	0	5.472624	7.054502	0.263985
100	1	0	3.329396	8.305345	0.235304
101	1	0	-3.412726	8.336734	0.145061
102	1	0	-5.567505	7.105901	0.116213
103	1	0	-8.965747	1.282223	0.070695
104	1	0	-8.977299	-1.199454	0.070527
105	1	0	-5.633418	-7.054520	0.115253
106	1	0	-3.490191	-8.305363	0.143934
107	1	0	3.251931	-8.336752	0.234177
108	1	0	5.406710	-7.105919	0.263025
109	1	0	8.799803	-3.761365	0.308460
110	1	0	8.834433	3.678499	0.308964
111	1	0	7.616840	5.810481	0.292678
112	1	0	1.191621	9.560406	0.206697
113	1	0	-1.263361	9.571836	0.173837
114	1	0	-7.723210	5.881899	0.087352
115	1	0	-8.960598	3.761346	0.070778

116	1	0	-8.995229	-3.678517	0.070274
117	1	0	-7.777635	-5.810499	0.086560
118	1	0	-1.352416	-9.560425	0.172541
119	1	0	1.102565	-9.571854	0.205401
120	1	0	7.562415	-5.881917	0.291886
121	6	0	1.022240	-1.127347	-3.100942
122	6	0	1.005265	1.122715	-3.101041
123	6	0	2.311192	-0.705736	-3.344889
124	6	0	2.300420	0.720498	-3.345048
125	1	0	0.604545	-2.117657	-2.994030
126	1	0	0.572882	2.106815	-2.995039
127	1	0	3.168154	-1.347751	-3.497812
128	1	0	3.147391	1.375858	-3.497000
129	7	0	0.234957	-0.008146	-2.964361
130	1	0	-0.733890	-0.015573	-2.685466

Flat-on pyridine

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.219644	-1.324825	0.000000
2	6	0	-0.219644	-0.613225	1.232527
3	6	0	-0.219644	0.809975	1.232527
4	6	0	-0.219644	1.521575	0.000000
5	6	0	-0.219644	0.809975	-1.232527
6	6	0	-0.219644	-0.613225	-1.232527
7	6	0	-0.219644	-2.744125	0.000000
8	6	0	-0.219644	-1.322875	2.461677
9	6	0	-0.219644	1.519625	2.461677
10	6	0	-0.219644	2.940875	0.000000
11	6	0	-0.219644	1.519625	-2.461677
12	6	0	-0.219644	-1.322875	-2.461677
13	6	0	-0.219644	-3.455017	-1.233398
14	6	0	-0.219644	-3.455017	1.233398
15	6	0	-0.219644	-2.746475	2.460629
16	6	0	-0.219644	-0.610168	3.694026

17	6	0	-0.219644	0.806917	3.694026
18	6	0	-0.219644	2.943224	2.460629
19	6	0	-0.219644	3.651766	1.233398
20	6	0	-0.219644	3.651766	-1.233398
21	6	0	-0.219644	2.943224	-2.460629
22	6	0	-0.219644	0.806917	-3.694026
23	6	0	-0.219644	-0.610168	-3.694026
24	6	0	-0.219644	-2.746475	-2.460629
25	6	0	-0.219644	-4.882417	-1.232765
26	6	0	-0.219644	-4.882417	1.232765
27	6	0	-0.219644	-3.459627	3.697110
28	6	0	-0.219644	-1.324416	4.929875
29	6	0	-0.219644	1.521165	4.929875
30	6	0	-0.219644	3.656376	3.697110
31	6	0	-0.219644	5.079166	1.232765
32	6	0	-0.219644	5.079166	-1.232765
33	6	0	-0.219644	3.656376	-3.697110
34	6	0	-0.219644	1.521165	-4.929875
35	6	0	-0.219644	-1.324416	-4.929875
36	6	0	-0.219644	-3.459627	-3.697110
37	6	0	-0.219644	-5.592025	0.000000
38	6	0	-0.219644	-2.746825	4.928031
39	6	0	-0.219644	2.943575	4.928031
40	6	0	-0.219644	5.788775	0.000000
41	6	0	-0.219644	2.943575	-4.928031
42	6	0	-0.219644	-2.746825	-4.928031
43	6	0	-0.219644	-5.589626	-2.463782
44	6	0	-0.219644	-5.589626	2.463782
45	6	0	-0.219644	-4.879324	3.694062
46	6	0	-0.219644	-0.611928	6.157844
47	6	0	-0.219644	0.808677	6.157844
48	6	0	-0.219644	5.076073	3.694062
49	6	0	-0.219644	5.786375	2.463782
50	6	0	-0.219644	5.786375	-2.463782
51	6	0	-0.219644	5.076073	-3.694062
52	6	0	-0.219644	0.808677	-6.157844
53	6	0	-0.219644	-0.611928	-6.157844
54	6	0	-0.219644	-4.879324	-3.694062

55	6	0	-0.219644	-7.024825	0.000000
56	6	0	-0.219644	-3.463225	6.168872
57	6	0	-0.219644	3.659975	6.168872
58	6	0	-0.219644	7.221575	0.000000
59	6	0	-0.219644	3.659975	-6.168872
60	6	0	-0.219644	-3.463225	-6.168872
61	6	0	-0.219644	-7.027799	-2.454947
62	6	0	-0.219644	-7.027799	2.454947
63	6	0	-0.219644	-5.590758	4.943974
64	6	0	-0.219644	-1.338666	7.398921
65	6	0	-0.219644	1.535415	7.398921
66	6	0	-0.219644	5.787507	4.943974
67	6	0	-0.219644	7.224548	2.454947
68	6	0	-0.219644	7.224548	-2.454947
69	6	0	-0.219644	5.787507	-4.943974
70	6	0	-0.219644	1.535415	-7.398921
71	6	0	-0.219644	-1.338666	-7.398921
72	6	0	-0.219644	-5.590758	-4.943974
73	6	0	-0.219644	-7.705644	-1.241703
74	6	0	-0.219644	-7.705644	1.241703
75	6	0	-0.219644	-4.878981	6.137627
76	6	0	-0.219644	-2.728289	7.379329
77	6	0	-0.219644	2.925038	7.379329
78	6	0	-0.219644	5.075730	6.137627
79	6	0	-0.219644	7.902393	1.241703
80	6	0	-0.219644	7.902393	-1.241703
81	6	0	-0.219644	5.075730	-6.137627
82	6	0	-0.219644	2.925038	-7.379329
83	6	0	-0.219644	-2.728289	-7.379329
84	6	0	-0.219644	-4.878981	-6.137627
85	6	0	-0.219644	-7.712746	-3.725024
86	6	0	-0.219644	-7.712746	3.725024
87	6	0	-0.219644	-7.033151	4.902117
88	6	0	-0.219644	-0.581221	8.627141
89	6	0	-0.219644	0.777970	8.627141
90	6	0	-0.219644	7.229900	4.902117
91	6	0	-0.219644	7.909495	3.725024
92	6	0	-0.219644	7.909495	-3.725024

93	6	0	-0.219644	7.229900	-4.902117
94	6	0	-0.219644	0.777970	-8.627141
95	6	0	-0.219644	-0.581221	-8.627141
96	6	0	-0.219644	-7.033151	-4.902117
97	1	0	-0.219644	-8.793643	-1.240852
98	1	0	-0.219644	-8.793643	1.240852
99	1	0	-0.219644	-5.422244	7.080287
100	1	0	-0.219644	-3.273025	8.321139
101	1	0	-0.219644	3.469774	8.321139
102	1	0	-0.219644	5.618993	7.080287
103	1	0	-0.219644	8.990393	1.240852
104	1	0	-0.219644	8.990393	-1.240852
105	1	0	-0.219644	5.618993	-7.080287
106	1	0	-0.219644	3.469774	-8.321139
107	1	0	-0.219644	-3.273025	-8.321139
108	1	0	-0.219644	-5.422244	-7.080287
109	1	0	-0.219644	-8.800034	-3.719972
110	1	0	-0.219644	-8.800034	3.719972
111	1	0	-0.219644	-7.572420	5.846262
112	1	0	-0.219644	-1.129240	9.566234
113	1	0	-0.219644	1.325989	9.566234
114	1	0	-0.219644	7.769169	5.846262
115	1	0	-0.219644	8.996784	3.719972
116	1	0	-0.219644	8.996784	-3.719972
117	1	0	-0.219644	7.769169	-5.846262
118	1	0	-0.219644	1.325989	-9.566234
119	1	0	-0.219644	-1.129240	-9.566234
120	1	0	-0.219644	-7.572420	-5.846262
121	7	0	3.152604	0.016237	0.000000
122	6	0	3.145736	-0.683778	1.141715
123	6	0	3.145736	-0.683778	-1.141715
124	6	0	3.135011	-2.078467	1.198306
125	6	0	3.135011	-2.078467	-1.198306
126	6	0	3.128115	-2.790651	0.000000
127	1	0	3.133503	-0.097872	2.059528
128	1	0	3.133503	-0.097872	-2.059528
129	1	0	3.109072	-2.587520	2.156921
130	1	0	3.109072	-2.587520	-2.156921

131	1	0	3.095570	-3.876757	0.000000
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Benzothiophene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.899978	-0.805827	-0.395520
2	6	0	-0.399620	-1.383975	-0.347700
3	6	0	-1.549521	-0.546818	-0.298757
4	6	0	-1.399824	0.868486	-0.297633
5	6	0	-0.100225	1.446634	-0.345453
6	6	0	1.049675	0.609478	-0.394396
7	6	0	2.046728	-1.640689	-0.444329
8	6	0	-0.548908	-2.795401	-0.348821
9	6	0	-2.845558	-1.123383	-0.251068
10	6	0	-2.546573	1.703348	-0.248824
11	6	0	0.049062	2.858061	-0.344332
12	6	0	2.345713	1.186042	-0.442085
13	6	0	3.346266	-1.061421	-0.492141
14	6	0	1.895946	-3.056282	-0.445412
15	6	0	0.601932	-3.631946	-0.397798
16	6	0	-1.849297	-3.372754	-0.300966
17	6	0	-2.994256	-2.539195	-0.252233
18	6	0	-3.995165	-0.285144	-0.202131
19	6	0	-3.846111	1.124079	-0.201012
20	6	0	-2.395791	3.118940	-0.247741
21	6	0	-1.101777	3.694604	-0.295355
22	6	0	1.349451	3.435413	-0.392187
23	6	0	2.494410	2.601854	-0.440920
24	6	0	3.495320	0.347802	-0.491022
25	6	0	4.499188	-1.901559	-0.541217
26	6	0	3.049612	-3.895397	-0.494512
27	6	0	0.451164	-5.051361	-0.398900
28	6	0	-1.998808	-4.792302	-0.302118
29	6	0	-4.297947	-3.118472	-0.204260
30	6	0	-5.298342	-0.865577	-0.154183

31	6	0	-4.999033	1.964218	-0.151936
32	6	0	-3.549457	3.958055	-0.198641
33	6	0	-0.951009	5.114019	-0.294253
34	6	0	1.498962	4.854961	-0.391035
35	6	0	3.798101	3.181131	-0.488893
36	6	0	4.798497	0.928235	-0.538970
37	6	0	4.347741	-3.315885	-0.542267
38	6	0	-0.848461	-5.627503	-0.351069
39	6	0	-5.446125	-2.280289	-0.155378
40	6	0	-4.847587	3.378544	-0.150885
41	6	0	0.348615	5.690162	-0.342084
42	6	0	4.946279	2.342948	-0.537775
43	6	0	5.794351	-1.322050	-0.588857
44	6	0	2.897255	-5.306897	-0.495513
45	6	0	1.600027	-5.883992	-0.447780
46	6	0	-3.296443	-5.366243	-0.254354
47	6	0	-4.444247	-4.530613	-0.205500
48	6	0	-6.443621	-0.028016	-0.105418
49	6	0	-6.294196	1.384708	-0.104296
50	6	0	-3.397100	5.369556	-0.197640
51	6	0	-2.099872	5.946650	-0.245372
52	6	0	2.796598	5.428901	-0.438799
53	6	0	3.944402	4.593271	-0.487653
54	6	0	5.943776	0.090674	-0.587735
55	6	0	5.505398	-4.158688	-0.591541
56	6	0	-0.999168	-7.052354	-0.352200
57	6	0	-6.754490	-2.862337	-0.107236
58	6	0	-6.005244	4.221347	-0.101612
59	6	0	0.499322	7.115013	-0.340952
60	6	0	6.254644	2.924996	-0.585917
61	6	0	6.951155	-2.175158	-0.638148
62	6	0	4.064448	-6.145717	-0.545139
63	6	0	1.439974	-7.313258	-0.448569
64	6	0	-3.438936	-6.797366	-0.255837
65	6	0	-5.761103	-5.106770	-0.156998
66	6	0	-7.753307	-0.620320	-0.057274
67	6	0	-7.451000	2.237817	-0.055005
68	6	0	-4.564293	6.208375	-0.148014

69	6	0	-1.939820	7.375917	-0.244584
70	6	0	2.939091	6.860024	-0.437316
71	6	0	5.261258	5.169429	-0.536155
72	6	0	7.253461	0.682979	-0.635879
73	6	0	6.785521	-3.555013	-0.638476
74	6	0	5.325436	-5.563307	-0.591432
75	6	0	0.163088	-7.859865	-0.401480
76	6	0	-2.304646	-7.598927	-0.303996
77	6	0	-6.872356	-4.273521	-0.109580
78	6	0	-7.880005	-2.004292	-0.059141
79	6	0	-7.285366	3.617672	-0.054677
80	6	0	-5.825281	5.625965	-0.101721
81	6	0	-0.662933	7.922523	-0.291673
82	6	0	1.804800	7.661586	-0.389157
83	6	0	6.372510	4.336180	-0.583573
84	6	0	7.380160	2.066951	-0.634012
85	6	0	8.251295	-1.550966	-0.685762
86	6	0	3.871139	-7.575709	-0.544634
87	6	0	2.629991	-8.127855	-0.498965
88	6	0	-4.773044	-7.345063	-0.206522
89	6	0	-5.871227	-6.545559	-0.159780
90	6	0	-8.894105	0.261975	-0.008464
91	6	0	-8.751141	1.613625	-0.007391
92	6	0	-4.370985	7.638368	-0.148518
93	6	0	-3.129836	8.190513	-0.194187
94	6	0	4.273198	7.407722	-0.486631
95	6	0	5.371381	6.608218	-0.533373
96	6	0	8.394260	-0.199316	-0.684689
97	1	0	7.664090	-4.195686	-0.675876
98	1	0	6.205005	-6.202603	-0.628864
99	1	0	0.047803	-8.941739	-0.402305
100	1	0	-2.418241	-8.680981	-0.304889
101	1	0	-7.866210	-4.714723	-0.073006
102	1	0	-8.873169	-2.447048	-0.022601
103	1	0	-8.163936	4.258345	-0.017277
104	1	0	-6.704851	6.265262	-0.064289
105	1	0	-0.547648	9.004397	-0.290848
106	1	0	1.918396	8.743639	-0.388264

107	1	0	7.366365	4.777382	-0.620147
108	1	0	8.373324	2.509707	-0.670552
109	1	0	9.126819	-2.194618	-0.723058
110	1	0	4.752603	-8.211190	-0.582122
111	1	0	2.510606	-9.208580	-0.499626
112	1	0	-4.882389	-8.426850	-0.207579
113	1	0	-6.866136	-6.982633	-0.123144
114	1	0	-9.884916	-0.184331	0.027967
115	1	0	-9.626665	2.257277	0.029905
116	1	0	-5.252449	8.273849	-0.111031
117	1	0	-3.010452	9.271239	-0.193527
118	1	0	4.382543	8.489509	-0.485574
119	1	0	6.366290	7.045292	-0.570009
120	1	0	9.385070	0.246990	-0.721120
121	16	0	0.137570	-0.032350	3.082112
122	6	0	1.875968	0.220168	3.015353
123	6	0	0.361187	-1.768885	3.011501
124	6	0	2.568345	-1.015137	2.947142
125	6	0	1.665635	-2.137841	2.944176
126	1	0	-0.507975	-2.413547	3.002018
127	1	0	1.994559	-3.168578	2.871028
128	6	0	2.554697	1.442807	2.997229
129	6	0	3.972374	-1.001132	2.865995
130	6	0	4.646835	0.211057	2.852133
131	1	0	5.729473	0.224284	2.767190
132	6	0	3.942239	1.427023	2.915651
133	1	0	4.486294	2.366317	2.879145
134	1	0	2.009900	2.381814	3.025556
135	1	0	4.516582	-1.938672	2.792069

Benzofuran

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.921587	-0.775251	-0.357231
2	6	0	-0.361325	-1.389745	-0.309673

3	6	0	-1.534224	-0.585595	-0.259246
4	6	0	-1.424636	0.833371	-0.257143
5	6	0	-0.141923	1.448091	-0.304701
6	6	0	1.031133	0.643954	-0.354659
7	6	0	2.091485	-1.577100	-0.406739
8	6	0	-0.470185	-2.804861	-0.311245
9	6	0	-2.813429	-1.198639	-0.211903
10	6	0	-2.594532	1.635415	-0.207374
11	6	0	-0.032628	2.863176	-0.302512
12	6	0	2.310223	1.256481	-0.401996
13	6	0	3.374113	-0.961352	-0.454281
14	6	0	1.980779	-2.996446	-0.408989
15	6	0	0.703593	-3.608580	-0.361579
16	6	0	-1.753938	-3.418884	-0.263726
17	6	0	-2.922016	-2.618090	-0.214239
18	6	0	-3.986277	-0.393300	-0.161999
19	6	0	-3.877150	1.019575	-0.159747
20	6	0	-2.483858	3.054705	-0.205153
21	6	0	-1.206659	3.666786	-0.252583
22	6	0	1.250895	3.477125	-0.350218
23	6	0	2.419041	2.676325	-0.399769
24	6	0	3.483353	0.451726	-0.452165
25	6	0	4.550320	-1.768479	-0.504328
26	6	0	3.157749	-3.802563	-0.458850
27	6	0	0.593064	-5.031657	-0.363622
28	6	0	-1.863237	-4.842092	-0.266208
29	6	0	-4.208783	-3.234056	-0.166404
30	6	0	-5.272500	-1.010407	-0.114237
31	6	0	-5.053367	1.826721	-0.109716
32	6	0	-3.660789	3.860806	-0.155098
33	6	0	-1.096107	5.089897	-0.250340
34	6	0	1.360188	4.900333	-0.347890
35	6	0	3.705734	3.292298	-0.447677
36	6	0	4.769456	1.068647	-0.499756
37	6	0	4.438944	-3.186522	-0.506537
38	6	0	-0.689733	-5.644374	-0.316069
39	6	0	-5.380202	-2.428732	-0.116569
40	6	0	-4.941992	3.244764	-0.107529

41	6	0	0.186685	5.702616	-0.297988
42	6	0	4.877154	2.486973	-0.497487
43	6	0	5.828557	-1.152523	-0.551794
44	6	0	3.045376	-5.217809	-0.461121
45	6	0	1.765007	-5.831412	-0.413545
46	6	0	-3.144102	-5.452553	-0.218585
47	6	0	-4.315075	-4.649770	-0.168780
48	6	0	-6.441003	-0.205622	-0.064520
49	6	0	-6.331604	1.210762	-0.062263
50	6	0	-3.548424	5.276051	-0.152964
51	6	0	-2.268054	5.889653	-0.200511
52	6	0	2.641056	5.510793	-0.395472
53	6	0	3.812028	4.708010	-0.445277
54	6	0	5.937956	0.263862	-0.549537
55	6	0	5.619970	-3.996196	-0.556760
56	6	0	-0.800071	-7.072918	-0.318345
57	6	0	-6.671565	-3.047600	-0.068614
58	6	0	-6.123017	4.054437	-0.057297
59	6	0	0.297023	7.131158	-0.295711
60	6	0	6.168517	3.105842	-0.545443
61	6	0	7.009021	-1.972521	-0.602052
62	6	0	4.235821	-6.023233	-0.511677
63	6	0	1.645452	-7.264633	-0.415481
64	6	0	-3.246052	-6.887132	-0.221220
65	6	0	-5.615092	-5.262990	-0.120457
66	6	0	-7.733397	-0.834780	-0.016571
67	6	0	-7.512068	2.030763	-0.012005
68	6	0	-4.738868	6.081473	-0.102380
69	6	0	-2.148500	7.322874	-0.198576
70	6	0	2.743005	6.945373	-0.392837
71	6	0	5.112046	5.321231	-0.493600
72	6	0	7.230350	0.893021	-0.597486
73	6	0	6.882490	-3.356510	-0.603485
74	6	0	5.479816	-5.405344	-0.557773
75	6	0	0.384552	-7.847183	-0.368556
76	6	0	-2.089552	-7.656243	-0.270298
77	6	0	-6.749462	-4.461552	-0.072099
78	6	0	-7.820892	-2.221780	-0.019554

79	6	0	-7.385536	3.414750	-0.010572
80	6	0	-5.982863	5.463584	-0.056284
81	6	0	-0.887599	7.905423	-0.245501
82	6	0	1.586504	7.714485	-0.343759
83	6	0	6.246414	4.519793	-0.541958
84	6	0	7.317845	2.280021	-0.594503
85	6	0	8.290970	-1.311759	-0.649443
86	6	0	4.083045	-7.458121	-0.512312
87	6	0	2.858025	-8.045197	-0.466820
88	6	0	-4.564119	-7.472393	-0.172057
89	6	0	-5.684469	-6.704316	-0.124405
90	6	0	-8.898686	0.014848	0.033227
91	6	0	-8.794018	1.370000	0.035386
92	6	0	-4.586093	7.516363	-0.101744
93	6	0	-3.361072	8.103436	-0.147236
94	6	0	4.061071	7.530635	-0.442000
95	6	0	5.181422	6.762557	-0.489652
96	6	0	8.395639	0.043393	-0.647284
97	1	0	7.778823	-3.972040	-0.641613
98	1	0	6.377110	-6.019470	-0.595933
99	1	0	0.299919	-8.931885	-0.370250
100	1	0	-2.172489	-8.741077	-0.272061
101	1	0	-7.730427	-4.930723	-0.035666
102	1	0	-8.801124	-2.692486	0.016844
103	1	0	-8.281871	4.030281	0.027556
104	1	0	-6.880158	6.077711	-0.018124
105	1	0	-0.802966	8.990125	-0.243807
106	1	0	1.669442	8.799317	-0.341996
107	1	0	7.227380	4.988965	-0.578391
108	1	0	8.298077	2.750727	-0.630900
109	1	0	9.184344	-1.930354	-0.687470
110	1	0	4.982124	-8.068380	-0.550525
111	1	0	2.769262	-9.128865	-0.468348
112	1	0	-4.642817	-8.556839	-0.173984
113	1	0	-6.666606	-7.169392	-0.087906
114	1	0	-9.876466	-0.459340	0.069513
115	1	0	-9.687392	1.988595	0.073413
116	1	0	-5.485172	8.126620	-0.063532

117	1	0	-3.272310	9.187106	-0.145709
118	1	0	4.139769	8.615081	-0.440073
119	1	0	6.163558	7.227633	-0.526151
120	1	0	9.373418	0.517580	-0.683569
121	6	0	1.861473	0.117252	2.992239
122	6	0	0.471007	-1.579045	2.985150
123	6	0	2.645688	-1.052593	2.989252
124	6	0	1.702217	-2.145587	2.986537
125	1	0	-0.525476	-1.993873	2.961868
126	1	0	1.920555	-3.203752	2.962799
127	6	0	2.391587	1.401186	2.973127
128	6	0	4.042785	-0.928658	2.961755
129	6	0	4.594258	0.348677	2.941824
130	1	0	5.673413	0.464379	2.899223
131	6	0	3.781547	1.498306	2.948495
132	1	0	4.244902	2.479659	2.910090
133	1	0	1.748862	2.274687	2.951949
134	1	0	4.677313	-1.809708	2.935284
135	8	0	0.528906	-0.205112	2.990702

Indole

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.893139	-0.836166	-0.354377
2	6	0	-0.420951	-1.380775	-0.308122
3	6	0	-1.549085	-0.514633	-0.261424
4	6	0	-1.363318	0.896405	-0.261376
5	6	0	-0.049313	1.441163	-0.307515
6	6	0	1.078887	0.574987	-0.354002
7	6	0	2.018300	-1.699959	-0.400415
8	6	0	-0.605860	-2.787953	-0.307886
9	6	0	-2.859477	-1.057885	-0.215413
10	6	0	-2.488468	1.760298	-0.215153
11	6	0	0.135933	2.848322	-0.307472
12	6	0	2.389191	1.117732	-0.399918

13	6	0	3.332289	-1.154148	-0.446572
14	6	0	1.831413	-3.111285	-0.400488
15	6	0	0.523092	-3.653751	-0.354451
16	6	0	-1.920842	-3.332012	-0.261587
17	6	0	-3.044253	-2.469442	-0.215637
18	6	0	-3.987399	-0.190544	-0.169067
19	6	0	-3.802438	1.214418	-0.168937
20	6	0	-2.301618	3.171583	-0.215061
21	6	0	-0.993263	3.714000	-0.261085
22	6	0	1.450703	3.392264	-0.353764
23	6	0	2.574140	2.529715	-0.399758
24	6	0	3.517374	0.250987	-0.446473
25	6	0	4.463475	-2.023467	-0.492986
26	6	0	2.963427	-3.979628	-0.446847
27	6	0	0.336184	-5.068832	-0.354337
28	6	0	-2.106537	-4.747258	-0.261875
29	6	0	-4.362372	-3.015225	-0.169214
30	6	0	-5.305036	-0.737494	-0.122720
31	6	0	-4.933625	2.083744	-0.122457
32	6	0	-3.433574	4.039904	-0.168558
33	6	0	-0.806329	5.129107	-0.260978
34	6	0	1.636386	4.807536	-0.353573
35	6	0	3.892220	3.075502	-0.446260
36	6	0	4.834890	0.797770	-0.492646
37	6	0	4.275991	-3.433469	-0.493067
38	6	0	-0.977799	-5.611582	-0.308258
39	6	0	-5.488866	-2.147975	-0.122920
40	6	0	-4.746143	3.493746	-0.122395
41	6	0	0.507647	5.671860	-0.307210
42	6	0	5.018714	2.208252	-0.492548
43	6	0	5.773077	-1.477236	-0.539062
44	6	0	2.775102	-5.386781	-0.446949
45	6	0	1.463498	-5.930547	-0.400787
46	6	0	-3.418469	-5.287861	-0.215729
47	6	0	-4.544654	-4.423174	-0.169459
48	6	0	-6.428648	0.129059	-0.076537
49	6	0	-6.243227	1.537511	-0.076406
50	6	0	-3.245254	5.447059	-0.168542

51	6	0	-1.933649	5.990823	-0.214680
52	6	0	2.948318	5.348137	-0.399739
53	6	0	4.074504	4.483449	-0.446009
54	6	0	5.958497	-0.068783	-0.538931
55	6	0	5.411844	-4.305579	-0.539739
56	6	0	-1.164811	-7.032125	-0.308389
57	6	0	-6.811732	-2.696408	-0.076385
58	6	0	-5.881996	4.365856	-0.075728
59	6	0	0.694660	7.092402	-0.307077
60	6	0	6.341581	2.756685	-0.539083
61	6	0	6.907814	-2.359626	-0.585739
62	6	0	3.920591	-6.255153	-0.493933
63	6	0	1.267030	-7.355265	-0.400587
64	6	0	-3.597429	-6.714883	-0.216193
65	6	0	-5.875858	-4.965500	-0.122583
66	6	0	-7.753096	-0.429592	-0.029993
67	6	0	-7.377964	2.419902	-0.029729
68	6	0	-4.390741	6.315429	-0.121535
69	6	0	-1.737182	7.415541	-0.214880
70	6	0	3.127278	6.775159	-0.399274
71	6	0	5.405708	5.025777	-0.492884
72	6	0	7.282944	0.489869	-0.585474
73	6	0	6.707027	-3.734804	-0.585131
74	6	0	5.196101	-5.705148	-0.538696
75	6	0	-0.023460	-7.869072	-0.355086
76	6	0	-2.483886	-7.545168	-0.261819
77	6	0	-6.965563	-4.104126	-0.077689
78	6	0	-7.915062	-1.809882	-0.030858
79	6	0	-7.177177	3.795082	-0.030337
80	6	0	-5.666252	5.765425	-0.076773
81	6	0	-0.446691	7.929347	-0.260382
82	6	0	2.013734	7.605445	-0.353648
83	6	0	6.495411	4.164404	-0.537779
84	6	0	7.444912	1.870159	-0.584610
85	6	0	8.223531	-1.768852	-0.631795
86	6	0	3.690857	-7.679747	-0.492493
87	6	0	2.435954	-8.200004	-0.448349
88	6	0	-4.945154	-7.228319	-0.168557

89	6	0	-6.022653	-6.401013	-0.124289
90	6	0	-8.871086	0.481566	0.016203
91	6	0	-8.693683	1.829129	0.016328
92	6	0	-4.161009	7.740023	-0.122974
93	6	0	-2.906105	8.260280	-0.167118
94	6	0	4.475003	7.288595	-0.446911
95	6	0	5.552501	6.461290	-0.491180
96	6	0	8.400936	-0.421289	-0.631670
97	1	0	7.569021	-4.397719	-0.620552
98	1	0	6.059130	-6.366711	-0.574148
99	1	0	-0.166311	-8.947652	-0.355154
100	1	0	-2.625050	-8.623971	-0.261952
101	1	0	-7.970407	-4.519794	-0.042336
102	1	0	-8.919257	-2.227121	0.004463
103	1	0	-8.039173	4.457996	0.005084
104	1	0	-6.529282	6.426989	-0.041320
105	1	0	-0.303839	9.007928	-0.260314
106	1	0	2.154901	8.684248	-0.353516
107	1	0	7.500257	4.580071	-0.573131
108	1	0	8.449106	2.287398	-0.619930
109	1	0	9.082405	-2.434666	-0.667115
110	1	0	4.555878	-8.337544	-0.528002
111	1	0	2.289033	-9.277332	-0.448260
112	1	0	-5.082065	-8.306964	-0.168848
113	1	0	-7.028447	-6.812526	-0.088879
114	1	0	-9.873019	0.060719	0.051421
115	1	0	-9.552556	2.494943	0.051646
116	1	0	-5.026030	8.397822	-0.087466
117	1	0	-2.759185	9.337608	-0.167208
118	1	0	4.611913	8.367241	-0.446621
119	1	0	6.558296	6.872804	-0.526588
120	1	0	9.402868	-0.000441	-0.666889
121	6	0	1.717863	0.158139	2.960030
122	6	0	0.240112	-1.543682	2.949237
123	6	0	2.444986	-1.063552	3.041012
124	6	0	1.476801	-2.125374	3.036760
125	1	0	-0.739744	-1.995766	2.890514
126	1	0	1.678266	-3.186857	3.074060

127	6	0	2.350472	1.403850	2.915185
128	6	0	3.849335	-1.012644	3.071619
129	6	0	4.481768	0.222720	3.022188
130	1	0	5.567158	0.271544	3.024979
131	6	0	3.739517	1.419607	2.946317
132	1	0	4.262666	2.369851	2.888893
133	1	0	1.777781	2.323241	2.828506
134	1	0	4.429363	-1.930855	3.113639
135	7	0	0.376471	-0.167335	2.919276
136	1	0	-0.370597	0.482788	2.730707

Quinoline

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.574779	-1.143386	-0.370867
2	6	0	-0.846664	-1.202671	-0.329535
3	6	0	-1.608368	-0.000899	-0.296217
4	6	0	-0.948543	1.260155	-0.303998
5	6	0	0.472775	1.319333	-0.345207
6	6	0	1.234453	0.117531	-0.378748
7	6	0	1.334191	-2.341896	-0.404240
8	6	0	-1.504617	-2.460231	-0.321875
9	6	0	-3.025780	-0.059906	-0.255172
10	6	0	-1.708068	2.458665	-0.270696
11	6	0	1.130780	2.576923	-0.352951
12	6	0	2.651876	0.176651	-0.419671
13	6	0	2.755930	-2.281726	-0.445339
14	6	0	0.673274	-3.602812	-0.396343
15	6	0	-0.741936	-3.661764	-0.355349
16	6	0	-2.926458	-2.518399	-0.280676
17	6	0	-3.684797	-1.321759	-0.247423
18	6	0	-3.786720	1.142795	-0.221773
19	6	0	-3.129795	2.398390	-0.229514
20	6	0	-1.047194	3.719546	-0.278506
21	6	0	0.368070	3.778502	-0.319511

22	6	0	2.552593	2.635102	-0.394152
23	6	0	3.310933	1.438463	-0.427378
24	6	0	3.412900	-1.026143	-0.452980
25	6	0	3.519255	-3.487376	-0.478805
26	6	0	1.437722	-4.807853	-0.429818
27	6	0	-1.404203	-4.926239	-0.347502
28	6	0	-3.587605	-3.783427	-0.272907
29	6	0	-5.110389	-1.380512	-0.206112
30	6	0	-5.212260	1.082779	-0.180476
31	6	0	-3.893120	3.604079	-0.196021
32	6	0	-1.811586	4.924557	-0.244988
33	6	0	1.030336	5.042942	-0.327328
34	6	0	3.213740	3.900129	-0.401931
35	6	0	4.736524	1.497215	-0.468725
36	6	0	4.838396	-0.966096	-0.494342
37	6	0	2.858228	-4.746834	-0.470990
38	6	0	-2.824861	-4.983574	-0.306333
39	6	0	-5.870021	-0.178389	-0.172761
40	6	0	-3.232093	4.863537	-0.203848
41	6	0	2.450996	5.100278	-0.368506
42	6	0	5.496157	0.295092	-0.502041
43	6	0	4.937001	-3.425266	-0.519865
44	6	0	0.776887	-6.064350	-0.422001
45	6	0	-0.641892	-6.123451	-0.380887
46	6	0	-5.005604	-3.839446	-0.231795
47	6	0	-5.765826	-2.639834	-0.198448
48	6	0	-5.969423	2.283256	-0.147212
49	6	0	-5.310866	3.541970	-0.154973
50	6	0	-1.150752	6.181053	-0.252836
51	6	0	0.268028	6.240155	-0.293943
52	6	0	4.631739	3.956149	-0.443043
53	6	0	5.391961	2.756537	-0.476388
54	6	0	5.595557	-2.166552	-0.527665
55	6	0	3.624976	-5.956744	-0.504621
56	6	0	-3.489071	-6.253094	-0.298504
57	6	0	-7.300980	-0.237998	-0.131302
58	6	0	-3.998841	6.073447	-0.170216
59	6	0	3.115206	6.369798	-0.376334

60	6	0	6.927115	0.354701	-0.543536
61	6	0	5.699165	-4.644445	-0.553447
62	6	0	1.553970	-7.274064	-0.455934
63	6	0	-1.316419	-7.393637	-0.372771
64	6	0	-5.664481	-5.117821	-0.224204
65	6	0	-7.202516	-2.690840	-0.156742
66	6	0	-7.405383	2.214595	-0.105689
67	6	0	-6.073031	4.761148	-0.121390
68	6	0	-1.927835	7.390768	-0.218902
69	6	0	0.942553	7.510340	-0.302067
70	6	0	5.290615	5.234524	-0.450632
71	6	0	6.828651	2.807543	-0.518096
72	6	0	7.031518	-2.097892	-0.569149
73	6	0	5.037622	-5.866626	-0.545262
74	6	0	2.940998	-7.196678	-0.495942
75	6	0	-2.705065	-7.431876	-0.332356
76	6	0	-4.904298	-6.280777	-0.257212
77	6	0	-7.929618	-1.506898	-0.124513
78	6	0	-8.032228	0.974252	-0.098690
79	6	0	-5.411486	5.983330	-0.129574
80	6	0	-3.314863	7.313381	-0.178896
81	6	0	2.331199	7.548579	-0.342481
82	6	0	4.530433	6.397481	-0.417625
83	6	0	7.555754	1.623602	-0.550325
84	6	0	7.658363	-0.857549	-0.576147
85	6	0	7.137976	-4.542617	-0.594749
86	6	0	0.848246	-8.532682	-0.446788
87	6	0	-0.509199	-8.589229	-0.407459
88	6	0	-7.106750	-5.136010	-0.182033
89	6	0	-7.834106	-3.988260	-0.150129
90	6	0	-8.141927	3.455023	-0.072663
91	6	0	-7.511840	4.659321	-0.080088
92	6	0	-1.222111	8.649385	-0.228049
93	6	0	0.135334	8.705932	-0.267379
94	6	0	6.732885	5.252713	-0.492805
95	6	0	7.460241	4.104963	-0.524709
96	6	0	7.768062	-3.338319	-0.602175
97	1	0	5.619136	-6.785829	-0.570785

98	1	0	3.523947	-8.114970	-0.521497
99	1	0	-3.210188	-8.395494	-0.326386
100	1	0	-5.407915	-7.245184	-0.251295
101	1	0	-9.016256	-1.551312	-0.093021
102	1	0	-9.118795	0.928138	-0.067217
103	1	0	-5.993001	6.902533	-0.104053
104	1	0	-3.897813	8.231673	-0.153341
105	1	0	2.836323	8.512197	-0.348450
106	1	0	5.034050	7.361887	-0.423543
107	1	0	8.642391	1.668016	-0.581816
108	1	0	8.744930	-0.811434	-0.607621
109	1	0	7.715561	-5.463470	-0.620171
110	1	0	1.434362	-9.448123	-0.472411
111	1	0	-1.017713	-9.550269	-0.401366
112	1	0	-7.606315	-6.101734	-0.176245
113	1	0	-8.920206	-4.028447	-0.118614
114	1	0	-9.227609	3.404741	-0.041253
115	1	0	-8.089426	5.580173	-0.054667
116	1	0	-1.808227	9.564827	-0.202427
117	1	0	0.643847	9.666972	-0.273471
118	1	0	7.232450	6.218437	-0.498592
119	1	0	8.546341	4.145151	-0.556223
120	1	0	8.853745	-3.288037	-0.633584
121	6	0	1.390656	-2.379688	2.957093
122	6	0	1.228330	0.050312	3.016934
123	6	0	2.048073	-1.123620	2.975182
124	6	0	-0.698615	-1.198015	3.017786
125	6	0	0.017543	-2.421235	2.980566
126	1	0	1.981201	-3.291442	2.904859
127	1	0	-1.788235	-1.216390	3.015653
128	1	0	-0.521348	-3.362789	2.945775
129	6	0	1.853048	1.324874	3.011498
130	6	0	3.459200	-0.982123	2.927098
131	6	0	3.224609	1.428936	2.963358
132	1	0	3.694137	2.408326	2.935343
133	6	0	4.035386	0.267552	2.921712
134	1	0	5.115028	0.369227	2.861415
135	1	0	1.211895	2.200439	3.024934

136	1	0	4.074893	-1.876808	2.871678
137	7	0	-0.136774	-0.006217	3.037743

Dibenzothiophene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.079604	-0.000127	-0.528964
2	6	0	0.368834	-1.232529	-0.491270
3	6	0	-1.052392	-1.232324	-0.416024
4	6	0	-1.762810	0.000310	-0.378374
5	6	0	-1.052016	1.232730	-0.415945
6	6	0	0.369165	1.232528	-0.491314
7	6	0	2.496967	-0.000419	-0.604002
8	6	0	1.077286	-2.461754	-0.528909
9	6	0	-1.761234	-2.461367	-0.378498
10	6	0	-3.180121	0.000523	-0.303292
11	6	0	-1.760491	2.461987	-0.378457
12	6	0	1.078143	2.461595	-0.528824
13	6	0	3.206925	1.233050	-0.641778
14	6	0	3.206732	-1.233847	-0.641655
15	6	0	2.498899	-2.461017	-0.604102
16	6	0	0.365362	-3.694033	-0.491225
17	6	0	-1.049711	-3.693824	-0.416216
18	6	0	-3.182840	-2.460105	-0.303187
19	6	0	-3.890204	-1.232768	-0.265695
20	6	0	-3.889831	1.234029	-0.265674
21	6	0	-3.182095	2.461153	-0.303147
22	6	0	-1.048590	3.694229	-0.416088
23	6	0	0.366462	3.693989	-0.491088
24	6	0	2.499621	2.460329	-0.604256
25	6	0	4.632395	1.232020	-0.717261
26	6	0	4.632025	-1.233384	-0.717226
27	6	0	3.210855	-3.697550	-0.641988
28	6	0	1.078405	-4.929935	-0.528830
29	6	0	-1.763146	-4.929566	-0.378437

30	6	0	-3.895180	-3.696479	-0.265472
31	6	0	-5.315606	-1.231919	-0.190184
32	6	0	-5.315232	1.233611	-0.190163
33	6	0	-3.894062	3.697742	-0.265411
34	6	0	-1.761654	4.930184	-0.378356
35	6	0	1.079936	4.929756	-0.528969
36	6	0	3.211918	3.696906	-0.641977
37	6	0	5.340838	-0.000759	-0.754645
38	6	0	2.498869	-4.928357	-0.604200
39	6	0	-3.183564	-4.927507	-0.303190
40	6	0	-6.024035	0.000953	-0.152634
41	6	0	-3.182073	4.928555	-0.303109
42	6	0	2.500376	4.927708	-0.604139
43	6	0	5.338848	2.463056	-0.754573
44	6	0	5.338060	-2.464543	-0.754596
45	6	0	4.628568	-3.694716	-0.717019
46	6	0	0.366807	-6.157875	-0.491308
47	6	0	-1.051843	-6.157642	-0.416166
48	6	0	-5.312889	-3.693216	-0.190369
49	6	0	-6.022011	-2.462830	-0.152782
50	6	0	-6.021265	2.464735	-0.152741
51	6	0	-5.311772	3.694907	-0.190306
52	6	0	-1.049978	6.158046	-0.416037
53	6	0	0.368637	6.157832	-0.491189
54	6	0	4.629644	3.693044	-0.716815
55	6	0	6.771623	-0.000977	-0.830483
56	6	0	3.214078	-6.169313	-0.642113
57	6	0	-3.899149	-6.168241	-0.265301
58	6	0	-7.454828	0.001169	-0.076838
59	6	0	-3.897282	6.169503	-0.265200
60	6	0	3.215946	6.168431	-0.641981
61	6	0	6.774968	2.453970	-0.830548
62	6	0	6.774222	-2.455925	-0.830667
63	6	0	5.338816	-4.944736	-0.754665
64	6	0	1.092308	-7.399043	-0.529720
65	6	0	-1.777750	-7.398608	-0.377703
66	6	0	-6.023517	-4.943022	-0.152742
67	6	0	-7.458169	-2.453778	-0.076701

68	6	0	-7.457425	2.456116	-0.076661
69	6	0	-6.022022	4.944927	-0.152662
70	6	0	-1.775511	7.399233	-0.377581
71	6	0	1.094546	7.398800	-0.529624
72	6	0	5.340248	4.943251	-0.754490
73	6	0	7.451676	1.240623	-0.866494
74	6	0	7.451301	-1.242783	-0.866514
75	6	0	4.627856	-6.138282	-0.717021
76	6	0	2.479986	-7.379659	-0.603257
77	6	0	-3.165424	-7.378808	-0.304190
78	6	0	-5.312917	-6.136781	-0.190407
79	6	0	-8.134880	-1.240431	-0.040832
80	6	0	-8.134505	1.242974	-0.040812
81	6	0	-5.311059	6.138472	-0.190305
82	6	0	-3.163191	7.379849	-0.304070
83	6	0	2.482219	7.378999	-0.603137
84	6	0	4.629712	6.136972	-0.716922
85	6	0	7.459144	3.723943	-0.866849
86	6	0	7.458017	-3.726104	-0.866911
87	6	0	6.779196	-4.903096	-0.830969
88	6	0	0.335735	-8.627147	-0.489686
89	6	0	-1.021552	-8.626943	-0.417783
90	6	0	-7.463884	-4.900947	-0.076438
91	6	0	-8.142350	-3.723752	-0.040477
92	6	0	-8.141223	3.726296	-0.040416
93	6	0	-7.462399	4.903286	-0.076357
94	6	0	-1.018941	8.627338	-0.417641
95	6	0	0.338346	8.627135	-0.489543
96	6	0	6.780680	4.901139	-0.830877
97	1	0	8.538152	1.239607	-0.924051
98	1	0	8.537777	-1.242096	-0.924070
99	1	0	5.170215	-7.081023	-0.745768
100	1	0	3.023817	-8.321552	-0.632083
101	1	0	-3.709540	-8.320535	-0.275381
102	1	0	-5.855562	-7.079360	-0.161675
103	1	0	-9.221358	-1.239417	0.016724
104	1	0	-9.220982	1.242287	0.016744
105	1	0	-5.853419	7.081214	-0.161558

106	1	0	-3.707022	8.321742	-0.275244
107	1	0	3.026336	8.320727	-0.631945
108	1	0	5.172357	7.079551	-0.745652
109	1	0	8.544909	3.718727	-0.924368
110	1	0	8.543783	-3.721218	-0.924430
111	1	0	7.317566	-5.847322	-0.859505
112	1	0	0.882845	-9.566323	-0.518685
113	1	0	-1.568945	-9.565954	-0.388799
114	1	0	-8.002541	-5.845011	-0.047917
115	1	0	-9.228115	-3.718535	0.017042
116	1	0	-9.226989	3.721408	0.017104
117	1	0	-8.000772	5.847513	-0.047821
118	1	0	-1.566050	9.566514	-0.388642
119	1	0	0.885739	9.566144	-0.518527
120	1	0	7.319337	5.845202	-0.859409
121	16	0	0.166877	0.000292	2.970369
122	6	0	1.405169	1.259404	2.898684
123	6	0	1.404040	-1.259935	2.898782
124	6	0	2.712141	0.725843	2.826934
125	6	0	2.711490	-0.727554	2.826997
126	6	0	1.177512	2.637272	2.884830
127	6	0	3.799861	1.607305	2.743446
128	6	0	3.578136	2.979035	2.732595
129	1	0	4.419311	3.660181	2.645663
130	6	0	2.273333	3.491396	2.802611
131	1	0	2.112613	4.564951	2.769036
132	1	0	0.166856	3.033086	2.916620
133	1	0	4.809767	1.214542	2.666321
134	6	0	1.175147	-2.637597	2.885029
135	6	0	3.798415	-1.609999	2.743605
136	6	0	2.270198	-3.492715	2.802891
137	1	0	2.108511	-4.566127	2.769398
138	1	0	4.808676	-1.218153	2.666478
139	1	0	0.164135	-3.032503	2.916833
140	6	0	3.575463	-2.981534	2.732864
141	1	0	4.416019	-3.663448	2.646018

Dibenzofuran

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.072230	0.005407	-0.493919
2	6	0	-0.350174	1.231232	-0.456264
3	6	0	1.070900	1.217981	-0.379335
4	6	0	1.769880	-0.021121	-0.339964
5	6	0	1.047800	-1.246963	-0.377495
6	6	0	-0.373228	-1.233717	-0.454547
7	6	0	-2.489441	0.018709	-0.570634
8	6	0	-1.047220	2.466907	-0.495620
9	6	0	1.790997	2.440465	-0.341849
10	6	0	3.187040	-0.034343	-0.263204
11	6	0	1.744869	-2.482671	-0.338290
12	6	0	-1.093462	-2.456223	-0.492017
13	6	0	-3.210694	-1.208191	-0.608369
14	6	0	-3.187761	1.258599	-0.610009
15	6	0	-2.468689	2.479219	-0.572494
16	6	0	-0.324011	3.692599	-0.457974
17	6	0	1.090910	3.679400	-0.381289
18	6	0	3.212441	2.426155	-0.264855
19	6	0	3.908416	1.192377	-0.225648
20	6	0	3.885304	-1.274312	-0.223865
21	6	0	3.166331	-2.494886	-0.261298
22	6	0	1.021684	-3.708326	-0.375883
23	6	0	-0.393216	-3.695097	-0.452558
24	6	0	-2.514778	-2.441909	-0.569132
25	6	0	-4.636004	-1.194076	-0.685540
26	6	0	-4.612907	1.271218	-0.687266
27	6	0	-3.169171	3.722234	-0.612107
28	6	0	-1.025586	4.934993	-0.497306
29	6	0	1.815662	4.908541	-0.343550
30	6	0	3.936104	3.655937	-0.227180
31	6	0	5.333661	1.178444	-0.148449
32	6	0	5.310559	-1.286977	-0.146667
33	6	0	3.866823	-3.737958	-0.221836

34	6	0	1.723279	-4.950773	-0.336424
35	6	0	-1.118007	-4.924263	-0.490400
36	6	0	-3.238399	-3.671895	-0.606813
37	6	0	-5.333008	0.045153	-0.724643
38	6	0	-2.445915	4.946454	-0.574356
39	6	0	3.235911	4.893444	-0.266620
40	6	0	6.030650	-0.060878	-0.109180
41	6	0	3.143564	-4.962183	-0.259496
42	6	0	-2.538278	-4.909176	-0.567252
43	6	0	-5.353730	-2.418575	-0.722808
44	6	0	-5.307519	2.508806	-0.726351
45	6	0	-4.586761	3.732413	-0.688813
46	6	0	-0.302743	6.156349	-0.459819
47	6	0	1.115754	6.143093	-0.382999
48	6	0	5.353633	3.639660	-0.150397
49	6	0	6.051338	2.402818	-0.111091
50	6	0	6.005168	-2.524530	-0.107529
51	6	0	5.284410	-3.748137	-0.145055
52	6	0	1.000360	-6.172051	-0.374069
53	6	0	-0.418103	-6.158815	-0.450901
54	6	0	-4.655940	-3.655020	-0.683331
55	6	0	-6.763640	0.058504	-0.802174
56	6	0	-3.149608	6.193921	-0.614002
57	6	0	3.962858	6.127556	-0.228771
58	6	0	7.461290	-0.074228	-0.031690
59	6	0	3.847257	-6.209643	-0.219854
60	6	0	-3.265211	-6.143278	-0.605055
61	6	0	-6.789615	-2.396308	-0.800489
62	6	0	-6.743608	2.513371	-0.804116
63	6	0	-5.285411	4.988899	-0.728194
64	6	0	-1.016726	7.404123	-0.499977
65	6	0	1.853025	7.377343	-0.344563
66	6	0	6.075707	4.882891	-0.112822
67	6	0	7.487261	2.380585	-0.033304
68	6	0	7.441256	-2.529093	-0.029756
69	6	0	5.983061	-5.004623	-0.105677
70	6	0	1.714374	-7.419844	-0.333868
71	6	0	-1.155376	-7.393067	-0.489308

72	6	0	-5.377993	-4.898651	-0.720953
73	6	0	-7.455067	-1.176800	-0.838103
74	6	0	-7.431799	1.306496	-0.839897
75	6	0	-4.563523	6.175869	-0.690561
76	6	0	-2.404437	7.397477	-0.575142
77	6	0	3.240370	7.344807	-0.269393
78	6	0	5.376187	6.083121	-0.152181
79	6	0	8.152715	1.161077	0.004234
80	6	0	8.129448	-1.322218	0.006028
81	6	0	5.261171	-6.191590	-0.143308
82	6	0	3.102087	-7.413199	-0.258728
83	6	0	-2.542720	-7.360529	-0.564478
84	6	0	-4.678537	-6.098843	-0.681692
85	6	0	-7.485426	-3.659946	-0.836692
86	6	0	-7.415622	3.789772	-0.842077
87	6	0	-6.726023	4.960483	-0.806173
88	6	0	-0.248912	8.625229	-0.459925
89	6	0	1.108229	8.612567	-0.386415
90	6	0	7.515534	4.827596	-0.034784
91	6	0	8.183077	3.644224	0.002823
92	6	0	8.113273	-3.805496	0.008207
93	6	0	7.423671	-4.976204	-0.027697
94	6	0	0.946563	-8.640952	-0.373946
95	6	0	-0.410579	-8.628291	-0.447454
96	6	0	-6.817885	-4.843319	-0.799076
97	1	0	-8.541419	-1.165812	-0.896946
98	1	0	-8.518166	1.315781	-0.898739
99	1	0	-5.097134	7.123548	-0.720624
100	1	0	-2.939528	8.344322	-0.605285
101	1	0	3.793110	8.281499	-0.240613
102	1	0	5.927463	7.020679	-0.123480
103	1	0	9.239069	1.150091	0.063075
104	1	0	9.215816	-1.331503	0.064869
105	1	0	5.794783	-7.139270	-0.113245
106	1	0	3.637178	-8.360043	-0.228586
107	1	0	-3.095461	-8.297222	-0.593257
108	1	0	-5.229814	-7.036401	-0.710391
109	1	0	-8.571028	-3.644764	-0.895499

110	1	0	-8.501319	3.794853	-0.900878
111	1	0	-7.255631	5.909610	-0.836021
112	1	0	-0.787307	9.569387	-0.490243
113	1	0	1.664221	9.546513	-0.357455
114	1	0	8.062837	5.766675	-0.006300
115	1	0	9.268679	3.629040	0.061630
116	1	0	9.198970	-3.810574	0.067008
117	1	0	7.953282	-5.925332	0.002151
118	1	0	1.484956	-9.585110	-0.343628
119	1	0	-0.966570	-9.562235	-0.476415
120	1	0	-7.365188	-5.782398	-0.827570
121	6	0	-1.596537	-1.075523	2.888885
122	6	0	-1.518257	1.124279	2.889688
123	6	0	-2.939226	-0.652479	2.847926
124	6	0	-2.887641	0.797767	2.848348
125	6	0	-1.218213	-2.410180	2.882828
126	6	0	-3.953466	-1.614352	2.795291
127	6	0	-3.594975	-2.960831	2.789264
128	1	0	-4.367777	-3.721135	2.727251
129	6	0	-2.246481	-3.352614	2.833811
130	1	0	-1.995687	-4.408769	2.804570
131	1	0	-0.171989	-2.695767	2.891163
132	1	0	-4.996342	-1.316233	2.739995
133	6	0	-1.046100	2.428622	2.884832
134	6	0	-3.830949	1.829315	2.796975
135	6	0	-2.004738	3.441880	2.836243
136	1	0	-1.679501	4.477541	2.807750
137	1	0	-4.892389	1.606178	2.741547
138	1	0	0.017815	2.639059	2.892967
139	6	0	-3.377641	3.146923	2.791791
140	1	0	-4.094541	3.960223	2.730388
141	8	0	-0.728629	-0.005157	2.913761

Carbazole

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

1	6	0	1.101483	-0.052867	-0.490566
2	6	0	0.327505	-1.246678	-0.455854
3	6	0	-1.091999	-1.172639	-0.384635
4	6	0	-1.737486	0.095234	-0.348028
5	6	0	-0.963485	1.289062	-0.382617
6	6	0	0.455975	1.215029	-0.453959
7	6	0	2.517123	-0.126791	-0.561588
8	6	0	0.971207	-2.511045	-0.492452
9	6	0	-1.863876	-2.363195	-0.350083
10	6	0	-3.153080	0.169077	-0.276962
11	6	0	-1.607206	2.553462	-0.346170
12	6	0	1.227989	2.405602	-0.488495
13	6	0	3.290346	1.068127	-0.596383
14	6	0	3.161918	-1.395424	-0.598200
15	6	0	2.391146	-2.584162	-0.563617
16	6	0	0.196083	-3.704672	-0.457754
17	6	0	-1.217274	-3.630950	-0.386754
18	6	0	-3.283705	-2.288083	-0.278799
19	6	0	-3.926417	-1.025657	-0.242346
20	6	0	-3.797815	1.437785	-0.240385
21	6	0	-3.027143	2.626482	-0.274888
22	6	0	-0.832109	3.747054	-0.380815
23	6	0	0.581228	3.673301	-0.451806
24	6	0	2.647690	2.330492	-0.559900
25	6	0	4.714046	0.993045	-0.667829
26	6	0	4.585519	-1.469006	-0.669733
27	6	0	3.037968	-3.856009	-0.600458
28	6	0	0.844022	-4.975946	-0.494310
29	6	0	-1.994087	-4.827957	-0.351968
30	6	0	-4.059456	-3.485778	-0.244074
31	6	0	-5.350058	-0.950759	-0.170873
32	6	0	-5.221521	1.511417	-0.168912
33	6	0	-3.673971	3.898386	-0.238197
34	6	0	-1.480066	5.018382	-0.344132
35	6	0	1.358081	4.870332	-0.486694
36	6	0	3.423409	3.528392	-0.594631
37	6	0	5.357552	-0.274871	-0.704175

38	6	0	2.262859	-5.048163	-0.565655
39	6	0	-3.412688	-4.752110	-0.280743
40	6	0	-5.993547	0.317249	-0.134360
41	6	0	-2.898859	5.090547	-0.272910
42	6	0	2.776703	4.794494	-0.557842
43	6	0	5.483640	2.185715	-0.702171
44	6	0	5.226705	-2.735179	-0.706070
45	6	0	4.454121	-3.926830	-0.671470
46	6	0	0.069450	-6.165258	-0.459770
47	6	0	-1.347478	-6.091325	-0.388647
48	6	0	-5.475288	-3.408869	-0.172985
49	6	0	-6.119598	-2.143307	-0.136440
50	6	0	-5.862708	2.777555	-0.132523
51	6	0	-5.090122	3.969206	-0.167111
52	6	0	-0.705420	6.207611	-0.378831
53	6	0	0.711476	6.133700	-0.449964
54	6	0	4.839227	3.450884	-0.665456
55	6	0	6.786604	-0.349418	-0.775959
56	6	0	2.912699	-6.324598	-0.602517
57	6	0	-4.191908	-5.953991	-0.245857
58	6	0	-7.422606	0.391795	-0.062618
59	6	0	-3.548700	6.366972	-0.236052
60	6	0	3.555907	5.996365	-0.592681
61	6	0	6.917558	2.102035	-0.774085
62	6	0	6.661586	-2.801182	-0.778066
63	6	0	5.098535	-5.212057	-0.708087
64	6	0	0.729559	-7.442437	-0.497102
65	6	0	-2.137020	-7.292902	-0.353216
66	6	0	-6.250028	-4.620067	-0.138354
67	6	0	-7.553556	-2.059658	-0.064420
68	6	0	-7.297586	2.843557	-0.060518
69	6	0	-5.734538	5.254432	-0.130496
70	6	0	-1.365560	7.484811	-0.341455
71	6	0	1.501019	7.335278	-0.485367
72	6	0	5.613963	4.662484	-0.700135
73	6	0	7.530379	0.855173	-0.809067
74	6	0	7.400912	-1.624855	-0.811041
75	6	0	4.326388	-6.367054	-0.673395

76	6	0	2.116574	-7.495170	-0.566692
77	6	0	-3.521994	-7.201038	-0.283619
78	6	0	-5.602338	-5.849128	-0.174944
79	6	0	-8.166380	-0.812797	-0.029515
80	6	0	-8.036913	1.667230	-0.027541
81	6	0	-4.962388	6.409428	-0.165187
82	6	0	-2.752577	7.537545	-0.271891
83	6	0	2.885992	7.243414	-0.554964
84	6	0	4.966336	5.891503	-0.663641
85	6	0	7.666927	3.334747	-0.807449
86	6	0	7.278531	-4.105167	-0.813371
87	6	0	6.539345	-5.245302	-0.780277
88	6	0	-0.089942	-8.629576	-0.460177
89	6	0	-1.445584	-8.558861	-0.392119
90	6	0	-7.686474	-4.503221	-0.066097
91	6	0	-8.302930	-3.292372	-0.031133
92	6	0	-7.914534	4.147543	-0.025212
93	6	0	-7.175345	5.287676	-0.058305
94	6	0	-0.546061	8.671952	-0.378406
95	6	0	0.809581	8.601237	-0.446463
96	6	0	7.050472	4.545597	-0.772474
97	1	0	8.615494	0.797715	-0.863547
98	1	0	8.486115	-1.680612	-0.865518
99	1	0	4.819088	-7.336696	-0.701347
100	1	0	2.610788	-8.464042	-0.594718
101	1	0	-4.114408	-8.113224	-0.257092
102	1	0	-6.193327	-6.762242	-0.148490
103	1	0	-9.251497	-0.755341	0.024964
104	1	0	-9.122117	1.722987	0.026936
105	1	0	-5.455089	7.379072	-0.137235
106	1	0	-3.246791	8.506416	-0.243865
107	1	0	3.478407	8.155602	-0.581490
108	1	0	5.557325	6.804617	-0.690093
109	1	0	8.751112	3.273132	-0.861896
110	1	0	8.363244	-4.156694	-0.867810
111	1	0	7.027984	-6.216220	-0.808030
112	1	0	0.407689	-9.595905	-0.488364
113	1	0	-2.041130	-9.468165	-0.365424

114	1	0	-8.273556	-5.418025	-0.039844
115	1	0	-9.387116	-3.230756	0.023314
116	1	0	-8.999247	4.199068	0.029228
117	1	0	-7.663987	6.258595	-0.030552
118	1	0	-1.043691	9.638280	-0.350219
119	1	0	1.405126	9.510539	-0.473158
120	1	0	7.637556	5.460400	-0.798738
121	6	0	1.413421	1.059277	2.869007
122	6	0	1.215641	-1.198776	2.871524
123	6	0	2.733086	0.533309	2.892444
124	6	0	2.606724	-0.910052	2.893992
125	6	0	1.168546	2.433116	2.839852
126	6	0	3.821264	1.412997	2.882580
127	6	0	3.583218	2.783994	2.851456
128	1	0	4.419496	3.476252	2.822677
129	6	0	2.269551	3.285478	2.831581
130	1	0	2.108034	4.358626	2.784976
131	1	0	0.155443	2.822841	2.796902
132	1	0	4.837218	1.027348	2.879506
133	6	0	0.735846	-2.509098	2.845306
134	6	0	3.525486	-1.965370	2.886459
135	6	0	1.672083	-3.539879	2.838721
136	1	0	1.326496	-4.568728	2.794553
137	1	0	4.593001	-1.762167	2.882785
138	1	0	-0.329546	-2.717016	2.802398
139	6	0	3.052820	-3.274292	2.858078
140	1	0	3.756131	-4.101378	2.831157
141	7	0	0.517491	0.000083	2.871672
142	1	0	-0.474330	0.086810	2.712153

Acridine

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.035912	-1.225514	-0.495878
2	6	0	-1.217987	-0.552728	-0.473436

3	6	0	-1.261870	0.869176	-0.429414
4	6	0	-0.051845	1.618121	-0.407795
5	6	0	1.202054	0.945224	-0.430192
6	6	0	1.245901	-0.476626	-0.474254
7	6	0	0.079640	-2.643494	-0.539811
8	6	0	-2.424665	-1.299564	-0.495061
9	6	0	-2.512290	1.540232	-0.407111
10	6	0	-0.095596	3.036066	-0.363886
11	6	0	2.408721	1.692114	-0.408604
12	6	0	2.496336	-1.147663	-0.496550
13	6	0	1.334360	-3.315670	-0.562129
14	6	0	-1.131256	-3.391763	-0.561400
15	6	0	-2.379739	-2.721764	-0.539145
16	6	0	-3.678402	-0.625546	-0.472610
17	6	0	-3.722083	0.790188	-0.428795
18	6	0	-2.555125	2.962506	-0.363073
19	6	0	-1.350320	3.708231	-0.341521
20	6	0	1.115302	3.784330	-0.342263
21	6	0	2.363790	3.114322	-0.364554
22	6	0	3.662454	1.018103	-0.431017
23	6	0	3.706150	-0.397636	-0.474852
24	6	0	2.539172	-2.569936	-0.540573
25	6	0	1.377737	-4.741732	-0.606267
26	6	0	-1.086619	-4.817791	-0.605533
27	6	0	-3.593648	-3.472381	-0.560792
28	6	0	-4.891645	-1.377236	-0.494363
29	6	0	-4.979361	1.465628	-0.406325
30	6	0	-3.813001	3.636832	-0.340638
31	6	0	-1.393686	5.134288	-0.297360
32	6	0	1.070670	5.210349	-0.298102
33	6	0	3.577699	3.864939	-0.342862
34	6	0	4.875695	1.769794	-0.409283
35	6	0	4.963408	-1.073076	-0.497323
36	6	0	3.797049	-3.244280	-0.563009
37	6	0	0.167433	-5.488691	-0.627877
38	6	0	-4.845956	-2.798232	-0.538370
39	6	0	-5.021364	2.886738	-0.362319
40	6	0	-0.183382	5.881250	-0.275778

41	6	0	4.830006	3.190791	-0.365285
42	6	0	5.005415	-2.494180	-0.541346
43	6	0	2.629969	-5.410289	-0.628544
44	6	0	-2.295250	-5.562300	-0.627062
45	6	0	-3.546839	-4.890629	-0.604716
46	6	0	-6.140992	-0.703311	-0.471950
47	6	0	-6.184783	0.715938	-0.428000
48	6	0	-3.853717	5.055269	-0.296716
49	6	0	-2.645918	5.802847	-0.275110
50	6	0	2.279301	5.954859	-0.276593
51	6	0	3.530890	5.283187	-0.298938
52	6	0	6.125043	1.095868	-0.431705
53	6	0	6.168833	-0.323381	-0.475651
54	6	0	3.837767	-4.662711	-0.606927
55	6	0	0.211599	-6.920124	-0.672205
56	6	0	-6.064123	-3.552227	-0.560161
57	6	0	-6.283698	3.564175	-0.339783
58	6	0	-0.227549	7.312682	-0.231450
59	6	0	6.048174	3.944786	-0.343494
60	6	0	6.267749	-3.171618	-0.563872
61	6	0	2.665469	-6.847362	-0.673035
62	6	0	-2.242087	-6.998828	-0.671558
63	6	0	-4.774226	-5.639944	-0.626351
64	6	0	-7.359077	-1.467641	-0.494061
65	6	0	-7.447670	1.403697	-0.405142
66	6	0	-5.124964	5.727466	-0.274329
67	6	0	-2.681419	7.239920	-0.230619
68	6	0	2.226137	7.391387	-0.232097
69	6	0	4.758277	6.032502	-0.277304
70	6	0	7.343127	1.860200	-0.409594
71	6	0	7.431721	-1.011139	-0.498513
72	6	0	5.109015	-5.334907	-0.629325
73	6	0	1.473697	-7.561987	-0.693642
74	6	0	-1.008526	-7.638599	-0.692895
75	6	0	-5.989252	-4.965669	-0.603971
76	6	0	-7.296659	-2.855334	-0.537058
77	6	0	-7.470924	2.792598	-0.362156
78	6	0	-6.296108	4.979544	-0.295991

79	6	0	-1.489647	7.954546	-0.210013
80	6	0	0.992576	8.031157	-0.210760
81	6	0	5.973302	5.358226	-0.299684
82	6	0	7.280709	3.247892	-0.366595
83	6	0	7.454975	-2.400040	-0.541499
84	6	0	6.280158	-4.586986	-0.607663
85	6	0	3.956056	-7.492475	-0.694609
86	6	0	-3.490446	-7.722303	-0.692368
87	6	0	-4.687928	-7.079669	-0.670988
88	6	0	-8.610060	-0.748809	-0.470257
89	6	0	-8.651958	0.609085	-0.428207
90	6	0	-5.127589	7.169774	-0.229717
91	6	0	-3.972005	7.885033	-0.209046
92	6	0	3.474497	8.114861	-0.211287
93	6	0	4.671979	7.472227	-0.232667
94	6	0	8.594111	1.141367	-0.433397
95	6	0	8.636008	-0.216526	-0.475448
96	6	0	5.111639	-6.777215	-0.673937
97	1	0	1.506385	-8.648976	-0.727302
98	1	0	-0.974138	-8.725534	-0.726555
99	1	0	-6.914718	-5.537494	-0.620495
100	1	0	-8.221229	-3.428605	-0.553629
101	1	0	-8.429078	3.307761	-0.345020
102	1	0	-7.255066	5.493209	-0.278900
103	1	0	-1.522334	9.041533	-0.176353
104	1	0	0.958188	9.118092	-0.177100
105	1	0	6.898769	5.930051	-0.283160
106	1	0	8.205280	3.821163	-0.350026
107	1	0	8.413128	-2.915203	-0.558635
108	1	0	7.239116	-5.100650	-0.624754
109	1	0	3.984522	-8.578881	-0.728245
110	1	0	-3.451881	-8.808398	-0.726007
111	1	0	-5.615001	-7.647550	-0.687388
112	1	0	-9.531815	-1.325275	-0.486930
113	1	0	-9.607497	1.127611	-0.410969
114	1	0	-6.087908	7.679402	-0.212749
115	1	0	-4.000472	8.971440	-0.175409
116	1	0	3.435932	9.200956	-0.177647

117	1	0	5.599051	8.040108	-0.216267
118	1	0	9.515864	1.717833	-0.416725
119	1	0	9.591548	-0.735052	-0.492685
120	1	0	6.071958	-7.286844	-0.690905
121	6	0	0.071041	-2.696775	2.844388
122	6	0	1.195171	-0.541808	2.928460
123	6	0	1.272797	-1.984429	2.874568
124	6	0	-1.112683	-0.574009	2.929348
125	6	0	-1.149970	-2.018291	2.874623
126	6	0	2.414083	0.204804	2.936274
127	6	0	3.624811	-0.434353	2.895179
128	6	0	2.555241	-2.610441	2.832177
129	6	0	3.699053	-1.857461	2.844530
130	6	0	-2.352288	0.138050	2.938851
131	6	0	-3.544505	-0.534850	2.897995
132	6	0	-2.414446	-2.680069	2.831779
133	6	0	-3.578834	-1.959595	2.845598
134	1	0	0.086127	-3.783438	2.782645
135	1	0	2.335898	1.286994	2.956845
136	1	0	4.544186	0.144506	2.878913
137	1	0	2.603344	-3.694969	2.769569
138	1	0	4.670818	-2.339253	2.790520
139	1	0	-2.304537	1.221982	2.960803
140	1	0	-4.479883	0.017785	2.883302
141	1	0	-2.431979	-3.765421	2.767667
142	1	0	-4.536726	-2.468368	2.791214
143	7	0	0.031539	0.129733	2.953177

Edge-on thiophene_1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	1.423200	-0.307011
2	6	0	1.232527	0.711600	-0.307011
3	6	0	1.232527	-0.711600	-0.307011

4	6	0	0.000000	-1.423200	-0.307011
5	6	0	-1.232527	-0.711600	-0.307011
6	6	0	-1.232527	0.711600	-0.307011
7	6	0	0.000000	2.842500	-0.307011
8	6	0	2.461677	1.421250	-0.307011
9	6	0	2.461677	-1.421250	-0.307011
10	6	0	0.000000	-2.842500	-0.307011
11	6	0	-2.461677	-1.421250	-0.307011
12	6	0	-2.461677	1.421250	-0.307011
13	6	0	-1.233398	3.553392	-0.307011
14	6	0	1.233398	3.553392	-0.307011
15	6	0	2.460629	2.844850	-0.307011
16	6	0	3.694026	0.708542	-0.307011
17	6	0	3.694026	-0.708542	-0.307011
18	6	0	2.460629	-2.844850	-0.307011
19	6	0	1.233398	-3.553392	-0.307011
20	6	0	-1.233398	-3.553392	-0.307011
21	6	0	-2.460629	-2.844850	-0.307011
22	6	0	-3.694026	-0.708542	-0.307011
23	6	0	-3.694026	0.708542	-0.307011
24	6	0	-2.460629	2.844850	-0.307011
25	6	0	-1.232765	4.980792	-0.307011
26	6	0	1.232765	4.980792	-0.307011
27	6	0	3.697110	3.558002	-0.307011
28	6	0	4.929875	1.422790	-0.307011
29	6	0	4.929875	-1.422790	-0.307011
30	6	0	3.697110	-3.558002	-0.307011
31	6	0	1.232765	-4.980792	-0.307011
32	6	0	-1.232765	-4.980792	-0.307011
33	6	0	-3.697110	-3.558002	-0.307011
34	6	0	-4.929875	-1.422790	-0.307011
35	6	0	-4.929875	1.422790	-0.307011
36	6	0	-3.697110	3.558002	-0.307011
37	6	0	0.000000	5.690400	-0.307011
38	6	0	4.928031	2.845200	-0.307011
39	6	0	4.928031	-2.845200	-0.307011
40	6	0	0.000000	-5.690400	-0.307011
41	6	0	-4.928031	-2.845200	-0.307011

42	6	0	-4.928031	2.845200	-0.307011
43	6	0	-2.463782	5.688001	-0.307011
44	6	0	2.463782	5.688001	-0.307011
45	6	0	3.694062	4.977698	-0.307011
46	6	0	6.157844	0.710302	-0.307011
47	6	0	6.157844	-0.710302	-0.307011
48	6	0	3.694062	-4.977698	-0.307011
49	6	0	2.463782	-5.688001	-0.307011
50	6	0	-2.463782	-5.688001	-0.307011
51	6	0	-3.694062	-4.977698	-0.307011
52	6	0	-6.157844	-0.710302	-0.307011
53	6	0	-6.157844	0.710302	-0.307011
54	6	0	-3.694062	4.977698	-0.307011
55	6	0	0.000000	7.123200	-0.307011
56	6	0	6.168872	3.561600	-0.307011
57	6	0	6.168872	-3.561600	-0.307011
58	6	0	0.000000	-7.123200	-0.307011
59	6	0	-6.168872	-3.561600	-0.307011
60	6	0	-6.168872	3.561600	-0.307011
61	6	0	-2.454947	7.126173	-0.307011
62	6	0	2.454947	7.126173	-0.307011
63	6	0	4.943974	5.689133	-0.307011
64	6	0	7.398921	1.437041	-0.307011
65	6	0	7.398921	-1.437041	-0.307011
66	6	0	4.943974	-5.689133	-0.307011
67	6	0	2.454947	-7.126173	-0.307011
68	6	0	-2.454947	-7.126173	-0.307011
69	6	0	-4.943974	-5.689133	-0.307011
70	6	0	-7.398921	-1.437041	-0.307011
71	6	0	-7.398921	1.437041	-0.307011
72	6	0	-4.943974	5.689133	-0.307011
73	6	0	-1.241703	7.804018	-0.307011
74	6	0	1.241703	7.804018	-0.307011
75	6	0	6.137627	4.977355	-0.307011
76	6	0	7.379329	2.826663	-0.307011
77	6	0	7.379329	-2.826663	-0.307011
78	6	0	6.137627	-4.977355	-0.307011
79	6	0	1.241703	-7.804018	-0.307011

80	6	0	-1.241703	-7.804018	-0.307011
81	6	0	-6.137627	-4.977355	-0.307011
82	6	0	-7.379329	-2.826663	-0.307011
83	6	0	-7.379329	2.826663	-0.307011
84	6	0	-6.137627	4.977355	-0.307011
85	6	0	-3.725024	7.811121	-0.307011
86	6	0	3.725024	7.811121	-0.307011
87	6	0	4.902117	7.131526	-0.307011
88	6	0	8.627141	0.679595	-0.307011
89	6	0	8.627141	-0.679595	-0.307011
90	6	0	4.902117	-7.131526	-0.307011
91	6	0	3.725024	-7.811121	-0.307011
92	6	0	-3.725024	-7.811121	-0.307011
93	6	0	-4.902117	-7.131526	-0.307011
94	6	0	-8.627141	-0.679595	-0.307011
95	6	0	-8.627141	0.679595	-0.307011
96	6	0	-4.902117	7.131526	-0.307011
97	1	0	-1.240852	8.892018	-0.307011
98	1	0	1.240852	8.892018	-0.307011
99	1	0	7.080287	5.520618	-0.307011
100	1	0	8.321139	3.371400	-0.307011
101	1	0	8.321139	-3.371400	-0.307011
102	1	0	7.080287	-5.520618	-0.307011
103	1	0	1.240852	-8.892018	-0.307011
104	1	0	-1.240852	-8.892018	-0.307011
105	1	0	-7.080287	-5.520618	-0.307011
106	1	0	-8.321139	-3.371400	-0.307011
107	1	0	-8.321139	3.371400	-0.307011
108	1	0	-7.080287	5.520618	-0.307011
109	1	0	-3.719972	8.898409	-0.307011
110	1	0	3.719972	8.898409	-0.307011
111	1	0	5.846262	7.670795	-0.307011
112	1	0	9.566234	1.227614	-0.307011
113	1	0	9.566234	-1.227614	-0.307011
114	1	0	5.846262	-7.670795	-0.307011
115	1	0	3.719972	-8.898409	-0.307011
116	1	0	-3.719972	-8.898409	-0.307011
117	1	0	-5.846262	-7.670795	-0.307011

118	1	0	-9.566234	-1.227614	-0.307011
119	1	0	-9.566234	1.227614	-0.307011
120	1	0	-5.846262	7.670795	-0.307011
121	16	0	0.000000	0.000000	2.987071
122	6	0	0.000000	-1.242827	4.197333
123	6	0	0.000000	1.242827	4.197333
124	6	0	0.000000	-0.714980	5.459778
125	6	0	0.000000	0.714980	5.459778
126	1	0	0.000000	-2.284403	3.904205
127	1	0	0.000000	2.284403	3.904205
128	1	0	0.000000	-1.320388	6.359920
129	1	0	0.000000	1.320388	6.359920

Edge-on thiophene_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.293886	1.507878	0.000000
2	6	0	0.293886	0.796278	1.232527
3	6	0	0.293886	-0.626922	1.232527
4	6	0	0.293886	-1.338522	0.000000
5	6	0	0.293886	-0.626922	-1.232527
6	6	0	0.293886	0.796278	-1.232527
7	6	0	0.293886	2.927178	0.000000
8	6	0	0.293886	1.505928	2.461677
9	6	0	0.293886	-1.336572	2.461677
10	6	0	0.293886	-2.757822	0.000000
11	6	0	0.293886	-1.336572	-2.461677
12	6	0	0.293886	1.505928	-2.461677
13	6	0	0.293886	3.638070	-1.233398
14	6	0	0.293886	3.638070	1.233398
15	6	0	0.293886	2.929528	2.460629
16	6	0	0.293886	0.793220	3.694026
17	6	0	0.293886	-0.623864	3.694026
18	6	0	0.293886	-2.760172	2.460629

19	6	0	0.293886	-3.468714	1.233398
20	6	0	0.293886	-3.468714	-1.233398
21	6	0	0.293886	-2.760172	-2.460629
22	6	0	0.293886	-0.623864	-3.694026
23	6	0	0.293886	0.793220	-3.694026
24	6	0	0.293886	2.929528	-2.460629
25	6	0	0.293886	5.065470	-1.232765
26	6	0	0.293886	5.065470	1.232765
27	6	0	0.293886	3.642680	3.697110
28	6	0	0.293886	1.507468	4.929875
29	6	0	0.293886	-1.338112	4.929875
30	6	0	0.293886	-3.473323	3.697110
31	6	0	0.293886	-4.896114	1.232765
32	6	0	0.293886	-4.896114	-1.232765
33	6	0	0.293886	-3.473323	-3.697110
34	6	0	0.293886	-1.338112	-4.929875
35	6	0	0.293886	1.507468	-4.929875
36	6	0	0.293886	3.642680	-3.697110
37	6	0	0.293886	5.775078	0.000000
38	6	0	0.293886	2.929878	4.928031
39	6	0	0.293886	-2.760522	4.928031
40	6	0	0.293886	-5.605722	0.000000
41	6	0	0.293886	-2.760522	-4.928031
42	6	0	0.293886	2.929878	-4.928031
43	6	0	0.293886	5.772679	-2.463782
44	6	0	0.293886	5.772679	2.463782
45	6	0	0.293886	5.062376	3.694062
46	6	0	0.293886	0.794980	6.157844
47	6	0	0.293886	-0.625624	6.157844
48	6	0	0.293886	-4.893020	3.694062
49	6	0	0.293886	-5.603322	2.463782
50	6	0	0.293886	-5.603322	-2.463782
51	6	0	0.293886	-4.893020	-3.694062
52	6	0	0.293886	-0.625624	-6.157844
53	6	0	0.293886	0.794980	-6.157844
54	6	0	0.293886	5.062376	-3.694062
55	6	0	0.293886	7.207878	0.000000
56	6	0	0.293886	3.646278	6.168872

57	6	0	0.293886	-3.476922	6.168872
58	6	0	0.293886	-7.038522	0.000000
59	6	0	0.293886	-3.476922	-6.168872
60	6	0	0.293886	3.646278	-6.168872
61	6	0	0.293886	7.210851	-2.454947
62	6	0	0.293886	7.210851	2.454947
63	6	0	0.293886	5.773811	4.943974
64	6	0	0.293886	1.521719	7.398921
65	6	0	0.293886	-1.352363	7.398921
66	6	0	0.293886	-5.604455	4.943974
67	6	0	0.293886	-7.041495	2.454947
68	6	0	0.293886	-7.041495	-2.454947
69	6	0	0.293886	-5.604455	-4.943974
70	6	0	0.293886	-1.352363	-7.398921
71	6	0	0.293886	1.521719	-7.398921
72	6	0	0.293886	5.773811	-4.943974
73	6	0	0.293886	7.888696	-1.241703
74	6	0	0.293886	7.888696	1.241703
75	6	0	0.293886	5.062033	6.137627
76	6	0	0.293886	2.911341	7.379329
77	6	0	0.293886	-2.741985	7.379329
78	6	0	0.293886	-4.892677	6.137627
79	6	0	0.293886	-7.719340	1.241703
80	6	0	0.293886	-7.719340	-1.241703
81	6	0	0.293886	-4.892677	-6.137627
82	6	0	0.293886	-2.741985	-7.379329
83	6	0	0.293886	2.911341	-7.379329
84	6	0	0.293886	5.062033	-6.137627
85	6	0	0.293886	7.895799	-3.725024
86	6	0	0.293886	7.895799	3.725024
87	6	0	0.293886	7.216204	4.902117
88	6	0	0.293886	0.764273	8.627141
89	6	0	0.293886	-0.594917	8.627141
90	6	0	0.293886	-7.046848	4.902117
91	6	0	0.293886	-7.726443	3.725024
92	6	0	0.293886	-7.726443	-3.725024
93	6	0	0.293886	-7.046848	-4.902117
94	6	0	0.293886	-0.594917	-8.627141

95	6	0	0.293886	0.764273	-8.627141
96	6	0	0.293886	7.216204	-4.902117
97	1	0	0.293886	8.976696	-1.240852
98	1	0	0.293886	8.976696	1.240852
99	1	0	0.293886	5.605296	7.080287
100	1	0	0.293886	3.456078	8.321139
101	1	0	0.293886	-3.286722	8.321139
102	1	0	0.293886	-5.435940	7.080287
103	1	0	0.293886	-8.807340	1.240852
104	1	0	0.293886	-8.807340	-1.240852
105	1	0	0.293886	-5.435940	-7.080287
106	1	0	0.293886	-3.286722	-8.321139
107	1	0	0.293886	3.456078	-8.321139
108	1	0	0.293886	5.605296	-7.080287
109	1	0	0.293886	8.983087	-3.719972
110	1	0	0.293886	8.983087	3.719972
111	1	0	0.293886	7.755473	5.846262
112	1	0	0.293886	1.312292	9.566234
113	1	0	0.293886	-1.142936	9.566234
114	1	0	0.293886	-7.586117	5.846262
115	1	0	0.293886	-8.813731	3.719972
116	1	0	0.293886	-8.813731	-3.719972
117	1	0	0.293886	-7.586117	-5.846262
118	1	0	0.293886	-1.142936	-9.566234
119	1	0	0.293886	1.312292	-9.566234
120	1	0	0.293886	7.755473	-5.846262
121	16	0	-3.137305	-1.982091	0.000000
122	6	0	-4.872931	-2.047194	0.000000
123	6	0	-3.159128	-0.245589	0.000000
124	6	0	-5.423779	-0.795178	0.000000
125	6	0	-4.437101	0.240210	0.000000
126	1	0	-5.381451	-3.002295	0.000000
127	1	0	-2.232245	0.308720	0.000000
128	1	0	-6.493230	-0.613033	0.000000
129	1	0	-4.669882	1.299732	0.000000

Edge-on thiophene_3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.232530	0.711602	-0.307012
2	6	0	0.000000	1.423203	-0.307013
3	6	0	1.232530	0.711602	-0.307012
4	6	0	1.232530	-0.711602	-0.307012
5	6	0	0.000000	-1.423203	-0.307013
6	6	0	-1.232530	-0.711602	-0.307012
7	6	0	-2.461677	1.421251	-0.307013
8	6	0	0.000000	2.842500	-0.307013
9	6	0	2.461677	1.421251	-0.307013
10	6	0	2.461677	-1.421251	-0.307013
11	6	0	0.000000	-2.842500	-0.307013
12	6	0	-2.461677	-1.421251	-0.307013
13	6	0	-3.694026	0.708542	-0.307013
14	6	0	-2.460629	2.844850	-0.307013
15	6	0	-1.233398	3.553392	-0.307013
16	6	0	1.233398	3.553392	-0.307013
17	6	0	2.460629	2.844850	-0.307013
18	6	0	3.694026	0.708542	-0.307013
19	6	0	3.694026	-0.708542	-0.307013
20	6	0	2.460629	-2.844850	-0.307013
21	6	0	1.233398	-3.553392	-0.307013
22	6	0	-1.233398	-3.553392	-0.307013
23	6	0	-2.460629	-2.844850	-0.307013
24	6	0	-3.694026	-0.708542	-0.307013
25	6	0	-4.929875	1.422790	-0.307013
26	6	0	-3.697110	3.558002	-0.307013
27	6	0	-1.232765	4.980792	-0.307013
28	6	0	1.232765	4.980792	-0.307013
29	6	0	3.697110	3.558002	-0.307013
30	6	0	4.929875	1.422790	-0.307013
31	6	0	4.929875	-1.422790	-0.307013
32	6	0	3.697110	-3.558002	-0.307013
33	6	0	1.232765	-4.980792	-0.307013

34	6	0	-1.232765	-4.980792	-0.307013
35	6	0	-3.697110	-3.558002	-0.307013
36	6	0	-4.929875	-1.422790	-0.307013
37	6	0	-4.928031	2.845200	-0.307013
38	6	0	0.000000	5.690400	-0.307013
39	6	0	4.928031	2.845200	-0.307013
40	6	0	4.928031	-2.845200	-0.307013
41	6	0	0.000000	-5.690400	-0.307013
42	6	0	-4.928031	-2.845200	-0.307013
43	6	0	-6.157844	0.710302	-0.307013
44	6	0	-3.694062	4.977698	-0.307013
45	6	0	-2.463782	5.688001	-0.307013
46	6	0	2.463782	5.688001	-0.307013
47	6	0	3.694062	4.977698	-0.307013
48	6	0	6.157844	0.710302	-0.307013
49	6	0	6.157844	-0.710302	-0.307013
50	6	0	3.694062	-4.977698	-0.307013
51	6	0	2.463782	-5.688001	-0.307013
52	6	0	-2.463782	-5.688001	-0.307013
53	6	0	-3.694062	-4.977698	-0.307013
54	6	0	-6.157844	-0.710302	-0.307013
55	6	0	-6.168872	3.561600	-0.307013
56	6	0	0.000000	7.123200	-0.307013
57	6	0	6.168872	3.561600	-0.307013
58	6	0	6.168872	-3.561600	-0.307013
59	6	0	0.000000	-7.123200	-0.307013
60	6	0	-6.168872	-3.561600	-0.307013
61	6	0	-7.398921	1.437041	-0.307013
62	6	0	-4.943974	5.689133	-0.307013
63	6	0	-2.454947	7.126173	-0.307013
64	6	0	2.454947	7.126173	-0.307013
65	6	0	4.943974	5.689133	-0.307013
66	6	0	7.398921	1.437041	-0.307013
67	6	0	7.398921	-1.437041	-0.307013
68	6	0	4.943974	-5.689133	-0.307013
69	6	0	2.454947	-7.126173	-0.307013
70	6	0	-2.454947	-7.126173	-0.307013
71	6	0	-4.943974	-5.689133	-0.307013

72	6	0	-7.398921	-1.437041	-0.307013
73	6	0	-7.379329	2.826663	-0.307013
74	6	0	-6.137627	4.977355	-0.307013
75	6	0	-1.241703	7.804018	-0.307013
76	6	0	1.241703	7.804018	-0.307013
77	6	0	6.137627	4.977355	-0.307013
78	6	0	7.379329	2.826663	-0.307013
79	6	0	7.379329	-2.826663	-0.307013
80	6	0	6.137627	-4.977355	-0.307013
81	6	0	1.241703	-7.804018	-0.307013
82	6	0	-1.241703	-7.804018	-0.307013
83	6	0	-6.137627	-4.977355	-0.307013
84	6	0	-7.379329	-2.826663	-0.307013
85	6	0	-8.627141	0.679595	-0.307013
86	6	0	-4.902117	7.131526	-0.307013
87	6	0	-3.725024	7.811121	-0.307013
88	6	0	3.725024	7.811121	-0.307013
89	6	0	4.902117	7.131526	-0.307013
90	6	0	8.627141	0.679595	-0.307013
91	6	0	8.627141	-0.679595	-0.307013
92	6	0	4.902117	-7.131526	-0.307013
93	6	0	3.725024	-7.811121	-0.307013
94	6	0	-3.725024	-7.811121	-0.307013
95	6	0	-4.902117	-7.131526	-0.307013
96	6	0	-8.627141	-0.679595	-0.307013
97	1	0	-8.321139	3.371400	-0.307013
98	1	0	-7.080287	5.520618	-0.307013
99	1	0	-1.240852	8.892018	-0.307013
100	1	0	1.240852	8.892018	-0.307013
101	1	0	7.080287	5.520618	-0.307013
102	1	0	8.321139	3.371400	-0.307013
103	1	0	8.321139	-3.371400	-0.307013
104	1	0	7.080287	-5.520618	-0.307013
105	1	0	1.240852	-8.892018	-0.307013
106	1	0	-1.240852	-8.892018	-0.307013
107	1	0	-7.080287	-5.520618	-0.307013
108	1	0	-8.321139	-3.371400	-0.307013
109	1	0	-9.566234	1.227614	-0.307013

110	1	0	-5.846262	7.670795	-0.307013
111	1	0	-3.719972	8.898409	-0.307013
112	1	0	3.719972	8.898409	-0.307013
113	1	0	5.846262	7.670795	-0.307013
114	1	0	9.566234	1.227614	-0.307013
115	1	0	9.566234	-1.227614	-0.307013
116	1	0	5.846262	-7.670795	-0.307013
117	1	0	3.719972	-8.898409	-0.307013
118	1	0	-3.719972	-8.898409	-0.307013
119	1	0	-5.846262	-7.670795	-0.307013
120	1	0	-9.566234	-1.227614	-0.307013
121	16	0	0.000000	0.000000	2.987079
122	6	0	1.242827	0.000000	4.197372
123	6	0	-1.242827	0.000000	4.197372
124	6	0	0.714997	0.000000	5.459797
125	6	0	-0.714997	0.000000	5.459797
126	1	0	2.284403	0.000000	3.904228
127	1	0	-2.284403	0.000000	3.904228
128	1	0	1.320342	0.000000	6.359981
129	1	0	-1.320342	0.000000	6.359981

Edge-on furan_1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	1.422998	-0.227754
2	6	0	1.232257	0.711246	-0.227738
3	6	0	1.232257	-0.711246	-0.227738
4	6	0	0.000000	-1.422998	-0.227754
5	6	0	-1.232257	-0.711246	-0.227738
6	6	0	-1.232257	0.711246	-0.227738
7	6	0	0.000000	2.842500	-0.227529
8	6	0	2.461605	1.421375	-0.227512
9	6	0	2.461605	-1.421375	-0.227512
10	6	0	0.000000	-2.842500	-0.227529

11	6	0	-2.461605	-1.421375	-0.227512
12	6	0	-2.461605	1.421375	-0.227512
13	6	0	-1.233398	3.553392	-0.227647
14	6	0	1.233398	3.553392	-0.227647
15	6	0	2.460629	2.844850	-0.227643
16	6	0	3.694026	0.708542	-0.227642
17	6	0	3.694026	-0.708542	-0.227642
18	6	0	2.460629	-2.844850	-0.227643
19	6	0	1.233398	-3.553392	-0.227647
20	6	0	-1.233398	-3.553392	-0.227647
21	6	0	-2.460629	-2.844850	-0.227643
22	6	0	-3.694026	-0.708542	-0.227642
23	6	0	-3.694026	0.708542	-0.227642
24	6	0	-2.460629	2.844850	-0.227643
25	6	0	-1.232765	4.980792	-0.227637
26	6	0	1.232765	4.980792	-0.227637
27	6	0	3.697110	3.558002	-0.227637
28	6	0	4.929875	1.422790	-0.227637
29	6	0	4.929875	-1.422790	-0.227637
30	6	0	3.697110	-3.558002	-0.227637
31	6	0	1.232765	-4.980792	-0.227637
32	6	0	-1.232765	-4.980792	-0.227637
33	6	0	-3.697110	-3.558002	-0.227637
34	6	0	-4.929875	-1.422790	-0.227637
35	6	0	-4.929875	1.422790	-0.227637
36	6	0	-3.697110	3.558002	-0.227637
37	6	0	0.000000	5.690400	-0.227637
38	6	0	4.928031	2.845200	-0.227637
39	6	0	4.928031	-2.845200	-0.227637
40	6	0	0.000000	-5.690400	-0.227637
41	6	0	-4.928031	-2.845200	-0.227637
42	6	0	-4.928031	2.845200	-0.227637
43	6	0	-2.463782	5.688001	-0.227637
44	6	0	2.463782	5.688001	-0.227637
45	6	0	3.694062	4.977698	-0.227637
46	6	0	6.157844	0.710302	-0.227637
47	6	0	6.157844	-0.710302	-0.227637
48	6	0	3.694062	-4.977698	-0.227637

49	6	0	2.463782	-5.688001	-0.227637
50	6	0	-2.463782	-5.688001	-0.227637
51	6	0	-3.694062	-4.977698	-0.227637
52	6	0	-6.157844	-0.710302	-0.227637
53	6	0	-6.157844	0.710302	-0.227637
54	6	0	-3.694062	4.977698	-0.227637
55	6	0	0.000000	7.123200	-0.227637
56	6	0	6.168872	3.561600	-0.227637
57	6	0	6.168872	-3.561600	-0.227637
58	6	0	0.000000	-7.123200	-0.227637
59	6	0	-6.168872	-3.561600	-0.227637
60	6	0	-6.168872	3.561600	-0.227637
61	6	0	-2.454947	7.126173	-0.227637
62	6	0	2.454947	7.126173	-0.227637
63	6	0	4.943974	5.689133	-0.227637
64	6	0	7.398921	1.437041	-0.227637
65	6	0	7.398921	-1.437041	-0.227637
66	6	0	4.943974	-5.689133	-0.227637
67	6	0	2.454947	-7.126173	-0.227637
68	6	0	-2.454947	-7.126173	-0.227637
69	6	0	-4.943974	-5.689133	-0.227637
70	6	0	-7.398921	-1.437041	-0.227637
71	6	0	-7.398921	1.437041	-0.227637
72	6	0	-4.943974	5.689133	-0.227637
73	6	0	-1.241703	7.804018	-0.227637
74	6	0	1.241703	7.804018	-0.227637
75	6	0	6.137627	4.977355	-0.227637
76	6	0	7.379329	2.826663	-0.227637
77	6	0	7.379329	-2.826663	-0.227637
78	6	0	6.137627	-4.977355	-0.227637
79	6	0	1.241703	-7.804018	-0.227637
80	6	0	-1.241703	-7.804018	-0.227637
81	6	0	-6.137627	-4.977355	-0.227637
82	6	0	-7.379329	-2.826663	-0.227637
83	6	0	-7.379329	2.826663	-0.227637
84	6	0	-6.137627	4.977355	-0.227637
85	6	0	-3.725024	7.811121	-0.227637
86	6	0	3.725024	7.811121	-0.227637

87	6	0	4.902117	7.131526	-0.227637
88	6	0	8.627141	0.679595	-0.227637
89	6	0	8.627141	-0.679595	-0.227637
90	6	0	4.902117	-7.131526	-0.227637
91	6	0	3.725024	-7.811121	-0.227637
92	6	0	-3.725024	-7.811121	-0.227637
93	6	0	-4.902117	-7.131526	-0.227637
94	6	0	-8.627141	-0.679595	-0.227637
95	6	0	-8.627141	0.679595	-0.227637
96	6	0	-4.902117	7.131526	-0.227637
97	1	0	-1.240852	8.892018	-0.227637
98	1	0	1.240852	8.892018	-0.227637
99	1	0	7.080287	5.520618	-0.227637
100	1	0	8.321139	3.371400	-0.227637
101	1	0	8.321139	-3.371400	-0.227637
102	1	0	7.080287	-5.520618	-0.227637
103	1	0	1.240852	-8.892018	-0.227637
104	1	0	-1.240852	-8.892018	-0.227637
105	1	0	-7.080287	-5.520618	-0.227637
106	1	0	-8.321139	-3.371400	-0.227637
107	1	0	-8.321139	3.371400	-0.227637
108	1	0	-7.080287	5.520618	-0.227637
109	1	0	-3.719972	8.898409	-0.227637
110	1	0	3.719972	8.898409	-0.227637
111	1	0	5.846262	7.670795	-0.227637
112	1	0	9.566234	1.227614	-0.227637
113	1	0	9.566234	-1.227614	-0.227637
114	1	0	5.846262	-7.670795	-0.227637
115	1	0	3.719972	-8.898409	-0.227637
116	1	0	-3.719972	-8.898409	-0.227637
117	1	0	-5.846262	-7.670795	-0.227637
118	1	0	-9.566234	-1.227614	-0.227637
119	1	0	-9.566234	1.227614	-0.227637
120	1	0	-5.846262	7.670795	-0.227637
121	6	0	0.000000	-1.096322	3.445558
122	6	0	0.000000	1.096322	3.445558
123	6	0	0.000000	-0.718525	4.753696
124	6	0	0.000000	0.718525	4.753696

125	1	0	0.000000	-2.048480	2.936557
126	1	0	0.000000	2.048480	2.936557
127	1	0	0.000000	-1.373916	5.613576
128	1	0	0.000000	1.373916	5.613576
129	8	0	0.000000	0.000000	2.636346

Edge-on furan_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.236649	1.503743	0.000000
2	6	0	0.236673	0.792106	1.232465
3	6	0	0.236653	-0.631078	1.232554
4	6	0	0.236680	-1.342678	0.000000
5	6	0	0.236653	-0.631078	-1.232554
6	6	0	0.236673	0.792106	-1.232465
7	6	0	0.236669	2.923022	0.000000
8	6	0	0.236653	1.501778	2.461674
9	6	0	0.236651	-1.340728	2.461677
10	6	0	0.236659	-2.761978	0.000000
11	6	0	0.236651	-1.340728	-2.461677
12	6	0	0.236653	1.501778	-2.461674
13	6	0	0.236660	3.633914	-1.233398
14	6	0	0.236660	3.633914	1.233398
15	6	0	0.236655	2.925372	2.460629
16	6	0	0.236658	0.789064	3.694026
17	6	0	0.236659	-0.628020	3.694026
18	6	0	0.236659	-2.764328	2.460629
19	6	0	0.236659	-3.472870	1.233398
20	6	0	0.236659	-3.472870	-1.233398
21	6	0	0.236659	-2.764328	-2.460629
22	6	0	0.236659	-0.628020	-3.694026
23	6	0	0.236658	0.789064	-3.694026
24	6	0	0.236655	2.925372	-2.460629
25	6	0	0.236659	5.061314	-1.232765

26	6	0	0.236659	5.061314	1.232765
27	6	0	0.236659	3.638524	3.697110
28	6	0	0.236659	1.503312	4.929875
29	6	0	0.236659	-1.342268	4.929875
30	6	0	0.236659	-3.477479	3.697110
31	6	0	0.236659	-4.900270	1.232765
32	6	0	0.236659	-4.900270	-1.232765
33	6	0	0.236659	-3.477479	-3.697110
34	6	0	0.236659	-1.342268	-4.929875
35	6	0	0.236659	1.503312	-4.929875
36	6	0	0.236659	3.638524	-3.697110
37	6	0	0.236659	5.770922	0.000000
38	6	0	0.236659	2.925722	4.928031
39	6	0	0.236659	-2.764678	4.928031
40	6	0	0.236659	-5.609878	0.000000
41	6	0	0.236659	-2.764678	-4.928031
42	6	0	0.236659	2.925722	-4.928031
43	6	0	0.236659	5.768523	-2.463782
44	6	0	0.236659	5.768523	2.463782
45	6	0	0.236659	5.058220	3.694062
46	6	0	0.236659	0.790824	6.157844
47	6	0	0.236659	-0.629780	6.157844
48	6	0	0.236659	-4.897176	3.694062
49	6	0	0.236659	-5.607478	2.463782
50	6	0	0.236659	-5.607478	-2.463782
51	6	0	0.236659	-4.897176	-3.694062
52	6	0	0.236659	-0.629780	-6.157844
53	6	0	0.236659	0.790824	-6.157844
54	6	0	0.236659	5.058220	-3.694062
55	6	0	0.236659	7.203722	0.000000
56	6	0	0.236659	3.642122	6.168872
57	6	0	0.236659	-3.481078	6.168872
58	6	0	0.236659	-7.042678	0.000000
59	6	0	0.236659	-3.481078	-6.168872
60	6	0	0.236659	3.642122	-6.168872
61	6	0	0.236659	7.206695	-2.454947
62	6	0	0.236659	7.206695	2.454947
63	6	0	0.236659	5.769655	4.943974

64	6	0	0.236659	1.517563	7.398921
65	6	0	0.236659	-1.356519	7.398921
66	6	0	0.236659	-5.608611	4.943974
67	6	0	0.236659	-7.045651	2.454947
68	6	0	0.236659	-7.045651	-2.454947
69	6	0	0.236659	-5.608611	-4.943974
70	6	0	0.236659	-1.356519	-7.398921
71	6	0	0.236659	1.517563	-7.398921
72	6	0	0.236659	5.769655	-4.943974
73	6	0	0.236659	7.884540	-1.241703
74	6	0	0.236659	7.884540	1.241703
75	6	0	0.236659	5.057877	6.137627
76	6	0	0.236659	2.907185	7.379329
77	6	0	0.236659	-2.746141	7.379329
78	6	0	0.236659	-4.896833	6.137627
79	6	0	0.236659	-7.723496	1.241703
80	6	0	0.236659	-7.723496	-1.241703
81	6	0	0.236659	-4.896833	-6.137627
82	6	0	0.236659	-2.746141	-7.379329
83	6	0	0.236659	2.907185	-7.379329
84	6	0	0.236659	5.057877	-6.137627
85	6	0	0.236659	7.891643	-3.725024
86	6	0	0.236659	7.891643	3.725024
87	6	0	0.236659	7.212048	4.902117
88	6	0	0.236659	0.760117	8.627141
89	6	0	0.236659	-0.599073	8.627141
90	6	0	0.236659	-7.051004	4.902117
91	6	0	0.236659	-7.730599	3.725024
92	6	0	0.236659	-7.730599	-3.725024
93	6	0	0.236659	-7.051004	-4.902117
94	6	0	0.236659	-0.599073	-8.627141
95	6	0	0.236659	0.760117	-8.627141
96	6	0	0.236659	7.212048	-4.902117
97	1	0	0.236659	8.972540	-1.240852
98	1	0	0.236659	8.972540	1.240852
99	1	0	0.236659	5.601140	7.080287
100	1	0	0.236659	3.451922	8.321139
101	1	0	0.236659	-3.290878	8.321139

102	1	0	0.236659	-5.440096	7.080287
103	1	0	0.236659	-8.811496	1.240852
104	1	0	0.236659	-8.811496	-1.240852
105	1	0	0.236659	-5.440096	-7.080287
106	1	0	0.236659	-3.290878	-8.321139
107	1	0	0.236659	3.451922	-8.321139
108	1	0	0.236659	5.601140	-7.080287
109	1	0	0.236659	8.978931	-3.719972
110	1	0	0.236659	8.978931	3.719972
111	1	0	0.236659	7.751317	5.846262
112	1	0	0.236659	1.308136	9.566234
113	1	0	0.236659	-1.147092	9.566234
114	1	0	0.236659	-7.590273	5.846262
115	1	0	0.236659	-8.817887	3.719972
116	1	0	0.236659	-8.817887	-3.719972
117	1	0	0.236659	-7.590273	-5.846262
118	1	0	0.236659	-1.147092	-9.566234
119	1	0	0.236659	1.308136	-9.566234
120	1	0	0.236659	7.751317	-5.846262
121	6	0	-4.056284	-2.486103	0.000000
122	6	0	-3.192549	-0.471357	0.000000
123	6	0	-5.110040	-1.624273	0.000000
124	6	0	-4.543276	-0.304081	0.000000
125	1	0	-3.968763	-3.562119	0.000000
126	1	0	-2.354434	0.207501	0.000000
127	1	0	-6.158416	-1.888712	0.000000
128	1	0	-5.073693	0.638039	0.000000
129	8	0	-2.878402	-1.799150	0.000000

Edge-on furan_3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.232304	0.711418	-0.227968
2	6	0	0.000000	1.422962	-0.227862

3	6	0	1.232304	0.711418	-0.227968
4	6	0	1.232304	-0.711418	-0.227968
5	6	0	0.000000	-1.422962	-0.227862
6	6	0	-1.232304	-0.711418	-0.227968
7	6	0	-2.461714	1.421187	-0.227733
8	6	0	0.000000	2.842500	-0.227743
9	6	0	2.461714	1.421187	-0.227733
10	6	0	2.461714	-1.421187	-0.227733
11	6	0	0.000000	-2.842500	-0.227743
12	6	0	-2.461714	-1.421187	-0.227733
13	6	0	-3.694026	0.708542	-0.227839
14	6	0	-2.460629	2.844850	-0.227837
15	6	0	-1.233398	3.553392	-0.227840
16	6	0	1.233398	3.553392	-0.227840
17	6	0	2.460629	2.844850	-0.227837
18	6	0	3.694026	0.708542	-0.227839
19	6	0	3.694026	-0.708542	-0.227839
20	6	0	2.460629	-2.844850	-0.227837
21	6	0	1.233398	-3.553392	-0.227840
22	6	0	-1.233398	-3.553392	-0.227840
23	6	0	-2.460629	-2.844850	-0.227837
24	6	0	-3.694026	-0.708542	-0.227839
25	6	0	-4.929875	1.422790	-0.227834
26	6	0	-3.697110	3.558002	-0.227834
27	6	0	-1.232765	4.980792	-0.227834
28	6	0	1.232765	4.980792	-0.227834
29	6	0	3.697110	3.558002	-0.227834
30	6	0	4.929875	1.422790	-0.227834
31	6	0	4.929875	-1.422790	-0.227834
32	6	0	3.697110	-3.558002	-0.227834
33	6	0	1.232765	-4.980792	-0.227834
34	6	0	-1.232765	-4.980792	-0.227834
35	6	0	-3.697110	-3.558002	-0.227834
36	6	0	-4.929875	-1.422790	-0.227834
37	6	0	-4.928031	2.845200	-0.227834
38	6	0	0.000000	5.690400	-0.227834
39	6	0	4.928031	2.845200	-0.227834
40	6	0	4.928031	-2.845200	-0.227834

41	6	0	0.000000	-5.690400	-0.227834
42	6	0	-4.928031	-2.845200	-0.227834
43	6	0	-6.157844	0.710302	-0.227834
44	6	0	-3.694062	4.977698	-0.227834
45	6	0	-2.463782	5.688001	-0.227834
46	6	0	2.463782	5.688001	-0.227834
47	6	0	3.694062	4.977698	-0.227834
48	6	0	6.157844	0.710302	-0.227834
49	6	0	6.157844	-0.710302	-0.227834
50	6	0	3.694062	-4.977698	-0.227834
51	6	0	2.463782	-5.688001	-0.227834
52	6	0	-2.463782	-5.688001	-0.227834
53	6	0	-3.694062	-4.977698	-0.227834
54	6	0	-6.157844	-0.710302	-0.227834
55	6	0	-6.168872	3.561600	-0.227834
56	6	0	0.000000	7.123200	-0.227834
57	6	0	6.168872	3.561600	-0.227834
58	6	0	6.168872	-3.561600	-0.227834
59	6	0	0.000000	-7.123200	-0.227834
60	6	0	-6.168872	-3.561600	-0.227834
61	6	0	-7.398921	1.437041	-0.227834
62	6	0	-4.943974	5.689133	-0.227834
63	6	0	-2.454947	7.126173	-0.227834
64	6	0	2.454947	7.126173	-0.227834
65	6	0	4.943974	5.689133	-0.227834
66	6	0	7.398921	1.437041	-0.227834
67	6	0	7.398921	-1.437041	-0.227834
68	6	0	4.943974	-5.689133	-0.227834
69	6	0	2.454947	-7.126173	-0.227834
70	6	0	-2.454947	-7.126173	-0.227834
71	6	0	-4.943974	-5.689133	-0.227834
72	6	0	-7.398921	-1.437041	-0.227834
73	6	0	-7.379329	2.826663	-0.227834
74	6	0	-6.137627	4.977355	-0.227834
75	6	0	-1.241703	7.804018	-0.227834
76	6	0	1.241703	7.804018	-0.227834
77	6	0	6.137627	4.977355	-0.227834
78	6	0	7.379329	2.826663	-0.227834

79	6	0	7.379329	-2.826663	-0.227834
80	6	0	6.137627	-4.977355	-0.227834
81	6	0	1.241703	-7.804018	-0.227834
82	6	0	-1.241703	-7.804018	-0.227834
83	6	0	-6.137627	-4.977355	-0.227834
84	6	0	-7.379329	-2.826663	-0.227834
85	6	0	-8.627141	0.679595	-0.227834
86	6	0	-4.902117	7.131526	-0.227834
87	6	0	-3.725024	7.811121	-0.227834
88	6	0	3.725024	7.811121	-0.227834
89	6	0	4.902117	7.131526	-0.227834
90	6	0	8.627141	0.679595	-0.227834
91	6	0	8.627141	-0.679595	-0.227834
92	6	0	4.902117	-7.131526	-0.227834
93	6	0	3.725024	-7.811121	-0.227834
94	6	0	-3.725024	-7.811121	-0.227834
95	6	0	-4.902117	-7.131526	-0.227834
96	6	0	-8.627141	-0.679595	-0.227834
97	1	0	-8.321139	3.371400	-0.227834
98	1	0	-7.080287	5.520618	-0.227834
99	1	0	-1.240852	8.892018	-0.227834
100	1	0	1.240852	8.892018	-0.227834
101	1	0	7.080287	5.520618	-0.227834
102	1	0	8.321139	3.371400	-0.227834
103	1	0	8.321139	-3.371400	-0.227834
104	1	0	7.080287	-5.520618	-0.227834
105	1	0	1.240852	-8.892018	-0.227834
106	1	0	-1.240852	-8.892018	-0.227834
107	1	0	-7.080287	-5.520618	-0.227834
108	1	0	-8.321139	-3.371400	-0.227834
109	1	0	-9.566234	1.227614	-0.227834
110	1	0	-5.846262	7.670795	-0.227834
111	1	0	-3.719972	8.898409	-0.227834
112	1	0	3.719972	8.898409	-0.227834
113	1	0	5.846262	7.670795	-0.227834
114	1	0	9.566234	1.227614	-0.227834
115	1	0	9.566234	-1.227614	-0.227834
116	1	0	5.846262	-7.670795	-0.227834

117	1	0	3.719972	-8.898409	-0.227834
118	1	0	-3.719972	-8.898409	-0.227834
119	1	0	-5.846262	-7.670795	-0.227834
120	1	0	-9.566234	-1.227614	-0.227834
121	6	0	1.096263	0.000000	3.448855
122	6	0	-1.096263	0.000000	3.448855
123	6	0	0.718516	0.000000	4.756964
124	6	0	-0.718516	0.000000	4.756964
125	1	0	2.048785	0.000000	2.940663
126	1	0	-2.048785	0.000000	2.940663
127	1	0	1.373983	0.000000	5.616782
128	1	0	-1.373983	0.000000	5.616782
129	8	0	0.000000	0.000000	2.639518

Edge-on pyrrole_1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	1.423200	-0.251319
2	6	0	1.232527	0.711600	-0.251319
3	6	0	1.232527	-0.711600	-0.251319
4	6	0	0.000000	-1.423200	-0.251319
5	6	0	-1.232527	-0.711600	-0.251319
6	6	0	-1.232527	0.711600	-0.251319
7	6	0	0.000000	2.842500	-0.251319
8	6	0	2.461677	1.421250	-0.251319
9	6	0	2.461677	-1.421250	-0.251319
10	6	0	0.000000	-2.842500	-0.251319
11	6	0	-2.461677	-1.421250	-0.251319
12	6	0	-2.461677	1.421250	-0.251319
13	6	0	-1.233398	3.553392	-0.251319
14	6	0	1.233398	3.553392	-0.251319
15	6	0	2.460629	2.844850	-0.251319
16	6	0	3.694026	0.708542	-0.251319
17	6	0	3.694026	-0.708542	-0.251319

18	6	0	2.460629	-2.844850	-0.251319
19	6	0	1.233398	-3.553392	-0.251319
20	6	0	-1.233398	-3.553392	-0.251319
21	6	0	-2.460629	-2.844850	-0.251319
22	6	0	-3.694026	-0.708542	-0.251319
23	6	0	-3.694026	0.708542	-0.251319
24	6	0	-2.460629	2.844850	-0.251319
25	6	0	-1.232765	4.980792	-0.251319
26	6	0	1.232765	4.980792	-0.251319
27	6	0	3.697110	3.558002	-0.251319
28	6	0	4.929875	1.422790	-0.251319
29	6	0	4.929875	-1.422790	-0.251319
30	6	0	3.697110	-3.558002	-0.251319
31	6	0	1.232765	-4.980792	-0.251319
32	6	0	-1.232765	-4.980792	-0.251319
33	6	0	-3.697110	-3.558002	-0.251319
34	6	0	-4.929875	-1.422790	-0.251319
35	6	0	-4.929875	1.422790	-0.251319
36	6	0	-3.697110	3.558002	-0.251319
37	6	0	0.000000	5.690400	-0.251319
38	6	0	4.928031	2.845200	-0.251319
39	6	0	4.928031	-2.845200	-0.251319
40	6	0	0.000000	-5.690400	-0.251319
41	6	0	-4.928031	-2.845200	-0.251319
42	6	0	-4.928031	2.845200	-0.251319
43	6	0	-2.463782	5.688001	-0.251319
44	6	0	2.463782	5.688001	-0.251319
45	6	0	3.694062	4.977698	-0.251319
46	6	0	6.157844	0.710302	-0.251319
47	6	0	6.157844	-0.710302	-0.251319
48	6	0	3.694062	-4.977698	-0.251319
49	6	0	2.463782	-5.688001	-0.251319
50	6	0	-2.463782	-5.688001	-0.251319
51	6	0	-3.694062	-4.977698	-0.251319
52	6	0	-6.157844	-0.710302	-0.251319
53	6	0	-6.157844	0.710302	-0.251319
54	6	0	-3.694062	4.977698	-0.251319
55	6	0	0.000000	7.123200	-0.251319

56	6	0	6.168872	3.561600	-0.251319
57	6	0	6.168872	-3.561600	-0.251319
58	6	0	0.000000	-7.123200	-0.251319
59	6	0	-6.168872	-3.561600	-0.251319
60	6	0	-6.168872	3.561600	-0.251319
61	6	0	-2.454947	7.126173	-0.251319
62	6	0	2.454947	7.126173	-0.251319
63	6	0	4.943974	5.689133	-0.251319
64	6	0	7.398921	1.437041	-0.251319
65	6	0	7.398921	-1.437041	-0.251319
66	6	0	4.943974	-5.689133	-0.251319
67	6	0	2.454947	-7.126173	-0.251319
68	6	0	-2.454947	-7.126173	-0.251319
69	6	0	-4.943974	-5.689133	-0.251319
70	6	0	-7.398921	-1.437041	-0.251319
71	6	0	-7.398921	1.437041	-0.251319
72	6	0	-4.943974	5.689133	-0.251319
73	6	0	-1.241703	7.804018	-0.251319
74	6	0	1.241703	7.804018	-0.251319
75	6	0	6.137627	4.977355	-0.251319
76	6	0	7.379329	2.826663	-0.251319
77	6	0	7.379329	-2.826663	-0.251319
78	6	0	6.137627	-4.977355	-0.251319
79	6	0	1.241703	-7.804018	-0.251319
80	6	0	-1.241703	-7.804018	-0.251319
81	6	0	-6.137627	-4.977355	-0.251319
82	6	0	-7.379329	-2.826663	-0.251319
83	6	0	-7.379329	2.826663	-0.251319
84	6	0	-6.137627	4.977355	-0.251319
85	6	0	-3.725024	7.811121	-0.251319
86	6	0	3.725024	7.811121	-0.251319
87	6	0	4.902117	7.131526	-0.251319
88	6	0	8.627141	0.679595	-0.251319
89	6	0	8.627141	-0.679595	-0.251319
90	6	0	4.902117	-7.131526	-0.251319
91	6	0	3.725024	-7.811121	-0.251319
92	6	0	-3.725024	-7.811121	-0.251319
93	6	0	-4.902117	-7.131526	-0.251319

94	6	0	-8.627141	-0.679595	-0.251319
95	6	0	-8.627141	0.679595	-0.251319
96	6	0	-4.902117	7.131526	-0.251319
97	1	0	-1.240852	8.892018	-0.251319
98	1	0	1.240852	8.892018	-0.251319
99	1	0	7.080287	5.520618	-0.251319
100	1	0	8.321139	3.371400	-0.251319
101	1	0	8.321139	-3.371400	-0.251319
102	1	0	7.080287	-5.520618	-0.251319
103	1	0	1.240852	-8.892018	-0.251319
104	1	0	-1.240852	-8.892018	-0.251319
105	1	0	-7.080287	-5.520618	-0.251319
106	1	0	-8.321139	-3.371400	-0.251319
107	1	0	-8.321139	3.371400	-0.251319
108	1	0	-7.080287	5.520618	-0.251319
109	1	0	-3.719972	8.898409	-0.251319
110	1	0	3.719972	8.898409	-0.251319
111	1	0	5.846262	7.670795	-0.251319
112	1	0	9.566234	1.227614	-0.251319
113	1	0	9.566234	-1.227614	-0.251319
114	1	0	5.846262	-7.670795	-0.251319
115	1	0	3.719972	-8.898409	-0.251319
116	1	0	-3.719972	-8.898409	-0.251319
117	1	0	-5.846262	-7.670795	-0.251319
118	1	0	-9.566234	-1.227614	-0.251319
119	1	0	-9.566234	1.227614	-0.251319
120	1	0	-5.846262	7.670795	-0.251319
121	6	0	0.000000	-1.124710	3.856002
122	6	0	0.000000	1.124710	3.856002
123	6	0	0.000000	-0.712973	5.172746
124	6	0	0.000000	0.712973	5.172746
125	1	0	0.000000	-2.110741	3.413901
126	1	0	0.000000	2.110741	3.413901
127	1	0	0.000000	-1.361635	6.038606
128	1	0	0.000000	1.361635	6.038606
129	7	0	0.000000	0.000000	3.068464
130	1	0	0.000000	0.000000	2.062242

Edge-on pyrrole_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.244959	1.500870	0.000000
2	6	0	0.245010	0.789271	1.232224
3	6	0	0.244919	-0.633982	1.232630
4	6	0	0.245010	-1.345582	0.000000
5	6	0	0.244919	-0.633982	-1.232630
6	6	0	0.245010	0.789271	-1.232224
7	6	0	0.245091	2.920118	0.000000
8	6	0	0.245023	1.498809	2.461711
9	6	0	0.245016	-1.343632	2.461677
10	6	0	0.245191	-2.764916	0.000000
11	6	0	0.245016	-1.343632	-2.461677
12	6	0	0.245023	1.498809	-2.461711
13	6	0	0.244999	3.631010	-1.233398
14	6	0	0.244999	3.631010	1.233398
15	6	0	0.245048	2.922468	2.460629
16	6	0	0.244949	0.786160	3.694026
17	6	0	0.245008	-0.630924	3.694026
18	6	0	0.245013	-2.767232	2.460629
19	6	0	0.244986	-3.475776	1.233397
20	6	0	0.244986	-3.475776	-1.233397
21	6	0	0.245013	-2.767232	-2.460629
22	6	0	0.245008	-0.630924	-3.694026
23	6	0	0.244949	0.786160	-3.694026
24	6	0	0.245048	2.922468	-2.460629
25	6	0	0.245008	5.058410	-1.232765
26	6	0	0.245008	5.058410	1.232765
27	6	0	0.245008	3.635620	3.697110
28	6	0	0.245008	1.500408	4.929875
29	6	0	0.245008	-1.345172	4.929875
30	6	0	0.245008	-3.480383	3.697110
31	6	0	0.245008	-4.903174	1.232765

32	6	0	0.245008	-4.903174	-1.232765
33	6	0	0.245008	-3.480383	-3.697110
34	6	0	0.245008	-1.345172	-4.929875
35	6	0	0.245008	1.500408	-4.929875
36	6	0	0.245008	3.635620	-3.697110
37	6	0	0.245008	5.768018	0.000000
38	6	0	0.245008	2.922818	4.928031
39	6	0	0.245008	-2.767582	4.928031
40	6	0	0.245008	-5.612782	0.000000
41	6	0	0.245008	-2.767582	-4.928031
42	6	0	0.245008	2.922818	-4.928031
43	6	0	0.245008	5.765619	-2.463782
44	6	0	0.245008	5.765619	2.463782
45	6	0	0.245008	5.055316	3.694062
46	6	0	0.245008	0.787920	6.157844
47	6	0	0.245008	-0.632684	6.157844
48	6	0	0.245008	-4.900080	3.694062
49	6	0	0.245008	-5.610382	2.463782
50	6	0	0.245008	-5.610382	-2.463782
51	6	0	0.245008	-4.900080	-3.694062
52	6	0	0.245008	-0.632684	-6.157844
53	6	0	0.245008	0.787920	-6.157844
54	6	0	0.245008	5.055316	-3.694062
55	6	0	0.245008	7.200818	0.000000
56	6	0	0.245008	3.639218	6.168872
57	6	0	0.245008	-3.483982	6.168872
58	6	0	0.245008	-7.045582	0.000000
59	6	0	0.245008	-3.483982	-6.168872
60	6	0	0.245008	3.639218	-6.168872
61	6	0	0.245008	7.203791	-2.454947
62	6	0	0.245008	7.203791	2.454947
63	6	0	0.245008	5.766751	4.943974
64	6	0	0.245008	1.514659	7.398921
65	6	0	0.245008	-1.359423	7.398921
66	6	0	0.245008	-5.611515	4.943974
67	6	0	0.245008	-7.048555	2.454947
68	6	0	0.245008	-7.048555	-2.454947
69	6	0	0.245008	-5.611515	-4.943974

70	6	0	0.245008	-1.359423	-7.398921
71	6	0	0.245008	1.514659	-7.398921
72	6	0	0.245008	5.766751	-4.943974
73	6	0	0.245008	7.881636	-1.241703
74	6	0	0.245008	7.881636	1.241703
75	6	0	0.245008	5.054973	6.137627
76	6	0	0.245008	2.904281	7.379329
77	6	0	0.245008	-2.749045	7.379329
78	6	0	0.245008	-4.899737	6.137627
79	6	0	0.245008	-7.726400	1.241703
80	6	0	0.245008	-7.726400	-1.241703
81	6	0	0.245008	-4.899737	-6.137627
82	6	0	0.245008	-2.749045	-7.379329
83	6	0	0.245008	2.904281	-7.379329
84	6	0	0.245008	5.054973	-6.137627
85	6	0	0.245008	7.888739	-3.725024
86	6	0	0.245008	7.888739	3.725024
87	6	0	0.245008	7.209144	4.902117
88	6	0	0.245008	0.757213	8.627141
89	6	0	0.245008	-0.601977	8.627141
90	6	0	0.245008	-7.053908	4.902117
91	6	0	0.245008	-7.733503	3.725024
92	6	0	0.245008	-7.733503	-3.725024
93	6	0	0.245008	-7.053908	-4.902117
94	6	0	0.245008	-0.601977	-8.627141
95	6	0	0.245008	0.757213	-8.627141
96	6	0	0.245008	7.209144	-4.902117
97	1	0	0.245008	8.969636	-1.240852
98	1	0	0.245008	8.969636	1.240852
99	1	0	0.245008	5.598236	7.080287
100	1	0	0.245008	3.449018	8.321139
101	1	0	0.245008	-3.293782	8.321139
102	1	0	0.245008	-5.443000	7.080287
103	1	0	0.245008	-8.814400	1.240852
104	1	0	0.245008	-8.814400	-1.240852
105	1	0	0.245008	-5.443000	-7.080287
106	1	0	0.245008	-3.293782	-8.321139
107	1	0	0.245008	3.449018	-8.321139

108	1	0	0.245008	5.598236	-7.080287
109	1	0	0.245008	8.976027	-3.719972
110	1	0	0.245008	8.976027	3.719972
111	1	0	0.245008	7.748413	5.846262
112	1	0	0.245008	1.305232	9.566234
113	1	0	0.245008	-1.149996	9.566234
114	1	0	0.245008	-7.593177	5.846262
115	1	0	0.245008	-8.820791	3.719972
116	1	0	0.245008	-8.820791	-3.719972
117	1	0	0.245008	-7.593177	-5.846262
118	1	0	0.245008	-1.149996	-9.566234
119	1	0	0.245008	1.305232	-9.566234
120	1	0	0.245008	7.748413	-5.846262
121	6	0	-4.343059	-2.437163	0.000000
122	6	0	-3.244163	-0.474346	0.000000
123	6	0	-5.290896	-1.435229	0.000000
124	6	0	-4.593730	-0.191397	0.000000
125	1	0	-4.442620	-3.513190	0.000000
126	1	0	-2.379970	0.172064	0.000000
127	1	0	-6.363319	-1.578284	0.000000
128	1	0	-5.031570	0.797939	0.000000
129	7	0	-3.104775	-1.841471	0.000000
130	1	0	-2.222885	-2.330357	0.000000

Edge-on pyrrole_3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.232530	0.711602	-0.251336
2	6	0	0.000000	1.423203	-0.251337
3	6	0	1.232530	0.711602	-0.251336
4	6	0	1.232530	-0.711602	-0.251336
5	6	0	0.000000	-1.423203	-0.251337
6	6	0	-1.232530	-0.711602	-0.251336
7	6	0	-2.461677	1.421251	-0.251337

8	6	0	0.000000	2.842500	-0.251337
9	6	0	2.461677	1.421251	-0.251337
10	6	0	2.461677	-1.421251	-0.251337
11	6	0	0.000000	-2.842500	-0.251337
12	6	0	-2.461677	-1.421251	-0.251337
13	6	0	-3.694026	0.708542	-0.251337
14	6	0	-2.460629	2.844850	-0.251337
15	6	0	-1.233398	3.553392	-0.251337
16	6	0	1.233398	3.553392	-0.251337
17	6	0	2.460629	2.844850	-0.251337
18	6	0	3.694026	0.708542	-0.251337
19	6	0	3.694026	-0.708542	-0.251337
20	6	0	2.460629	-2.844850	-0.251337
21	6	0	1.233398	-3.553392	-0.251337
22	6	0	-1.233398	-3.553392	-0.251337
23	6	0	-2.460629	-2.844850	-0.251337
24	6	0	-3.694026	-0.708542	-0.251337
25	6	0	-4.929875	1.422790	-0.251337
26	6	0	-3.697110	3.558002	-0.251337
27	6	0	-1.232765	4.980792	-0.251337
28	6	0	1.232765	4.980792	-0.251337
29	6	0	3.697110	3.558002	-0.251337
30	6	0	4.929875	1.422790	-0.251337
31	6	0	4.929875	-1.422790	-0.251337
32	6	0	3.697110	-3.558002	-0.251337
33	6	0	1.232765	-4.980792	-0.251337
34	6	0	-1.232765	-4.980792	-0.251337
35	6	0	-3.697110	-3.558002	-0.251337
36	6	0	-4.929875	-1.422790	-0.251337
37	6	0	-4.928031	2.845200	-0.251337
38	6	0	0.000000	5.690400	-0.251337
39	6	0	4.928031	2.845200	-0.251337
40	6	0	4.928031	-2.845200	-0.251337
41	6	0	0.000000	-5.690400	-0.251337
42	6	0	-4.928031	-2.845200	-0.251337
43	6	0	-6.157844	0.710302	-0.251337
44	6	0	-3.694062	4.977698	-0.251337
45	6	0	-2.463782	5.688001	-0.251337

46	6	0	2.463782	5.688001	-0.251337
47	6	0	3.694062	4.977698	-0.251337
48	6	0	6.157844	0.710302	-0.251337
49	6	0	6.157844	-0.710302	-0.251337
50	6	0	3.694062	-4.977698	-0.251337
51	6	0	2.463782	-5.688001	-0.251337
52	6	0	-2.463782	-5.688001	-0.251337
53	6	0	-3.694062	-4.977698	-0.251337
54	6	0	-6.157844	-0.710302	-0.251337
55	6	0	-6.168872	3.561600	-0.251337
56	6	0	0.000000	7.123200	-0.251337
57	6	0	6.168872	3.561600	-0.251337
58	6	0	6.168872	-3.561600	-0.251337
59	6	0	0.000000	-7.123200	-0.251337
60	6	0	-6.168872	-3.561600	-0.251337
61	6	0	-7.398921	1.437041	-0.251337
62	6	0	-4.943974	5.689133	-0.251337
63	6	0	-2.454947	7.126173	-0.251337
64	6	0	2.454947	7.126173	-0.251337
65	6	0	4.943974	5.689133	-0.251337
66	6	0	7.398921	1.437041	-0.251337
67	6	0	7.398921	-1.437041	-0.251337
68	6	0	4.943974	-5.689133	-0.251337
69	6	0	2.454947	-7.126173	-0.251337
70	6	0	-2.454947	-7.126173	-0.251337
71	6	0	-4.943974	-5.689133	-0.251337
72	6	0	-7.398921	-1.437041	-0.251337
73	6	0	-7.379329	2.826663	-0.251337
74	6	0	-6.137627	4.977355	-0.251337
75	6	0	-1.241703	7.804018	-0.251337
76	6	0	1.241703	7.804018	-0.251337
77	6	0	6.137627	4.977355	-0.251337
78	6	0	7.379329	2.826663	-0.251337
79	6	0	7.379329	-2.826663	-0.251337
80	6	0	6.137627	-4.977355	-0.251337
81	6	0	1.241703	-7.804018	-0.251337
82	6	0	-1.241703	-7.804018	-0.251337
83	6	0	-6.137627	-4.977355	-0.251337

84	6	0	-7.379329	-2.826663	-0.251337
85	6	0	-8.627141	0.679595	-0.251337
86	6	0	-4.902117	7.131526	-0.251337
87	6	0	-3.725024	7.811121	-0.251337
88	6	0	3.725024	7.811121	-0.251337
89	6	0	4.902117	7.131526	-0.251337
90	6	0	8.627141	0.679595	-0.251337
91	6	0	8.627141	-0.679595	-0.251337
92	6	0	4.902117	-7.131526	-0.251337
93	6	0	3.725024	-7.811121	-0.251337
94	6	0	-3.725024	-7.811121	-0.251337
95	6	0	-4.902117	-7.131526	-0.251337
96	6	0	-8.627141	-0.679595	-0.251337
97	1	0	-8.321139	3.371400	-0.251337
98	1	0	-7.080287	5.520618	-0.251337
99	1	0	-1.240852	8.892018	-0.251337
100	1	0	1.240852	8.892018	-0.251337
101	1	0	7.080287	5.520618	-0.251337
102	1	0	8.321139	3.371400	-0.251337
103	1	0	8.321139	-3.371400	-0.251337
104	1	0	7.080287	-5.520618	-0.251337
105	1	0	1.240852	-8.892018	-0.251337
106	1	0	-1.240852	-8.892018	-0.251337
107	1	0	-7.080287	-5.520618	-0.251337
108	1	0	-8.321139	-3.371400	-0.251337
109	1	0	-9.566234	1.227614	-0.251337
110	1	0	-5.846262	7.670795	-0.251337
111	1	0	-3.719972	8.898409	-0.251337
112	1	0	3.719972	8.898409	-0.251337
113	1	0	5.846262	7.670795	-0.251337
114	1	0	9.566234	1.227614	-0.251337
115	1	0	9.566234	-1.227614	-0.251337
116	1	0	5.846262	-7.670795	-0.251337
117	1	0	3.719972	-8.898409	-0.251337
118	1	0	-3.719972	-8.898409	-0.251337
119	1	0	-5.846262	-7.670795	-0.251337
120	1	0	-9.566234	-1.227614	-0.251337
121	6	0	1.124697	0.000000	3.856308

122	6	0	-1.124697	0.000000	3.856308
123	6	0	0.712979	0.000000	5.173040
124	6	0	-0.712979	0.000000	5.173040
125	1	0	2.110796	0.000000	3.414380
126	1	0	-2.110796	0.000000	3.414380
127	1	0	1.361675	0.000000	6.038871
128	1	0	-1.361675	0.000000	6.038871
129	7	0	0.000000	0.000000	3.068720
130	1	0	0.000000	0.000000	2.062487

Edge-on pyridine_1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	1.423111	-0.285726
2	6	0	1.232455	0.711523	-0.285722
3	6	0	1.232455	-0.711523	-0.285722
4	6	0	0.000000	-1.423111	-0.285726
5	6	0	-1.232455	-0.711523	-0.285722
6	6	0	-1.232455	0.711523	-0.285722
7	6	0	0.000000	2.842500	-0.285699
8	6	0	2.461685	1.421236	-0.285699
9	6	0	2.461685	-1.421236	-0.285699
10	6	0	0.000000	-2.842500	-0.285699
11	6	0	-2.461685	-1.421236	-0.285699
12	6	0	-2.461685	1.421236	-0.285699
13	6	0	-1.233398	3.553392	-0.285707
14	6	0	1.233398	3.553392	-0.285707
15	6	0	2.460629	2.844850	-0.285708
16	6	0	3.694026	0.708542	-0.285706
17	6	0	3.694026	-0.708542	-0.285706
18	6	0	2.460629	-2.844850	-0.285708
19	6	0	1.233398	-3.553392	-0.285707
20	6	0	-1.233398	-3.553392	-0.285707
21	6	0	-2.460629	-2.844850	-0.285708

22	6	0	-3.694026	-0.708542	-0.285706
23	6	0	-3.694026	0.708542	-0.285706
24	6	0	-2.460629	2.844850	-0.285708
25	6	0	-1.232765	4.980792	-0.285709
26	6	0	1.232765	4.980792	-0.285709
27	6	0	3.697110	3.558002	-0.285709
28	6	0	4.929875	1.422790	-0.285709
29	6	0	4.929875	-1.422790	-0.285709
30	6	0	3.697110	-3.558002	-0.285709
31	6	0	1.232765	-4.980792	-0.285709
32	6	0	-1.232765	-4.980792	-0.285709
33	6	0	-3.697110	-3.558002	-0.285709
34	6	0	-4.929875	-1.422790	-0.285709
35	6	0	-4.929875	1.422790	-0.285709
36	6	0	-3.697110	3.558002	-0.285709
37	6	0	0.000000	5.690400	-0.285709
38	6	0	4.928031	2.845200	-0.285709
39	6	0	4.928031	-2.845200	-0.285709
40	6	0	0.000000	-5.690400	-0.285709
41	6	0	-4.928031	-2.845200	-0.285709
42	6	0	-4.928031	2.845200	-0.285709
43	6	0	-2.463782	5.688001	-0.285709
44	6	0	2.463782	5.688001	-0.285709
45	6	0	3.694062	4.977698	-0.285709
46	6	0	6.157844	0.710302	-0.285709
47	6	0	6.157844	-0.710302	-0.285709
48	6	0	3.694062	-4.977698	-0.285709
49	6	0	2.463782	-5.688001	-0.285709
50	6	0	-2.463782	-5.688001	-0.285709
51	6	0	-3.694062	-4.977698	-0.285709
52	6	0	-6.157844	-0.710302	-0.285709
53	6	0	-6.157844	0.710302	-0.285709
54	6	0	-3.694062	4.977698	-0.285709
55	6	0	0.000000	7.123200	-0.285709
56	6	0	6.168872	3.561600	-0.285709
57	6	0	6.168872	-3.561600	-0.285709
58	6	0	0.000000	-7.123200	-0.285709
59	6	0	-6.168872	-3.561600	-0.285709

60	6	0	-6.168872	3.561600	-0.285709
61	6	0	-2.454947	7.126173	-0.285709
62	6	0	2.454947	7.126173	-0.285709
63	6	0	4.943974	5.689133	-0.285709
64	6	0	7.398921	1.437041	-0.285709
65	6	0	7.398921	-1.437041	-0.285709
66	6	0	4.943974	-5.689133	-0.285709
67	6	0	2.454947	-7.126173	-0.285709
68	6	0	-2.454947	-7.126173	-0.285709
69	6	0	-4.943974	-5.689133	-0.285709
70	6	0	-7.398921	-1.437041	-0.285709
71	6	0	-7.398921	1.437041	-0.285709
72	6	0	-4.943974	5.689133	-0.285709
73	6	0	-1.241703	7.804018	-0.285709
74	6	0	1.241703	7.804018	-0.285709
75	6	0	6.137627	4.977355	-0.285709
76	6	0	7.379329	2.826663	-0.285709
77	6	0	7.379329	-2.826663	-0.285709
78	6	0	6.137627	-4.977355	-0.285709
79	6	0	1.241703	-7.804018	-0.285709
80	6	0	-1.241703	-7.804018	-0.285709
81	6	0	-6.137627	-4.977355	-0.285709
82	6	0	-7.379329	-2.826663	-0.285709
83	6	0	-7.379329	2.826663	-0.285709
84	6	0	-6.137627	4.977355	-0.285709
85	6	0	-3.725024	7.811121	-0.285709
86	6	0	3.725024	7.811121	-0.285709
87	6	0	4.902117	7.131526	-0.285709
88	6	0	8.627141	0.679595	-0.285709
89	6	0	8.627141	-0.679595	-0.285709
90	6	0	4.902117	-7.131526	-0.285709
91	6	0	3.725024	-7.811121	-0.285709
92	6	0	-3.725024	-7.811121	-0.285709
93	6	0	-4.902117	-7.131526	-0.285709
94	6	0	-8.627141	-0.679595	-0.285709
95	6	0	-8.627141	0.679595	-0.285709
96	6	0	-4.902117	7.131526	-0.285709
97	1	0	-1.240852	8.892018	-0.285709

98	1	0	1.240852	8.892018	-0.285709
99	1	0	7.080287	5.520618	-0.285709
100	1	0	8.321139	3.371400	-0.285709
101	1	0	8.321139	-3.371400	-0.285709
102	1	0	7.080287	-5.520618	-0.285709
103	1	0	1.240852	-8.892018	-0.285709
104	1	0	-1.240852	-8.892018	-0.285709
105	1	0	-7.080287	-5.520618	-0.285709
106	1	0	-8.321139	-3.371400	-0.285709
107	1	0	-8.321139	3.371400	-0.285709
108	1	0	-7.080287	5.520618	-0.285709
109	1	0	-3.719972	8.898409	-0.285709
110	1	0	3.719972	8.898409	-0.285709
111	1	0	5.846262	7.670795	-0.285709
112	1	0	9.566234	1.227614	-0.285709
113	1	0	9.566234	-1.227614	-0.285709
114	1	0	5.846262	-7.670795	-0.285709
115	1	0	3.719972	-8.898409	-0.285709
116	1	0	-3.719972	-8.898409	-0.285709
117	1	0	-5.846262	-7.670795	-0.285709
118	1	0	-9.566234	-1.227614	-0.285709
119	1	0	-9.566234	1.227614	-0.285709
120	1	0	-5.846262	7.670795	-0.285709
121	7	0	0.000000	0.000000	2.665463
122	6	0	-1.143576	0.000000	3.358888
123	6	0	1.143576	0.000000	3.358888
124	6	0	-1.200164	0.000000	4.754298
125	6	0	1.200164	0.000000	4.754298
126	6	0	0.000000	0.000000	5.465700
127	1	0	-2.057560	0.000000	2.765928
128	1	0	2.057560	0.000000	2.765928
129	1	0	-2.158719	0.000000	5.265128
130	1	0	2.158719	0.000000	5.265128
131	1	0	0.000000	0.000000	6.552645

Edge-on pyridine_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.232546	0.711609	-0.285848
2	6	0	0.000000	1.423214	-0.285853
3	6	0	1.232546	0.711609	-0.285848
4	6	0	1.232546	-0.711609	-0.285848
5	6	0	0.000000	-1.423214	-0.285853
6	6	0	-1.232546	-0.711609	-0.285848
7	6	0	-2.461678	1.421248	-0.285855
8	6	0	0.000000	2.842500	-0.285856
9	6	0	2.461678	1.421248	-0.285855
10	6	0	2.461678	-1.421248	-0.285855
11	6	0	0.000000	-2.842500	-0.285856
12	6	0	-2.461678	-1.421248	-0.285855
13	6	0	-3.694026	0.708542	-0.285854
14	6	0	-2.460629	2.844850	-0.285854
15	6	0	-1.233398	3.553392	-0.285854
16	6	0	1.233398	3.553392	-0.285854
17	6	0	2.460629	2.844850	-0.285854
18	6	0	3.694026	0.708542	-0.285854
19	6	0	3.694026	-0.708542	-0.285854
20	6	0	2.460629	-2.844850	-0.285854
21	6	0	1.233398	-3.553392	-0.285854
22	6	0	-1.233398	-3.553392	-0.285854
23	6	0	-2.460629	-2.844850	-0.285854
24	6	0	-3.694026	-0.708542	-0.285854
25	6	0	-4.929875	1.422790	-0.285854
26	6	0	-3.697110	3.558002	-0.285854
27	6	0	-1.232765	4.980792	-0.285854
28	6	0	1.232765	4.980792	-0.285854
29	6	0	3.697110	3.558002	-0.285854
30	6	0	4.929875	1.422790	-0.285854
31	6	0	4.929875	-1.422790	-0.285854
32	6	0	3.697110	-3.558002	-0.285854
33	6	0	1.232765	-4.980792	-0.285854
34	6	0	-1.232765	-4.980792	-0.285854

35	6	0	-3.697110	-3.558002	-0.285854
36	6	0	-4.929875	-1.422790	-0.285854
37	6	0	-4.928031	2.845200	-0.285854
38	6	0	0.000000	5.690400	-0.285854
39	6	0	4.928031	2.845200	-0.285854
40	6	0	4.928031	-2.845200	-0.285854
41	6	0	0.000000	-5.690400	-0.285854
42	6	0	-4.928031	-2.845200	-0.285854
43	6	0	-6.157844	0.710302	-0.285854
44	6	0	-3.694062	4.977698	-0.285854
45	6	0	-2.463782	5.688001	-0.285854
46	6	0	2.463782	5.688001	-0.285854
47	6	0	3.694062	4.977698	-0.285854
48	6	0	6.157844	0.710302	-0.285854
49	6	0	6.157844	-0.710302	-0.285854
50	6	0	3.694062	-4.977698	-0.285854
51	6	0	2.463782	-5.688001	-0.285854
52	6	0	-2.463782	-5.688001	-0.285854
53	6	0	-3.694062	-4.977698	-0.285854
54	6	0	-6.157844	-0.710302	-0.285854
55	6	0	-6.168872	3.561600	-0.285854
56	6	0	0.000000	7.123200	-0.285854
57	6	0	6.168872	3.561600	-0.285854
58	6	0	6.168872	-3.561600	-0.285854
59	6	0	0.000000	-7.123200	-0.285854
60	6	0	-6.168872	-3.561600	-0.285854
61	6	0	-7.398920	1.437041	-0.285854
62	6	0	-4.943974	5.689133	-0.285854
63	6	0	-2.454947	7.126173	-0.285854
64	6	0	2.454947	7.126173	-0.285854
65	6	0	4.943974	5.689133	-0.285854
66	6	0	7.398920	1.437041	-0.285854
67	6	0	7.398920	-1.437041	-0.285854
68	6	0	4.943974	-5.689133	-0.285854
69	6	0	2.454947	-7.126173	-0.285854
70	6	0	-2.454947	-7.126173	-0.285854
71	6	0	-4.943974	-5.689133	-0.285854
72	6	0	-7.398920	-1.437041	-0.285854

73	6	0	-7.379329	2.826663	-0.285854
74	6	0	-6.137627	4.977355	-0.285854
75	6	0	-1.241703	7.804018	-0.285854
76	6	0	1.241703	7.804018	-0.285854
77	6	0	6.137627	4.977355	-0.285854
78	6	0	7.379329	2.826663	-0.285854
79	6	0	7.379329	-2.826663	-0.285854
80	6	0	6.137627	-4.977355	-0.285854
81	6	0	1.241703	-7.804018	-0.285854
82	6	0	-1.241703	-7.804018	-0.285854
83	6	0	-6.137627	-4.977355	-0.285854
84	6	0	-7.379329	-2.826663	-0.285854
85	6	0	-8.627141	0.679595	-0.285854
86	6	0	-4.902117	7.131526	-0.285854
87	6	0	-3.725024	7.811121	-0.285854
88	6	0	3.725024	7.811121	-0.285854
89	6	0	4.902117	7.131526	-0.285854
90	6	0	8.627141	0.679595	-0.285854
91	6	0	8.627141	-0.679595	-0.285854
92	6	0	4.902117	-7.131526	-0.285854
93	6	0	3.725024	-7.811121	-0.285854
94	6	0	-3.725024	-7.811121	-0.285854
95	6	0	-4.902117	-7.131526	-0.285854
96	6	0	-8.627141	-0.679595	-0.285854
97	1	0	-8.321139	3.371400	-0.285854
98	1	0	-7.080287	5.520618	-0.285854
99	1	0	-1.240852	8.892018	-0.285854
100	1	0	1.240852	8.892018	-0.285854
101	1	0	7.080287	5.520618	-0.285854
102	1	0	8.321139	3.371400	-0.285854
103	1	0	8.321139	-3.371400	-0.285854
104	1	0	7.080287	-5.520618	-0.285854
105	1	0	1.240852	-8.892018	-0.285854
106	1	0	-1.240852	-8.892018	-0.285854
107	1	0	-7.080287	-5.520618	-0.285854
108	1	0	-8.321139	-3.371400	-0.285854
109	1	0	-9.566234	1.227614	-0.285854
110	1	0	-5.846262	7.670795	-0.285854

111	1	0	-3.719972	8.898409	-0.285854
112	1	0	3.719972	8.898409	-0.285854
113	1	0	5.846262	7.670795	-0.285854
114	1	0	9.566234	1.227614	-0.285854
115	1	0	9.566234	-1.227614	-0.285854
116	1	0	5.846262	-7.670795	-0.285854
117	1	0	3.719972	-8.898409	-0.285854
118	1	0	-3.719972	-8.898409	-0.285854
119	1	0	-5.846262	-7.670795	-0.285854
120	1	0	-9.566234	-1.227614	-0.285854
121	7	0	0.000000	0.000000	2.667260
122	6	0	0.000000	-1.143585	3.361046
123	6	0	0.000000	1.143585	3.361046
124	6	0	0.000000	-1.200162	4.756399
125	6	0	0.000000	1.200162	4.756399
126	6	0	0.000000	0.000000	5.467941
127	1	0	0.000000	-2.057385	2.767679
128	1	0	0.000000	2.057385	2.767679
129	1	0	0.000000	-2.158820	5.267037
130	1	0	0.000000	2.158820	5.267037
131	1	0	0.000000	0.000000	6.554869

Edge-on pyridine_3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	1.423200	-0.317544
2	6	0	1.232527	0.711600	-0.317544
3	6	0	1.232527	-0.711600	-0.317544
4	6	0	0.000000	-1.423200	-0.317544
5	6	0	-1.232527	-0.711600	-0.317544
6	6	0	-1.232527	0.711600	-0.317544
7	6	0	0.000000	2.842500	-0.317544
8	6	0	2.461677	1.421250	-0.317544
9	6	0	2.461677	-1.421250	-0.317544

10	6	0	0.000000	-2.842500	-0.317544
11	6	0	-2.461677	-1.421250	-0.317544
12	6	0	-2.461677	1.421250	-0.317544
13	6	0	-1.233398	3.553392	-0.317544
14	6	0	1.233398	3.553392	-0.317544
15	6	0	2.460629	2.844850	-0.317544
16	6	0	3.694026	0.708542	-0.317544
17	6	0	3.694026	-0.708542	-0.317544
18	6	0	2.460629	-2.844850	-0.317544
19	6	0	1.233398	-3.553392	-0.317544
20	6	0	-1.233398	-3.553392	-0.317544
21	6	0	-2.460629	-2.844850	-0.317544
22	6	0	-3.694026	-0.708542	-0.317544
23	6	0	-3.694026	0.708542	-0.317544
24	6	0	-2.460629	2.844850	-0.317544
25	6	0	-1.232765	4.980792	-0.317544
26	6	0	1.232765	4.980792	-0.317544
27	6	0	3.697110	3.558002	-0.317544
28	6	0	4.929875	1.422790	-0.317544
29	6	0	4.929875	-1.422790	-0.317544
30	6	0	3.697110	-3.558002	-0.317544
31	6	0	1.232765	-4.980792	-0.317544
32	6	0	-1.232765	-4.980792	-0.317544
33	6	0	-3.697110	-3.558002	-0.317544
34	6	0	-4.929875	-1.422790	-0.317544
35	6	0	-4.929875	1.422790	-0.317544
36	6	0	-3.697110	3.558002	-0.317544
37	6	0	0.000000	5.690400	-0.317544
38	6	0	4.928031	2.845200	-0.317544
39	6	0	4.928031	-2.845200	-0.317544
40	6	0	0.000000	-5.690400	-0.317544
41	6	0	-4.928031	-2.845200	-0.317544
42	6	0	-4.928031	2.845200	-0.317544
43	6	0	-2.463782	5.688001	-0.317544
44	6	0	2.463782	5.688001	-0.317544
45	6	0	3.694062	4.977698	-0.317544
46	6	0	6.157844	0.710302	-0.317544
47	6	0	6.157844	-0.710302	-0.317544

48	6	0	3.694062	-4.977698	-0.317544
49	6	0	2.463782	-5.688001	-0.317544
50	6	0	-2.463782	-5.688001	-0.317544
51	6	0	-3.694062	-4.977698	-0.317544
52	6	0	-6.157844	-0.710302	-0.317544
53	6	0	-6.157844	0.710302	-0.317544
54	6	0	-3.694062	4.977698	-0.317544
55	6	0	0.000000	7.123200	-0.317544
56	6	0	6.168872	3.561600	-0.317544
57	6	0	6.168872	-3.561600	-0.317544
58	6	0	0.000000	-7.123200	-0.317544
59	6	0	-6.168872	-3.561600	-0.317544
60	6	0	-6.168872	3.561600	-0.317544
61	6	0	-2.454947	7.126173	-0.317544
62	6	0	2.454947	7.126173	-0.317544
63	6	0	4.943974	5.689133	-0.317544
64	6	0	7.398921	1.437041	-0.317544
65	6	0	7.398921	-1.437041	-0.317544
66	6	0	4.943974	-5.689133	-0.317544
67	6	0	2.454947	-7.126173	-0.317544
68	6	0	-2.454947	-7.126173	-0.317544
69	6	0	-4.943974	-5.689133	-0.317544
70	6	0	-7.398921	-1.437041	-0.317544
71	6	0	-7.398921	1.437041	-0.317544
72	6	0	-4.943974	5.689133	-0.317544
73	6	0	-1.241703	7.804018	-0.317544
74	6	0	1.241703	7.804018	-0.317544
75	6	0	6.137627	4.977355	-0.317544
76	6	0	7.379329	2.826663	-0.317544
77	6	0	7.379329	-2.826663	-0.317544
78	6	0	6.137627	-4.977355	-0.317544
79	6	0	1.241703	-7.804018	-0.317544
80	6	0	-1.241703	-7.804018	-0.317544
81	6	0	-6.137627	-4.977355	-0.317544
82	6	0	-7.379329	-2.826663	-0.317544
83	6	0	-7.379329	2.826663	-0.317544
84	6	0	-6.137627	4.977355	-0.317544
85	6	0	-3.725024	7.811121	-0.317544

86	6	0	3.725024	7.811121	-0.317544
87	6	0	4.902117	7.131526	-0.317544
88	6	0	8.627141	0.679595	-0.317544
89	6	0	8.627141	-0.679595	-0.317544
90	6	0	4.902117	-7.131526	-0.317544
91	6	0	3.725024	-7.811121	-0.317544
92	6	0	-3.725024	-7.811121	-0.317544
93	6	0	-4.902117	-7.131526	-0.317544
94	6	0	-8.627141	-0.679595	-0.317544
95	6	0	-8.627141	0.679595	-0.317544
96	6	0	-4.902117	7.131526	-0.317544
97	1	0	-1.240852	8.892018	-0.317544
98	1	0	1.240852	8.892018	-0.317544
99	1	0	7.080287	5.520618	-0.317544
100	1	0	8.321139	3.371400	-0.317544
101	1	0	8.321139	-3.371400	-0.317544
102	1	0	7.080287	-5.520618	-0.317544
103	1	0	1.240852	-8.892018	-0.317544
104	1	0	-1.240852	-8.892018	-0.317544
105	1	0	-7.080287	-5.520618	-0.317544
106	1	0	-8.321139	-3.371400	-0.317544
107	1	0	-8.321139	3.371400	-0.317544
108	1	0	-7.080287	5.520618	-0.317544
109	1	0	-3.719972	8.898409	-0.317544
110	1	0	3.719972	8.898409	-0.317544
111	1	0	5.846262	7.670795	-0.317544
112	1	0	9.566234	1.227614	-0.317544
113	1	0	9.566234	-1.227614	-0.317544
114	1	0	5.846262	-7.670795	-0.317544
115	1	0	3.719972	-8.898409	-0.317544
116	1	0	-3.719972	-8.898409	-0.317544
117	1	0	-5.846262	-7.670795	-0.317544
118	1	0	-9.566234	-1.227614	-0.317544
119	1	0	-9.566234	1.227614	-0.317544
120	1	0	-5.846262	7.670795	-0.317544
121	7	0	0.000000	0.000000	5.957908
122	6	0	1.142607	0.000000	5.258137
123	6	0	-1.142607	0.000000	5.258137

124	6	0	1.199053	0.000000	3.862880
125	6	0	-1.199053	0.000000	3.862880
126	6	0	0.000000	0.000000	3.151986
127	1	0	2.060101	0.000000	5.845273
128	1	0	-2.060101	0.000000	5.845273
129	1	0	2.155575	0.000000	3.347966
130	1	0	-2.155575	0.000000	3.347966
131	1	0	0.000000	0.000000	2.070413

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

Thiophene

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	16	0	0.212046	-0.000899	-2.457117
122	6	0	1.423097	-1.244800	-2.400000
123	6	0	1.423303	1.242800	-2.400000
124	6	0	2.682891	-0.716176	-2.340592
125	6	0	2.683010	0.713966	-2.340592
126	1	0	1.132516	-2.286857	-2.413699
127	1	0	1.132896	2.284905	-2.413699
128	1	0	3.582268	-1.321070	-2.298176
129	1	0	3.582488	1.318711	-2.298176

Furan

Center	Atomic	Atomic	Coordinates (Angstroms)		
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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	8	0	0.609224	-0.000932	-2.315792
122	6	0	1.423291	1.094100	-2.330000
123	6	0	1.423109	-1.096100	-2.330000
124	6	0	2.730651	0.716824	-2.352821
125	6	0	2.730532	-0.719042	-2.352821
126	1	0	0.921942	2.050077	-2.321248
127	1	0	0.921601	-2.051994	-2.321248
128	1	0	3.589826	1.372852	-2.367817
129	1	0	3.589597	-1.375212	-2.367817

Pyrrole

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	7	0	0.280796	0.000000	-2.154513
122	6	0	1.058198	-1.125501	-2.300000
123	6	0	1.058202	1.125499	-2.300000
124	6	0	2.350812	-0.712776	-2.541906
125	6	0	2.350814	0.712769	-2.541906
126	1	0	0.629267	-2.113962	-2.219728
127	1	0	0.629275	2.113961	-2.219728
128	1	0	3.201960	-1.361042	-2.701194

129	1	0	3.201965	1.361032	-2.701194
130	1	0	-0.709904	0.000002	-1.969108

Pyridine

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	7	0	0.100900	0.000100	-2.400000
122	6	0	0.800754	1.142085	-2.400000
123	6	0	0.800564	-1.142002	-2.400000
124	6	0	2.196246	1.198628	-2.400000
125	6	0	2.196046	-1.198776	-2.400000
126	6	0	2.909200	-0.000134	-2.400000
127	1	0	0.214463	2.059910	-2.400000
128	1	0	0.214120	-2.059729	-2.400000
129	1	0	2.705515	2.158042	-2.400000
130	1	0	2.705156	-2.158275	-2.400000
131	1	0	3.996100	-0.000224	-2.400000
