

Table S3. Cartesian Coordinates of all Species in Table S2 Optimized at the M06-2X/6-31G(d) level

CH4 Td cc3-ch4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	1	0	0.629802	0.629802	0.629802
3	1	0	-0.629802	-0.629802	0.629802
4	1	0	-0.629802	0.629802	-0.629802
5	1	0	0.629802	-0.629802	-0.629802

HCCl3 C3v cc3-hccl3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.455182
2	1	0	0.000000	0.000000	1.540927
3	17	0	0.000000	1.686735	-0.083765
4	17	0	-1.460756	-0.843368	-0.083765
5	17	0	1.460756	-0.843368	-0.083765

CO2 Dih cc3-co2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	0.000000	0.000000	1.162697
2	6	0	0.000000	0.000000	0.000000
3	8	0	0.000000	0.000000	-1.162697

C2H2 Dih cc3-rcc

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.601088
2	1	0	0.000000	0.000000	1.667979
3	6	0	0.000000	0.000000	-0.601088
4	1	0	0.000000	0.000000	-1.667979

H2O C2v cc3-h2o

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	0.000000	0.000000	0.118351

2	1	0	-0.000000	0.762602	-0.473403
3	1	0	-0.000000	-0.762602	-0.473403

SF6 Oh cc3-sf6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	16	0	0.000000	0.000000	0.000000
2	9	0	-0.000000	-0.000000	1.579653
3	9	0	-0.000000	1.579653	-0.000000
4	9	0	-0.000000	-0.000000	-1.579653
5	9	0	-1.579653	-0.000000	-0.000000
6	9	0	-0.000000	-1.579653	0.000000
7	9	0	1.579653	-0.000000	0.000000

15-Crown-5 D5 crown4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.067045	2.385528	0.542942
2	1	0	0.700296	1.617475	1.236394
3	1	0	1.670334	3.085911	1.125807
4	6	0	-1.939037	1.751988	0.542942
5	1	0	-1.321907	1.165848	1.236394
6	1	0	-2.418714	2.542180	1.125807
7	6	0	-2.265435	-1.302739	0.542942
8	1	0	-1.517279	-0.896941	1.236394
9	1	0	-3.165181	-1.514757	1.125807
10	6	0	0.538921	-2.557126	0.542942
11	1	0	0.384177	-1.720189	1.236394
12	1	0	0.462525	-3.478352	1.125807
13	6	0	2.598507	-0.277651	0.542942
14	1	0	1.754714	-0.166194	1.236394
15	1	0	3.451037	-0.634983	1.125807
16	8	0	-0.000000	3.138123	-0.000000
17	8	0	2.984532	0.969733	-0.000000
18	8	0	1.844542	-2.538795	-0.000000
19	8	0	-1.844542	-2.538795	-0.000000
20	8	0	-2.984532	0.969733	-0.000000
21	6	0	-0.538921	-2.557126	-0.542942
22	1	0	-0.384177	-1.720189	-1.236394
23	1	0	-0.462525	-3.478352	-1.125807
24	6	0	1.939037	1.751988	-0.542942
25	1	0	1.321907	1.165848	-1.236394
26	1	0	2.418714	2.542180	-1.125807
27	6	0	-1.067045	2.385528	-0.542942
28	1	0	-0.700296	1.617475	-1.236394
29	1	0	-1.670334	3.085911	-1.125807
30	6	0	-2.598507	-0.277651	-0.542942
31	1	0	-1.754714	-0.166194	-1.236394
32	1	0	-3.451037	-0.634983	-1.125807
33	6	0	2.265435	-1.302739	-0.542942
34	1	0	1.517279	-0.896941	-1.236394

35 1 0 3.165181 -1.514757 -1.125807

15-Crown-5 C1 crown22

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-2.313406	1.383053	0.548775
2	8	0	1.074876	2.748788	0.194577
3	8	0	-2.077367	-1.392094	-0.567671
4	8	0	3.319041	-0.138855	0.008779
5	8	0	0.600712	-1.591784	0.101842
6	6	0	-0.897759	1.374086	0.595444
7	6	0	-2.874603	0.902530	-0.655719
8	6	0	-0.319214	2.655716	0.001501
9	6	0	-3.230044	-0.573235	-0.578058
10	6	0	1.842566	1.762319	-0.469138
11	6	0	-1.679811	-1.840328	0.707037
12	6	0	2.404000	0.786582	0.564924
13	6	0	-0.344454	-2.532824	0.550956
14	6	0	2.766511	-1.135621	-0.819716
15	6	0	1.882197	-2.144554	-0.104427
16	1	0	-1.589204	-1.005508	1.414861
17	1	0	-0.037749	-2.967313	1.515589
18	1	0	-3.848407	-0.754688	0.312104
19	1	0	-2.191188	1.058502	-1.502148
20	1	0	2.343210	-2.432027	0.853656
21	1	0	2.191306	-0.707731	-1.653268
22	1	0	1.586625	0.275684	1.086550
23	1	0	-0.613980	1.320490	1.652658
24	1	0	1.238074	1.242536	-1.225607
25	1	0	-0.761429	3.518343	0.506743
26	1	0	-2.412512	-2.554490	1.115115
27	1	0	-0.438981	-3.350285	-0.180463
28	1	0	1.798802	-3.048729	-0.729213
29	1	0	-3.815593	-0.848625	-1.463664
30	1	0	3.626293	-1.664730	-1.241494
31	1	0	-3.786060	1.482681	-0.842025
32	1	0	2.971584	1.363328	1.300172
33	1	0	-0.493882	0.489794	0.087127
34	1	0	-0.568352	2.725345	-1.069839
35	1	0	2.674256	2.256534	-0.984107

Mesitylene C3v cc3-mes2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.199694	0.692644	-0.011796
2	6	0	0.000000	1.404735	-0.009247
3	6	0	-1.199694	0.692644	-0.011796
4	6	0	-1.216536	-0.702367	-0.009247
5	6	0	-0.000000	-1.385288	-0.011796
6	6	0	1.216536	-0.702367	-0.009247
7	1	0	2.142466	1.236954	-0.024022

8	1	0	-2.142466	1.236954	-0.024022
9	1	0	-0.000000	-2.473907	-0.024022
10	6	0	-2.522562	-1.456402	0.012907
11	1	0	-2.848152	-1.644382	1.042255
12	1	0	-3.315643	-0.890952	-0.484710
13	1	0	-2.429409	-2.425955	-0.484710
14	6	0	0.000000	2.912803	0.012907
15	1	0	-0.886234	3.316907	-0.484710
16	1	0	0.000000	3.288763	1.042255
17	1	0	0.886234	3.316907	-0.484710
18	6	0	2.522562	-1.456402	0.012907
19	1	0	3.315643	-0.890952	-0.484710
20	1	0	2.848152	-1.644382	1.042255
21	1	0	2.429409	-2.425955	-0.484710

5-tBu-m-xylene Cs cc3-dpe10

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.268169	-2.323292	0.000000
2	6	0	1.399534	-1.518500	0.000000
3	6	0	1.240096	-0.125900	0.000000
4	6	0	-0.020030	0.465072	0.000000
5	6	0	-1.139999	-0.381329	0.000000
6	6	0	-1.015548	-1.764952	0.000000
7	1	0	0.379491	-3.406323	0.000000
8	1	0	2.134337	0.490515	0.000000
9	1	0	-2.139180	0.049315	0.000000
10	6	0	-0.225186	1.982820	0.000000
11	6	0	-1.015548	2.390359	1.254823
12	6	0	1.102231	2.747513	0.000000
13	6	0	-1.015548	2.390359	-1.254823
14	1	0	-1.997754	1.909303	1.286749
15	1	0	-0.472250	2.108529	2.162632
16	1	0	-1.170861	3.475170	1.268378
17	1	0	1.699780	2.516691	-0.888166
18	1	0	0.904580	3.824386	0.000000
19	1	0	1.699780	2.516691	0.888166
20	1	0	-1.170861	3.475170	-1.268378
21	1	0	-0.472250	2.108529	-2.162632
22	1	0	-1.997754	1.909303	-1.286749
23	6	0	2.784305	-2.116512	0.000000
24	6	0	-2.230228	-2.658912	0.000000
25	1	0	3.350759	-1.799149	0.881787
26	1	0	2.744978	-3.208778	0.000000
27	1	0	3.350759	-1.799149	-0.881787
28	1	0	-3.153685	-2.074246	0.000000
29	1	0	-2.241678	-3.308160	-0.881737
30	1	0	-2.241678	-3.308160	0.881737

CC3-R T cc3-r

Standard orientation:

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

1	7	0	-1.124432	-0.902806	5.552609
2	7	0	1.124432	0.902806	5.552609
3	7	0	0.902806	5.552609	1.124432
4	7	0	-0.902806	5.552609	-1.124432
5	6	0	-2.750819	-1.328371	3.218686
6	1	0	-2.983002	-0.476489	3.852668
7	6	0	-1.639580	-2.119879	3.541811
8	6	0	-0.818491	-1.818789	4.731235
9	1	0	0.069627	-2.454586	4.871341
10	6	0	-0.271235	-0.718923	6.710127
11	1	0	0.598645	-1.400085	6.684638
12	6	0	0.271235	0.718923	6.710127
13	1	0	-0.598645	1.400085	6.684638
14	6	0	1.088303	0.985190	7.979368
15	1	0	1.449229	2.019204	7.956556
16	1	0	1.974687	0.337812	7.958187
17	6	0	0.270266	0.715422	9.242580
18	1	0	0.884081	0.895420	10.131460
19	1	0	-0.571825	1.419340	9.289561
20	6	0	-0.270266	-0.715422	9.242580
21	1	0	-0.884081	-0.895420	10.131460
22	1	0	0.571825	-1.419340	9.289561
23	6	0	-1.088303	-0.985190	7.979368
24	1	0	-1.974687	-0.337812	7.958187
25	1	0	-1.449229	-2.019204	7.956556
26	6	0	0.818491	1.818789	4.731235
27	1	0	-0.069627	2.454586	4.871341
28	6	0	1.639580	2.119879	3.541811
29	6	0	2.750819	1.328371	3.218686
30	1	0	2.983002	0.476489	3.852668
31	6	0	3.541811	1.639580	2.119879
32	6	0	3.218686	2.750819	1.328371
33	1	0	3.852668	2.983002	0.476489
34	6	0	2.119879	3.541811	1.639580
35	6	0	1.328371	3.218686	2.750819
36	1	0	0.476489	3.852668	2.983002
37	6	0	1.818789	4.731235	0.818491
38	1	0	2.454586	4.871341	-0.069627
39	6	0	0.718923	6.710127	0.271235
40	1	0	1.400085	6.684638	-0.598645
41	6	0	-0.718923	6.710127	-0.271235
42	1	0	-1.400085	6.684638	0.598645
43	6	0	-0.985190	7.979368	-1.088303
44	1	0	-2.019204	7.956556	-1.449229
45	1	0	-0.337812	7.958187	-1.974687
46	6	0	-0.715422	9.242580	-0.270266
47	1	0	-1.419340	9.289561	0.571825
48	1	0	-0.895420	10.131460	-0.884081
49	6	0	0.715422	9.242580	0.270266
50	1	0	1.419340	9.289561	-0.571825
51	1	0	0.895420	10.131460	0.884081
52	6	0	0.985190	7.979368	1.088303
53	1	0	0.337812	7.958187	1.974687
54	1	0	2.019204	7.956556	1.449229
55	6	0	-1.818789	4.731235	-0.818491
56	1	0	-2.454586	4.871341	0.069627
57	7	0	-0.902806	-5.552609	1.124432
58	7	0	0.902806	-5.552609	-1.124432

59	7	0	5.552609	-1.124432	-0.902806
60	7	0	5.552609	1.124432	0.902806
61	6	0	-1.328371	-3.218686	2.750819
62	1	0	-0.476489	-3.852668	2.983002
63	6	0	-2.119879	-3.541811	1.639580
64	6	0	-1.818789	-4.731235	0.818491
65	1	0	-2.454586	-4.871341	-0.069627
66	6	0	-0.718923	-6.710127	0.271235
67	1	0	-1.400085	-6.684638	-0.598645
68	6	0	0.718923	-6.710127	-0.271235
69	1	0	1.400085	-6.684638	0.598645
70	6	0	0.985190	-7.979368	-1.088303
71	1	0	2.019204	-7.956556	-1.449229
72	1	0	0.337812	-7.958187	-1.974687
73	6	0	0.715422	-9.242580	-0.270266
74	1	0	0.895420	-10.131460	-0.884081
75	1	0	1.419340	-9.289561	0.571825
76	6	0	-0.715422	-9.242580	0.270266
77	1	0	-0.895420	-10.131460	0.884081
78	1	0	-1.419340	-9.289561	-0.571825
79	6	0	-0.985190	-7.979368	1.088303
80	1	0	-0.337812	-7.958187	1.974687
81	1	0	-2.019204	-7.956556	1.449229
82	6	0	1.818789	-4.731235	-0.818491
83	1	0	2.454586	-4.871341	0.069627
84	6	0	2.119879	-3.541811	-1.639580
85	6	0	1.328371	-3.218686	-2.750819
86	1	0	0.476489	-3.852668	-2.983002
87	6	0	1.639580	-2.119879	-3.541811
88	6	0	2.750819	-1.328371	-3.218686
89	1	0	2.983002	-0.476489	-3.852668
90	6	0	3.541811	-1.639580	-2.119879
91	6	0	3.218686	-2.750819	-1.328371
92	1	0	3.852668	-2.983002	-0.476489
93	6	0	4.731235	-0.818491	-1.818789
94	1	0	4.871341	0.069627	-2.454586
95	6	0	6.710127	-0.271235	-0.718923
96	1	0	6.684638	0.598645	-1.400085
97	6	0	6.710127	0.271235	0.718923
98	1	0	6.684638	-0.598645	1.400085
99	6	0	7.979368	1.088303	0.985190
100	1	0	7.956556	1.449229	2.019204
101	1	0	7.958187	1.974687	0.337812
102	6	0	9.242580	0.270266	0.715422
103	1	0	9.289561	-0.571825	1.419340
104	1	0	10.131460	0.884081	0.895420
105	6	0	9.242580	-0.270266	-0.715422
106	1	0	9.289561	0.571825	-1.419340
107	1	0	10.131460	-0.884081	-0.895420
108	6	0	7.979368	-1.088303	-0.985190
109	1	0	7.958187	-1.974687	-0.337812
110	1	0	7.956556	-1.449229	-2.019204
111	6	0	4.731235	0.818491	1.818789
112	1	0	4.871341	-0.069627	2.454586
113	7	0	-5.552609	-1.124432	0.902806
114	7	0	-5.552609	1.124432	-0.902806
115	7	0	-1.124432	0.902806	-5.552609
116	7	0	1.124432	-0.902806	-5.552609
117	6	0	-3.218686	-2.750819	1.328371

118	1	0	-3.852668	-2.983002	0.476489
119	6	0	-3.541811	-1.639580	2.119879
120	6	0	-4.731235	-0.818491	1.818789
121	1	0	-4.871341	0.069627	2.454586
122	6	0	-6.710127	-0.271235	0.718923
123	1	0	-6.684638	0.598645	1.400085
124	6	0	-6.710127	0.271235	-0.718923
125	1	0	-6.684638	-0.598645	-1.400085
126	6	0	-7.979368	1.088303	-0.985190
127	1	0	-7.956556	1.449229	-2.019204
128	1	0	-7.958187	1.974687	-0.337812
129	6	0	-9.242580	0.270266	-0.715422
130	1	0	-10.131460	0.884081	-0.895420
131	1	0	-9.289561	-0.571825	-1.419340
132	6	0	-9.242580	-0.270266	0.715422
133	1	0	-10.131460	-0.884081	0.895420
134	1	0	-9.289561	0.571825	1.419340
135	6	0	-7.979368	-1.088303	0.985190
136	1	0	-7.958187	-1.974687	0.337812
137	1	0	-7.956556	-1.449229	2.019204
138	6	0	-4.731235	0.818491	-1.818789
139	1	0	-4.871341	-0.069627	-2.454586
140	6	0	-3.541811	1.639580	-2.119879
141	6	0	-3.218686	2.750819	-1.328371
142	1	0	-3.852668	2.983002	-0.476489
143	6	0	-2.119879	3.541811	-1.639580
144	6	0	-1.328371	3.218686	-2.750819
145	1	0	-0.476489	3.852668	-2.983002
146	6	0	-1.639580	2.119879	-3.541811
147	6	0	-2.750819	1.328371	-3.218686
148	1	0	-2.983002	0.476489	-3.852668
149	6	0	-0.818491	1.818789	-4.731235
150	1	0	0.069627	2.454586	-4.871341
151	6	0	-0.271235	0.718923	-6.710127
152	1	0	0.598645	1.400085	-6.684638
153	6	0	0.271235	-0.718923	-6.710127
154	1	0	-0.598645	-1.400085	-6.684638
155	6	0	1.088303	-0.985190	-7.979368
156	1	0	1.449229	-2.019204	-7.956556
157	1	0	1.974687	-0.337812	-7.958187
158	6	0	0.270266	-0.715422	-9.242580
159	1	0	-0.571825	-1.419340	-9.289561
160	1	0	0.884081	-0.895420	-10.131460
161	6	0	-0.270266	0.715422	-9.242580
162	1	0	0.571825	1.419340	-9.289561
163	1	0	-0.884081	0.895420	-10.131460
164	6	0	-1.088303	0.985190	-7.979368
165	1	0	-1.974687	0.337812	-7.958187
166	1	0	-1.449229	2.019204	-7.956556
167	6	0	0.818491	-1.818789	-4.731235
168	1	0	-0.069627	-2.454586	-4.871341

Xe@CC3 T cc3-xex

Standard orientation:

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

1	7	0	-1.112383	-0.903515	5.533892
2	7	0	1.112383	0.903515	5.533892
3	7	0	0.903515	5.533892	1.112383
4	7	0	-0.903515	5.533892	-1.112383
5	6	0	-2.680457	-1.260717	3.152781
6	1	0	-2.915018	-0.413734	3.792422
7	6	0	-1.571133	-2.055670	3.474603
8	6	0	-0.764808	-1.771833	4.678125
9	1	0	0.145371	-2.379542	4.799410
10	6	0	-0.266795	-0.721060	6.696307
11	1	0	0.608090	-1.395719	6.671542
12	6	0	0.266795	0.721060	6.696307
13	1	0	-0.608090	1.395719	6.671542
14	6	0	1.083692	0.991683	7.963876
15	1	0	1.439282	2.027524	7.941854
16	1	0	1.973141	0.348681	7.941899
17	6	0	0.266807	0.716859	9.226954
18	1	0	0.879350	0.899552	10.116126
19	1	0	-0.578884	1.416469	9.274085
20	6	0	-0.266807	-0.716859	9.226954
21	1	0	-0.879350	-0.899552	10.116126
22	1	0	0.578884	-1.416469	9.274085
23	6	0	-1.083692	-0.991683	7.963876
24	1	0	-1.973141	-0.348681	7.941899
25	1	0	-1.439282	-2.027524	7.941854
26	6	0	0.764808	1.771833	4.678125
27	1	0	-0.145371	2.379542	4.799410
28	6	0	1.571133	2.055670	3.474603
29	6	0	2.680457	1.260717	3.152781
30	1	0	2.915018	0.413734	3.792422
31	6	0	3.474603	1.571133	2.055670
32	6	0	3.152781	2.680457	1.260717
33	1	0	3.792422	2.915018	0.413734
34	6	0	2.055670	3.474603	1.571133
35	6	0	1.260717	3.152781	2.680457
36	1	0	0.413734	3.792422	2.915018
37	6	0	1.771833	4.678125	0.764808
38	1	0	2.379542	4.799410	-0.145371
39	6	0	0.721060	6.696307	0.266795
40	1	0	1.395719	6.671542	-0.608090
41	6	0	-0.721060	6.696307	-0.266795
42	1	0	-1.395719	6.671542	0.608090
43	6	0	-0.991683	7.963876	-1.083692
44	1	0	-2.027524	7.941854	-1.439282
45	1	0	-0.348681	7.941899	-1.973141
46	6	0	-0.716859	9.226954	-0.266807
47	1	0	-1.416469	9.274085	0.578884
48	1	0	-0.899552	10.116126	-0.879350
49	6	0	0.716859	9.226954	0.266807
50	1	0	1.416469	9.274085	-0.578884
51	1	0	0.899552	10.116126	0.879350
52	6	0	0.991683	7.963876	1.083692
53	1	0	0.348681	7.941899	1.973141
54	1	0	2.027524	7.941854	1.439282
55	6	0	-1.771833	4.678125	-0.764808
56	1	0	-2.379542	4.799410	0.145371
57	7	0	-0.903515	-5.533892	1.112383
58	7	0	0.903515	-5.533892	-1.112383
59	7	0	5.533892	-1.112383	-0.903515

60	7	0	5.533892	1.112383	0.903515
61	6	0	-1.260717	-3.152781	2.680457
62	1	0	-0.413734	-3.792422	2.915018
63	6	0	-2.055670	-3.474603	1.571133
64	6	0	-1.771833	-4.678125	0.764808
65	1	0	-2.379542	-4.799410	-0.145371
66	6	0	-0.721060	-6.696307	0.266795
67	1	0	-1.395719	-6.671542	-0.608090
68	6	0	0.721060	-6.696307	-0.266795
69	1	0	1.395719	-6.671542	0.608090
70	6	0	0.991683	-7.963876	-1.083692
71	1	0	2.027524	-7.941854	-1.439282
72	1	0	0.348681	-7.941899	-1.973141
73	6	0	0.716859	-9.226954	-0.266807
74	1	0	0.899552	-10.116126	-0.879350
75	1	0	1.416469	-9.274085	0.578884
76	6	0	-0.716859	-9.226954	0.266807
77	1	0	-0.899552	-10.116126	0.879350
78	1	0	-1.416469	-9.274085	-0.578884
79	6	0	-0.991683	-7.963876	1.083692
80	1	0	-0.348681	-7.941899	1.973141
81	1	0	-2.027524	-7.941854	1.439282
82	6	0	1.771833	-4.678125	-0.764808
83	1	0	2.379542	-4.799410	0.145371
84	6	0	2.055670	-3.474603	-1.571133
85	6	0	1.260717	-3.152781	-2.680457
86	1	0	0.413734	-3.792422	-2.915018
87	6	0	1.571133	-2.055670	-3.474603
88	6	0	2.680457	-1.260717	-3.152781
89	1	0	2.915018	-0.413734	-3.792422
90	6	0	3.474603	-1.571133	-2.055670
91	6	0	3.152781	-2.680457	-1.260717
92	1	0	3.792422	-2.915018	-0.413734
93	6	0	4.678125	-0.764808	-1.771833
94	1	0	4.799410	0.145371	-2.379542
95	6	0	6.696307	-0.266795	-0.721060
96	1	0	6.671542	0.608090	-1.395719
97	6	0	6.696307	0.266795	0.721060
98	1	0	6.671542	-0.608090	1.395719
99	6	0	7.963876	1.083692	0.991683
100	1	0	7.941854	1.439282	2.027524
101	1	0	7.941899	1.973141	0.348681
102	6	0	9.226954	0.266807	0.716859
103	1	0	9.274085	-0.578884	1.416469
104	1	0	10.116126	0.879350	0.899552
105	6	0	9.226954	-0.266807	-0.716859
106	1	0	9.274085	0.578884	-1.416469
107	1	0	10.116126	-0.879350	-0.899552
108	6	0	7.963876	-1.083692	-0.991683
109	1	0	7.941899	-1.973141	-0.348681
110	1	0	7.941854	-1.439282	-2.027524
111	6	0	4.678125	0.764808	1.771833
112	1	0	4.799410	-0.145371	2.379542
113	7	0	-5.533892	-1.112383	0.903515
114	7	0	-5.533892	1.112383	-0.903515
115	7	0	-1.112383	0.903515	-5.533892
116	7	0	1.112383	-0.903515	-5.533892
117	6	0	-3.152781	-2.680457	1.260717
118	1	0	-3.792422	-2.915018	0.413734

119	6	0	-3.474603	-1.571133	2.055670
120	6	0	-4.678125	-0.764808	1.771833
121	1	0	-4.799410	0.145371	2.379542
122	6	0	-6.696307	-0.266795	0.721060
123	1	0	-6.671542	0.608090	1.395719
124	6	0	-6.696307	0.266795	-0.721060
125	1	0	-6.671542	-0.608090	-1.395719
126	6	0	-7.963876	1.083692	-0.991683
127	1	0	-7.941854	1.439282	-2.027524
128	1	0	-7.941899	1.973141	-0.348681
129	6	0	-9.226954	0.266807	-0.716859
130	1	0	-10.116126	0.879350	-0.899552
131	1	0	-9.274085	-0.578884	-1.416469
132	6	0	-9.226954	-0.266807	0.716859
133	1	0	-10.116126	-0.879350	0.899552
134	1	0	-9.274085	0.578884	1.416469
135	6	0	-7.963876	-1.083692	0.991683
136	1	0	-7.941899	-1.973141	0.348681
137	1	0	-7.941854	-1.439282	2.027524
138	6	0	-4.678125	0.764808	-1.771833
139	1	0	-4.799410	-0.145371	-2.379542
140	6	0	-3.474603	1.571133	-2.055670
141	6	0	-3.152781	2.680457	-1.260717
142	1	0	-3.792422	2.915018	-0.413734
143	6	0	-2.055670	3.474603	-1.571133
144	6	0	-1.260717	3.152781	-2.680457
145	1	0	-0.413734	3.792422	-2.915018
146	6	0	-1.571133	2.055670	-3.474603
147	6	0	-2.680457	1.260717	-3.152781
148	1	0	-2.915018	0.413734	-3.792422
149	6	0	-0.764808	1.771833	-4.678125
150	1	0	0.145371	2.379542	-4.799410
151	6	0	-0.266795	0.721060	-6.696307
152	1	0	0.608090	1.395719	-6.671542
153	6	0	0.266795	-0.721060	-6.696307
154	1	0	-0.608090	-1.395719	-6.671542
155	6	0	1.083692	-0.991683	-7.963876
156	1	0	1.439282	-2.027524	-7.941854
157	1	0	1.973141	-0.348681	-7.941899
158	6	0	0.266807	-0.716859	-9.226954
159	1	0	-0.578884	-1.416469	-9.274085
160	1	0	0.879350	-0.899552	-10.116126
161	6	0	-0.266807	0.716859	-9.226954
162	1	0	0.578884	1.416469	-9.274085
163	1	0	-0.879350	0.899552	-10.116126
164	6	0	-1.083692	0.991683	-7.963876
165	1	0	-1.973141	0.348681	-7.941899
166	1	0	-1.439282	2.027524	-7.941854
167	6	0	0.764808	-1.771833	-4.678125
168	1	0	-0.145371	-2.379542	-4.799410
169	54	0	0.000000	0.000000	0.000000

3Xe@CC3 C3 cc3-rcj

Standard orientation:

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

1	7	0	-4.041853	2.684805	3.265148
2	7	0	-1.697082	4.363664	3.528595
3	7	0	1.763906	5.084029	-1.845795
4	7	0	1.477724	3.410987	-4.197463
5	6	0	-4.358570	0.648826	1.260101
6	1	0	-4.628983	1.669190	0.999104
7	6	0	-3.831806	0.400993	2.535330
8	6	0	-3.672500	1.497069	3.511395
9	1	0	-3.228964	1.214008	4.478847
10	6	0	-3.893509	3.670954	4.317675
11	1	0	-3.378149	3.247693	5.198790
12	6	0	-3.039183	4.838709	3.802277
13	1	0	-3.525197	5.227454	2.889177
14	6	0	-2.963007	5.953924	4.851959
15	1	0	-2.361017	6.775888	4.449404
16	1	0	-2.425892	5.564456	5.726630
17	6	0	-4.353165	6.439832	5.262356
18	1	0	-4.266569	7.220834	6.025125
19	1	0	-4.851793	6.894937	4.395757
20	6	0	-5.202227	5.276532	5.777056
21	1	0	-6.208653	5.620002	6.038561
22	1	0	-4.751862	4.880402	6.697407
23	6	0	-5.285136	4.163921	4.731818
24	1	0	-5.800750	4.527620	3.833459
25	1	0	-5.863219	3.312548	5.107399
26	6	0	-1.233195	4.541898	2.362175
27	1	0	-1.825208	5.021030	1.566015
28	6	0	0.138373	4.145401	1.986848
29	6	0	0.964553	3.463511	2.890891
30	1	0	0.569445	3.221572	3.874262
31	6	0	2.263173	3.117944	2.535330
32	6	0	2.741185	3.450220	1.260101
33	1	0	3.760053	3.174221	0.999104
34	6	0	1.925554	4.112670	0.350756
35	6	0	0.622338	4.466773	0.724293
36	1	0	0.000000	4.993005	0.004456
37	6	0	2.444858	4.440380	-0.991393
38	1	0	3.470746	4.098348	-1.201882
39	6	0	2.392535	5.394322	-3.114935
40	1	0	3.384376	4.915186	-3.202381
41	6	0	1.519323	4.859112	-4.259032
42	1	0	0.512041	5.297573	-4.140431
43	6	0	2.097412	5.276078	-5.617040
44	1	0	1.445623	4.892463	-6.409606
45	1	0	3.071443	4.784789	-5.739961
46	6	0	2.256356	6.792839	-5.722095
47	1	0	1.267133	7.268003	-5.673297
48	1	0	2.688076	7.057455	-6.693109
49	6	0	3.126654	7.325431	-4.582821
50	1	0	4.143077	6.921673	-4.685896
51	1	0	3.210878	8.415810	-4.639497
52	6	0	2.551971	6.915566	-3.226814
53	1	0	1.565682	7.374878	-3.080210
54	1	0	3.189815	7.263774	-2.407045
55	6	0	0.338676	2.855132	-4.155402
56	1	0	-0.594509	3.440363	-4.133479
57	7	0	-2.930503	-3.651548	3.528595
58	7	0	-0.304183	-4.842750	3.265148
59	7	0	4.627585	-0.712116	3.528595

60	7	0	4.346036	2.157945	3.265148
61	6	0	-3.481765	-0.896428	2.890891
62	1	0	-3.074686	-1.117633	3.874262
63	6	0	-3.659209	-1.952866	1.986848
64	6	0	-3.316801	-3.338927	2.362175
65	1	0	-3.435736	-4.091192	1.566015
66	6	0	-2.670853	-5.051364	3.802277
67	1	0	-2.764509	-5.666637	2.889177
68	6	0	-1.232385	-5.207355	4.317675
69	1	0	-1.123510	-4.549409	5.198790
70	6	0	-0.963493	-6.659023	4.731818
71	1	0	0.062859	-6.733971	5.107399
72	1	0	-1.020659	-7.287407	3.833459
73	6	0	-1.968497	-7.143526	5.777056
74	1	0	-1.762738	-8.186853	6.038561
75	1	0	-1.850621	-6.555434	6.697407
76	6	0	-3.400475	-6.989867	5.262356
77	1	0	-4.120141	-7.305375	6.025125
78	1	0	-3.545294	-7.649245	4.395757
79	6	0	-3.674746	-5.543001	4.851959
80	1	0	-3.606014	-4.883112	5.726630
81	1	0	-4.687583	-5.432644	4.449404
82	6	0	0.539750	-3.929013	3.511395
83	1	0	0.563121	-3.403369	4.478847
84	6	0	1.568632	-3.518938	2.535330
85	6	0	1.617386	-4.099045	1.260101
86	1	0	0.868930	-4.843412	0.999104
87	6	0	2.598900	-3.723914	0.350756
88	6	0	3.557170	-2.772347	0.724293
89	1	0	4.324069	-2.496502	0.004456
90	6	0	3.520837	-2.192535	1.986848
91	6	0	2.517212	-2.567083	2.890891
92	1	0	2.505241	-2.103940	3.874262
93	6	0	4.549996	-1.202971	2.362175
94	1	0	5.260944	-0.929839	1.566015
95	6	0	5.710036	0.212655	3.802277
96	1	0	6.289707	0.439183	2.889177
97	6	0	5.125894	1.536400	4.317675
98	1	0	4.501659	1.301716	5.198790
99	6	0	6.248629	2.495102	4.731818
100	1	0	5.800360	3.421423	5.107399
101	1	0	6.821409	2.759787	3.833459
102	6	0	7.170724	1.866994	5.777056
103	1	0	6.602483	1.675032	6.697407
104	1	0	7.971391	2.566850	6.038561
105	6	0	7.753640	0.550036	5.262356
106	1	0	8.397087	0.754308	4.395757
107	1	0	8.386711	0.084540	6.025125
108	6	0	6.637753	-0.410922	4.851959
109	1	0	6.031906	-0.681344	5.726630
110	1	0	7.048599	-1.343243	4.449404
111	6	0	3.132750	2.431944	3.511395
112	1	0	2.665844	2.189361	4.478847
113	7	0	-5.284852	-1.014427	-1.845795
114	7	0	-3.692864	-0.425747	-4.197463
115	7	0	2.215140	-2.985240	-4.197463
116	7	0	3.520945	-4.069602	-1.845795
117	6	0	-4.179507	-1.694426	0.724293
118	1	0	-4.324069	-2.496502	0.004456

119	6	0	-4.524454	-0.388756	0.350756
120	6	0	-5.067911	-0.102881	-0.991393
121	1	0	-5.284646	0.956580	-1.201882
122	6	0	-5.867887	-0.625165	-3.114935
123	1	0	-5.948864	0.473363	-3.202381
124	6	0	-4.967776	-1.113784	-4.259032
125	1	0	-4.843854	-2.205346	-4.140431
126	6	0	-5.617924	-0.821627	-5.617040
127	1	0	-4.959808	-1.194285	-6.409606
128	1	0	-5.679470	0.267553	-5.739961
129	6	0	-7.010949	-1.442358	-5.722095
130	1	0	-7.455973	-1.200785	-6.693109
131	1	0	-6.927842	-2.536632	-5.673297
132	6	0	-7.907336	-0.954954	-4.582821
133	1	0	-8.893744	-1.427203	-4.639497
134	1	0	-8.065883	0.127174	-4.685896
135	6	0	-7.265041	-1.247711	-3.226814
136	1	0	-7.169673	-2.331518	-3.080210
137	1	0	-7.885520	-0.869426	-2.407045
138	6	0	-2.641955	-1.134264	-4.155402
139	1	0	-2.682187	-2.235042	-4.133479
140	6	0	-1.288456	-0.545639	-4.152656
141	6	0	-1.107248	0.843601	-4.156113
142	1	0	-1.986935	1.482844	-4.157094
143	6	0	0.171690	1.388655	-4.152656
144	6	0	1.284204	0.537104	-4.156113
145	1	0	2.277648	0.979314	-4.157094
146	6	0	1.116765	-0.843016	-4.152656
147	6	0	-0.176956	-1.380706	-4.156113
148	1	0	-0.290713	-2.462158	-4.157094
149	6	0	2.303279	-1.720868	-4.155402
150	1	0	3.276697	-1.205321	-4.133479
151	6	0	3.448453	-3.745328	-4.259032
152	1	0	4.331812	-3.092227	-4.140431
153	6	0	3.475353	-4.769157	-3.114935
154	1	0	2.564488	-5.388548	-3.202381
155	6	0	4.713070	-5.667854	-3.226814
156	1	0	4.695706	-6.394348	-2.407045
157	1	0	5.603990	-5.043359	-3.080210
158	6	0	4.780682	-6.370477	-4.582821
159	1	0	3.922806	-7.048847	-4.685896
160	1	0	5.682866	-6.988607	-4.639497
161	6	0	4.754593	-5.350481	-5.722095
162	1	0	5.660708	-4.731371	-5.673297
163	1	0	4.767897	-5.856670	-6.693109
164	6	0	3.520511	-4.454451	-5.617040
165	1	0	2.608027	-5.052342	-5.739961
166	1	0	3.514185	-3.698178	-6.409606
167	6	0	2.623053	-4.337499	-0.991393
168	1	0	1.813900	-5.054928	-1.201882
169	54	0	-0.861859	-2.247724	-0.679513
170	54	0	-1.515657	1.870253	-0.679513
171	54	0	2.377515	0.377471	-0.679513

4Xe@CC3 T cc3-rc

Standard orientation:

Center Atomic Atomic Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	7	0	-5.565537	-1.133104	0.904947
2	7	0	-5.565537	1.133104	-0.904947
3	7	0	-1.133104	0.904947	-5.565537
4	7	0	1.133104	-0.904947	-5.565537
5	6	0	-3.289567	-2.823902	1.400177
6	1	0	-3.918407	-3.054870	0.543633
7	6	0	-3.611541	-1.709899	2.186879
8	6	0	-4.781503	-0.869208	1.866004
9	1	0	-4.940701	-0.001908	2.526505
10	6	0	-6.717443	-0.272796	0.717633
11	1	0	-6.690053	0.594276	1.402032
12	6	0	-6.717443	0.272796	-0.717633
13	1	0	-6.690053	-0.594276	-1.402032
14	6	0	-7.988563	1.088918	-0.982936
15	1	0	-7.965093	1.450781	-2.016671
16	1	0	-7.968221	1.974738	-0.334762
17	6	0	-9.251821	0.270694	-0.715163
18	1	0	-10.140497	0.884845	-0.894945
19	1	0	-9.298295	-0.570823	-1.419743
20	6	0	-9.251821	-0.270694	0.715163
21	1	0	-10.140497	-0.884845	0.894945
22	1	0	-9.298295	0.570823	1.419743
23	6	0	-7.988563	-1.088918	0.982936
24	1	0	-7.968221	-1.974738	0.334762
25	1	0	-7.965093	-1.450781	2.016671
26	6	0	-4.781503	0.869208	-1.866004
27	1	0	-4.940701	0.001908	-2.526505
28	6	0	-3.611541	1.709899	-2.186879
29	6	0	-3.289567	2.823902	-1.400177
30	1	0	-3.918407	3.054870	-0.543633
31	6	0	-2.186879	3.611541	-1.709899
32	6	0	-1.400177	3.289567	-2.823902
33	1	0	-0.543633	3.918407	-3.054870
34	6	0	-1.709899	2.186879	-3.611541
35	6	0	-2.823902	1.400177	-3.289567
36	1	0	-3.054870	0.543633	-3.918407
37	6	0	-0.869208	1.866004	-4.781503
38	1	0	-0.001908	2.526505	-4.940701
39	6	0	-0.272796	0.717633	-6.717443
40	1	0	0.594276	1.402032	-6.690053
41	6	0	0.272796	-0.717633	-6.717443
42	1	0	-0.594276	-1.402032	-6.690053
43	6	0	1.088918	-0.982936	-7.988563
44	1	0	1.450781	-2.016671	-7.965093
45	1	0	1.974738	-0.334762	-7.968221
46	6	0	0.270694	-0.715163	-9.251821
47	1	0	-0.570823	-1.419743	-9.298295
48	1	0	0.884845	-0.894945	-10.140497
49	6	0	-0.270694	0.715163	-9.251821
50	1	0	0.570823	1.419743	-9.298295
51	1	0	-0.884845	0.894945	-10.140497
52	6	0	-1.088918	0.982936	-7.988563
53	1	0	-1.974738	0.334762	-7.968221
54	1	0	-1.450781	2.016671	-7.965093
55	6	0	0.869208	-1.866004	-4.781503
56	1	0	0.001908	-2.526505	-4.940701
57	7	0	-1.133104	-0.904947	5.565537

58	7	0	1.133104	0.904947	5.565537
59	7	0	0.904947	5.565537	1.133104
60	7	0	-0.904947	5.565537	-1.133104
61	6	0	-2.823902	-1.400177	3.289567
62	1	0	-3.054870	-0.543633	3.918407
63	6	0	-1.709899	-2.186879	3.611541
64	6	0	-0.869208	-1.866004	4.781503
65	1	0	-0.001908	-2.526505	4.940701
66	6	0	-0.272796	-0.717633	6.717443
67	1	0	0.594276	-1.402032	6.690053
68	6	0	0.272796	0.717633	6.717443
69	1	0	-0.594276	1.402032	6.690053
70	6	0	1.088918	0.982936	7.988563
71	1	0	1.450781	2.016671	7.965093
72	1	0	1.974738	0.334762	7.968221
73	6	0	0.270694	0.715163	9.251821
74	1	0	0.884845	0.894945	10.140497
75	1	0	-0.570823	1.419743	9.298295
76	6	0	-0.270694	-0.715163	9.251821
77	1	0	-0.884845	-0.894945	10.140497
78	1	0	0.570823	-1.419743	9.298295
79	6	0	-1.088918	-0.982936	7.988563
80	1	0	-1.974738	-0.334762	7.968221
81	1	0	-1.450781	-2.016671	7.965093
82	6	0	0.869208	1.866004	4.781503
83	1	0	0.001908	2.526505	4.940701
84	6	0	1.709899	2.186879	3.611541
85	6	0	2.823902	1.400177	3.289567
86	1	0	3.054870	0.543633	3.918407
87	6	0	3.611541	1.709899	2.186879
88	6	0	3.289567	2.823902	1.400177
89	1	0	3.918407	3.054870	0.543633
90	6	0	2.186879	3.611541	1.709899
91	6	0	1.400177	3.289567	2.823902
92	1	0	0.543633	3.918407	3.054870
93	6	0	1.866004	4.781503	0.869208
94	1	0	2.526505	4.940701	0.001908
95	6	0	0.717633	6.717443	0.272796
96	1	0	1.402032	6.690053	-0.594276
97	6	0	-0.717633	6.717443	-0.272796
98	1	0	-1.402032	6.690053	0.594276
99	6	0	-0.982936	7.988563	-1.088918
100	1	0	-2.016671	7.965093	-1.450781
101	1	0	-0.334762	7.968221	-1.974738
102	6	0	-0.715163	9.251821	-0.270694
103	1	0	-1.419743	9.298295	0.570823
104	1	0	-0.894945	10.140497	-0.884845
105	6	0	0.715163	9.251821	0.270694
106	1	0	1.419743	9.298295	-0.570823
107	1	0	0.894945	10.140497	0.884845
108	6	0	0.982936	7.988563	1.088918
109	1	0	0.334762	7.968221	1.974738
110	1	0	2.016671	7.965093	1.450781
111	6	0	-1.866004	4.781503	-0.869208
112	1	0	-2.526505	4.940701	-0.001908
113	7	0	-0.904947	-5.565537	1.133104
114	7	0	0.904947	-5.565537	-1.133104
115	7	0	5.565537	-1.133104	-0.904947
116	7	0	5.565537	1.133104	0.904947

117	6	0	-1.400177	-3.289567	2.823902
118	1	0	-0.543633	-3.918407	3.054870
119	6	0	-2.186879	-3.611541	1.709899
120	6	0	-1.866004	-4.781503	0.869208
121	1	0	-2.526505	-4.940701	0.001908
122	6	0	-0.717633	-6.717443	0.272796
123	1	0	-1.402032	-6.690053	-0.594276
124	6	0	0.717633	-6.717443	-0.272796
125	1	0	1.402032	-6.690053	0.594276
126	6	0	0.982936	-7.988563	-1.088918
127	1	0	2.016671	-7.965093	-1.450781
128	1	0	0.334762	-7.968221	-1.974738
129	6	0	0.715163	-9.251821	-0.270694
130	1	0	0.894945	-10.140497	-0.884845
131	1	0	1.419743	-9.298295	0.570823
132	6	0	-0.715163	-9.251821	0.270694
133	1	0	-0.894945	-10.140497	0.884845
134	1	0	-1.419743	-9.298295	-0.570823
135	6	0	-0.982936	-7.988563	1.088918
136	1	0	-0.334762	-7.968221	1.974738
137	1	0	-2.016671	-7.965093	1.450781
138	6	0	1.866004	-4.781503	-0.869208
139	1	0	2.526505	-4.940701	-0.001908
140	6	0	2.186879	-3.611541	-1.709899
141	6	0	1.400177	-3.289567	-2.823902
142	1	0	0.543633	-3.918407	-3.054870
143	6	0	1.709899	-2.186879	-3.611541
144	6	0	2.823902	-1.400177	-3.289567
145	1	0	3.054870	-0.543633	-3.918407
146	6	0	3.611541	-1.709899	-2.186879
147	6	0	3.289567	-2.823902	-1.400177
148	1	0	3.918407	-3.054870	-0.543633
149	6	0	4.781503	-0.869208	-1.866004
150	1	0	4.940701	-0.001908	-2.526505
151	6	0	6.717443	-0.272796	-0.717633
152	1	0	6.690053	0.594276	-1.402032
153	6	0	6.717443	0.272796	0.717633
154	1	0	6.690053	-0.594276	1.402032
155	6	0	7.988563	1.088918	0.982936
156	1	0	7.965093	1.450781	2.016671
157	1	0	7.968221	1.974738	0.334762
158	6	0	9.251821	0.270694	0.715163
159	1	0	9.298295	-0.570823	1.419743
160	1	0	10.140497	0.884845	0.894945
161	6	0	9.251821	-0.270694	-0.715163
162	1	0	9.298295	0.570823	-1.419743
163	1	0	10.140497	-0.884845	-0.894945
164	6	0	7.988563	-1.088918	-0.982936
165	1	0	7.968221	-1.974738	-0.334762
166	1	0	7.965093	-1.450781	-2.016671
167	6	0	4.781503	0.869208	1.866004
168	1	0	4.940701	0.001908	2.526505
169	54	0	1.470786	-1.470786	1.470786
170	54	0	-1.470786	1.470786	1.470786
171	54	0	-1.470786	-1.470786	-1.470786
172	54	0	1.470786	1.470786	-1.470786

4Xe@CC3 C1 cc3-rcx

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-4.804906	0.715158	3.068899
2	7	0	-3.383492	3.228672	3.334169
3	7	0	-0.557616	5.354259	-2.044085
4	7	0	-0.112445	3.718109	-4.395865
5	6	0	-4.241532	-1.271260	1.062192
6	1	0	-4.912088	-0.457309	0.797208
7	6	0	-3.679236	-1.285805	2.345357
8	6	0	-3.990993	-0.223717	3.321803
9	1	0	-3.481189	-0.306721	4.295031
10	6	0	-5.082565	1.670619	4.123205
11	1	0	-4.436219	1.500734	5.003226
12	6	0	-4.800089	3.090157	3.610818
13	1	0	-5.406149	3.240672	2.699243
14	6	0	-5.199348	4.131525	4.663485
15	1	0	-4.999676	5.131410	4.262844
16	1	0	-4.547631	4.002302	5.537424
17	6	0	-6.664637	3.986377	5.074546
18	1	0	-6.914213	4.729717	5.839022
19	1	0	-7.308956	4.191349	4.208787
20	6	0	-6.944996	2.572763	5.586215
21	1	0	-8.002396	2.460116	5.848170
22	1	0	-6.369406	2.400847	6.505956
23	6	0	-6.552412	1.531097	4.538561
24	1	0	-7.174039	1.645531	3.640947
25	1	0	-6.717576	0.514602	4.912144
26	6	0	-3.042659	3.612444	2.174655
27	1	0	-3.784598	3.808716	1.384149
28	6	0	-1.634229	3.846539	1.800007
29	6	0	-0.598219	3.602290	2.710757
30	1	0	-0.852512	3.227985	3.699127
31	6	0	0.726078	3.829215	2.345357
32	6	0	1.019823	4.308905	1.062192
33	1	0	2.060003	4.482648	0.797208
34	6	0	0.000000	4.552264	0.155885
35	6	0	-1.330789	4.323772	0.530247
36	1	0	-2.116725	4.524579	-0.193864
37	6	0	0.331756	5.060093	-1.189503
38	1	0	1.406124	5.182629	-1.400865
39	6	0	-0.119477	5.900836	-3.313459
40	1	0	0.981804	5.883956	-3.402246
41	6	0	-0.687072	5.047743	-4.457074
42	1	0	-1.785064	5.019919	-4.336673
43	6	0	-0.340504	5.669792	-5.815294
44	1	0	-0.770789	5.047465	-6.607558
45	1	0	0.749690	5.635060	-5.939422
46	6	0	-0.835749	7.112373	-5.919358
47	1	0	-1.932977	7.126492	-5.868804
48	1	0	-0.557215	7.534456	-6.890755
49	6	0	-0.269069	7.961805	-4.780832
50	1	0	0.822658	8.023555	-4.885667
51	1	0	-0.651977	8.986247	-4.836682
52	6	0	-0.615689	7.347812	-3.424408
53	1	0	-1.703519	7.349159	-3.276303
54	1	0	-0.182838	7.932094	-2.604988

55	6	0	-0.908409	2.732252	-4.346521
56	1	0	-2.001567	2.866400	-4.317984
57	7	0	-1.104366	-4.544526	3.334169
58	7	0	1.783108	-4.518750	3.068899
59	7	0	4.487858	1.315854	3.334169
60	7	0	3.021798	3.803592	3.068899
61	6	0	-2.820565	-2.319218	2.710757
62	1	0	-2.369261	-2.352289	3.699127
63	6	0	-2.514086	-3.338553	1.800007
64	6	0	-1.607139	-4.441242	2.174655
65	1	0	-1.406145	-5.181916	1.384149
66	6	0	-0.276110	-5.702078	3.610818
67	1	0	-0.103429	-6.302198	2.699243
68	6	0	1.094484	-5.236940	4.123205
69	1	0	0.918435	-4.592246	5.003226
70	6	0	1.950237	-6.440104	4.538561
71	1	0	2.913130	-6.074892	4.912144
72	1	0	2.161948	-7.035665	3.640947
73	6	0	1.244420	-7.300924	5.586215
74	1	0	1.870675	-8.160336	5.848170
75	1	0	1.105508	-6.716491	6.505956
76	6	0	-0.119985	-7.764934	5.074546
77	1	0	-0.638949	-8.352742	5.839022
78	1	0	0.024663	-8.425416	4.208787
79	6	0	-0.978332	-6.568530	4.663485
80	1	0	-1.192280	-5.939515	5.537424
81	1	0	-1.944094	-6.895551	4.262844
82	6	0	2.189241	-3.344443	3.321803
83	1	0	2.006223	-2.861437	4.295031
84	6	0	2.953158	-2.543410	2.345357
85	6	0	3.221710	-3.037645	1.062192
86	1	0	2.852085	-4.025339	0.797208
87	6	0	3.942376	-2.276132	0.155885
88	6	0	4.409891	-1.009389	0.530247
89	1	0	4.976763	-0.429153	-0.193864
90	6	0	4.148315	-0.507986	1.800007
91	6	0	3.418784	-1.283072	2.710757
92	1	0	3.221773	-0.875696	3.699127
93	6	0	4.649798	0.828798	2.174655
94	1	0	5.190744	1.373200	1.384149
95	6	0	5.076199	2.611920	3.610818
96	1	0	5.509578	3.061527	2.699243
97	6	0	3.988081	3.566321	4.123205
98	1	0	3.517784	3.091511	5.003226
99	6	0	4.602175	4.909007	4.538561
100	1	0	3.804446	5.560291	4.912144
101	1	0	5.012091	5.390135	3.640947
102	6	0	5.700576	4.728162	5.586215
103	1	0	5.263898	4.315644	6.505956
104	1	0	6.131721	5.700220	5.848170
105	6	0	6.784622	3.778557	5.074546
106	1	0	7.284293	4.234067	4.208787
107	1	0	7.553161	3.623025	5.839022
108	6	0	6.177680	2.437005	4.663485
109	1	0	5.739911	1.937213	5.537424
110	1	0	6.943769	1.764141	4.262844
111	6	0	1.801752	3.568160	3.321803
112	1	0	1.474966	3.168159	4.295031
113	7	0	-4.358117	-3.160040	-2.044085

114	7	0	-3.163755	-1.956435	-4.395865
115	7	0	3.276199	-1.761675	-4.395865
116	7	0	4.915733	-2.194220	-2.044085
117	6	0	-3.079102	-3.314383	0.530247
118	1	0	-2.860039	-4.095427	-0.193864
119	6	0	-3.942376	-2.276132	0.155885
120	6	0	-4.548047	-2.242738	-1.189503
121	1	0	-5.191350	-1.373575	-1.400865
122	6	0	-5.050535	-3.053888	-3.313459
123	1	0	-5.586557	-2.091711	-3.402246
124	6	0	-4.027938	-3.118893	-4.457074
125	1	0	-3.454846	-4.055870	-4.336673
126	6	0	-4.739932	-3.129781	-5.815294
127	1	0	-3.985839	-3.191255	-6.607558
128	1	0	-5.254950	-2.168280	-5.939422
129	6	0	-5.741621	-4.279966	-5.919358
130	1	0	-6.246423	-4.249790	-6.890755
131	1	0	-5.205235	-5.237253	-5.868804
132	6	0	-6.760591	-4.213923	-4.780832
133	1	0	-7.456330	-5.057752	-4.836682
134	1	0	-7.359932	-3.299335	-4.885667
135	6	0	-6.055547	-4.207109	-3.424408
136	1	0	-5.512799	-5.149870	-3.276303
137	1	0	-6.777976	-4.124390	-2.604988
138	6	0	-1.911995	-2.152831	-4.346521
139	1	0	-1.481592	-3.166608	-4.317984
140	6	0	-0.932976	-1.037691	-4.346204
141	6	0	-1.361236	0.296131	-4.347461
142	1	0	-2.429340	0.499852	-4.348970
143	6	0	-0.432179	1.326826	-4.346204
144	6	0	0.937075	1.030799	-4.347461
145	1	0	1.647554	1.853945	-4.348970
146	6	0	1.365155	-0.289135	-4.346204
147	6	0	0.424161	-1.326930	-4.347461
148	1	0	0.781786	-2.353796	-4.348970
149	6	0	2.820404	-0.579420	-4.346521
150	1	0	3.483159	0.300208	-4.317984
151	6	0	4.715010	-1.928850	-4.457074
152	1	0	5.239910	-0.964049	-4.336673
153	6	0	5.170012	-2.846948	-3.313459
154	1	0	4.604754	-3.792245	-3.402246
155	6	0	6.671237	-3.140703	-3.424408
156	1	0	6.960814	-3.807704	-2.604988
157	1	0	7.216318	-2.199289	-3.276303
158	6	0	7.029660	-3.747882	-4.780832
159	1	0	6.537274	-4.724220	-4.885667
160	1	0	8.108306	-3.928495	-4.836682
161	6	0	6.577370	-2.832406	-5.919358
162	1	0	7.138212	-1.889239	-5.868804
163	1	0	6.803638	-3.284666	-6.890755
164	6	0	5.080436	-2.540011	-5.815294
165	1	0	4.505260	-3.466780	-5.939422
166	1	0	4.756627	-1.856210	-6.607558
167	6	0	4.216291	-2.817355	-1.189503
168	1	0	3.785226	-3.809053	-1.400865
169	54	0	0.178304	-2.390153	-0.861816
170	54	0	0.000000	0.000000	2.696002
171	54	0	-2.159085	1.040661	-0.861816
172	54	0	1.980781	1.349492	-0.861816

5Xe@CC3 T cc3-xexx

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-5.545360	-1.125960	0.887581
2	7	0	-5.545360	1.125960	-0.887581
3	7	0	-1.125960	0.887581	-5.545360
4	7	0	1.125960	-0.887581	-5.545360
5	6	0	-3.206034	-2.744408	1.317485
6	1	0	-3.848223	-2.991553	0.476042
7	6	0	-3.531616	-1.630916	2.104601
8	6	0	-4.731587	-0.823598	1.811687
9	1	0	-4.889759	0.050100	2.463760
10	6	0	-6.710771	-0.282165	0.714348
11	1	0	-6.692993	0.577176	1.409008
12	6	0	-6.710771	0.282165	-0.714348
13	1	0	-6.692993	-0.577176	-1.409008
14	6	0	-7.976675	1.109324	-0.962886
15	1	0	-7.954631	1.490625	-1.989584
16	1	0	-7.952984	1.982212	-0.297577
17	6	0	-9.240650	0.286847	-0.709072
18	1	0	-10.129169	0.905449	-0.873516
19	1	0	-9.289483	-0.538688	-1.432150
20	6	0	-9.240650	-0.286847	0.709072
21	1	0	-10.129169	-0.905449	0.873516
22	1	0	-9.289483	0.538688	1.432150
23	6	0	-7.976675	-1.109324	0.962886
24	1	0	-7.952984	-1.982212	0.297577
25	1	0	-7.954631	-1.490625	1.989584
26	6	0	-4.731587	0.823598	-1.811687
27	1	0	-4.889759	-0.050100	-2.463760
28	6	0	-3.531616	1.630916	-2.104601
29	6	0	-3.206034	2.744408	-1.317485
30	1	0	-3.848223	2.991553	-0.476042
31	6	0	-2.104601	3.531616	-1.630916
32	6	0	-1.317485	3.206034	-2.744408
33	1	0	-0.476042	3.848223	-2.991553
34	6	0	-1.630916	2.104601	-3.531616
35	6	0	-2.744408	1.317485	-3.206034
36	1	0	-2.991553	0.476042	-3.848223
37	6	0	-0.823598	1.811687	-4.731587
38	1	0	0.050100	2.463760	-4.889759
39	6	0	-0.282165	0.714348	-6.710771
40	1	0	0.577176	1.409008	-6.692993
41	6	0	0.282165	-0.714348	-6.710771
42	1	0	-0.577176	-1.409008	-6.692993
43	6	0	1.109324	-0.962886	-7.976675
44	1	0	1.490625	-1.989584	-7.954631
45	1	0	1.982212	-0.297577	-7.952984
46	6	0	0.286847	-0.709072	-9.240650
47	1	0	-0.538688	-1.432150	-9.289483
48	1	0	0.905449	-0.873516	-10.129169
49	6	0	-0.286847	0.709072	-9.240650
50	1	0	0.538688	1.432150	-9.289483
51	1	0	-0.905449	0.873516	-10.129169

52	6	0	-1.109324	0.962886	-7.976675
53	1	0	-1.982212	0.297577	-7.952984
54	1	0	-1.490625	1.989584	-7.954631
55	6	0	0.823598	-1.811687	-4.731587
56	1	0	-0.050100	-2.463760	-4.889759
57	7	0	-1.125960	-0.887581	5.545360
58	7	0	1.125960	0.887581	5.545360
59	7	0	0.887581	5.545360	1.125960
60	7	0	-0.887581	5.545360	-1.125960
61	6	0	-2.744408	-1.317485	3.206034
62	1	0	-2.991553	-0.476042	3.848223
63	6	0	-1.630916	-2.104601	3.531616
64	6	0	-0.823598	-1.811687	4.731587
65	1	0	0.050100	-2.463760	4.889759
66	6	0	-0.282165	-0.714348	6.710771
67	1	0	0.577176	-1.409008	6.692993
68	6	0	0.282165	0.714348	6.710771
69	1	0	-0.577176	1.409008	6.692993
70	6	0	1.109324	0.962886	7.976675
71	1	0	1.490625	1.989584	7.954631
72	1	0	1.982212	0.297577	7.952984
73	6	0	0.286847	0.709072	9.240650
74	1	0	0.905449	0.873516	10.129169
75	1	0	-0.538688	1.432150	9.289483
76	6	0	-0.286847	-0.709072	9.240650
77	1	0	-0.905449	-0.873516	10.129169
78	1	0	0.538688	-1.432150	9.289483
79	6	0	-1.109324	-0.962886	7.976675
80	1	0	-1.982212	-0.297577	7.952984
81	1	0	-1.490625	-1.989584	7.954631
82	6	0	0.823598	1.811687	4.731587
83	1	0	-0.050100	2.463760	4.889759
84	6	0	1.630916	2.104601	3.531616
85	6	0	2.744408	1.317485	3.206034
86	1	0	2.991553	0.476042	3.848223
87	6	0	3.531616	1.630916	2.104601
88	6	0	3.206034	2.744408	1.317485
89	1	0	3.848223	2.991553	0.476042
90	6	0	2.104601	3.531616	1.630916
91	6	0	1.317485	3.206034	2.744408
92	1	0	0.476042	3.848223	2.991553
93	6	0	1.811687	4.731587	0.823598
94	1	0	2.463760	4.889759	-0.050100
95	6	0	0.714348	6.710771	0.282165
96	1	0	1.409008	6.692993	-0.577176
97	6	0	-0.714348	6.710771	-0.282165
98	1	0	-1.409008	6.692993	0.577176
99	6	0	-0.962886	7.976675	-1.109324
100	1	0	-1.989584	7.954631	-1.490625
101	1	0	-0.297577	7.952984	-1.982212
102	6	0	-0.709072	9.240650	-0.286847
103	1	0	-1.432150	9.289483	0.538688
104	1	0	-0.873516	10.129169	-0.905449
105	6	0	0.709072	9.240650	0.286847
106	1	0	1.432150	9.289483	-0.538688
107	1	0	0.873516	10.129169	0.905449
108	6	0	0.962886	7.976675	1.109324
109	1	0	0.297577	7.952984	1.982212
110	1	0	1.989584	7.954631	1.490625

111	6	0	-1.811687	4.731587	-0.823598
112	1	0	-2.463760	4.889759	0.050100
113	7	0	-0.887581	-5.545360	1.125960
114	7	0	0.887581	-5.545360	-1.125960
115	7	0	5.545360	-1.125960	-0.887581
116	7	0	5.545360	1.125960	0.887581
117	6	0	-1.317485	-3.206034	2.744408
118	1	0	-0.476042	-3.848223	2.991553
119	6	0	-2.104601	-3.531616	1.630916
120	6	0	-1.811687	-4.731587	0.823598
121	1	0	-2.463760	-4.889759	-0.050100
122	6	0	-0.714348	-6.710771	0.282165
123	1	0	-1.409008	-6.692993	-0.577176
124	6	0	0.714348	-6.710771	-0.282165
125	1	0	1.409008	-6.692993	0.577176
126	6	0	0.962886	-7.976675	-1.109324
127	1	0	1.989584	-7.954631	-1.490625
128	1	0	0.297577	-7.952984	-1.982212
129	6	0	0.709072	-9.240650	-0.286847
130	1	0	0.873516	-10.129169	-0.905449
131	1	0	1.432150	-9.289483	0.538688
132	6	0	-0.709072	-9.240650	0.286847
133	1	0	-0.873516	-10.129169	0.905449
134	1	0	-1.432150	-9.289483	-0.538688
135	6	0	-0.962886	-7.976675	1.109324
136	1	0	-0.297577	-7.952984	1.982212
137	1	0	-1.989584	-7.954631	1.490625
138	6	0	1.811687	-4.731587	-0.823598
139	1	0	2.463760	-4.889759	0.050100
140	6	0	2.104601	-3.531616	-1.630916
141	6	0	1.317485	-3.206034	-2.744408
142	1	0	0.476042	-3.848223	-2.991553
143	6	0	1.630916	-2.104601	-3.531616
144	6	0	2.744408	-1.317485	-3.206034
145	1	0	2.991553	-0.476042	-3.848223
146	6	0	3.531616	-1.630916	-2.104601
147	6	0	3.206034	-2.744408	-1.317485
148	1	0	3.848223	-2.991553	-0.476042
149	6	0	4.731587	-0.823598	-1.811687
150	1	0	4.889759	0.050100	-2.463760
151	6	0	6.710771	-0.282165	-0.714348
152	1	0	6.692993	0.577176	-1.409008
153	6	0	6.710771	0.282165	0.714348
154	1	0	6.692993	-0.577176	1.409008
155	6	0	7.976675	1.109324	0.962886
156	1	0	7.954631	1.490625	1.989584
157	1	0	7.952984	1.982212	0.297577
158	6	0	9.240650	0.286847	0.709072
159	1	0	9.289483	-0.538688	1.432150
160	1	0	10.129169	0.905449	0.873516
161	6	0	9.240650	-0.286847	-0.709072
162	1	0	9.289483	0.538688	-1.432150
163	1	0	10.129169	-0.905449	-0.873516
164	6	0	7.976675	-1.109324	-0.962886
165	1	0	7.952984	-1.982212	-0.297577
166	1	0	7.954631	-1.490625	-1.989584
167	6	0	4.731587	0.823598	1.811687
168	1	0	4.889759	-0.050100	2.463760
169	54	0	2.361199	-2.361199	2.361199

170	54	0	-2.361199	2.361199	2.361199
171	54	0	-2.361199	-2.361199	-2.361199
172	54	0	2.361199	2.361199	-2.361199
173	54	0	0.000000	0.000000	0.000000

5Xe@CC3 C1 cc3-xexxqq

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-2.906564	-0.153895	-4.926692
2	7	0	-3.445488	2.452311	-3.863531
3	7	0	1.635315	5.341718	-1.194560
4	7	0	4.076452	4.023035	-0.457960
5	6	0	-0.748182	-1.790946	-3.954217
6	1	0	-0.526234	-1.069860	-4.736679
7	6	0	-2.050760	-1.840497	-3.438177
8	6	0	-3.105489	-0.950710	-3.960701
9	1	0	-4.089118	-1.039421	-3.472640
10	6	0	-4.027216	0.644957	-5.380754
11	1	0	-4.923135	0.473539	-4.756794
12	6	0	-3.661201	2.131916	-5.260293
13	1	0	-2.745830	2.296271	-5.857273
14	6	0	-4.791160	3.007122	-5.812995
15	1	0	-4.500568	4.059458	-5.722902
16	1	0	-5.676688	2.865017	-5.179952
17	6	0	-5.116550	2.649160	-7.263719
18	1	0	-5.939069	3.273554	-7.628104
19	1	0	-4.246107	2.868396	-7.896997
20	6	0	-5.470278	1.166248	-7.392029
21	1	0	-5.665855	0.906624	-8.437753
22	1	0	-6.396630	0.967005	-6.836194
23	6	0	-4.347292	0.289237	-6.836556
24	1	0	-3.434100	0.421400	-7.431308
25	1	0	-4.612771	-0.772109	-6.891736
26	6	0	-2.310443	2.911094	-3.533562
27	1	0	-1.506315	3.061015	-4.271519
28	6	0	-1.988518	3.306229	-2.148732
29	6	0	-2.918366	3.124317	-1.115175
30	1	0	-3.876539	2.669018	-1.351988
31	6	0	-2.629182	3.549097	0.175788
32	6	0	-1.397170	4.163394	0.441161
33	1	0	-1.197264	4.512722	1.450936
34	6	0	-0.468522	4.349331	-0.575596
35	6	0	-0.771461	3.917944	-1.874597
36	1	0	-0.045995	4.097433	-2.663894
37	6	0	0.796330	5.053231	-0.288654
38	1	0	0.955610	5.336964	0.763831
39	6	0	2.821536	6.076897	-0.803076
40	1	0	2.858699	6.228050	0.291037
41	6	0	4.066493	5.268919	-1.198212
42	1	0	4.012548	5.089573	-2.287342
43	6	0	5.340356	6.058324	-0.877297
44	1	0	6.210226	5.463394	-1.176288
45	1	0	5.400225	6.186727	0.211289
46	6	0	5.342725	7.421372	-1.570387
47	1	0	5.360205	7.276218	-2.659134

48	1	0	6.252125	7.972680	-1.309157
49	6	0	4.098636	8.226698	-1.190670
50	1	0	4.130919	8.455359	-0.116709
51	1	0	4.085366	9.185859	-1.718882
52	6	0	2.825010	7.440091	-1.503527
53	1	0	2.740275	7.270862	-2.584866
54	1	0	1.933110	7.997695	-1.197562
55	6	0	4.104322	2.944087	-1.123420
56	1	0	4.112556	2.940002	-2.225038
57	7	0	-2.914950	-4.890761	-0.585775
58	7	0	-2.759614	-4.486149	2.245308
59	7	0	-3.615864	1.591880	4.144578
60	7	0	-3.477397	3.863839	2.405730
61	6	0	-2.365353	-2.778869	-2.462884
62	1	0	-3.374346	-2.854825	-2.065936
63	6	0	-1.391160	-3.671901	-1.994680
64	6	0	-1.731769	-4.712240	-1.005198
65	1	0	-0.893561	-5.343497	-0.669613
66	6	0	-3.138745	-5.967757	0.357657
67	1	0	-2.192446	-6.472163	0.624810
68	6	0	-3.728650	-5.384369	1.650523
69	1	0	-4.658195	-4.851774	1.379133
70	6	0	-4.057305	-6.505848	2.641763
71	1	0	-4.483252	-6.063428	3.548861
72	1	0	-3.117551	-6.991947	2.934459
73	6	0	-5.013023	-7.530608	2.029206
74	1	0	-5.215214	-8.331007	2.748674
75	1	0	-5.975325	-7.047127	1.812430
76	6	0	-4.436773	-8.105868	0.733967
77	1	0	-5.141078	-8.810494	0.279382
78	1	0	-3.524611	-8.672562	0.965416
79	6	0	-4.102202	-6.989279	-0.255962
80	1	0	-5.017104	-6.461881	-0.555774
81	1	0	-3.654130	-7.394777	-1.169629
82	6	0	-3.107483	-3.280322	2.425291
83	1	0	-4.107462	-2.914453	2.142868
84	6	0	-2.216506	-2.285272	3.052385
85	6	0	-0.906057	-2.624450	3.417562
86	1	0	-0.555149	-3.633057	3.214780
87	6	0	-0.089746	-1.698741	4.055865
88	6	0	-0.586308	-0.417748	4.335568
89	1	0	0.055247	0.285838	4.859845
90	6	0	-1.884134	-0.071255	3.979668
91	6	0	-2.698468	-1.013057	3.335046
92	1	0	-3.719919	-0.735145	3.088117
93	6	0	-2.407454	1.260782	4.339114
94	1	0	-1.685332	1.945239	4.812132
95	6	0	-4.028145	2.913482	4.572871
96	1	0	-3.178256	3.486127	4.986508
97	6	0	-4.556258	3.690319	3.357457
98	1	0	-5.385526	3.102546	2.923670
99	6	0	-5.080082	5.064463	3.788255
100	1	0	-5.457278	5.592593	2.905769
101	1	0	-4.234702	5.649303	4.173476
102	6	0	-6.165299	4.937930	4.858282
103	1	0	-7.034899	4.416965	4.434999
104	1	0	-6.508559	5.932157	5.162998
105	6	0	-5.649432	4.154058	6.066595
106	1	0	-4.842209	4.723010	6.547673

107	1	0	-6.441303	4.033881	6.813374
108	6	0	-5.119920	2.784063	5.640351
109	1	0	-5.934447	2.175156	5.226925
110	1	0	-4.714629	2.234707	6.497030
111	6	0	-3.643668	3.401265	1.236959
112	1	0	-4.569516	2.881616	0.943062
113	7	0	2.470361	-3.486217	-3.800772
114	7	0	4.660398	-1.955401	-2.753392
115	7	0	4.393432	-0.958845	3.593368
116	7	0	2.018342	-1.332113	5.160408
117	6	0	-0.103110	-3.613167	-2.512786
118	1	0	0.662452	-4.312420	-2.186612
119	6	0	0.225708	-2.670222	-3.496724
120	6	0	1.572921	-2.641196	-4.098146
121	1	0	1.743305	-1.850169	-4.845739
122	6	0	3.741554	-3.386652	-4.490234
123	1	0	3.767712	-2.508743	-5.160949
124	6	0	4.861907	-3.207290	-3.455105
125	1	0	4.815281	-4.068312	-2.763907
126	6	0	6.229821	-3.185768	-4.145917
127	1	0	7.008670	-3.065813	-3.384971
128	1	0	6.274897	-2.299109	-4.791639
129	6	0	6.458919	-4.452181	-4.971819
130	1	0	7.432684	-4.403134	-5.470385
131	1	0	6.487359	-5.323089	-4.302904
132	6	0	5.339461	-4.642609	-5.997037
133	1	0	5.487598	-5.569895	-6.560391
134	1	0	5.372528	-3.819810	-6.724132
135	6	0	3.972160	-4.659460	-5.312291
136	1	0	3.896966	-5.522478	-4.638005
137	1	0	3.165393	-4.757745	-6.046783
138	6	0	4.544913	-2.000654	-1.491559
139	1	0	4.587866	-2.951635	-0.936980
140	6	0	4.369733	-0.788817	-0.668413
141	6	0	4.277379	0.477048	-1.263823
142	1	0	4.326552	0.546512	-2.347485
143	6	0	4.153458	1.617375	-0.479619
144	6	0	4.124380	1.495447	0.916722
145	1	0	4.051897	2.399708	1.515538
146	6	0	4.215404	0.245964	1.517522
147	6	0	4.341205	-0.897627	0.716511
148	1	0	4.437706	-1.864781	1.203057
149	6	0	4.226172	0.143316	2.989347
150	1	0	4.097539	1.091960	3.534493
151	6	0	4.416065	-0.935072	5.042211
152	1	0	4.219730	0.080392	5.431614
153	6	0	3.306168	-1.853867	5.573465
154	1	0	3.483956	-2.861982	5.157061
155	6	0	3.355387	-1.922332	7.103819
156	1	0	2.560818	-2.590235	7.453958
157	1	0	3.130727	-0.923523	7.500088
158	6	0	4.724481	-2.390825	7.598586
159	1	0	4.901814	-3.420135	7.258294
160	1	0	4.739931	-2.411566	8.693368
161	6	0	5.835640	-1.486159	7.062620
162	1	0	5.713097	-0.477765	7.480798
163	1	0	6.816551	-1.847720	7.388615
164	6	0	5.786516	-1.411361	5.536017
165	1	0	5.983428	-2.400249	5.101892

166	1	0	6.556753	-0.734806	5.150032
167	6	0	1.263693	-2.097594	4.487789
168	1	0	1.569933	-3.118887	4.210477
169	54	0	1.690044	-3.600105	0.822643
170	54	0	-4.164027	-0.349659	-0.122848
171	54	0	1.384919	1.318948	-3.556642
172	54	0	1.093251	2.646350	2.873653
173	54	0	-0.110126	-0.017207	0.010127

Kr@CC3 T cc3-krx

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-1.116843	-0.902661	5.540784
2	7	0	1.116843	0.902661	5.540784
3	7	0	0.902661	5.540784	1.116843
4	7	0	-0.902661	5.540784	-1.116843
5	6	0	-2.704301	-1.283430	3.174928
6	1	0	-2.938042	-0.434762	3.812605
7	6	0	-1.594389	-2.077187	3.497433
8	6	0	-0.783241	-1.787359	4.696277
9	1	0	0.119431	-2.404880	4.823887
10	6	0	-0.268765	-0.720182	6.701724
11	1	0	0.603985	-1.397624	6.676907
12	6	0	0.268765	0.720182	6.701724
13	1	0	-0.603985	1.397624	6.676907
14	6	0	1.086050	0.988685	7.969732
15	1	0	1.444239	2.023640	7.947429
16	1	0	1.973950	0.343510	7.947977
17	6	0	0.268628	0.716161	9.232905
18	1	0	0.881792	0.897422	10.121954
19	1	0	-0.575265	1.417923	9.280027
20	6	0	-0.268628	-0.716161	9.232905
21	1	0	-0.881792	-0.897422	10.121954
22	1	0	0.575265	-1.417923	9.280027
23	6	0	-1.086050	-0.988685	7.969732
24	1	0	-1.973950	-0.343510	7.947977
25	1	0	-1.444239	-2.023640	7.947429
26	6	0	0.783241	1.787359	4.696277
27	1	0	-0.119431	2.404880	4.823887
28	6	0	1.594389	2.077187	3.497433
29	6	0	2.704301	1.283430	3.174928
30	1	0	2.938042	0.434762	3.812605
31	6	0	3.497433	1.594389	2.077187
32	6	0	3.174928	2.704301	1.283430
33	1	0	3.812605	2.938042	0.434762
34	6	0	2.077187	3.497433	1.594389
35	6	0	1.283430	3.174928	2.704301
36	1	0	0.434762	3.812605	2.938042
37	6	0	1.787359	4.696277	0.783241
38	1	0	2.404880	4.823887	-0.119431
39	6	0	0.720182	6.701724	0.268765
40	1	0	1.397624	6.676907	-0.603985
41	6	0	-0.720182	6.701724	-0.268765
42	1	0	-1.397624	6.676907	0.603985
43	6	0	-0.988685	7.969732	-1.086050

44	1	0	-2.023640	7.947429	-1.444239
45	1	0	-0.343510	7.947977	-1.973950
46	6	0	-0.716161	9.232905	-0.268628
47	1	0	-1.417923	9.280027	0.575265
48	1	0	-0.897422	10.121954	-0.881792
49	6	0	0.716161	9.232905	0.268628
50	1	0	1.417923	9.280027	-0.575265
51	1	0	0.897422	10.121954	0.881792
52	6	0	0.988685	7.969732	1.086050
53	1	0	0.343510	7.947977	1.973950
54	1	0	2.023640	7.947429	1.444239
55	6	0	-1.787359	4.696277	-0.783241
56	1	0	-2.404880	4.823887	0.119431
57	7	0	-0.902661	-5.540784	1.116843
58	7	0	0.902661	-5.540784	-1.116843
59	7	0	5.540784	-1.116843	-0.902661
60	7	0	5.540784	1.116843	0.902661
61	6	0	-1.283430	-3.174928	2.704301
62	1	0	-0.434762	-3.812605	2.938042
63	6	0	-2.077187	-3.497433	1.594389
64	6	0	-1.787359	-4.696277	0.783241
65	1	0	-2.404880	-4.823887	-0.119431
66	6	0	-0.720182	-6.701724	0.268765
67	1	0	-1.397624	-6.676907	-0.603985
68	6	0	0.720182	-6.701724	-0.268765
69	1	0	1.397624	-6.676907	0.603985
70	6	0	0.988685	-7.969732	-1.086050
71	1	0	2.023640	-7.947429	-1.444239
72	1	0	0.343510	-7.947977	-1.973950
73	6	0	0.716161	-9.232905	-0.268628
74	1	0	0.897422	-10.121954	-0.881792
75	1	0	1.417923	-9.280027	0.575265
76	6	0	-0.716161	-9.232905	0.268628
77	1	0	-0.897422	-10.121954	0.881792
78	1	0	-1.417923	-9.280027	-0.575265
79	6	0	-0.988685	-7.969732	1.086050
80	1	0	-0.343510	-7.947977	1.973950
81	1	0	-2.023640	-7.947429	1.444239
82	6	0	1.787359	-4.696277	-0.783241
83	1	0	2.404880	-4.823887	0.119431
84	6	0	2.077187	-3.497433	-1.594389
85	6	0	1.283430	-3.174928	-2.704301
86	1	0	0.434762	-3.812605	-2.938042
87	6	0	1.594389	-2.077187	-3.497433
88	6	0	2.704301	-1.283430	-3.174928
89	1	0	2.938042	-0.434762	-3.812605
90	6	0	3.497433	-1.594389	-2.077187
91	6	0	3.174928	-2.704301	-1.283430
92	1	0	3.812605	-2.938042	-0.434762
93	6	0	4.696277	-0.783241	-1.787359
94	1	0	4.823887	0.119431	-2.404880
95	6	0	6.701724	-0.268765	-0.720182
96	1	0	6.676907	0.603985	-1.397624
97	6	0	6.701724	0.268765	0.720182
98	1	0	6.676907	-0.603985	1.397624
99	6	0	7.969732	1.086050	0.988685
100	1	0	7.947429	1.444239	2.023640
101	1	0	7.947977	1.973950	0.343510
102	6	0	9.232905	0.268628	0.716161

103	1	0	9.280027	-0.575265	1.417923
104	1	0	10.121954	0.881792	0.897422
105	6	0	9.232905	-0.268628	-0.716161
106	1	0	9.280027	0.575265	-1.417923
107	1	0	10.121954	-0.881792	-0.897422
108	6	0	7.969732	-1.086050	-0.988685
109	1	0	7.947977	-1.973950	-0.343510
110	1	0	7.947429	-1.444239	-2.023640
111	6	0	4.696277	0.783241	1.787359
112	1	0	4.823887	-0.119431	2.404880
113	7	0	-5.540784	-1.116843	0.902661
114	7	0	-5.540784	1.116843	-0.902661
115	7	0	-1.116843	0.902661	-5.540784
116	7	0	1.116843	-0.902661	-5.540784
117	6	0	-3.174928	-2.704301	1.283430
118	1	0	-3.812605	-2.938042	0.434762
119	6	0	-3.497433	-1.594389	2.077187
120	6	0	-4.696277	-0.783241	1.787359
121	1	0	-4.823887	0.119431	2.404880
122	6	0	-6.701724	-0.268765	0.720182
123	1	0	-6.676907	0.603985	1.397624
124	6	0	-6.701724	0.268765	-0.720182
125	1	0	-6.676907	-0.603985	-1.397624
126	6	0	-7.969732	1.086050	-0.988685
127	1	0	-7.947429	1.444239	-2.023640
128	1	0	-7.947977	1.973950	-0.343510
129	6	0	-9.232905	0.268628	-0.716161
130	1	0	-10.121954	0.881792	-0.897422
131	1	0	-9.280027	-0.575265	-1.417923
132	6	0	-9.232905	-0.268628	0.716161
133	1	0	-10.121954	-0.881792	0.897422
134	1	0	-9.280027	0.575265	1.417923
135	6	0	-7.969732	-1.086050	0.988685
136	1	0	-7.947977	-1.973950	0.343510
137	1	0	-7.947429	-1.444239	2.023640
138	6	0	-4.696277	0.783241	-1.787359
139	1	0	-4.823887	-0.119431	-2.404880
140	6	0	-3.497433	1.594389	-2.077187
141	6	0	-3.174928	2.704301	-1.283430
142	1	0	-3.812605	2.938042	-0.434762
143	6	0	-2.077187	3.497433	-1.594389
144	6	0	-1.283430	3.174928	-2.704301
145	1	0	-0.434762	3.812605	-2.938042
146	6	0	-1.594389	2.077187	-3.497433
147	6	0	-2.704301	1.283430	-3.174928
148	1	0	-2.938042	0.434762	-3.812605
149	6	0	-0.783241	1.787359	-4.696277
150	1	0	0.119431	2.404880	-4.823887
151	6	0	-0.268765	0.720182	-6.701724
152	1	0	0.603985	1.397624	-6.676907
153	6	0	0.268765	-0.720182	-6.701724
154	1	0	-0.603985	-1.397624	-6.676907
155	6	0	1.086050	-0.988685	-7.969732
156	1	0	1.444239	-2.023640	-7.947429
157	1	0	1.973950	-0.343510	-7.947977
158	6	0	0.268628	-0.716161	-9.232905
159	1	0	-0.575265	-1.417923	-9.280027
160	1	0	0.881792	-0.897422	-10.121954
161	6	0	-0.268628	0.716161	-9.232905

162	1	0	0.575265	1.417923	-9.280027
163	1	0	-0.881792	0.897422	-10.121954
164	6	0	-1.086050	0.988685	-7.969732
165	1	0	-1.973950	0.343510	-7.947977
166	1	0	-1.444239	2.023640	-7.947429
167	6	0	0.783241	-1.787359	-4.696277
168	1	0	-0.119431	-2.404880	-4.823887
169	36	0	0.000000	0.000000	0.000000

4Kr@CC3 T cc3-re

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-5.552021	-1.121895	0.907504
2	7	0	-5.552021	1.121895	-0.907504
3	7	0	-1.121895	0.907504	-5.552021
4	7	0	1.121895	-0.907504	-5.552021
5	6	0	-3.220987	-2.749537	1.329663
6	1	0	-3.854025	-2.978832	0.475843
7	6	0	-3.541080	-1.637823	2.121013
8	6	0	-4.724328	-0.809786	1.815679
9	1	0	-4.854766	0.086589	2.442253
10	6	0	-6.707247	-0.266764	0.720455
11	1	0	-6.678850	0.607059	1.396272
12	6	0	-6.707247	0.266764	-0.720455
13	1	0	-6.678850	-0.607059	-1.396272
14	6	0	-7.977280	1.080641	-0.993292
15	1	0	-7.954299	1.433878	-2.029955
16	1	0	-7.956745	1.971743	-0.352487
17	6	0	-9.240189	0.264246	-0.717693
18	1	0	-10.129245	0.876183	-0.903012
19	1	0	-9.286489	-0.583767	-1.414499
20	6	0	-9.240189	-0.264246	0.717693
21	1	0	-10.129245	-0.876183	0.903012
22	1	0	-9.286489	0.583767	1.414499
23	6	0	-7.977280	-1.080641	0.993292
24	1	0	-7.956745	-1.971743	0.352487
25	1	0	-7.954299	-1.433878	2.029955
26	6	0	-4.724328	0.809786	-1.815679
27	1	0	-4.854766	-0.086589	-2.442253
28	6	0	-3.541080	1.637823	-2.121013
29	6	0	-3.220987	2.749537	-1.329663
30	1	0	-3.854025	2.978832	-0.475843
31	6	0	-2.121013	3.541080	-1.637823
32	6	0	-1.329663	3.220987	-2.749537
33	1	0	-0.475843	3.854025	-2.978832
34	6	0	-1.637823	2.121013	-3.541080
35	6	0	-2.749537	1.329663	-3.220987
36	1	0	-2.978832	0.475843	-3.854025
37	6	0	-0.809786	1.815679	-4.724328
38	1	0	0.086589	2.442253	-4.854766
39	6	0	-0.266764	0.720455	-6.707247
40	1	0	0.607059	1.396272	-6.678850
41	6	0	0.266764	-0.720455	-6.707247
42	1	0	-0.607059	-1.396272	-6.678850
43	6	0	1.080641	-0.993292	-7.977280

44	1	0	1.433878	-2.029955	-7.954299
45	1	0	1.971743	-0.352487	-7.956745
46	6	0	0.264246	-0.717693	-9.240189
47	1	0	-0.583767	-1.414499	-9.286489
48	1	0	0.876183	-0.903012	-10.129245
49	6	0	-0.264246	0.717693	-9.240189
50	1	0	0.583767	1.414499	-9.286489
51	1	0	-0.876183	0.903012	-10.129245
52	6	0	-1.080641	0.993292	-7.977280
53	1	0	-1.971743	0.352487	-7.956745
54	1	0	-1.433878	2.029955	-7.954299
55	6	0	0.809786	-1.815679	-4.724328
56	1	0	-0.086589	-2.442253	-4.854766
57	7	0	-1.121895	-0.907504	5.552021
58	7	0	1.121895	0.907504	5.552021
59	7	0	0.907504	5.552021	1.121895
60	7	0	-0.907504	5.552021	-1.121895
61	6	0	-2.749537	-1.329663	3.220987
62	1	0	-2.978832	-0.475843	3.854025
63	6	0	-1.637823	-2.121013	3.541080
64	6	0	-0.809786	-1.815679	4.724328
65	1	0	0.086589	-2.442253	4.854766
66	6	0	-0.266764	-0.720455	6.707247
67	1	0	0.607059	-1.396272	6.678850
68	6	0	0.266764	0.720455	6.707247
69	1	0	-0.607059	1.396272	6.678850
70	6	0	1.080641	0.993292	7.977280
71	1	0	1.433878	2.029955	7.954299
72	1	0	1.971743	0.352487	7.956745
73	6	0	0.264246	0.717693	9.240189
74	1	0	0.876183	0.903012	10.129245
75	1	0	-0.583767	1.414499	9.286489
76	6	0	-0.264246	-0.717693	9.240189
77	1	0	-0.876183	-0.903012	10.129245
78	1	0	0.583767	-1.414499	9.286489
79	6	0	-1.080641	-0.993292	7.977280
80	1	0	-1.971743	-0.352487	7.956745
81	1	0	-1.433878	-2.029955	7.954299
82	6	0	0.809786	1.815679	4.724328
83	1	0	-0.086589	2.442253	4.854766
84	6	0	1.637823	2.121013	3.541080
85	6	0	2.749537	1.329663	3.220987
86	1	0	2.978832	0.475843	3.854025
87	6	0	3.541080	1.637823	2.121013
88	6	0	3.220987	2.749537	1.329663
89	1	0	3.854025	2.978832	0.475843
90	6	0	2.121013	3.541080	1.637823
91	6	0	1.329663	3.220987	2.749537
92	1	0	0.475843	3.854025	2.978832
93	6	0	1.815679	4.724328	0.809786
94	1	0	2.442253	4.854766	-0.086589
95	6	0	0.720455	6.707247	0.266764
96	1	0	1.396272	6.678850	-0.607059
97	6	0	-0.720455	6.707247	-0.266764
98	1	0	-1.396272	6.678850	0.607059
99	6	0	-0.993292	7.977280	-1.080641
100	1	0	-2.029955	7.954299	-1.433878
101	1	0	-0.352487	7.956745	-1.971743
102	6	0	-0.717693	9.240189	-0.264246

103	1	0	-1.414499	9.286489	0.583767
104	1	0	-0.903012	10.129245	-0.876183
105	6	0	0.717693	9.240189	0.264246
106	1	0	1.414499	9.286489	-0.583767
107	1	0	0.903012	10.129245	0.876183
108	6	0	0.993292	7.977280	1.080641
109	1	0	0.352487	7.956745	1.971743
110	1	0	2.029955	7.954299	1.433878
111	6	0	-1.815679	4.724328	-0.809786
112	1	0	-2.442253	4.854766	0.086589
113	7	0	-0.907504	-5.552021	1.121895
114	7	0	0.907504	-5.552021	-1.121895
115	7	0	5.552021	-1.121895	-0.907504
116	7	0	5.552021	1.121895	0.907504
117	6	0	-1.329663	-3.220987	2.749537
118	1	0	-0.475843	-3.854025	2.978832
119	6	0	-2.121013	-3.541080	1.637823
120	6	0	-1.815679	-4.724328	0.809786
121	1	0	-2.442253	-4.854766	-0.086589
122	6	0	-0.720455	-6.707247	0.266764
123	1	0	-1.396272	-6.678850	-0.607059
124	6	0	0.720455	-6.707247	-0.266764
125	1	0	1.396272	-6.678850	0.607059
126	6	0	0.993292	-7.977280	-1.080641
127	1	0	2.029955	-7.954299	-1.433878
128	1	0	0.352487	-7.956745	-1.971743
129	6	0	0.717693	-9.240189	-0.264246
130	1	0	0.903012	-10.129245	-0.876183
131	1	0	1.414499	-9.286489	0.583767
132	6	0	-0.717693	-9.240189	0.264246
133	1	0	-0.903012	-10.129245	0.876183
134	1	0	-1.414499	-9.286489	-0.583767
135	6	0	-0.993292	-7.977280	1.080641
136	1	0	-0.352487	-7.956745	1.971743
137	1	0	-2.029955	-7.954299	1.433878
138	6	0	1.815679	-4.724328	-0.809786
139	1	0	2.442253	-4.854766	0.086589
140	6	0	2.121013	-3.541080	-1.637823
141	6	0	1.329663	-3.220987	-2.749537
142	1	0	0.475843	-3.854025	-2.978832
143	6	0	1.637823	-2.121013	-3.541080
144	6	0	2.749537	-1.329663	-3.220987
145	1	0	2.978832	-0.475843	-3.854025
146	6	0	3.541080	-1.637823	-2.121013
147	6	0	3.220987	-2.749537	-1.329663
148	1	0	3.854025	-2.978832	-0.475843
149	6	0	4.724328	-0.809786	-1.815679
150	1	0	4.854766	0.086589	-2.442253
151	6	0	6.707247	-0.266764	-0.720455
152	1	0	6.678850	0.607059	-1.396272
153	6	0	6.707247	0.266764	0.720455
154	1	0	6.678850	-0.607059	1.396272
155	6	0	7.977280	1.080641	0.993292
156	1	0	7.954299	1.433878	2.029955
157	1	0	7.956745	1.971743	0.352487
158	6	0	9.240189	0.264246	0.717693
159	1	0	9.286489	-0.583767	1.414499
160	1	0	10.129245	0.876183	0.903012
161	6	0	9.240189	-0.264246	-0.717693

162	1	0	9.286489	0.583767	-1.414499
163	1	0	10.129245	-0.876183	-0.903012
164	6	0	7.977280	-1.080641	-0.993292
165	1	0	7.956745	-1.971743	-0.352487
166	1	0	7.954299	-1.433878	-2.029955
167	6	0	4.724328	0.809786	1.815679
168	1	0	4.854766	-0.086589	2.442253
169	36	0	1.370921	-1.370921	1.370921
170	36	0	-1.370921	1.370921	1.370921
171	36	0	-1.370921	-1.370921	-1.370921
172	36	0	1.370921	1.370921	-1.370921

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-5.538193	-1.115241	0.900606
2	7	0	-5.538193	1.115241	-0.900606
3	7	0	-1.115241	0.900606	-5.538193
4	7	0	1.115241	-0.900606	-5.538193
5	6	0	-3.180877	-2.708553	1.288972
6	1	0	-3.824650	-2.947506	0.446140
7	6	0	-3.500947	-1.597170	2.081993
8	6	0	-4.700279	-0.786675	1.793400
9	1	0	-4.834650	0.109315	2.419890
10	6	0	-6.700761	-0.269452	0.719655
11	1	0	-6.676912	0.602358	1.398290
12	6	0	-6.700761	0.269452	-0.719655
13	1	0	-6.676912	-0.602358	-1.398290
14	6	0	-7.968002	1.088538	-0.986469
15	1	0	-7.945817	1.448555	-2.020801
16	1	0	-7.945852	1.975139	-0.339535
17	6	0	-9.231223	0.270582	-0.715484
18	1	0	-10.120280	0.884285	-0.894775
19	1	0	-9.278623	-0.571449	-1.419428
20	6	0	-9.231223	-0.270582	0.715484
21	1	0	-10.120280	-0.884285	0.894775
22	1	0	-9.278623	0.571449	1.419428
23	6	0	-7.968002	-1.088538	0.986469
24	1	0	-7.945852	-1.975139	0.339535
25	1	0	-7.945817	-1.448555	-2.020801
26	6	0	-4.700279	0.786675	-1.793400
27	1	0	-4.834650	-0.109315	-2.419890
28	6	0	-3.500947	1.597170	-2.081993
29	6	0	-3.180877	2.708553	-1.288972
30	1	0	-3.824650	2.947506	-0.446140
31	6	0	-2.081993	3.500947	-1.597170
32	6	0	-1.288972	3.180877	-2.708553
33	1	0	-0.446140	3.824650	-2.947506
34	6	0	-1.597170	2.081993	-3.500947
35	6	0	-2.708553	1.288972	-3.180877
36	1	0	-2.947506	0.446140	-3.824650
37	6	0	-0.786675	1.793400	-4.700279
38	1	0	0.109315	2.419890	-4.834650
39	6	0	-0.269452	0.719655	-6.700761
40	1	0	0.602358	1.398290	-6.676912

41	6	0	0.269452	-0.719655	-6.700761
42	1	0	-0.602358	-1.398290	-6.676912
43	6	0	1.088538	-0.986469	-7.968002
44	1	0	1.448555	-2.020801	-7.945817
45	1	0	1.975139	-0.339535	-7.945852
46	6	0	0.270582	-0.715484	-9.231223
47	1	0	-0.571449	-1.419428	-9.278623
48	1	0	0.884285	-0.894775	-10.120280
49	6	0	-0.270582	0.715484	-9.231223
50	1	0	0.571449	1.419428	-9.278623
51	1	0	-0.884285	0.894775	-10.120280
52	6	0	-1.088538	0.986469	-7.968002
53	1	0	-1.975139	0.339535	-7.945852
54	1	0	-1.448555	2.020801	-7.945817
55	6	0	0.786675	-1.793400	-4.700279
56	1	0	-0.109315	-2.419890	-4.834650
57	7	0	-1.115241	-0.900606	5.538193
58	7	0	1.115241	0.900606	5.538193
59	7	0	0.900606	5.538193	1.115241
60	7	0	-0.900606	5.538193	-1.115241
61	6	0	-2.708553	-1.288972	3.180877
62	1	0	-2.947506	-0.446140	3.824650
63	6	0	-1.597170	-2.081993	3.500947
64	6	0	-0.786675	-1.793400	4.700279
65	1	0	0.109315	-2.419890	4.834650
66	6	0	-0.269452	-0.719655	6.700761
67	1	0	0.602358	-1.398290	6.676912
68	6	0	0.269452	0.719655	6.700761
69	1	0	-0.602358	1.398290	6.676912
70	6	0	1.088538	0.986469	7.968002
71	1	0	1.448555	2.020801	7.945817
72	1	0	1.975139	0.339535	7.945852
73	6	0	0.270582	0.715484	9.231223
74	1	0	0.884285	0.894775	10.120280
75	1	0	-0.571449	1.419428	9.278623
76	6	0	-0.270582	-0.715484	9.231223
77	1	0	-0.884285	-0.894775	10.120280
78	1	0	0.571449	-1.419428	9.278623
79	6	0	-1.088538	-0.986469	7.968002
80	1	0	-1.975139	-0.339535	7.945852
81	1	0	-1.448555	-2.020801	7.945817
82	6	0	0.786675	1.793400	4.700279
83	1	0	-0.109315	2.419890	4.834650
84	6	0	1.597170	2.081993	3.500947
85	6	0	2.708553	1.288972	3.180877
86	1	0	2.947506	0.446140	3.824650
87	6	0	3.500947	1.597170	2.081993
88	6	0	3.180877	2.708553	1.288972
89	1	0	3.824650	2.947506	0.446140
90	6	0	2.081993	3.500947	1.597170
91	6	0	1.288972	3.180877	2.708553
92	1	0	0.446140	3.824650	2.947506
93	6	0	1.793400	4.700279	0.786675
94	1	0	2.419890	4.834650	-0.109315
95	6	0	0.719655	6.700761	0.269452
96	1	0	1.398290	6.676912	-0.602358
97	6	0	-0.719655	6.700761	-0.269452
98	1	0	-1.398290	6.676912	0.602358
99	6	0	-0.986469	7.968002	-1.088538

100	1	0	-2.020801	7.945817	-1.448555
101	1	0	-0.339535	7.945852	-1.975139
102	6	0	-0.715484	9.231223	-0.270582
103	1	0	-1.419428	9.278623	0.571449
104	1	0	-0.894775	10.120280	-0.884285
105	6	0	0.715484	9.231223	0.270582
106	1	0	1.419428	9.278623	-0.571449
107	1	0	0.894775	10.120280	0.884285
108	6	0	0.986469	7.968002	1.088538
109	1	0	0.339535	7.945852	1.975139
110	1	0	2.020801	7.945817	1.448555
111	6	0	-1.793400	4.700279	-0.786675
112	1	0	-2.419890	4.834650	0.109315
113	7	0	-0.900606	-5.538193	1.115241
114	7	0	0.900606	-5.538193	-1.115241
115	7	0	5.538193	-1.115241	-0.900606
116	7	0	5.538193	1.115241	0.900606
117	6	0	-1.288972	-3.180877	2.708553
118	1	0	-0.446140	-3.824650	2.947506
119	6	0	-2.081993	-3.500947	1.597170
120	6	0	-1.793400	-4.700279	0.786675
121	1	0	-2.419890	-4.834650	-0.109315
122	6	0	-0.719655	-6.700761	0.269452
123	1	0	-1.398290	-6.676912	-0.602358
124	6	0	0.719655	-6.700761	-0.269452
125	1	0	1.398290	-6.676912	0.602358
126	6	0	0.986469	-7.968002	-1.088538
127	1	0	2.020801	-7.945817	-1.448555
128	1	0	0.339535	-7.945852	-1.975139
129	6	0	0.715484	-9.231223	-0.270582
130	1	0	0.894775	-10.120280	-0.884285
131	1	0	1.419428	-9.278623	0.571449
132	6	0	-0.715484	-9.231223	0.270582
133	1	0	-0.894775	-10.120280	0.884285
134	1	0	-1.419428	-9.278623	-0.571449
135	6	0	-0.986469	-7.968002	1.088538
136	1	0	-0.339535	-7.945852	1.975139
137	1	0	-2.020801	-7.945817	1.448555
138	6	0	1.793400	-4.700279	-0.786675
139	1	0	2.419890	-4.834650	0.109315
140	6	0	2.081993	-3.500947	-1.597170
141	6	0	1.288972	-3.180877	-2.708553
142	1	0	0.446140	-3.824650	-2.947506
143	6	0	1.597170	-2.081993	-3.500947
144	6	0	2.708553	-1.288972	-3.180877
145	1	0	2.947506	-0.446140	-3.824650
146	6	0	3.500947	-1.597170	-2.081993
147	6	0	3.180877	-2.708553	-1.288972
148	1	0	3.824650	-2.947506	-0.446140
149	6	0	4.700279	-0.786675	-1.793400
150	1	0	4.834650	0.109315	-2.419890
151	6	0	6.700761	-0.269452	-0.719655
152	1	0	6.676912	0.602358	-1.398290
153	6	0	6.700761	0.269452	0.719655
154	1	0	6.676912	-0.602358	1.398290
155	6	0	7.968002	1.088538	0.986469
156	1	0	7.945817	1.448555	2.020801
157	1	0	7.945852	1.975139	0.339535
158	6	0	9.231223	0.270582	0.715484

159	1	0	9.278623	-0.571449	1.419428
160	1	0	10.120280	0.884285	0.894775
161	6	0	9.231223	-0.270582	-0.715484
162	1	0	9.278623	0.571449	-1.419428
163	1	0	10.120280	-0.884285	-0.894775
164	6	0	7.968002	-1.088538	-0.986469
165	1	0	7.945852	-1.975139	-0.339535
166	1	0	7.945817	-1.448555	-2.020801
167	6	0	4.700279	0.786675	1.793400
168	1	0	4.834650	-0.109315	2.419890
169	36	0	2.180492	-2.180492	2.180492
170	36	0	-2.180492	2.180492	2.180492
171	36	0	-2.180492	-2.180492	-2.180492
172	36	0	2.180492	2.180492	-2.180492
173	36	0	0.000000	0.000000	0.000000

CH4@CC3 T cc3-rra

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-5.542871	-1.118596	0.902146
2	7	0	-5.542871	1.118596	-0.902146
3	7	0	-1.118596	0.902146	-5.542871
4	7	0	1.118596	-0.902146	-5.542871
5	6	0	-3.182833	-2.713252	1.291971
6	1	0	-3.819692	-2.946903	0.442618
7	6	0	-3.505700	-1.603064	2.085070
8	6	0	-4.702693	-0.790243	1.792920
9	1	0	-4.833210	0.109321	2.414454
10	6	0	-6.703127	-0.269560	0.719666
11	1	0	-6.678507	0.602350	1.398259
12	6	0	-6.703127	0.269560	-0.719666
13	1	0	-6.678507	-0.602350	-1.398259
14	6	0	-7.971050	1.086974	-0.987513
15	1	0	-7.948505	1.446272	-2.022086
16	1	0	-7.949291	1.974239	-0.341441
17	6	0	-9.234287	0.269332	-0.716207
18	1	0	-10.123238	0.882801	-0.896821
19	1	0	-9.281416	-0.573888	-1.418729
20	6	0	-9.234287	-0.269332	0.716207
21	1	0	-10.123238	-0.882801	0.896821
22	1	0	-9.281416	0.573888	1.418729
23	6	0	-7.971050	-1.086974	0.987513
24	1	0	-7.949291	-1.974239	0.341441
25	1	0	-7.948505	-1.446272	2.022086
26	6	0	-4.702693	0.790243	-1.792920
27	1	0	-4.833210	-0.109321	-2.414454
28	6	0	-3.505700	1.603064	-2.085070
29	6	0	-3.182833	2.713252	-1.291971
30	1	0	-3.819692	2.946903	-0.442618
31	6	0	-2.085070	3.505700	-1.603064
32	6	0	-1.291971	3.182833	-2.713252
33	1	0	-0.442618	3.819692	-2.946903
34	6	0	-1.603064	2.085070	-3.505700
35	6	0	-2.713252	1.291971	-3.182833
36	1	0	-2.946903	0.442618	-3.819692

37	6	0	-0.790243	1.792920	-4.702693
38	1	0	0.109321	2.414454	-4.833210
39	6	0	-0.269560	0.719666	-6.703127
40	1	0	0.602350	1.398259	-6.678507
41	6	0	0.269560	-0.719666	-6.703127
42	1	0	-0.602350	-1.398259	-6.678507
43	6	0	1.086974	-0.987513	-7.971050
44	1	0	1.446272	-2.022086	-7.948505
45	1	0	1.974239	-0.341441	-7.949291
46	6	0	0.269332	-0.716207	-9.234287
47	1	0	-0.573888	-1.418729	-9.281416
48	1	0	0.882801	-0.896821	-10.123238
49	6	0	-0.269332	0.716207	-9.234287
50	1	0	0.573888	1.418729	-9.281416
51	1	0	-0.882801	0.896821	-10.123238
52	6	0	-1.086974	0.987513	-7.971050
53	1	0	-1.974239	0.341441	-7.949291
54	1	0	-1.446272	2.022086	-7.948505
55	6	0	0.790243	-1.792920	-4.702693
56	1	0	-0.109321	-2.414454	-4.833210
57	7	0	-1.118596	-0.902146	5.542871
58	7	0	1.118596	0.902146	5.542871
59	7	0	0.902146	5.542871	1.118596
60	7	0	-0.902146	5.542871	-1.118596
61	6	0	-2.713252	-1.291971	3.182833
62	1	0	-2.946903	-0.442618	3.819692
63	6	0	-1.603064	-2.085070	3.505700
64	6	0	-0.790243	-1.792920	4.702693
65	1	0	0.109321	-2.414454	4.833210
66	6	0	-0.269560	-0.719666	6.703127
67	1	0	0.602350	-1.398259	6.678507
68	6	0	0.269560	0.719666	6.703127
69	1	0	-0.602350	1.398259	6.678507
70	6	0	1.086974	0.987513	7.971050
71	1	0	1.446272	2.022086	7.948505
72	1	0	1.974239	0.341441	7.949291
73	6	0	0.269332	0.716207	9.234287
74	1	0	0.882801	0.896821	10.123238
75	1	0	-0.573888	1.418729	9.281416
76	6	0	-0.269332	-0.716207	9.234287
77	1	0	-0.882801	-0.896821	10.123238
78	1	0	0.573888	-1.418729	9.281416
79	6	0	-1.086974	-0.987513	7.971050
80	1	0	-1.974239	-0.341441	7.949291
81	1	0	-1.446272	-2.022086	7.948505
82	6	0	0.790243	1.792920	4.702693
83	1	0	-0.109321	2.414454	4.833210
84	6	0	1.603064	2.085070	3.505700
85	6	0	2.713252	1.291971	3.182833
86	1	0	2.946903	0.442618	3.819692
87	6	0	3.505700	1.603064	2.085070
88	6	0	3.182833	2.713252	1.291971
89	1	0	3.819692	2.946903	0.442618
90	6	0	2.085070	3.505700	1.603064
91	6	0	1.291971	3.182833	2.713252
92	1	0	0.442618	3.819692	2.946903
93	6	0	1.792920	4.702693	0.790243
94	1	0	2.414454	4.833210	-0.109321
95	6	0	0.719666	6.703127	0.269560

96	1	0	1.398259	6.678507	-0.602350
97	6	0	-0.719666	6.703127	-0.269560
98	1	0	-1.398259	6.678507	0.602350
99	6	0	-0.987513	7.971050	-1.086974
100	1	0	-2.022086	7.948505	-1.446272
101	1	0	-0.341441	7.949291	-1.974239
102	6	0	-0.716207	9.234287	-0.269332
103	1	0	-1.418729	9.281416	0.573888
104	1	0	-0.896821	10.123238	-0.882801
105	6	0	0.716207	9.234287	0.269332
106	1	0	1.418729	9.281416	-0.573888
107	1	0	0.896821	10.123238	0.882801
108	6	0	0.987513	7.971050	1.086974
109	1	0	0.341441	7.949291	1.974239
110	1	0	2.022086	7.948505	1.446272
111	6	0	-1.792920	4.702693	-0.790243
112	1	0	-2.414454	4.833210	0.109321
113	7	0	-0.902146	-5.542871	1.118596
114	7	0	0.902146	-5.542871	-1.118596
115	7	0	5.542871	-1.118596	-0.902146
116	7	0	5.542871	1.118596	0.902146
117	6	0	-1.291971	-3.182833	2.713252
118	1	0	-0.442618	-3.819692	2.946903
119	6	0	-2.085070	-3.505700	1.603064
120	6	0	-1.792920	-4.702693	0.790243
121	1	0	-2.414454	-4.833210	-0.109321
122	6	0	-0.719666	-6.703127	0.269560
123	1	0	-1.398259	-6.678507	-0.602350
124	6	0	0.719666	-6.703127	-0.269560
125	1	0	1.398259	-6.678507	0.602350
126	6	0	0.987513	-7.971050	-1.086974
127	1	0	2.022086	-7.948505	-1.446272
128	1	0	0.341441	-7.949291	-1.974239
129	6	0	0.716207	-9.234287	-0.269332
130	1	0	0.896821	-10.123238	-0.882801
131	1	0	1.418729	-9.281416	0.573888
132	6	0	-0.716207	-9.234287	0.269332
133	1	0	-0.896821	-10.123238	0.882801
134	1	0	-1.418729	-9.281416	-0.573888
135	6	0	-0.987513	-7.971050	1.086974
136	1	0	-0.341441	-7.949291	1.974239
137	1	0	-2.022086	-7.948505	1.446272
138	6	0	1.792920	-4.702693	-0.790243
139	1	0	2.414454	-4.833210	0.109321
140	6	0	2.085070	-3.505700	-1.603064
141	6	0	1.291971	-3.182833	-2.713252
142	1	0	0.442618	-3.819692	-2.946903
143	6	0	1.603064	-2.085070	-3.505700
144	6	0	2.713252	-1.291971	-3.182833
145	1	0	2.946903	-0.442618	-3.819692
146	6	0	3.505700	-1.603064	-2.085070
147	6	0	3.182833	-2.713252	-1.291971
148	1	0	3.819692	-2.946903	-0.442618
149	6	0	4.702693	-0.790243	-1.792920
150	1	0	4.833210	0.109321	-2.414454
151	6	0	6.703127	-0.269560	-0.719666
152	1	0	6.678507	0.602350	-1.398259
153	6	0	6.703127	0.269560	0.719666
154	1	0	6.678507	-0.602350	1.398259

155	6	0	7.971050	1.086974	0.987513
156	1	0	7.948505	1.446272	2.022086
157	1	0	7.949291	1.974239	0.341441
158	6	0	9.234287	0.269332	0.716207
159	1	0	9.281416	-0.573888	1.418729
160	1	0	10.123238	0.882801	0.896821
161	6	0	9.234287	-0.269332	-0.716207
162	1	0	9.281416	0.573888	-1.418729
163	1	0	10.123238	-0.882801	-0.896821
164	6	0	7.971050	-1.086974	-0.987513
165	1	0	7.949291	-1.974239	-0.341441
166	1	0	7.948505	-1.446272	-2.022086
167	6	0	4.702693	0.790243	1.792920
168	1	0	4.833210	-0.109321	2.414454
169	6	0	0.000000	0.000000	0.000000
170	1	0	0.630261	-0.630261	0.630261
171	1	0	0.630261	0.630261	-0.630261
172	1	0	-0.630261	-0.630261	-0.630261
173	1	0	-0.630261	0.630261	0.630261

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-0.564623	5.327254	-2.085729
2	7	0	-0.116284	3.709011	-4.428972
3	7	0	-3.153955	-1.955210	-4.428972
4	7	0	-4.331226	-3.152605	-2.085729
5	6	0	-1.330643	4.186579	0.444210
6	1	0	-2.115898	4.393069	-0.278477
7	6	0	0.000000	4.425823	0.073421
8	6	0	0.327780	4.970410	-1.258940
9	1	0	1.401598	5.066514	-1.483279
10	6	0	-0.129022	5.889052	-3.349234
11	1	0	0.972386	5.878148	-3.438930
12	6	0	-0.691955	5.037756	-4.497990
13	1	0	-1.790460	5.009648	-4.380783
14	6	0	-0.341566	5.664261	-5.852275
15	1	0	-0.765879	5.043588	-6.648964
16	1	0	0.749322	5.634176	-5.971608
17	6	0	-0.842179	7.105521	-5.951908
18	1	0	-0.561609	7.533187	-6.920208
19	1	0	-1.939737	7.114642	-5.905936
20	6	0	-0.284385	7.953394	-4.807421
21	1	0	-0.672138	8.976111	-4.861412
22	1	0	0.807480	8.021241	-4.907595
23	6	0	-0.632672	7.332941	-3.454107
24	1	0	-1.720947	7.327424	-3.309907
25	1	0	-0.205738	7.916630	-2.631289
26	6	0	-0.909442	2.726989	-4.311393
27	1	0	-2.000489	2.863386	-4.250557
28	6	0	-0.437430	1.328779	-4.273324
29	6	0	0.933022	1.033339	-4.271443
30	1	0	1.641504	1.857688	-4.279643
31	6	0	1.369471	-0.285564	-4.273324
32	6	0	0.428387	-1.324690	-4.271443

33	1	0	0.788052	-2.350428	-4.279643
34	6	0	-0.932041	-1.043215	-4.273324
35	6	0	-1.361409	0.291351	-4.271443
36	1	0	-2.429557	0.492741	-4.279643
37	6	0	-1.906921	-2.151095	-4.311393
38	1	0	-1.479521	-3.164167	-4.250557
39	6	0	-4.016847	-3.118128	-4.497990
40	1	0	-3.443252	-4.055408	-4.380783
41	6	0	-5.035558	-3.056262	-3.349234
42	1	0	-5.576819	-2.096963	-3.438930
43	6	0	-6.034177	-4.214381	-3.454107
44	1	0	-6.753133	-4.136489	-2.631289
45	1	0	-5.485261	-5.154096	-3.309907
46	6	0	-6.745648	-4.222982	-4.807421
47	1	0	-7.350339	-3.311323	-4.907595
48	1	0	-7.437471	-5.070144	-4.861412
49	6	0	-5.732472	-4.282109	-5.951908
50	1	0	-5.191593	-5.237183	-5.905936
51	1	0	-6.243127	-4.252961	-6.920208
52	6	0	-4.734611	-3.127935	-5.852275
53	1	0	-5.254001	-2.168156	-5.971608
54	1	0	-3.984936	-3.185065	-6.648964
55	6	0	-4.468391	-2.201339	-1.258940
56	1	0	-5.088529	-1.319437	-1.483279
57	7	0	3.001595	3.800309	3.038149
58	7	0	4.459518	1.329059	3.285294
59	7	0	4.895849	-2.174649	-2.085729
60	7	0	3.270240	-1.753800	-4.428972
61	6	0	1.019676	4.178167	0.984192
62	1	0	2.059059	4.362619	0.724900
63	6	0	0.725154	3.696896	2.267413
64	6	0	1.797469	3.468652	3.255824
65	1	0	1.480645	3.008906	4.205224
66	6	0	3.967925	3.568695	4.093266
67	1	0	3.501226	3.086404	4.971200
68	6	0	5.057090	2.617902	3.573036
69	1	0	5.490060	3.075651	2.665184
70	6	0	6.157495	2.435137	4.624378
71	1	0	6.924238	1.765006	4.220571
72	1	0	5.718932	1.929923	5.494755
73	6	0	6.763253	3.774964	5.043536
74	1	0	7.531459	3.615547	5.807535
75	1	0	7.263395	4.235369	4.180560
76	6	0	5.679123	4.722412	5.560119
77	1	0	6.111022	5.692750	5.826809
78	1	0	5.242616	4.305304	6.477873
79	6	0	4.579955	4.909242	4.513867
80	1	0	4.989458	5.394562	3.618380
81	1	0	3.782758	5.558919	4.891178
82	6	0	4.560092	0.880602	2.103663
83	1	0	5.069826	1.445001	1.307248
84	6	0	4.030487	-0.440924	1.714070
85	6	0	3.297647	-1.214858	2.624608
86	1	0	3.105374	-0.809573	3.615001
87	6	0	2.839028	-2.476450	2.267413
88	6	0	3.108561	-2.972148	0.984192
89	1	0	2.748610	-3.964507	0.724900
90	6	0	3.832875	-2.212912	0.073421
91	6	0	4.291005	-0.940919	0.444210

92	1	0	4.862459	-0.364113	-0.278477
93	6	0	4.140612	-2.769071	-1.258940
94	1	0	3.686930	-3.747077	-1.483279
95	6	0	5.164579	-2.832790	-3.349234
96	1	0	4.604432	-3.781185	-3.438930
97	6	0	4.708802	-1.919628	-4.497990
98	1	0	5.233712	-0.954240	-4.380783
99	6	0	5.076176	-2.536326	-5.852275
100	1	0	4.750815	-1.858523	-6.648964
101	1	0	4.504679	-3.466020	-5.971608
102	6	0	6.574651	-2.823412	-5.951908
103	1	0	7.131330	-1.877460	-5.905936
104	1	0	6.804736	-3.280226	-6.920208
105	6	0	7.030034	-3.730412	-4.807421
106	1	0	6.542859	-4.709919	-4.907595
107	1	0	8.109609	-3.905967	-4.861412
108	6	0	6.666849	-3.118560	-3.454107
109	1	0	7.206209	-2.173328	-3.309907
110	1	0	6.958871	-3.780141	-2.631289
111	6	0	2.816363	-0.575894	-4.311393
112	1	0	3.480009	0.300781	-4.250557
113	7	0	-3.380758	3.197526	3.285294
114	7	0	-4.791962	0.699303	3.038149
115	7	0	-1.078760	-4.526586	3.285294
116	7	0	1.790367	-4.499612	3.038149
117	6	0	-0.596726	3.463275	2.624608
118	1	0	-0.851576	3.094119	3.615001
119	6	0	-1.633392	3.710967	1.714070
120	6	0	-3.042669	3.508854	2.103663
121	1	0	-3.786321	3.668097	1.307248
122	6	0	-4.795715	3.070618	3.573036
123	1	0	-5.408622	3.216706	2.665184
124	6	0	-5.074543	1.651977	4.093266
125	1	0	-4.423518	1.488949	4.971200
126	6	0	-6.541506	1.511736	4.513867
127	1	0	-6.705544	0.496505	4.891178
128	1	0	-7.166557	1.623717	3.618380
129	6	0	-6.929290	2.557059	5.560119
130	1	0	-7.985577	2.445926	5.826809
131	1	0	-6.349810	2.387587	6.477873
132	6	0	-6.650841	3.969667	5.043536
133	1	0	-6.896885	4.714661	5.807535
134	1	0	-7.299635	4.172600	4.180560
135	6	0	-5.187638	4.114979	4.624378
136	1	0	-4.530828	3.987778	5.494755
137	1	0	-4.990659	5.114063	4.220571
138	6	0	-3.902676	-0.177672	3.255824
139	1	0	-3.346111	-0.222176	4.205224
140	6	0	-3.564182	-1.220446	2.267413
141	6	0	-4.128237	-1.206019	0.984192
142	1	0	-4.807669	-0.398112	0.724900
143	6	0	-3.832875	-2.212912	0.073421
144	6	0	-2.960362	-3.245660	0.444210
145	1	0	-2.746560	-4.028956	-0.278477
146	6	0	-2.397095	-3.270042	1.714070
147	6	0	-2.700922	-2.248417	2.624608
148	1	0	-2.253798	-2.284546	3.615001
149	6	0	-1.517422	-4.389456	2.103663
150	1	0	-1.283505	-5.113098	1.307248

151	6	0	-0.261376	-5.688520	3.573036
152	1	0	-0.081438	-6.292357	2.665184
153	6	0	1.106617	-5.220672	4.093266
154	1	0	0.922291	-4.575353	4.971200
155	6	0	1.961551	-6.420978	4.513867
156	1	0	2.922786	-6.055424	4.891178
157	1	0	2.177099	-7.018279	3.618380
158	6	0	1.250167	-7.279471	5.560119
159	1	0	1.107195	-6.692890	6.477873
160	1	0	1.874555	-8.138675	5.826809
161	6	0	-0.112412	-7.744631	5.043536
162	1	0	0.036240	-8.407969	4.180560
163	1	0	-0.634574	-8.330208	5.807535
164	6	0	-0.969857	-6.550116	4.624378
165	1	0	-1.188103	-5.917702	5.494755
166	1	0	-1.933579	-6.879069	4.220571
167	6	0	2.105206	-3.290980	3.255824
168	1	0	1.865466	-2.786729	4.205224
169	6	0	0.000000	0.000000	2.854800
170	1	0	0.000000	0.000000	3.948206
171	1	0	0.066383	-1.027917	2.489888
172	1	0	-0.923393	0.456469	2.489888
173	1	0	0.857011	0.571447	2.489888

3CH4@CC3 C3 cc3-rbb

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-4.780043	-0.717485	-3.106630
2	7	0	-3.386840	-3.220823	-3.377127
3	7	0	-0.577006	-5.321288	1.990649
4	7	0	-0.147225	-3.700065	4.323246
5	6	0	-4.115255	1.196615	-1.065869
6	1	0	-4.789995	0.386071	-0.801789
7	6	0	-3.559407	1.213971	-2.352827
8	6	0	-3.907680	0.172748	-3.339130
9	1	0	-3.377112	0.231160	-4.302317
10	6	0	-5.078508	-1.663212	-4.164030
11	1	0	-4.435874	-1.498586	-5.047839
12	6	0	-4.803148	-3.086149	-3.653938
13	1	0	-5.409766	-3.232478	-2.741910
14	6	0	-5.209101	-4.123156	-4.706768
15	1	0	-5.012881	-5.125189	-4.310083
16	1	0	-4.559938	-3.994261	-5.582625
17	6	0	-6.675414	-3.968769	-5.111378
18	1	0	-6.932512	-4.708190	-5.877123
19	1	0	-7.317135	-4.173085	-4.243484
20	6	0	-6.951423	-2.552012	-5.617780
21	1	0	-8.009501	-2.434045	-5.874265
22	1	0	-6.379519	-2.380697	-6.539952
23	6	0	-6.548901	-1.513580	-4.569940
24	1	0	-7.166134	-1.627022	-3.669226
25	1	0	-6.711456	-0.495758	-4.940891
26	6	0	-3.041842	-3.509496	-2.191826
27	1	0	-3.780365	-3.648741	-1.386624
28	6	0	-1.631310	-3.707072	-1.805168

29	6	0	-0.593570	-3.461259	-2.714645
30	1	0	-0.848195	-3.102407	-3.708627
31	6	0	0.728374	-3.689523	-2.352827
32	6	0	1.021328	-4.162223	-1.065869
33	1	0	2.060650	-4.341292	-0.801789
34	6	0	0.000000	-4.407023	-0.156492
35	6	0	-1.330007	-4.174932	-0.532373
36	1	0	-2.117355	-4.379743	0.188800
37	6	0	0.321902	-4.948662	1.177970
38	1	0	1.394291	-5.033399	1.414245
39	6	0	-0.154305	-5.882544	3.257999
40	1	0	0.946101	-5.872210	3.359148
41	6	0	-0.728514	-5.025323	4.396641
42	1	0	-1.825341	-4.994854	4.265359
43	6	0	-0.395587	-5.645731	5.757641
44	1	0	-0.828127	-5.020899	6.546575
45	1	0	0.693823	-5.617283	5.889810
46	6	0	-0.900495	-7.085547	5.857021
47	1	0	-1.997449	-7.092570	5.798138
48	1	0	-0.632451	-7.509957	6.830291
49	6	0	-0.330942	-7.939613	4.722814
50	1	0	0.759494	-8.009478	4.836415
51	1	0	-0.721492	-8.961270	4.776822
52	6	0	-0.661607	-7.324912	3.362392
53	1	0	-1.747970	-7.318073	3.204774
54	1	0	-0.225622	-7.913093	2.547574
55	6	0	-0.931359	-2.718177	4.154434
56	1	0	-2.020630	-2.850161	4.057901
57	7	0	-1.095894	4.543501	-3.377127
58	7	0	1.768662	4.498381	-3.106630
59	7	0	4.482734	-1.322678	-3.377127
60	7	0	3.011382	-3.780896	-3.106630
61	6	0	-2.700753	2.244676	-2.714645
62	1	0	-2.262666	2.285762	-3.708627
63	6	0	-2.394763	3.266292	-1.805168
64	6	0	-1.518392	4.389061	-2.191826
65	1	0	-1.269720	5.098262	-1.386624
66	6	0	-0.271109	5.702722	-3.653938
67	1	0	-0.094525	6.301234	-2.741910
68	6	0	1.098871	5.229723	-4.164030
69	1	0	0.920123	4.590873	-5.047839
70	6	0	1.963651	6.428305	-4.569940
71	1	0	2.926390	6.060171	-4.940891
72	1	0	2.174025	7.019565	-3.669226
73	6	0	1.265604	7.296115	-5.617780
74	1	0	1.896806	8.153453	-5.874265
75	1	0	1.128016	6.715174	-6.539952
76	6	0	-0.099347	7.765463	-5.111378
77	1	0	-0.611156	8.357827	-5.877123
78	1	0	0.044569	8.423367	-4.243484
79	6	0	-0.966207	6.572792	-4.706768
80	1	0	-1.179162	5.946153	-5.582625
81	1	0	-1.932104	6.903877	-4.310083
82	6	0	2.103444	3.297776	-3.339130
83	1	0	1.888746	2.809085	-4.302317
84	6	0	2.831033	2.475552	-2.352827
85	6	0	3.093927	2.965607	-1.065869
86	1	0	2.729344	3.955222	-0.801789
87	6	0	3.816594	2.203512	-0.156492

88	6	0	4.280601	0.935646	-0.532373
89	1	0	4.851647	0.356188	0.188800
90	6	0	4.026073	0.440780	-1.805168
91	6	0	3.294323	1.216583	-2.714645
92	1	0	3.110861	0.816645	-3.708627
93	6	0	4.560234	-0.879564	-2.191826
94	1	0	5.050085	-1.449521	-1.386624
95	6	0	5.074257	-2.616573	-3.653938
96	1	0	5.504291	-3.068756	-2.741910
97	6	0	3.979637	-3.566511	-4.164030
98	1	0	3.515751	-3.092287	-5.047839
99	6	0	4.585250	-4.914724	-4.569940
100	1	0	3.785067	-5.564413	-4.940891
101	1	0	4.992109	-5.392543	-3.669226
102	6	0	5.685819	-4.744103	-5.617780
103	1	0	5.251503	-4.334478	-6.539952
104	1	0	6.112695	-5.719409	-5.874265
105	6	0	6.774762	-3.796694	-5.111378
106	1	0	7.272565	-4.250282	-4.243484
107	1	0	7.543668	-3.649636	-5.877123
108	6	0	6.175308	-2.449636	-4.706768
109	1	0	5.739100	-1.951892	-5.582625
110	1	0	6.944985	-1.778688	-4.310083
111	6	0	1.804236	-3.470524	-3.339130
112	1	0	1.488366	-3.040245	-4.302317
113	7	0	-4.319867	3.160346	1.990649
114	7	0	-3.130738	1.977533	4.323246
115	7	0	3.277963	1.722532	4.323246
116	7	0	4.896873	2.160942	1.990649
117	6	0	-2.950594	3.239286	-0.532373
118	1	0	-2.734292	4.023555	0.188800
119	6	0	-3.816594	2.203512	-0.156492
120	6	0	-4.446618	2.195556	1.177970
121	1	0	-5.056197	1.309208	1.414245
122	6	0	-5.017280	3.074904	3.257999
123	1	0	-5.558534	2.116758	3.359148
124	6	0	-3.987800	3.143573	4.396641
125	1	0	-3.413001	4.078219	4.265359
126	6	0	-4.691553	3.165454	5.757641
127	1	0	-3.934162	3.227628	6.546575
128	1	0	-5.211621	2.207773	5.889810
129	6	0	-5.686016	4.322625	5.857021
130	1	0	-6.187588	4.302697	6.830291
131	1	0	-5.143622	5.276126	5.798138
132	6	0	-6.710435	4.256411	4.722814
133	1	0	-7.399941	5.105466	4.776822
134	1	0	-7.316158	3.346998	4.836415
135	6	0	-6.012756	4.235425	3.362392
136	1	0	-5.463652	5.172823	3.204774
137	1	0	-6.740129	4.151941	2.547574
138	6	0	-1.888331	2.165669	4.154434
139	1	0	-1.457997	3.174998	4.057901
140	6	0	-0.922943	1.050687	4.107150
141	6	0	-1.363886	-0.279432	4.104941
142	1	0	-2.433637	-0.472534	4.113840
143	6	0	-0.448450	-1.324635	4.107150
144	6	0	0.923938	-1.041444	4.104941
145	1	0	1.626044	-1.871324	4.113840
146	6	0	1.371393	0.273949	4.107150

147	6	0	0.439948	1.320876	4.104941
148	1	0	0.807592	2.343858	4.113840
149	6	0	2.819690	0.552508	4.154434
150	1	0	3.478627	-0.324836	4.057901
151	6	0	4.716315	1.881750	4.396641
152	1	0	5.238341	0.916636	4.265359
153	6	0	5.171585	2.807639	3.257999
154	1	0	4.612433	3.755452	3.359148
155	6	0	6.674363	3.089487	3.362392
156	1	0	6.965751	3.761152	2.547574
157	1	0	7.211622	2.145250	3.204774
158	6	0	7.041377	3.683202	4.722814
159	1	0	6.556665	4.662480	4.836415
160	1	0	8.121434	3.855804	4.776822
161	6	0	6.586511	2.762922	5.857021
162	1	0	7.141070	1.816444	5.798138
163	1	0	6.820039	3.207260	6.830291
164	6	0	5.087140	2.480277	5.757641
165	1	0	4.517798	3.409510	5.889810
166	1	0	4.762289	1.793271	6.546575
167	6	0	4.124716	2.753106	1.177970
168	1	0	3.661906	3.724191	1.414245
169	6	0	0.275231	2.457368	0.888065
170	6	0	-2.265758	-0.990327	0.888065
171	1	0	0.224510	2.769806	-0.158109
172	1	0	-1.638895	-0.097373	0.950159
173	1	0	-2.510977	-1.190472	-0.158109
174	1	0	-1.726162	-1.843900	1.308097
175	1	0	-0.733783	2.416850	1.308097
176	1	0	0.735120	1.468012	0.950159
177	6	0	1.990528	-1.467041	0.888065
178	1	0	2.459945	-0.572950	1.308097
179	1	0	0.903776	-1.370638	0.950159
180	1	0	2.286467	-1.579334	-0.158109
181	1	0	-3.184520	-0.822114	1.456536
182	1	0	0.880289	3.168932	1.456536
183	1	0	2.304231	-2.346818	1.456536

4CH4@CC3-a T cc3-ra

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-0.892782	5.544633	-1.124480
2	7	0	0.892782	5.544633	1.124480
3	7	0	5.544633	1.124480	0.892782
4	7	0	5.544633	-1.124480	-0.892782
5	6	0	-1.307424	3.196024	-2.733540
6	1	0	-0.457586	3.830363	-2.972625
7	6	0	-2.095952	3.521623	-1.621649
8	6	0	-1.799406	4.716459	-0.808683
9	1	0	-2.433789	4.857449	0.080732
10	6	0	-0.716665	6.706676	-0.276443
11	1	0	-1.403934	6.684206	0.588657
12	6	0	0.716665	6.706676	0.276443
13	1	0	1.403934	6.684206	-0.588657
14	6	0	0.975254	7.974034	1.098211

15	1	0	2.005933	7.951650	1.468540
16	1	0	0.319558	7.951802	1.978371
17	6	0	0.712655	9.237465	0.277856
18	1	0	0.885575	10.126359	0.893631
19	1	0	1.425277	9.285138	-0.556828
20	6	0	-0.712655	9.237465	-0.277856
21	1	0	-0.885575	10.126359	-0.893631
22	1	0	-1.425277	9.285138	0.556828
23	6	0	-0.975254	7.974034	-1.098211
24	1	0	-0.319558	7.951802	-1.978371
25	1	0	-2.005933	7.951650	-1.468540
26	6	0	1.799406	4.716459	0.808683
27	1	0	2.433789	4.857449	-0.080732
28	6	0	2.095952	3.521623	1.621649
29	6	0	1.307424	3.196024	2.733540
30	1	0	0.457586	3.830363	2.972625
31	6	0	1.621649	2.095952	3.521623
32	6	0	2.733540	1.307424	3.196024
33	1	0	2.972625	0.457586	3.830363
34	6	0	3.521623	1.621649	2.095952
35	6	0	3.196024	2.733540	1.307424
36	1	0	3.830363	2.972625	0.457586
37	6	0	4.716459	0.808683	1.799406
38	1	0	4.857449	-0.080732	2.433789
39	6	0	6.706676	0.276443	0.716665
40	1	0	6.684206	-0.588657	1.403934
41	6	0	6.706676	-0.276443	-0.716665
42	1	0	6.684206	0.588657	-1.403934
43	6	0	7.974034	-1.098211	-0.975254
44	1	0	7.951650	-1.468540	-2.005933
45	1	0	7.951802	-1.978371	-0.319558
46	6	0	9.237465	-0.277856	-0.712655
47	1	0	9.285138	0.556828	-1.425277
48	1	0	10.126359	-0.893631	-0.885575
49	6	0	9.237465	0.277856	0.712655
50	1	0	9.285138	-0.556828	1.425277
51	1	0	10.126359	0.893631	0.885575
52	6	0	7.974034	1.098211	0.975254
53	1	0	7.951802	1.978371	0.319558
54	1	0	7.951650	1.468540	2.005933
55	6	0	4.716459	-0.808683	-1.799406
56	1	0	4.857449	0.080732	-2.433789
57	7	0	-5.544633	1.124480	-0.892782
58	7	0	-5.544633	-1.124480	0.892782
59	7	0	-1.124480	-0.892782	5.544633
60	7	0	1.124480	0.892782	5.544633
61	6	0	-3.196024	2.733540	-1.307424
62	1	0	-3.830363	2.972625	-0.457586
63	6	0	-3.521623	1.621649	-2.095952
64	6	0	-4.716459	0.808683	-1.799406
65	1	0	-4.857449	-0.080732	-2.433789
66	6	0	-6.706676	0.276443	-0.716665
67	1	0	-6.684206	-0.588657	-1.403934
68	6	0	-6.706676	-0.276443	0.716665
69	1	0	-6.684206	0.588657	1.403934
70	6	0	-7.974034	-1.098211	0.975254
71	1	0	-7.951650	-1.468540	2.005933
72	1	0	-7.951802	-1.978371	0.319558
73	6	0	-9.237465	-0.277856	0.712655

74	1	0	-10.126359	-0.893631	0.885575
75	1	0	-9.285138	0.556828	1.425277
76	6	0	-9.237465	0.277856	-0.712655
77	1	0	-10.126359	0.893631	-0.885575
78	1	0	-9.285138	-0.556828	-1.425277
79	6	0	-7.974034	1.098211	-0.975254
80	1	0	-7.951802	1.978371	-0.319558
81	1	0	-7.951650	1.468540	-2.005933
82	6	0	-4.716459	-0.808683	1.799406
83	1	0	-4.857449	0.080732	2.433789
84	6	0	-3.521623	-1.621649	2.095952
85	6	0	-3.196024	-2.733540	1.307424
86	1	0	-3.830363	-2.972625	0.457586
87	6	0	-2.095952	-3.521623	1.621649
88	6	0	-1.307424	-3.196024	2.733540
89	1	0	-0.457586	-3.830363	2.972625
90	6	0	-1.621649	-2.095952	3.521623
91	6	0	-2.733540	-1.307424	3.196024
92	1	0	-2.972625	-0.457586	3.830363
93	6	0	-0.808683	-1.799406	4.716459
94	1	0	0.080732	-2.433789	4.857449
95	6	0	-0.276443	-0.716665	6.706676
96	1	0	0.588657	-1.403934	6.684206
97	6	0	0.276443	0.716665	6.706676
98	1	0	-0.588657	1.403934	6.684206
99	6	0	1.098211	0.975254	7.974034
100	1	0	1.468540	2.005933	7.951650
101	1	0	1.978371	0.319558	7.951802
102	6	0	0.277856	0.712655	9.237465
103	1	0	-0.556828	1.425277	9.285138
104	1	0	0.893631	0.885575	10.126359
105	6	0	-0.277856	-0.712655	9.237465
106	1	0	0.556828	-1.425277	9.285138
107	1	0	-0.893631	-0.885575	10.126359
108	6	0	-1.098211	-0.975254	7.974034
109	1	0	-1.978371	-0.319558	7.951802
110	1	0	-1.468540	-2.005933	7.951650
111	6	0	0.808683	1.799406	4.716459
112	1	0	-0.080732	2.433789	4.857449
113	7	0	-1.124480	0.892782	-5.544633
114	7	0	1.124480	-0.892782	-5.544633
115	7	0	0.892782	-5.544633	-1.124480
116	7	0	-0.892782	-5.544633	1.124480
117	6	0	-2.733540	1.307424	-3.196024
118	1	0	-2.972625	0.457586	-3.830363
119	6	0	-1.621649	2.095952	-3.521623
120	6	0	-0.808683	1.799406	-4.716459
121	1	0	0.080732	2.433789	-4.857449
122	6	0	-0.276443	0.716665	-6.706676
123	1	0	0.588657	1.403934	-6.684206
124	6	0	0.276443	-0.716665	-6.706676
125	1	0	-0.588657	-1.403934	-6.684206
126	6	0	1.098211	-0.975254	-7.974034
127	1	0	1.468540	-2.005933	-7.951650
128	1	0	1.978371	-0.319558	-7.951802
129	6	0	0.277856	-0.712655	-9.237465
130	1	0	0.893631	-0.885575	-10.126359
131	1	0	-0.556828	-1.425277	-9.285138
132	6	0	-0.277856	0.712655	-9.237465

133	1	0	-0.893631	0.885575	-10.126359
134	1	0	0.556828	1.425277	-9.285138
135	6	0	-1.098211	0.975254	-7.974034
136	1	0	-1.978371	0.319558	-7.951802
137	1	0	-1.468540	2.005933	-7.951650
138	6	0	0.808683	-1.799406	-4.716459
139	1	0	-0.080732	-2.433789	-4.857449
140	6	0	1.621649	-2.095952	-3.521623
141	6	0	2.733540	-1.307424	-3.196024
142	1	0	2.972625	-0.457586	-3.830363
143	6	0	3.521623	-1.621649	-2.095952
144	6	0	3.196024	-2.733540	-1.307424
145	1	0	3.830363	-2.972625	-0.457586
146	6	0	2.095952	-3.521623	-1.621649
147	6	0	1.307424	-3.196024	-2.733540
148	1	0	0.457586	-3.830363	-2.972625
149	6	0	1.799406	-4.716459	-0.808683
150	1	0	2.433789	-4.857449	0.080732
151	6	0	0.716665	-6.706676	-0.276443
152	1	0	1.403934	-6.684206	0.588657
153	6	0	-0.716665	-6.706676	0.276443
154	1	0	-1.403934	-6.684206	-0.588657
155	6	0	-0.975254	-7.974034	1.098211
156	1	0	-2.005933	-7.951650	1.468540
157	1	0	-0.319558	-7.951802	1.978371
158	6	0	-0.712655	-9.237465	0.277856
159	1	0	-1.425277	-9.285138	-0.556828
160	1	0	-0.885575	-10.126359	0.893631
161	6	0	0.712655	-9.237465	-0.277856
162	1	0	1.425277	-9.285138	0.556828
163	1	0	0.885575	-10.126359	-0.893631
164	6	0	0.975254	-7.974034	-1.098211
165	1	0	0.319558	-7.951802	-1.978371
166	1	0	2.005933	-7.951650	-1.468540
167	6	0	-1.799406	-4.716459	0.808683
168	1	0	-2.433789	-4.857449	-0.080732
169	6	0	-1.603280	1.603280	1.603280
170	6	0	-1.603280	-1.603280	-1.603280
171	6	0	1.603280	1.603280	-1.603280
172	1	0	-2.653024	1.402186	1.373338
173	1	0	-2.653024	-1.402186	-1.373338
174	1	0	1.402186	1.373338	-2.653024
175	1	0	1.373338	2.653024	-1.402186
176	1	0	2.653024	1.402186	-1.373338
177	1	0	-1.402186	1.373338	2.653024
178	1	0	-1.373338	2.653024	1.402186
179	1	0	-1.402186	-1.373338	-2.653024
180	1	0	-1.373338	-2.653024	-1.402186
181	6	0	1.603280	-1.603280	1.603280
182	1	0	1.373338	-2.653024	1.402186
183	1	0	2.653024	-1.402186	1.373338
184	1	0	1.402186	-1.373338	2.653024
185	1	0	0.973148	-0.973148	0.973148
186	1	0	-0.973148	0.973148	0.973148
187	1	0	0.973148	0.973148	-0.973148
188	1	0	-0.973148	-0.973148	-0.973148

4CH4@CC3-b T cc3-rb

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-1.116297	-0.906117	5.543108
2	7	0	1.116297	0.906117	5.543108
3	7	0	0.906117	5.543108	1.116297
4	7	0	-0.906117	5.543108	-1.116297
5	6	0	-2.718410	-1.299175	3.191020
6	1	0	-2.947619	-0.445446	3.824076
7	6	0	-1.608429	-2.092535	3.511448
8	6	0	-0.787543	-1.795511	4.701473
9	1	0	0.117296	-2.411270	4.824516
10	6	0	-0.265621	-0.720839	6.701447
11	1	0	0.609499	-1.395069	6.674362
12	6	0	0.265621	0.720839	6.701447
13	1	0	-0.609499	1.395069	6.674362
14	6	0	1.080490	0.994578	7.970221
15	1	0	1.432968	2.031466	7.947499
16	1	0	1.971906	0.354268	7.949066
17	6	0	0.264189	0.717983	9.233139
18	1	0	0.875995	0.903205	10.122307
19	1	0	-0.583946	1.414636	9.279713
20	6	0	-0.264189	-0.717983	9.233139
21	1	0	-0.875995	-0.903205	10.122307
22	1	0	0.583946	-1.414636	9.279713
23	6	0	-1.080490	-0.994578	7.970221
24	1	0	-1.971906	-0.354268	7.949066
25	1	0	-1.432968	-2.031466	7.947499
26	6	0	0.787543	1.795511	4.701473
27	1	0	-0.117296	2.411270	4.824516
28	6	0	1.608429	2.092535	3.511448
29	6	0	2.718410	1.299175	3.191020
30	1	0	2.947619	0.445446	3.824076
31	6	0	3.511448	1.608429	2.092535
32	6	0	3.191020	2.718410	1.299175
33	1	0	3.824076	2.947619	0.445446
34	6	0	2.092535	3.511448	1.608429
35	6	0	1.299175	3.191020	2.718410
36	1	0	0.445446	3.824076	2.947619
37	6	0	1.795511	4.701473	0.787543
38	1	0	2.411270	4.824516	-0.117296
39	6	0	0.720839	6.701447	0.265621
40	1	0	1.395069	6.674362	-0.609499
41	6	0	-0.720839	6.701447	-0.265621
42	1	0	-1.395069	6.674362	0.609499
43	6	0	-0.994578	7.970221	-1.080490
44	1	0	-2.031466	7.947499	-1.432968
45	1	0	-0.354268	7.949066	-1.971906
46	6	0	-0.717983	9.233139	-0.264189
47	1	0	-1.414636	9.279713	0.583946
48	1	0	-0.903205	10.122307	-0.875995
49	6	0	0.717983	9.233139	0.264189
50	1	0	1.414636	9.279713	-0.583946
51	1	0	0.903205	10.122307	0.875995
52	6	0	0.994578	7.970221	1.080490
53	1	0	0.354268	7.949066	1.971906
54	1	0	2.031466	7.947499	1.432968

55	6	0	-1.795511	4.701473	-0.787543
56	1	0	-2.411270	4.824516	0.117296
57	7	0	-0.906117	-5.543108	1.116297
58	7	0	0.906117	-5.543108	-1.116297
59	7	0	5.543108	-1.116297	-0.906117
60	7	0	5.543108	1.116297	0.906117
61	6	0	-1.299175	-3.191020	2.718410
62	1	0	-0.445446	-3.824076	2.947619
63	6	0	-2.092535	-3.511448	1.608429
64	6	0	-1.795511	-4.701473	0.787543
65	1	0	-2.411270	-4.824516	-0.117296
66	6	0	-0.720839	-6.701447	0.265621
67	1	0	-1.395069	-6.674362	-0.609499
68	6	0	0.720839	-6.701447	-0.265621
69	1	0	1.395069	-6.674362	0.609499
70	6	0	0.994578	-7.970221	-1.080490
71	1	0	2.031466	-7.947499	-1.432968
72	1	0	0.354268	-7.949066	-1.971906
73	6	0	0.717983	-9.233139	-0.264189
74	1	0	0.903205	-10.122307	-0.875995
75	1	0	1.414636	-9.279713	0.583946
76	6	0	-0.717983	-9.233139	0.264189
77	1	0	-0.903205	-10.122307	0.875995
78	1	0	-1.414636	-9.279713	-0.583946
79	6	0	-0.994578	-7.970221	1.080490
80	1	0	-0.354268	-7.949066	1.971906
81	1	0	-2.031466	-7.947499	1.432968
82	6	0	1.795511	-4.701473	-0.787543
83	1	0	2.411270	-4.824516	0.117296
84	6	0	2.092535	-3.511448	-1.608429
85	6	0	1.299175	-3.191020	-2.718410
86	1	0	0.445446	-3.824076	-2.947619
87	6	0	1.608429	-2.092535	-3.511448
88	6	0	2.718410	-1.299175	-3.191020
89	1	0	2.947619	-0.445446	-3.824076
90	6	0	3.511448	-1.608429	-2.092535
91	6	0	3.191020	-2.718410	-1.299175
92	1	0	3.824076	-2.947619	-0.445446
93	6	0	4.701473	-0.787543	-1.795511
94	1	0	4.824516	0.117296	-2.411270
95	6	0	6.701447	-0.265621	-0.720839
96	1	0	6.674362	0.609499	-1.395069
97	6	0	6.701447	0.265621	0.720839
98	1	0	6.674362	-0.609499	1.395069
99	6	0	7.970221	1.080490	0.994578
100	1	0	7.947499	1.432968	2.031466
101	1	0	7.949066	1.971906	0.354268
102	6	0	9.233139	0.264189	0.717983
103	1	0	9.279713	-0.583946	1.414636
104	1	0	10.122307	0.875995	0.903205
105	6	0	9.233139	-0.264189	-0.717983
106	1	0	9.279713	0.583946	-1.414636
107	1	0	10.122307	-0.875995	-0.903205
108	6	0	7.970221	-1.080490	-0.994578
109	1	0	7.949066	-1.971906	-0.354268
110	1	0	7.947499	-1.432968	-2.031466
111	6	0	4.701473	0.787543	1.795511
112	1	0	4.824516	-0.117296	2.411270
113	7	0	-5.543108	-1.116297	0.906117

114	7	0	-5.543108	1.116297	-0.906117
115	7	0	-1.116297	0.906117	-5.543108
116	7	0	1.116297	-0.906117	-5.543108
117	6	0	-3.191020	-2.718410	1.299175
118	1	0	-3.824076	-2.947619	0.445446
119	6	0	-3.511448	-1.608429	2.092535
120	6	0	-4.701473	-0.787543	1.795511
121	1	0	-4.824516	0.117296	2.411270
122	6	0	-6.701447	-0.265621	0.720839
123	1	0	-6.674362	0.609499	1.395069
124	6	0	-6.701447	0.265621	-0.720839
125	1	0	-6.674362	-0.609499	-1.395069
126	6	0	-7.970221	1.080490	-0.994578
127	1	0	-7.947499	1.432968	-2.031466
128	1	0	-7.949066	1.971906	-0.354268
129	6	0	-9.233139	0.264189	-0.717983
130	1	0	-10.122307	0.875995	-0.903205
131	1	0	-9.279713	-0.583946	-1.414636
132	6	0	-9.233139	-0.264189	0.717983
133	1	0	-10.122307	-0.875995	0.903205
134	1	0	-9.279713	0.583946	1.414636
135	6	0	-7.970221	-1.080490	0.994578
136	1	0	-7.949066	-1.971906	0.354268
137	1	0	-7.947499	-1.432968	2.031466
138	6	0	-4.701473	0.787543	-1.795511
139	1	0	-4.824516	-0.117296	-2.411270
140	6	0	-3.511448	1.608429	-2.092535
141	6	0	-3.191020	2.718410	-1.299175
142	1	0	-3.824076	2.947619	-0.445446
143	6	0	-2.092535	3.511448	-1.608429
144	6	0	-1.299175	3.191020	-2.718410
145	1	0	-0.445446	3.824076	-2.947619
146	6	0	-1.608429	2.092535	-3.511448
147	6	0	-2.718410	1.299175	-3.191020
148	1	0	-2.947619	0.445446	-3.824076
149	6	0	-0.787543	1.795511	-4.701473
150	1	0	0.117296	2.411270	-4.824516
151	6	0	-0.265621	0.720839	-6.701447
152	1	0	0.609499	1.395069	-6.674362
153	6	0	0.265621	-0.720839	-6.701447
154	1	0	-0.609499	-1.395069	-6.674362
155	6	0	1.080490	-0.994578	-7.970221
156	1	0	1.432968	-2.031466	-7.947499
157	1	0	1.971906	-0.354268	-7.949066
158	6	0	0.264189	-0.717983	-9.233139
159	1	0	-0.583946	-1.414636	-9.279713
160	1	0	0.875995	-0.903205	-10.122307
161	6	0	-0.264189	0.717983	-9.233139
162	1	0	0.583946	1.414636	-9.279713
163	1	0	-0.875995	0.903205	-10.122307
164	6	0	-1.080490	0.994578	-7.970221
165	1	0	-1.971906	0.354268	-7.949066
166	1	0	-1.432968	2.031466	-7.947499
167	6	0	0.787543	-1.795511	-4.701473
168	1	0	-0.117296	-2.411270	-4.824516
169	6	0	1.598617	-1.598617	1.598617
170	6	0	-1.598617	-1.598617	-1.598617
171	6	0	-1.598617	1.598617	1.598617
172	1	0	0.960047	-2.229349	0.975003

173	1	0	-0.960047	-2.229349	-0.975003
174	1	0	-2.229349	0.975003	0.960047
175	1	0	-0.975003	0.960047	2.229349
176	1	0	-0.960047	2.229349	0.975003
177	1	0	2.229349	-0.975003	0.960047
178	1	0	0.975003	-0.960047	2.229349
179	1	0	-2.229349	-0.975003	-0.960047
180	1	0	-0.975003	-0.960047	-2.229349
181	6	0	1.598617	1.598617	-1.598617
182	1	0	0.975003	0.960047	-2.229349
183	1	0	0.960047	2.229349	-0.975003
184	1	0	2.229349	0.975003	-0.960047
185	1	0	-2.230056	2.230056	2.230056
186	1	0	2.230056	-2.230056	2.230056
187	1	0	-2.230056	-2.230056	-2.230056
188	1	0	2.230056	2.230056	-2.230056

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	0.899886	5.537063	1.115772
2	7	0	-0.899886	5.537063	-1.115772
3	7	0	-5.537063	1.115772	-0.899886
4	7	0	-5.537063	-1.115772	0.899886
5	6	0	1.279106	3.170143	2.700687
6	1	0	0.429167	3.805919	2.936221
7	6	0	2.071323	3.492546	1.590422
8	6	0	1.781669	4.690620	0.778890
9	1	0	2.397172	4.815649	-0.125905
10	6	0	0.719640	6.699166	0.269339
11	1	0	1.397961	6.674746	-0.602677
12	6	0	-0.719640	6.699166	-0.269339
13	1	0	-1.397961	6.674746	0.602677
14	6	0	-0.987256	7.966545	-1.087767
15	1	0	-2.021720	7.944319	-1.447327
16	1	0	-0.340762	7.944489	-1.974674
17	6	0	-0.715824	9.229694	-0.269853
18	1	0	-0.895809	10.118787	-0.883304
19	1	0	-1.419031	9.276950	0.572820
20	6	0	0.715824	9.229694	0.269853
21	1	0	0.895809	10.118787	0.883304
22	1	0	1.419031	9.276950	-0.572820
23	6	0	0.987256	7.966545	1.087767
24	1	0	0.340762	7.944489	1.974674
25	1	0	2.021720	7.944319	1.447327
26	6	0	-1.781669	4.690620	-0.778890
27	1	0	-2.397172	4.815649	0.125905
28	6	0	-2.071323	3.492546	-1.590422
29	6	0	-1.279106	3.170143	-2.700687
30	1	0	-0.429167	3.805919	-2.936221
31	6	0	-1.590422	2.071323	-3.492546
32	6	0	-2.700687	1.279106	-3.170143
33	1	0	-2.936221	0.429167	-3.805919
34	6	0	-3.492546	1.590422	-2.071323
35	6	0	-3.170143	2.700687	-1.279106

36	1	0	-3.805919	2.936221	-0.429167
37	6	0	-4.690620	0.778890	-1.781669
38	1	0	-4.815649	-0.125905	-2.397172
39	6	0	-6.699166	0.269339	-0.719640
40	1	0	-6.674746	-0.602677	-1.397961
41	6	0	-6.699166	-0.269339	0.719640
42	1	0	-6.674746	0.602677	1.397961
43	6	0	-7.966545	-1.087767	0.987256
44	1	0	-7.944319	-1.447327	2.021720
45	1	0	-7.944489	-1.974674	0.340762
46	6	0	-9.229694	-0.269853	0.715824
47	1	0	-9.276950	0.572820	1.419031
48	1	0	-10.118787	-0.883304	0.895809
49	6	0	-9.229694	0.269853	-0.715824
50	1	0	-9.276950	-0.572820	-1.419031
51	1	0	-10.118787	0.883304	-0.895809
52	6	0	-7.966545	1.087767	-0.987256
53	1	0	-7.944489	1.974674	-0.340762
54	1	0	-7.944319	1.447327	-2.021720
55	6	0	-4.690620	-0.778890	1.781669
56	1	0	-4.815649	0.125905	2.397172
57	7	0	5.537063	1.115772	0.899886
58	7	0	5.537063	-1.115772	-0.899886
59	7	0	1.115772	-0.899886	-5.537063
60	7	0	-1.115772	0.899886	-5.537063
61	6	0	3.170143	2.700687	1.279106
62	1	0	3.805919	2.936221	0.429167
63	6	0	3.492546	1.590422	2.071323
64	6	0	4.690620	0.778890	1.781669
65	1	0	4.815649	-0.125905	2.397172
66	6	0	6.699166	0.269339	0.719640
67	1	0	6.674746	-0.602677	1.397961
68	6	0	6.699166	-0.269339	-0.719640
69	1	0	6.674746	0.602677	-1.397961
70	6	0	7.966545	-1.087767	-0.987256
71	1	0	7.944319	-1.447327	-2.021720
72	1	0	7.944489	-1.974674	-0.340762
73	6	0	9.229694	-0.269853	-0.715824
74	1	0	10.118787	-0.883304	-0.895809
75	1	0	9.276950	0.572820	-1.419031
76	6	0	9.229694	0.269853	0.715824
77	1	0	10.118787	0.883304	0.895809
78	1	0	9.276950	-0.572820	1.419031
79	6	0	7.966545	1.087767	0.987256
80	1	0	7.944489	1.974674	0.340762
81	1	0	7.944319	1.447327	2.021720
82	6	0	4.690620	-0.778890	-1.781669
83	1	0	4.815649	0.125905	-2.397172
84	6	0	3.492546	-1.590422	-2.071323
85	6	0	3.170143	-2.700687	-1.279106
86	1	0	3.805919	-2.936221	-0.429167
87	6	0	2.071323	-3.492546	-1.590422
88	6	0	1.279106	-3.170143	-2.700687
89	1	0	0.429167	-3.805919	-2.936221
90	6	0	1.590422	-2.071323	-3.492546
91	6	0	2.700687	-1.279106	-3.170143
92	1	0	2.936221	-0.429167	-3.805919
93	6	0	0.778890	-1.781669	-4.690620
94	1	0	-0.125905	-2.397172	-4.815649

95	6	0	0.269339	-0.719640	-6.699166
96	1	0	-0.602677	-1.397961	-6.674746
97	6	0	-0.269339	0.719640	-6.699166
98	1	0	0.602677	1.397961	-6.674746
99	6	0	-1.087767	0.987256	-7.966545
100	1	0	-1.447327	2.021720	-7.944319
101	1	0	-1.974674	0.340762	-7.944489
102	6	0	-0.269853	0.715824	-9.229694
103	1	0	0.572820	1.419031	-9.276950
104	1	0	-0.883304	0.895809	-10.118787
105	6	0	0.269853	-0.715824	-9.229694
106	1	0	-0.572820	-1.419031	-9.276950
107	1	0	0.883304	-0.895809	-10.118787
108	6	0	1.087767	-0.987256	-7.966545
109	1	0	1.974674	-0.340762	-7.944489
110	1	0	1.447327	-2.021720	-7.944319
111	6	0	-0.778890	1.781669	-4.690620
112	1	0	0.125905	2.397172	-4.815649
113	7	0	1.115772	0.899886	5.537063
114	7	0	-1.115772	-0.899886	5.537063
115	7	0	-0.899886	-5.537063	1.115772
116	7	0	0.899886	-5.537063	-1.115772
117	6	0	2.700687	1.279106	3.170143
118	1	0	2.936221	0.429167	3.805919
119	6	0	1.590422	2.071323	3.492546
120	6	0	0.778890	1.781669	4.690620
121	1	0	-0.125905	2.397172	4.815649
122	6	0	0.269339	0.719640	6.699166
123	1	0	-0.602677	1.397961	6.674746
124	6	0	-0.269339	-0.719640	6.699166
125	1	0	0.602677	-1.397961	6.674746
126	6	0	-1.087767	-0.987256	7.966545
127	1	0	-1.447327	-2.021720	7.944319
128	1	0	-1.974674	-0.340762	7.944489
129	6	0	-0.269853	-0.715824	9.229694
130	1	0	-0.883304	-0.895809	10.118787
131	1	0	0.572820	-1.419031	9.276950
132	6	0	0.269853	0.715824	9.229694
133	1	0	0.883304	0.895809	10.118787
134	1	0	-0.572820	1.419031	9.276950
135	6	0	1.087767	0.987256	7.966545
136	1	0	1.974674	0.340762	7.944489
137	1	0	1.447327	2.021720	7.944319
138	6	0	-0.778890	-1.781669	4.690620
139	1	0	0.125905	-2.397172	4.815649
140	6	0	-1.590422	-2.071323	3.492546
141	6	0	-2.700687	-1.279106	3.170143
142	1	0	-2.936221	-0.429167	3.805919
143	6	0	-3.492546	-1.590422	2.071323
144	6	0	-3.170143	-2.700687	1.279106
145	1	0	-3.805919	-2.936221	0.429167
146	6	0	-2.071323	-3.492546	1.590422
147	6	0	-1.279106	-3.170143	2.700687
148	1	0	-0.429167	-3.805919	2.936221
149	6	0	-1.781669	-4.690620	0.778890
150	1	0	-2.397172	-4.815649	-0.125905
151	6	0	-0.719640	-6.699166	0.269339
152	1	0	-1.397961	-6.674746	-0.602677
153	6	0	0.719640	-6.699166	-0.269339

154	1	0	1.397961	-6.674746	0.602677
155	6	0	0.987256	-7.966545	-1.087767
156	1	0	2.021720	-7.944319	-1.447327
157	1	0	0.340762	-7.944489	-1.974674
158	6	0	0.715824	-9.229694	-0.269853
159	1	0	1.419031	-9.276950	0.572820
160	1	0	0.895809	-10.118787	-0.883304
161	6	0	-0.715824	-9.229694	0.269853
162	1	0	-1.419031	-9.276950	-0.572820
163	1	0	-0.895809	-10.118787	0.883304
164	6	0	-0.987256	-7.966545	1.087767
165	1	0	-0.340762	-7.944489	1.974674
166	1	0	-2.021720	-7.944319	1.447327
167	6	0	1.781669	-4.690620	-0.778890
168	1	0	2.397172	-4.815649	0.125905
169	6	0	1.892506	1.892506	-1.892506
170	6	0	1.892506	-1.892506	1.892506
171	6	0	-1.892506	1.892506	1.892506
172	1	0	2.517944	1.264719	-1.251726
173	1	0	2.517944	-1.264719	1.251726
174	1	0	-1.264719	1.251726	2.517944
175	1	0	-1.251726	2.517944	1.264719
176	1	0	-2.517944	1.264719	1.251726
177	1	0	1.264719	1.251726	-2.517944
178	1	0	1.251726	2.517944	-1.264719
179	1	0	1.264719	-1.251726	2.517944
180	1	0	1.251726	-2.517944	1.264719
181	6	0	-1.892506	-1.892506	-1.892506
182	1	0	-1.251726	-2.517944	-1.264719
183	1	0	-2.517944	-1.264719	-1.251726
184	1	0	-1.264719	-1.251726	-2.517944
185	1	0	-2.523822	2.523822	2.523822
186	1	0	2.523822	2.523822	-2.523822
187	1	0	2.523822	-2.523822	2.523822
188	1	0	-2.523822	-2.523822	-2.523822
189	6	0	0.000000	0.000000	0.000000
190	1	0	0.632198	0.632198	0.632198
191	1	0	-0.632198	0.632198	-0.632198
192	1	0	0.632198	-0.632198	-0.632198
193	1	0	-0.632198	-0.632198	0.632198

5CH4@CC3 C1 cc3-raarr

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-3.880601	1.363265	3.973830
2	7	0	-5.036700	2.255332	1.507378
3	7	0	-4.215180	-1.688315	-3.481072
4	7	0	-2.339543	-3.855527	-3.515186
5	6	0	-1.682394	-0.490285	3.984140
6	1	0	-2.686855	-0.898386	3.902881
7	6	0	-1.521173	0.901894	3.981747
8	6	0	-2.691379	1.798155	3.909150
9	1	0	-2.465616	2.872517	3.820304
10	6	0	-4.957254	2.332109	3.932188
11	1	0	-4.571343	3.362573	3.830683

12	6	0	-5.831390	2.046615	2.700891
13	1	0	-6.178783	1.000494	2.778607
14	6	0	-7.042243	2.984972	2.672552
15	1	0	-7.651651	2.750572	1.793012
16	1	0	-6.676818	4.011953	2.542854
17	6	0	-7.865222	2.877068	3.956765
18	1	0	-8.711496	3.571019	3.918514
19	1	0	-8.286618	1.865663	4.036172
20	6	0	-6.995802	3.156765	5.184045
21	1	0	-7.580235	3.044366	6.103291
22	1	0	-6.651021	4.199316	5.151867
23	6	0	-5.785777	2.222498	5.216327
24	1	0	-6.115104	1.180838	5.323738
25	1	0	-5.140786	2.442411	6.073965
26	6	0	-4.862302	1.266721	0.732912
27	1	0	-5.290186	0.274411	0.945848
28	6	0	-4.101953	1.379242	-0.526929
29	6	0	-3.418579	2.559486	-0.849734
30	1	0	-3.436600	3.382564	-0.139583
31	6	0	-2.751294	2.677361	-2.063072
32	6	0	-2.758138	1.603096	-2.963112
33	1	0	-2.240019	1.715658	-3.912315
34	6	0	-3.432909	0.428560	-2.652433
35	6	0	-4.102826	0.319701	-1.426225
36	1	0	-4.634441	-0.602121	-1.203244
37	6	0	-3.478056	-0.668753	-3.638260
38	1	0	-2.848875	-0.534219	-4.532202
39	6	0	-4.213696	-2.690772	-4.527330
40	1	0	-3.527421	-2.417660	-5.349233
41	6	0	-3.716064	-4.019566	-3.936997
42	1	0	-4.374005	-4.268604	-3.084834
43	6	0	-3.794130	-5.135410	-4.984034
44	1	0	-3.445451	-6.070338	-4.532100
45	1	0	-3.095491	-4.893393	-5.795440
46	6	0	-5.211609	-5.286696	-5.537081
47	1	0	-5.886591	-5.601648	-4.729598
48	1	0	-5.235225	-6.075864	-6.295937
49	6	0	-5.710505	-3.963879	-6.121589
50	1	0	-5.091769	-3.696714	-6.989120
51	1	0	-6.738340	-4.067168	-6.485037
52	6	0	-5.634088	-2.846988	-5.080030
53	1	0	-6.306240	-3.066434	-4.240327
54	1	0	-5.956563	-1.889849	-5.504067
55	6	0	-2.073158	-4.027680	-2.287594
56	1	0	-2.849843	-4.289401	-1.551801
57	7	0	2.413694	2.418610	4.585709
58	7	0	4.138413	3.129206	2.409524
59	7	0	1.154173	4.703666	-3.042526
60	7	0	-1.613520	4.171051	-3.564339
61	6	0	-0.247134	1.444710	4.097968
62	1	0	-0.097385	2.521513	4.109335
63	6	0	0.871460	0.609997	4.225012
64	6	0	2.221136	1.177957	4.408880
65	1	0	3.049355	0.451906	4.407775
66	6	0	3.775258	2.867838	4.795186
67	1	0	4.490375	2.026387	4.754578
68	6	0	4.151838	3.844193	3.669740
69	1	0	3.408301	4.661589	3.679862
70	6	0	5.549993	4.424147	3.907105

71	1	0	5.785454	5.123753	3.097770
72	1	0	6.276771	3.604076	3.841330
73	6	0	5.649128	5.107475	5.271415
74	1	0	6.661974	5.495133	5.423289
75	1	0	4.970818	5.971224	5.297014
76	6	0	5.270750	4.138246	6.392897
77	1	0	5.309314	4.640797	7.365092
78	1	0	6.005254	3.322075	6.427418
79	6	0	3.875874	3.556672	6.160051
80	1	0	3.122595	4.354295	6.197646
81	1	0	3.614319	2.834846	6.941377
82	6	0	3.328438	3.520816	1.516130
83	1	0	2.648062	4.372040	1.676087
84	6	0	3.259841	2.887509	0.184881
85	6	0	3.995431	1.728360	-0.096961
86	1	0	4.597090	1.288049	0.694369
87	6	0	3.969339	1.169855	-1.369254
88	6	0	3.194509	1.769083	-2.371615
89	1	0	3.193454	1.325430	-3.364215
90	6	0	2.461539	2.918674	-2.102228
91	6	0	2.494556	3.474103	-0.815908
92	1	0	1.923722	4.379465	-0.624727
93	6	0	1.699175	3.567945	-3.186318
94	1	0	1.654527	3.014007	-4.137252
95	6	0	0.461033	5.269625	-4.182174
96	1	0	0.494358	4.591825	-5.054278
97	6	0	-1.017218	5.468206	-3.812064
98	1	0	-1.048540	6.107303	-2.911141
99	6	0	-1.768818	6.160057	-4.953953
100	1	0	-2.814083	6.298894	-4.657203
101	1	0	-1.770144	5.486589	-5.820835
102	6	0	-1.120151	7.494221	-5.324566
103	1	0	-1.192241	8.184087	-4.472678
104	1	0	-1.664189	7.957332	-6.154478
105	6	0	0.352594	7.299103	-5.689641
106	1	0	0.420769	6.685324	-6.598183
107	1	0	0.822378	8.260908	-5.920816
108	6	0	1.106770	6.608769	-4.552642
109	1	0	1.109921	7.246471	-3.659122
110	1	0	2.153896	6.434437	-4.822919
111	6	0	-2.088043	3.949336	-2.409684
112	1	0	-2.053511	4.704199	-1.608370
113	7	0	0.167800	-3.585744	4.452389
114	7	0	0.291914	-5.291369	2.152363
115	7	0	3.973986	-3.153624	-2.641191
116	7	0	4.944326	-0.463827	-2.838927
117	6	0	0.701046	-0.769258	4.226315
118	1	0	1.551953	-1.437369	4.334300
119	6	0	-0.579572	-1.326586	4.109576
120	6	0	-0.776246	-2.787977	4.169695
121	1	0	-1.801963	-3.140348	3.977663
122	6	0	-0.140934	-4.999714	4.522861
123	1	0	-1.204592	-5.194059	4.294940
124	6	0	0.696610	-5.741083	3.469002
125	1	0	1.758290	-5.508169	3.668177
126	6	0	0.478034	-7.253789	3.575942
127	1	0	1.095468	-7.755133	2.822718
128	1	0	-0.568802	-7.467366	3.323812
129	6	0	0.797108	-7.768255	4.980089

130	1	0	0.614083	-8.846570	5.034339
131	1	0	1.864464	-7.615854	5.190681
132	6	0	-0.032837	-7.028657	6.031037
133	1	0	0.223534	-7.375476	7.037616
134	1	0	-1.096276	-7.257201	5.877136
135	6	0	0.182108	-5.518264	5.927926
136	1	0	1.227104	-5.268824	6.153349
137	1	0	-0.437133	-4.981471	6.654772
138	6	0	1.165742	-4.730376	1.424850
139	1	0	2.201659	-4.578706	1.766877
140	6	0	0.869771	-4.269158	0.054576
141	6	0	-0.437719	-4.306851	-0.448618
142	1	0	-1.235921	-4.657070	0.201246
143	6	0	-0.699345	-3.923751	-1.758635
144	6	0	0.353617	-3.490057	-2.575577
145	1	0	0.133327	-3.204032	-3.601122
146	6	0	1.653649	-3.449122	-2.086052
147	6	0	1.907001	-3.837582	-0.763507
148	1	0	2.931187	-3.809664	-0.399684
149	6	0	2.756858	-3.046571	-2.979867
150	1	0	2.456358	-2.670151	-3.970390
151	6	0	4.981010	-2.765748	-3.608167
152	1	0	4.523476	-2.400414	-4.545331
153	6	0	5.809466	-1.611653	-3.022147
154	1	0	6.228017	-1.961156	-2.061031
155	6	0	6.953478	-1.236283	-3.969692
156	1	0	7.532267	-0.421631	-3.521073
157	1	0	6.515740	-0.843661	-4.896669
158	6	0	7.844726	-2.440208	-4.276822
159	1	0	8.334531	-2.776714	-3.352878
160	1	0	8.641048	-2.149363	-4.969994
161	6	0	7.021180	-3.591572	-4.856827
162	1	0	6.607886	-3.286121	-5.827760
163	1	0	7.656796	-4.463651	-5.043036
164	6	0	5.877887	-3.969626	-3.914441
165	1	0	6.279570	-4.347822	-2.965406
166	1	0	5.263395	-4.769691	-4.341301
167	6	0	4.797082	-0.016419	-1.661770
168	1	0	5.299400	-0.474190	-0.795029
169	6	0	-0.482663	3.082112	1.001592
170	6	0	2.726069	-1.188232	1.389123
171	6	0	-2.567591	-1.846344	0.869573
172	1	0	0.418671	2.676638	1.469771
173	1	0	2.564096	-0.155868	1.711702
174	1	0	-1.654613	-2.243388	1.322242
175	1	0	-2.717704	-0.817915	1.210006
176	1	0	-2.458435	-1.850592	-0.218581
177	1	0	-0.361873	3.060481	-0.085129
178	1	0	-1.339699	2.461869	1.278701
179	1	0	1.864750	-1.794351	1.683681
180	1	0	2.824238	-1.211515	0.300161
181	6	0	0.326724	-0.046767	-3.265695
182	1	0	1.235079	-0.433450	-2.795178
183	1	0	-0.522260	-0.669435	-2.969919
184	1	0	0.155141	0.977812	-2.923918
185	1	0	-3.423627	-2.461938	1.159220
186	1	0	-0.644653	4.110274	1.336702
187	1	0	3.634182	-1.583759	1.852298
188	1	0	0.436882	-0.061671	-4.353484

189	6	0	0.001878	-0.002687	-0.001197
190	1	0	-0.107284	0.013973	1.088220
191	1	0	-0.907125	0.394329	-0.465114
192	1	0	0.859059	0.613763	-0.291593
193	1	0	0.162803	-1.032738	-0.336198

6CH4@CC3 T cc3-roo

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-5.595894	-1.156393	0.938899
2	7	0	-5.595894	1.156393	-0.938899
3	7	0	-1.156393	0.938899	-5.595894
4	7	0	1.156393	-0.938899	-5.595894
5	6	0	-3.476171	-3.014231	1.587480
6	1	0	-4.093046	-3.234810	0.719497
7	6	0	-3.800510	-1.896956	2.372367
8	6	0	-4.933541	-1.017279	2.012120
9	1	0	-5.155520	-0.213183	2.731916
10	6	0	-6.724589	-0.265924	0.721291
11	1	0	-6.684969	0.605923	1.398563
12	6	0	-6.724589	0.265924	-0.721291
13	1	0	-6.684969	-0.605923	-1.398563
14	6	0	-8.006491	1.065158	-1.001887
15	1	0	-7.980719	1.406042	-2.042826
16	1	0	-7.991263	1.965210	-0.373044
17	6	0	-9.269321	0.252753	-0.721037
18	1	0	-10.157462	0.862509	-0.917969
19	1	0	-9.312954	-0.605531	-1.405251
20	6	0	-9.269321	-0.252753	0.721037
21	1	0	-10.157462	-0.862509	0.917969
22	1	0	-9.312954	0.605531	1.405251
23	6	0	-8.006491	-1.065158	1.001887
24	1	0	-7.991263	-1.965210	0.373044
25	1	0	-7.980719	-1.406042	2.042826
26	6	0	-4.933541	1.017279	-2.012120
27	1	0	-5.155520	0.213183	-2.731916
28	6	0	-3.800510	1.896956	-2.372367
29	6	0	-3.476171	3.014231	-1.587480
30	1	0	-4.093046	3.234810	-0.719497
31	6	0	-2.372367	3.800510	-1.896956
32	6	0	-1.587480	3.476171	-3.014231
33	1	0	-0.719497	4.093046	-3.234810
34	6	0	-1.896956	2.372367	-3.800510
35	6	0	-3.014231	1.587480	-3.476171
36	1	0	-3.234810	0.719497	-4.093046
37	6	0	-1.017279	2.012120	-4.933541
38	1	0	-0.213183	2.731916	-5.155520
39	6	0	-0.265924	0.721291	-6.724589
40	1	0	0.605923	1.398563	-6.684969
41	6	0	0.265924	-0.721291	-6.724589
42	1	0	-0.605923	-1.398563	-6.684969
43	6	0	1.065158	-1.001887	-8.006491
44	1	0	1.406042	-2.042826	-7.980719
45	1	0	1.965210	-0.373044	-7.991263
46	6	0	0.252753	-0.721037	-9.269321

47	1	0	-0.605531	-1.405251	-9.312954
48	1	0	0.862509	-0.917969	-10.157462
49	6	0	-0.252753	0.721037	-9.269321
50	1	0	0.605531	1.405251	-9.312954
51	1	0	-0.862509	0.917969	-10.157462
52	6	0	-1.065158	1.001887	-8.006491
53	1	0	-1.965210	0.373044	-7.991263
54	1	0	-1.406042	2.042826	-7.980719
55	6	0	1.017279	-2.012120	-4.933541
56	1	0	0.213183	-2.731916	-5.155520
57	7	0	-1.156393	-0.938899	5.595894
58	7	0	1.156393	0.938899	5.595894
59	7	0	0.938899	5.595894	1.156393
60	7	0	-0.938899	5.595894	-1.156393
61	6	0	-3.014231	-1.587480	3.476171
62	1	0	-3.234810	-0.719497	4.093046
63	6	0	-1.896956	-2.372367	3.800510
64	6	0	-1.017279	-2.012120	4.933541
65	1	0	-0.213183	-2.731916	5.155520
66	6	0	-0.265924	-0.721291	6.724589
67	1	0	0.605923	-1.398563	6.684969
68	6	0	0.265924	0.721291	6.724589
69	1	0	-0.605923	1.398563	6.684969
70	6	0	1.065158	1.001887	8.006491
71	1	0	1.406042	2.042826	7.980719
72	1	0	1.965210	0.373044	7.991263
73	6	0	0.252753	0.721037	9.269321
74	1	0	0.862509	0.917969	10.157462
75	1	0	-0.605531	1.405251	9.312954
76	6	0	-0.252753	-0.721037	9.269321
77	1	0	-0.862509	-0.917969	10.157462
78	1	0	0.605531	-1.405251	9.312954
79	6	0	-1.065158	-1.001887	8.006491
80	1	0	-1.965210	-0.373044	7.991263
81	1	0	-1.406042	-2.042826	7.980719
82	6	0	1.017279	2.012120	4.933541
83	1	0	0.213183	2.731916	5.155520
84	6	0	1.896956	2.372367	3.800510
85	6	0	3.014231	1.587480	3.476171
86	1	0	3.234810	0.719497	4.093046
87	6	0	3.800510	1.896956	2.372367
88	6	0	3.476171	3.014231	1.587480
89	1	0	4.093046	3.234810	0.719497
90	6	0	2.372367	3.800510	1.896956
91	6	0	1.587480	3.476171	3.014231
92	1	0	0.719497	4.093046	3.234810
93	6	0	2.012120	4.933541	1.017279
94	1	0	2.731916	5.155520	0.213183
95	6	0	0.721291	6.724589	0.265924
96	1	0	1.398563	6.684969	-0.605923
97	6	0	-0.721291	6.724589	-0.265924
98	1	0	-1.398563	6.684969	0.605923
99	6	0	-1.001887	8.006491	-1.065158
100	1	0	-2.042826	7.980719	-1.406042
101	1	0	-0.373044	7.991263	-1.965210
102	6	0	-0.721037	9.269321	-0.252753
103	1	0	-1.405251	9.312954	0.605531
104	1	0	-0.917969	10.157462	-0.862509
105	6	0	0.721037	9.269321	0.252753

106	1	0	1.405251	9.312954	-0.605531
107	1	0	0.917969	10.157462	0.862509
108	6	0	1.001887	8.006491	1.065158
109	1	0	0.373044	7.991263	1.965210
110	1	0	2.042826	7.980719	1.406042
111	6	0	-2.012120	4.933541	-1.017279
112	1	0	-2.731916	5.155520	-0.213183
113	7	0	-0.938899	-5.595894	1.156393
114	7	0	0.938899	-5.595894	-1.156393
115	7	0	5.595894	-1.156393	-0.938899
116	7	0	5.595894	1.156393	0.938899
117	6	0	-1.587480	-3.476171	3.014231
118	1	0	-0.719497	-4.093046	3.234810
119	6	0	-2.372367	-3.800510	1.896956
120	6	0	-2.012120	-4.933541	1.017279
121	1	0	-2.731916	-5.155520	0.213183
122	6	0	-0.721291	-6.724589	0.265924
123	1	0	-1.398563	-6.684969	-0.605923
124	6	0	0.721291	-6.724589	-0.265924
125	1	0	1.398563	-6.684969	0.605923
126	6	0	1.001887	-8.006491	-1.065158
127	1	0	2.042826	-7.980719	-1.406042
128	1	0	0.373044	-7.991263	-1.965210
129	6	0	0.721037	-9.269321	-0.252753
130	1	0	0.917969	-10.157462	-0.862509
131	1	0	1.405251	-9.312954	0.605531
132	6	0	-0.721037	-9.269321	0.252753
133	1	0	-0.917969	-10.157462	0.862509
134	1	0	-1.405251	-9.312954	-0.605531
135	6	0	-1.001887	-8.006491	1.065158
136	1	0	-0.373044	-7.991263	1.965210
137	1	0	-2.042826	-7.980719	1.406042
138	6	0	2.012120	-4.933541	-1.017279
139	1	0	2.731916	-5.155520	-0.213183
140	6	0	2.372367	-3.800510	-1.896956
141	6	0	1.587480	-3.476171	-3.014231
142	1	0	0.719497	-4.093046	-3.234810
143	6	0	1.896956	-2.372367	-3.800510
144	6	0	3.014231	-1.587480	-3.476171
145	1	0	3.234810	-0.719497	-4.093046
146	6	0	3.800510	-1.896956	-2.372367
147	6	0	3.476171	-3.014231	-1.587480
148	1	0	4.093046	-3.234810	-0.719497
149	6	0	4.933541	-1.017279	-2.012120
150	1	0	5.155520	-0.213183	-2.731916
151	6	0	6.724589	-0.265924	-0.721291
152	1	0	6.684969	0.605923	-1.398563
153	6	0	6.724589	0.265924	0.721291
154	1	0	6.684969	-0.605923	1.398563
155	6	0	8.006491	1.065158	1.001887
156	1	0	7.980719	1.406042	2.042826
157	1	0	7.991263	1.965210	0.373044
158	6	0	9.269321	0.252753	0.721037
159	1	0	9.312954	-0.605531	1.405251
160	1	0	10.157462	0.862509	0.917969
161	6	0	9.269321	-0.252753	-0.721037
162	1	0	9.312954	0.605531	-1.405251
163	1	0	10.157462	-0.862509	-0.917969
164	6	0	8.006491	-1.065158	-1.001887

165	1	0	7.991263	-1.965210	-0.373044
166	1	0	7.980719	-1.406042	-2.042826
167	6	0	4.933541	1.017279	2.012120
168	1	0	5.155520	0.213183	2.731916
169	6	0	0.000000	0.000000	-2.606135
170	6	0	0.000000	2.606135	-0.000000
171	6	0	0.000000	0.000000	2.606135
172	6	0	-0.000000	-2.606135	0.000000
173	6	0	2.606135	-0.000000	0.000000
174	6	0	-2.606135	0.000000	-0.000000
175	1	0	0.849331	-0.254288	3.244409
176	1	0	-0.849331	0.254288	3.244409
177	1	0	0.251981	0.855462	1.978362
178	1	0	-0.849331	-0.254288	-3.244409
179	1	0	0.849331	0.254288	-3.244409
180	1	0	-0.251981	0.855462	-1.978362
181	1	0	0.855462	-1.978362	-0.251981
182	1	0	-0.254288	-3.244409	-0.849331
183	1	0	0.254288	-3.244409	0.849331
184	1	0	3.244409	-0.849331	0.254288
185	1	0	1.978362	-0.251981	-0.855462
186	1	0	3.244409	0.849331	-0.254288
187	1	0	-0.254288	3.244409	0.849331
188	1	0	0.254288	3.244409	-0.849331
189	1	0	-0.855462	1.978362	-0.251981
190	1	0	-3.244409	0.849331	0.254288
191	1	0	-3.244409	-0.849331	-0.254288
192	1	0	-1.978362	0.251981	-0.855462
193	1	0	0.855462	1.978362	0.251981
194	1	0	1.978362	0.251981	0.855462
195	1	0	0.251981	-0.855462	-1.978362
196	1	0	-0.855462	-1.978362	0.251981
197	1	0	-0.251981	-0.855462	1.978362
198	1	0	-1.978362	-0.251981	0.855462

6CH4@CC3 C1 cc3-rooxx

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-3.437564	-1.244179	4.491002
2	7	0	-3.813018	1.674383	4.024716
3	7	0	-4.109483	3.469217	-2.151626
4	7	0	-3.312308	1.719462	-4.427261
5	6	0	-2.330651	-3.272300	2.749239
6	1	0	-3.388518	-3.042046	2.646900
7	6	0	-1.602035	-2.633980	3.764657
8	6	0	-2.245040	-1.644685	4.656512
9	1	0	-1.610158	-1.258692	5.470071
10	6	0	-3.978279	-0.311957	5.467240
11	1	0	-3.176041	0.143284	6.075114
12	6	0	-4.734372	0.828626	4.766498
13	1	0	-5.485469	0.370420	4.098489
14	6	0	-5.449844	1.715111	5.797466
15	1	0	-5.995084	2.499149	5.260392
16	1	0	-4.684736	2.218983	6.402869
17	6	0	-6.386886	0.914391	6.699843

18	1	0	-6.862873	1.579383	7.428267
19	1	0	-7.191691	0.474980	6.094955
20	6	0	-5.621534	-0.203058	7.407265
21	1	0	-6.295697	-0.800082	8.030521
22	1	0	-4.873705	0.239697	8.079131
23	6	0	-4.922963	-1.100388	6.387342
24	1	0	-5.668088	-1.605420	5.758438
25	1	0	-4.344477	-1.886405	6.885318
26	6	0	-4.148437	2.024307	2.852127
27	1	0	-5.071897	1.655583	2.377570
28	6	0	-3.323606	2.926535	2.019532
29	6	0	-2.173370	3.539428	2.539825
30	1	0	-1.913668	3.356473	3.579848
31	6	0	-1.369224	4.336295	1.733032
32	6	0	-1.724545	4.536458	0.390236
33	1	0	-1.077732	5.151277	-0.231219
34	6	0	-2.861113	3.935464	-0.138539
35	6	0	-3.663555	3.133560	0.687561
36	1	0	-4.541564	2.659397	0.255312
37	6	0	-3.178105	4.107626	-1.572930
38	1	0	-2.534928	4.817473	-2.117336
39	6	0	-4.362120	3.765739	-3.552588
40	1	0	-3.517337	4.314795	-4.005598
41	6	0	-4.556560	2.468432	-4.354339
42	1	0	-5.349094	1.882916	-3.854944
43	6	0	-4.992825	2.783605	-5.793429
44	1	0	-5.143944	1.837079	-6.324186
45	1	0	-4.163697	3.299632	-6.295477
46	6	0	-6.251917	3.647185	-5.841640
47	1	0	-7.093493	3.093240	-5.403944
48	1	0	-6.518501	3.861535	-6.882009
49	6	0	-6.041134	4.942907	-5.059604
50	1	0	-5.257945	5.537629	-5.549097
51	1	0	-6.952103	5.550771	-5.064117
52	6	0	-5.625582	4.637245	-3.621753
53	1	0	-6.434195	4.106847	-3.101549
54	1	0	-5.440466	5.559980	-3.060736
55	6	0	-3.365946	0.467497	-4.228228
56	1	0	-4.304413	-0.036282	-3.946389
57	7	0	2.608823	-3.379959	3.912072
58	7	0	4.812471	-1.808297	2.666886
59	7	0	3.475135	4.382022	1.504701
60	7	0	0.724991	5.526385	1.570523
61	6	0	-0.244685	-2.901326	3.901337
62	1	0	0.346385	-2.409899	4.670560
63	6	0	0.400397	-3.789558	3.027077
64	6	0	1.856696	-4.029415	3.123127
65	1	0	2.254404	-4.801533	2.445189
66	6	0	4.015511	-3.745462	3.957752
67	1	0	4.299086	-4.360997	3.085382
68	6	0	4.902307	-2.489611	3.948360
69	1	0	4.566443	-1.837491	4.774362
70	6	0	6.374953	-2.867299	4.170410
71	1	0	6.970131	-1.947466	4.181185
72	1	0	6.711021	-3.452126	3.303908
73	6	0	6.580638	-3.669385	5.454081
74	1	0	7.638162	-3.931210	5.565756
75	1	0	6.311771	-3.049995	6.320541
76	6	0	5.710767	-4.925623	5.444148

77	1	0	5.830512	-5.487235	6.376689
78	1	0	6.037959	-5.585875	4.629471
79	6	0	4.242195	-4.556570	5.242815
80	1	0	3.885531	-3.957484	6.091154
81	1	0	3.613039	-5.452633	5.201765
82	6	0	4.686629	-0.545782	2.678419
83	1	0	4.583645	0.019272	3.618656
84	6	0	4.640652	0.265130	1.442337
85	6	0	4.855176	-0.321023	0.185431
86	1	0	5.081416	-1.383750	0.140685
87	6	0	4.749029	0.435520	-0.976005
88	6	0	4.437846	1.800732	-0.882389
89	1	0	4.344913	2.375578	-1.800804
90	6	0	4.222733	2.394556	0.356031
91	6	0	4.332949	1.618590	1.520140
92	1	0	4.148153	2.094767	2.480180
93	6	0	3.831086	3.819157	0.424701
94	1	0	3.848843	4.361074	-0.534440
95	6	0	3.167388	5.802386	1.456256
96	1	0	3.014628	6.145037	0.417223
97	6	0	1.879381	6.104714	2.239404
98	1	0	2.002563	5.692076	3.256701
99	6	0	1.648677	7.620752	2.334249
100	1	0	0.738071	7.796211	2.917740
101	1	0	1.454504	7.999765	1.322106
102	6	0	2.842236	8.351737	2.946228
103	1	0	2.982820	8.019774	3.983880
104	1	0	2.643732	9.428216	2.980458
105	6	0	4.112727	8.061390	2.148426
106	1	0	4.005155	8.471308	1.134977
107	1	0	4.977163	8.557414	2.602401
108	6	0	4.359281	6.556099	2.066133
109	1	0	4.541832	6.149739	3.069794
110	1	0	5.250646	6.335157	1.468553
111	6	0	-0.127223	4.917816	2.286959
112	1	0	0.022342	4.770375	3.368549
113	7	0	-1.940623	-5.455153	-0.144035
114	7	0	-2.259823	-4.453741	-2.931618
115	7	0	2.569796	-0.804743	-5.126659
116	7	0	4.682349	0.375193	-3.388504
117	6	0	-0.333786	-4.414869	2.025820
118	1	0	0.143985	-5.096714	1.326255
119	6	0	-1.704601	-4.154410	1.876023
120	6	0	-2.479406	-4.763664	0.773281
121	1	0	-3.562185	-4.560381	0.787705
122	6	0	-2.814289	-6.049615	-1.142916
123	1	0	-3.816228	-5.584604	-1.127987
124	6	0	-2.233878	-5.857598	-2.553553
125	1	0	-1.202305	-6.252755	-2.546833
126	6	0	-3.064170	-6.631901	-3.588776
127	1	0	-2.607098	-6.490548	-4.574452
128	1	0	-4.062458	-6.176759	-3.634123
129	6	0	-3.181209	-8.115797	-3.245558
130	1	0	-3.792376	-8.626218	-3.997440
131	1	0	-2.185483	-8.578740	-3.275502
132	6	0	-3.778239	-8.295881	-1.850555
133	1	0	-3.834136	-9.357410	-1.587092
134	1	0	-4.807021	-7.910835	-1.844823
135	6	0	-2.946684	-7.544294	-0.812711

136	1	0	-1.936785	-7.972080	-0.758925
137	1	0	-3.384426	-7.640230	0.187102
138	6	0	-1.224101	-3.973438	-3.485238
139	1	0	-0.308554	-4.570868	-3.622318
140	6	0	-1.148105	-2.576393	-3.964864
141	6	0	-2.274833	-1.740308	-3.935735
142	1	0	-3.215384	-2.149994	-3.575055
143	6	0	-2.180147	-0.410590	-4.329977
144	6	0	-0.946265	0.089950	-4.773143
145	1	0	-0.885574	1.135709	-5.065168
146	6	0	0.178096	-0.726884	-4.807223
147	6	0	0.067818	-2.067206	-4.406230
148	1	0	0.959502	-2.689370	-4.425784
149	6	0	1.481218	-0.159022	-5.215819
150	1	0	1.449420	0.877638	-5.587662
151	6	0	3.778895	-0.160171	-5.613551
152	1	0	3.630364	0.926826	-5.742842
153	6	0	4.935324	-0.356141	-4.619612
154	1	0	5.032661	-1.440084	-4.430080
155	6	0	6.250924	0.172892	-5.211179
156	1	0	7.052717	-0.005737	-4.486147
157	1	0	6.160962	1.261619	-5.322406
158	6	0	6.578174	-0.465168	-6.559971
159	1	0	6.739592	-1.543448	-6.426023
160	1	0	7.512173	-0.049836	-6.953072
161	6	0	5.431865	-0.246571	-7.546426
162	1	0	5.327436	0.828332	-7.747329
163	1	0	5.648050	-0.730084	-8.504999
164	6	0	4.123469	-0.787645	-6.973028
165	1	0	4.193460	-1.875190	-6.838357
166	1	0	3.288409	-0.607019	-7.658957
167	6	0	4.913959	-0.219433	-2.291831
168	1	0	5.234463	-1.273052	-2.258612
169	6	0	-1.727754	1.208746	-1.530847
170	6	0	0.978785	2.307017	0.715594
171	6	0	1.727440	-1.208069	1.532443
172	6	0	-0.977175	-2.307002	-0.715831
173	6	0	1.689366	-0.099332	-1.981362
174	6	0	-1.688466	0.101009	1.982263
175	1	0	2.607526	-1.757061	1.189685
176	1	0	1.697297	-1.248668	2.623716
177	1	0	1.790246	-0.168487	1.208590
178	1	0	-2.796578	1.313061	-1.330392
179	1	0	-1.505323	1.693340	-2.484319
180	1	0	-1.153857	1.687974	-0.736805
181	1	0	-0.352164	-1.668324	-1.341170
182	1	0	-1.943404	-2.468074	-1.199448
183	1	0	-0.490339	-3.275989	-0.583541
184	1	0	1.949096	-0.993419	-2.552833
185	1	0	0.621287	0.101487	-2.073228
186	1	0	2.254635	0.744770	-2.383126
187	1	0	1.616816	2.490198	1.583230
188	1	0	0.815223	3.255873	0.199505
189	1	0	0.024142	1.896141	1.046352
190	1	0	-1.616181	0.759312	2.851082
191	1	0	-2.586950	-0.511711	2.085829
192	1	0	-1.757723	0.696757	1.071318
193	1	0	1.466993	1.604567	0.038995
194	1	0	1.946212	-0.250966	-0.932284

195	1	0	-1.469305	0.150482	-1.584217
196	1	0	-1.130768	-1.834350	0.255031
197	1	0	0.828626	-1.668135	1.120113
198	1	0	-0.806819	-0.539435	1.936800

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-0.408120	4.812450	2.460781
2	7	0	2.359232	4.027454	2.705556
3	7	0	5.070293	1.765728	-2.666429
4	7	0	3.583063	0.962021	-5.003169
5	6	0	-2.126823	3.748866	0.406580
6	1	0	-1.487188	4.588363	0.146467
7	6	0	-2.020647	3.198867	1.692103
8	6	0	-1.079503	3.759835	2.681973
9	1	0	-1.009866	3.214690	3.635979
10	6	0	0.453761	5.299005	3.520421
11	1	0	0.449159	4.617095	4.390436
12	6	0	1.898100	5.369333	3.000636
13	1	0	1.894616	6.005337	2.096921
14	6	0	2.820879	5.989888	4.055845
15	1	0	3.837698	6.037672	3.651101
16	1	0	2.853602	5.314758	4.920934
17	6	0	2.334117	7.373243	4.487356
18	1	0	3.001500	7.783523	5.252531
19	1	0	2.373468	8.058619	3.629738
20	6	0	0.897790	7.301846	5.007802
21	1	0	0.538600	8.298424	5.285479
22	1	0	0.874413	6.689653	5.919661
23	6	0	-0.028828	6.686501	3.958478
24	1	0	-0.072820	7.329784	3.069970
25	1	0	-1.052346	6.599946	4.339165
26	6	0	2.745567	3.776890	1.524333
27	1	0	2.726799	4.539144	0.729880
28	6	0	3.269037	2.452714	1.134039
29	6	0	3.263744	1.389823	2.047595
30	1	0	2.857587	1.566072	3.039033
31	6	0	3.780624	0.150498	1.692103
32	6	0	4.310025	-0.032550	0.406580
33	1	0	4.717233	-1.006239	0.146467
34	6	0	4.323518	1.015463	-0.505636
35	6	0	3.795590	2.261120	-0.136744
36	1	0	3.818558	3.069985	-0.862532
37	6	0	4.923252	0.815788	-1.839792
38	1	0	5.253967	-0.209962	-2.065878
39	6	0	5.708897	1.467781	-3.933306
40	1	0	5.945553	0.392148	-4.024565
41	6	0	4.745700	1.825012	-5.076229
42	1	0	4.469217	2.888064	-4.954970
43	6	0	5.427367	1.629083	-6.435035
44	1	0	4.722070	1.904361	-7.226726
45	1	0	5.643771	0.559961	-6.558679
46	6	0	6.717483	2.442751	-6.540343
47	1	0	6.478583	3.513851	-6.490248

48	1	0	7.191561	2.268687	-7.512041
49	6	0	7.676281	2.087880	-5.402559
50	1	0	7.988150	1.039729	-5.507260
51	1	0	8.584879	2.696427	-5.460677
52	6	0	7.001466	2.284058	-4.044743
53	1	0	6.751678	3.342703	-3.896433
54	1	0	7.671353	1.997913	-3.226589
55	6	0	2.446218	1.510019	-4.882249
56	1	0	2.329970	2.603305	-4.820085
57	7	0	-4.667493	0.029428	2.705556
58	7	0	-3.963644	-2.759667	2.460781
59	7	0	2.308261	-4.056882	2.705556
60	7	0	4.371764	-2.052783	2.460781
61	6	0	-2.835494	2.131574	2.047595
62	1	0	-2.785052	1.691707	3.039033
63	6	0	-3.758631	1.604712	1.134039
64	6	0	-4.643666	0.489286	1.524333
65	1	0	-5.294414	0.091905	0.729880
66	6	0	-5.599029	-1.040864	3.000636
67	1	0	-6.148083	-1.361884	2.096921
68	6	0	-4.815953	-2.256534	3.520421
69	1	0	-4.223101	-1.919564	4.390436
70	6	0	-5.776266	-3.368216	3.958478
71	1	0	-5.189548	-4.211331	4.339165
72	1	0	-6.311369	-3.727956	3.069970
73	6	0	-6.772479	-2.873414	5.007802
74	1	0	-7.455947	-3.682770	5.285479
75	1	0	-6.230616	-2.587562	5.919661
76	6	0	-7.552474	-1.665217	4.487356
77	1	0	-8.241479	-1.292386	5.252531
78	1	0	-8.165703	-1.973826	3.629738
79	6	0	-6.597834	-0.551991	4.055845
80	1	0	-6.029516	-0.186087	4.920934
81	1	0	-7.147626	0.304708	3.651101
82	6	0	-2.716361	-2.814795	2.681973
83	1	0	-2.279070	-2.481915	3.635979
84	6	0	-1.759977	-3.349365	1.692103
85	6	0	-2.183202	-3.716316	0.406580
86	1	0	-3.230045	-3.582124	0.146467
87	6	0	-1.282342	-4.252008	-0.505636
88	6	0	0.060392	-4.417637	-0.136744
89	1	0	0.749406	-4.841961	-0.862532
90	6	0	0.489594	-4.057426	1.134039
91	6	0	-0.428250	-3.521397	2.047595
92	1	0	-0.072535	-3.257779	3.039033
93	6	0	1.898099	-4.266176	1.524333
94	1	0	2.567615	-4.631049	0.729880
95	6	0	3.700929	-4.328469	3.000636
96	1	0	4.253467	-4.643454	2.096921
97	6	0	4.362192	-3.042471	3.520421
98	1	0	3.773942	-2.697531	4.390436
99	6	0	5.805094	-3.318285	3.958478
100	1	0	6.241894	-2.388615	4.339165
101	1	0	6.384189	-3.601828	3.069970
102	6	0	5.874689	-4.428432	5.007802
103	1	0	5.356203	-4.102091	5.919661
104	1	0	6.917346	-4.615654	5.285479
105	6	0	5.218357	-5.708026	4.487356
106	1	0	5.792235	-6.084793	3.629738

107	1	0	5.239978	-6.491137	5.252531
108	6	0	3.776955	-5.437897	4.055845
109	1	0	3.175914	-5.128671	4.920934
110	1	0	3.309928	-6.342380	3.651101
111	6	0	3.795864	-0.945040	2.681973
112	1	0	3.288936	-0.732775	3.635979
113	7	0	-4.064312	3.508139	-2.666429
114	7	0	-2.624666	2.622013	-5.003169
115	7	0	-0.958397	-3.584034	-5.003169
116	7	0	-1.005981	-5.273867	-2.666429
117	6	0	-3.855982	2.156517	-0.136744
118	1	0	-4.567964	1.771976	-0.862532
119	6	0	-3.041176	3.236545	-0.505636
120	6	0	-3.168119	3.855767	-1.839792
121	1	0	-2.445151	4.655050	-2.065878
122	6	0	-4.125584	4.210159	-3.933306
123	1	0	-3.312387	4.952926	-4.024565
124	6	0	-3.953357	3.197391	-5.076229
125	1	0	-4.735745	2.426423	-4.954970
126	6	0	-4.124511	3.885696	-6.435035
127	1	0	-4.010260	3.137252	-7.226726
128	1	0	-3.306826	4.607669	-6.558679
129	6	0	-5.474227	4.596136	-6.540343
130	1	0	-5.560521	5.093731	-7.512041
131	1	0	-6.282375	3.853693	-6.490248
132	6	0	-5.646298	5.603914	-5.402559
133	1	0	-6.627614	6.086510	-5.460677
134	1	0	-4.894507	6.398076	-5.507260
135	6	0	-5.478785	4.921418	-4.044743
136	1	0	-6.270705	4.175773	-3.896433
137	1	0	-5.565920	5.644630	-3.226589
138	6	0	-2.530824	1.363477	-4.882249
139	1	0	-3.419513	0.716161	-4.820085
140	6	0	-1.229228	0.667909	-4.842594
141	6	0	-0.028621	1.391959	-4.840618
142	1	0	-0.077715	2.477798	-4.849272
143	6	0	1.193040	0.730588	-4.842594
144	6	0	1.219782	-0.671193	-4.840618
145	1	0	2.184693	-1.171596	-4.849272
146	6	0	0.036188	-1.398497	-4.842594
147	6	0	-1.191161	-0.720766	-4.840618
148	1	0	-2.106978	-1.306202	-4.849272
149	6	0	0.084606	-2.873496	-4.882249
150	1	0	1.089543	-3.319466	-4.820085
151	6	0	-0.792343	-5.022403	-5.076229
152	1	0	0.266528	-5.314487	-4.954970
153	6	0	-1.583313	-5.677940	-3.933306
154	1	0	-2.633166	-5.345074	-4.024565
155	6	0	-1.522681	-7.205476	-4.044743
156	1	0	-2.105433	-7.642543	-3.226589
157	1	0	-0.480973	-7.518476	-3.896433
158	6	0	-2.029983	-7.691794	-5.402559
159	1	0	-3.093643	-7.437805	-5.507260
160	1	0	-1.957265	-8.782937	-5.460677
161	6	0	-1.243257	-7.038887	-6.540343
162	1	0	-0.196208	-7.367543	-6.490248
163	1	0	-1.631040	-7.362418	-7.512041
164	6	0	-1.302856	-5.514779	-6.435035
165	1	0	-2.336945	-5.167630	-6.558679

166	1	0	-0.711810	-5.041613	-7.226726
167	6	0	-1.755133	-4.671555	-1.839792
168	1	0	-2.808816	-4.445088	-2.065878
169	16	0	-0.000000	0.000000	5.343874
170	9	0	-1.131206	-0.622586	6.253462
171	9	0	1.131293	0.619863	4.429532
172	9	0	-1.102464	0.669797	4.429532
173	9	0	-0.028829	-1.289660	4.429532
174	9	0	1.104778	-0.668360	6.253462
175	9	0	0.026428	1.290946	6.253462

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	2.223415	2.200169	4.476272
2	7	0	2.670737	4.127695	2.381106
3	7	0	-2.415610	5.276552	-1.380248
4	7	0	-4.784137	3.632232	-1.437156
5	6	0	0.161153	0.209916	4.342569
6	1	0	-0.105874	1.204471	4.690421
7	6	0	1.477659	-0.017798	3.917559
8	6	0	2.480862	1.064048	3.975366
9	1	0	3.475452	0.816881	3.576249
10	6	0	3.295929	3.174292	4.527496
11	1	0	4.208287	2.798126	4.029823
12	6	0	2.857494	4.444915	3.782934
13	1	0	1.917778	4.793646	4.248324
14	6	0	3.924751	5.537582	3.911163
15	1	0	3.579131	6.432881	3.382961
16	1	0	4.830831	5.193357	3.395691
17	6	0	4.238535	5.849270	5.374864
18	1	0	5.016322	6.617796	5.435483
19	1	0	3.343907	6.263139	5.859834
20	6	0	4.673074	4.584614	6.117440
21	1	0	4.863145	4.804170	7.173336
22	1	0	5.619457	4.223592	5.692186
23	6	0	3.610973	3.491879	5.993657
24	1	0	2.681357	3.811434	6.482412
25	1	0	3.932505	2.571321	6.492911
26	6	0	1.529748	4.340087	1.870802
27	1	0	0.692427	4.743923	2.461021
28	6	0	1.244478	4.078336	0.446092
29	6	0	2.216358	3.496440	-0.378983
30	1	0	3.177583	3.237336	0.055943
31	6	0	1.954316	3.266445	-1.723744
32	6	0	0.707002	3.622039	-2.255490
33	1	0	0.521084	3.440849	-3.311113
34	6	0	-0.260048	4.209132	-1.448602
35	6	0	0.013062	4.431290	-0.091193
36	1	0	-0.754942	4.893862	0.523383
37	6	0	-1.548349	4.625639	-2.037146
38	1	0	-1.700551	4.353576	-3.093308
39	6	0	-3.627195	5.675727	-2.068999
40	1	0	-3.646843	5.296411	-3.106776
41	6	0	-4.839598	5.077413	-1.338563

42	1	0	-4.791388	5.414002	-0.287086
43	6	0	-6.145955	5.570365	-1.970987
44	1	0	-6.989324	5.138883	-1.420931
45	1	0	-6.199519	5.178565	-2.995091
46	6	0	-6.222906	7.097206	-1.987305
47	1	0	-6.243615	7.473004	-0.955235
48	1	0	-7.155917	7.419935	-2.461214
49	6	0	-5.016139	7.692584	-2.714604
50	1	0	-5.046876	7.391860	-3.770743
51	1	0	-5.056114	8.786786	-2.695138
52	6	0	-3.710393	7.206126	-2.085274
53	1	0	-3.633660	7.564157	-1.050343
54	1	0	-2.842068	7.601336	-2.623614
55	6	0	-4.755015	2.965696	-0.359149
56	1	0	-4.758990	3.453321	0.628189
57	7	0	2.492889	-4.023482	2.786281
58	7	0	2.370190	-5.003198	0.084238
59	7	0	3.160982	-0.359274	-4.311840
60	7	0	2.852383	2.467549	-3.814499
61	6	0	1.847269	-1.283109	3.476235
62	1	0	2.862446	-1.486167	3.143955
63	6	0	0.914526	-2.330521	3.466964
64	6	0	1.298606	-3.696041	3.058515
65	1	0	0.475956	-4.427614	3.030088
66	6	0	2.742739	-5.412969	2.451852
67	1	0	1.806360	-5.999912	2.445699
68	6	0	3.342492	-5.497010	1.040019
69	1	0	4.261837	-4.883577	1.033262
70	6	0	3.699448	-6.947178	0.696147
71	1	0	4.132801	-6.975530	-0.309595
72	1	0	2.770080	-7.530425	0.659719
73	6	0	4.658418	-7.547304	1.725027
74	1	0	4.881242	-8.588059	1.467260
75	1	0	5.611344	-7.001474	1.696361
76	6	0	4.069836	-7.456803	3.134185
77	1	0	4.775281	-7.853570	3.871868
78	1	0	3.167686	-8.081261	3.188895
79	6	0	3.708205	-6.011888	3.480305
80	1	0	4.612986	-5.390658	3.504462
81	1	0	3.251442	-5.947589	4.473875
82	6	0	2.722103	-4.036340	-0.656804
83	1	0	3.721843	-3.585848	-0.582707
84	6	0	1.834919	-3.454373	-1.682265
85	6	0	0.538273	-3.951234	-1.874387
86	1	0	0.195551	-4.764979	-1.240367
87	6	0	-0.278724	-3.423850	-2.866407
88	6	0	0.198544	-2.379602	-3.670843
89	1	0	-0.451299	-1.984119	-4.447272
90	6	0	1.479810	-1.875135	-3.484974
91	6	0	2.297880	-2.417928	-2.484156
92	1	0	3.300949	-2.018522	-2.360275
93	6	0	1.975129	-0.804283	-4.372014
94	1	0	1.250747	-0.429060	-5.111643
95	6	0	3.545675	0.651148	-5.278899
96	1	0	2.697992	0.926093	-5.932492
97	6	0	3.984403	1.924458	-4.541468
98	1	0	4.806879	1.647337	-3.857696
99	6	0	4.488396	2.973545	-5.539495
100	1	0	4.804265	3.864235	-4.985357

101	1	0	3.645730	3.275532	-6.175122
102	6	0	5.628752	2.428527	-6.400003
103	1	0	6.492232	2.202510	-5.759596
104	1	0	5.955198	3.190582	-7.115544
105	6	0	5.197682	1.155114	-7.129633
106	1	0	4.397132	1.400089	-7.840912
107	1	0	6.028312	0.747300	-7.715312
108	6	0	4.692216	0.106828	-6.137960
109	1	0	5.504917	-0.203002	-5.467963
110	1	0	4.347990	-0.793762	-6.657959
111	6	0	3.006491	2.677343	-2.573587
112	1	0	3.951214	2.446543	-2.061021
113	7	0	-2.996623	-1.496913	4.949614
114	7	0	-5.209115	-0.716032	3.272418
115	7	0	-4.778342	-2.632459	-2.849515
116	7	0	-2.361331	-3.645493	-4.053455
117	6	0	-0.387282	-2.092515	3.890393
118	1	0	-1.126379	-2.889480	3.899492
119	6	0	-0.771257	-0.819279	4.332712
120	6	0	-2.140729	-0.570059	4.824375
121	1	0	-2.367103	0.472740	5.096377
122	6	0	-4.297662	-1.147547	5.485337
123	1	0	-4.381749	-0.060925	5.668180
124	6	0	-5.380446	-1.525775	4.462604
125	1	0	-5.264248	-2.602097	4.240713
126	6	0	-6.777351	-1.273438	5.040825
127	1	0	-7.525852	-1.564936	4.295979
128	1	0	-6.891297	-0.193409	5.201235
129	6	0	-6.987442	-2.025303	6.355541
130	1	0	-7.984710	-1.811051	6.754053
131	1	0	-6.945188	-3.106987	6.168471
132	6	0	-5.909160	-1.649046	7.373066
133	1	0	-6.041848	-2.214127	8.301687
134	1	0	-6.010801	-0.585869	7.630232
135	6	0	-4.513891	-1.902385	6.801782
136	1	0	-4.373357	-2.974010	6.609326
137	1	0	-3.736335	-1.602305	7.512673
138	6	0	-5.015335	-1.314404	2.171661
139	1	0	-4.964941	-2.412468	2.105967
140	6	0	-4.868007	-0.589327	0.894074
141	6	0	-4.841675	0.812185	0.864564
142	1	0	-4.913862	1.352181	1.805173
143	6	0	-4.740108	1.489590	-0.343967
144	6	0	-4.657362	0.761501	-1.539148
145	1	0	-4.584650	1.308350	-2.475737
146	6	0	-4.683059	-0.627269	-1.521467
147	6	0	-4.786187	-1.301025	-0.296214
148	1	0	-4.811341	-2.387713	-0.302027
149	6	0	-4.636706	-1.373852	-2.794043
150	1	0	-4.490860	-0.763681	-3.699096
151	6	0	-4.761129	-3.256499	-4.158030
152	1	0	-4.551419	-2.520219	-4.954996
153	6	0	-3.642483	-4.308820	-4.198247
154	1	0	-3.826415	-5.018222	-3.371105
155	6	0	-3.664768	-5.066022	-5.530804
156	1	0	-2.866237	-5.815894	-5.524312
157	1	0	-3.427769	-4.355001	-6.332944
158	6	0	-5.025794	-5.713824	-5.787113
159	1	0	-5.217431	-6.476262	-5.019796

160	1	0	-5.018734	-6.230247	-6.752769
161	6	0	-6.140673	-4.667335	-5.745027
162	1	0	-6.000477	-3.957393	-6.571552
163	1	0	-7.117554	-5.139178	-5.894371
164	6	0	-6.123205	-3.910304	-4.416789
165	1	0	-6.336564	-4.597257	-3.587487
166	1	0	-6.896860	-3.135066	-4.394685
167	6	0	-1.621841	-3.996116	-3.085231
168	1	0	-1.934130	-4.766740	-2.363216
169	16	0	4.826138	0.120651	-0.092030
170	9	0	4.463527	-1.418904	-0.098255
171	9	0	5.196217	1.661321	-0.077851
172	9	0	4.628218	0.156947	1.477823
173	9	0	3.306157	0.486024	-0.294455
174	9	0	5.025980	0.083008	-1.658663
175	9	0	6.351359	-0.241161	0.112472

SF6@CC3 T cc3-rsf6c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	5.535780	0.904140	-1.113576
2	7	0	5.535780	-0.904140	1.113576
3	7	0	1.113576	-5.535780	0.904140
4	7	0	-1.113576	-5.535780	-0.904140
5	6	0	3.164505	1.272750	-2.692203
6	1	0	3.802212	0.423579	-2.924050
7	6	0	3.486048	2.068279	-1.583240
8	6	0	4.684500	1.779236	-0.771924
9	1	0	4.807366	2.389847	0.136089
10	6	0	6.697084	0.720945	-0.266600
11	1	0	6.671828	1.395691	0.608224
12	6	0	6.697084	-0.720945	0.266600
13	1	0	6.671828	-1.395691	-0.608224
14	6	0	7.964933	-0.992156	1.083062
15	1	0	7.942747	-2.028178	1.438114
16	1	0	7.943161	-0.349664	1.972893
17	6	0	9.228002	-0.717049	0.266303
18	1	0	10.117149	-0.900253	0.878727
19	1	0	9.275032	-1.416049	-0.579890
20	6	0	9.228002	0.717049	-0.266303
21	1	0	10.117149	0.900253	-0.878727
22	1	0	9.275032	1.416049	0.579890
23	6	0	7.964933	0.992156	-1.083062
24	1	0	7.943161	0.349664	-1.972893
25	1	0	7.942747	2.028178	-1.438114
26	6	0	4.684500	-1.779236	0.771924
27	1	0	4.807366	-2.389847	-0.136089
28	6	0	3.486048	-2.068279	1.583240
29	6	0	3.164505	-1.272750	2.692203
30	1	0	3.802212	-0.423579	2.924050
31	6	0	2.068279	-1.583240	3.486048
32	6	0	1.272750	-2.692203	3.164505
33	1	0	0.423579	-2.924050	3.802212
34	6	0	1.583240	-3.486048	2.068279
35	6	0	2.692203	-3.164505	1.272750

36	1	0	2.924050	-3.802212	0.423579
37	6	0	0.771924	-4.684500	1.779236
38	1	0	-0.136089	-4.807366	2.389847
39	6	0	0.266600	-6.697084	0.720945
40	1	0	-0.608224	-6.671828	1.395691
41	6	0	-0.266600	-6.697084	-0.720945
42	1	0	0.608224	-6.671828	-1.395691
43	6	0	-1.083062	-7.964933	-0.992156
44	1	0	-1.438114	-7.942747	-2.028178
45	1	0	-1.972893	-7.943161	-0.349664
46	6	0	-0.266303	-9.228002	-0.717049
47	1	0	0.579890	-9.275032	-1.416049
48	1	0	-0.878727	-10.117149	-0.900253
49	6	0	0.266303	-9.228002	0.717049
50	1	0	-0.579890	-9.275032	1.416049
51	1	0	0.878727	-10.117149	0.900253
52	6	0	1.083062	-7.964933	0.992156
53	1	0	1.972893	-7.943161	0.349664
54	1	0	1.438114	-7.942747	2.028178
55	6	0	-0.771924	-4.684500	-1.779236
56	1	0	0.136089	-4.807366	-2.389847
57	7	0	1.113576	5.535780	-0.904140
58	7	0	-1.113576	5.535780	0.904140
59	7	0	-0.904140	1.113576	5.535780
60	7	0	0.904140	-1.113576	5.535780
61	6	0	2.692203	3.164505	-1.272750
62	1	0	2.924050	3.802212	-0.423579
63	6	0	1.583240	3.486048	-2.068279
64	6	0	0.771924	4.684500	-1.779236
65	1	0	-0.136089	4.807366	-2.389847
66	6	0	0.266600	6.697084	-0.720945
67	1	0	-0.608224	6.671828	-1.395691
68	6	0	-0.266600	6.697084	0.720945
69	1	0	0.608224	6.671828	1.395691
70	6	0	-1.083062	7.964933	0.992156
71	1	0	-1.438114	7.942747	2.028178
72	1	0	-1.972893	7.943161	0.349664
73	6	0	-0.266303	9.228002	0.717049
74	1	0	-0.878727	10.117149	0.900253
75	1	0	0.579890	9.275032	1.416049
76	6	0	0.266303	9.228002	-0.717049
77	1	0	0.878727	10.117149	-0.900253
78	1	0	-0.579890	9.275032	-1.416049
79	6	0	1.083062	7.964933	-0.992156
80	1	0	1.972893	7.943161	-0.349664
81	1	0	1.438114	7.942747	-2.028178
82	6	0	-0.771924	4.684500	1.779236
83	1	0	0.136089	4.807366	2.389847
84	6	0	-1.583240	3.486048	2.068279
85	6	0	-2.692203	3.164505	1.272750
86	1	0	-2.924050	3.802212	0.423579
87	6	0	-3.486048	2.068279	1.583240
88	6	0	-3.164505	1.272750	2.692203
89	1	0	-3.802212	0.423579	2.924050
90	6	0	-2.068279	1.583240	3.486048
91	6	0	-1.272750	2.692203	3.164505
92	1	0	-0.423579	2.924050	3.802212
93	6	0	-1.779236	0.771924	4.684500
94	1	0	-2.389847	-0.136089	4.807366

95	6	0	-0.720945	0.266600	6.697084
96	1	0	-1.395691	-0.608224	6.671828
97	6	0	0.720945	-0.266600	6.697084
98	1	0	1.395691	0.608224	6.671828
99	6	0	0.992156	-1.083062	7.964933
100	1	0	2.028178	-1.438114	7.942747
101	1	0	0.349664	-1.972893	7.943161
102	6	0	0.717049	-0.266303	9.228002
103	1	0	1.416049	0.579890	9.275032
104	1	0	0.900253	-0.878727	10.117149
105	6	0	-0.717049	0.266303	9.228002
106	1	0	-1.416049	-0.579890	9.275032
107	1	0	-0.900253	0.878727	10.117149
108	6	0	-0.992156	1.083062	7.964933
109	1	0	-0.349664	1.972893	7.943161
110	1	0	-2.028178	1.438114	7.942747
111	6	0	1.779236	-0.771924	4.684500
112	1	0	2.389847	0.136089	4.807366
113	7	0	0.904140	1.113576	-5.535780
114	7	0	-0.904140	-1.113576	-5.535780
115	7	0	-5.535780	-0.904140	-1.113576
116	7	0	-5.535780	0.904140	1.113576
117	6	0	1.272750	2.692203	-3.164505
118	1	0	0.423579	2.924050	-3.802212
119	6	0	2.068279	1.583240	-3.486048
120	6	0	1.779236	0.771924	-4.684500
121	1	0	2.389847	-0.136089	-4.807366
122	6	0	0.720945	0.266600	-6.697084
123	1	0	1.395691	-0.608224	-6.671828
124	6	0	-0.720945	-0.266600	-6.697084
125	1	0	-1.395691	0.608224	-6.671828
126	6	0	-0.992156	-1.083062	-7.964933
127	1	0	-2.028178	-1.438114	-7.942747
128	1	0	-0.349664	-1.972893	-7.943161
129	6	0	-0.717049	-0.266303	-9.228002
130	1	0	-0.900253	-0.878727	-10.117149
131	1	0	-1.416049	0.579890	-9.275032
132	6	0	0.717049	0.266303	-9.228002
133	1	0	0.900253	0.878727	-10.117149
134	1	0	1.416049	-0.579890	-9.275032
135	6	0	0.992156	1.083062	-7.964933
136	1	0	0.349664	1.972893	-7.943161
137	1	0	2.028178	1.438114	-7.942747
138	6	0	-1.779236	-0.771924	-4.684500
139	1	0	-2.389847	0.136089	-4.807366
140	6	0	-2.068279	-1.583240	-3.486048
141	6	0	-1.272750	-2.692203	-3.164505
142	1	0	-0.423579	-2.924050	-3.802212
143	6	0	-1.583240	-3.486048	-2.068279
144	6	0	-2.692203	-3.164505	-1.272750
145	1	0	-2.924050	-3.802212	-0.423579
146	6	0	-3.486048	-2.068279	-1.583240
147	6	0	-3.164505	-1.272750	-2.692203
148	1	0	-3.802212	-0.423579	-2.924050
149	6	0	-4.684500	-1.779236	-0.771924
150	1	0	-4.807366	-2.389847	0.136089
151	6	0	-6.697084	-0.720945	-0.266600
152	1	0	-6.671828	-1.395691	0.608224
153	6	0	-6.697084	0.720945	0.266600

154	1	0	-6.671828	1.395691	-0.608224
155	6	0	-7.964933	0.992156	1.083062
156	1	0	-7.942747	2.028178	1.438114
157	1	0	-7.943161	0.349664	1.972893
158	6	0	-9.228002	0.717049	0.266303
159	1	0	-9.275032	1.416049	-0.579890
160	1	0	-10.117149	0.900253	0.878727
161	6	0	-9.228002	-0.717049	-0.266303
162	1	0	-9.275032	-1.416049	0.579890
163	1	0	-10.117149	-0.900253	-0.878727
164	6	0	-7.964933	-0.992156	-1.083062
165	1	0	-7.943161	-0.349664	-1.972893
166	1	0	-7.942747	-2.028178	-1.438114
167	6	0	-4.684500	1.779236	0.771924
168	1	0	-4.807366	2.389847	-0.136089
169	16	0	0.000000	0.000000	0.000000
170	9	0	-0.000000	1.581528	0.000000
171	9	0	-0.000000	-1.581528	-0.000000
172	9	0	0.000000	0.000000	-1.581528
173	9	0	-1.581528	0.000000	-0.000000
174	9	0	0.000000	-0.000000	1.581528
175	9	0	1.581528	-0.000000	-0.000000

4SF6@CC3 T cc3-rsf6by

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	0.883652	5.561970	-1.143318
2	7	0	-0.883652	5.561970	1.143318
3	7	0	-5.561970	1.143318	0.883652
4	7	0	-5.561970	-1.143318	-0.883652
5	6	0	1.392104	3.277977	-2.825184
6	1	0	0.543629	3.911482	-3.067485
7	6	0	2.175269	3.608651	-1.710862
8	6	0	1.859349	4.793192	-0.888871
9	1	0	2.536763	4.975953	-0.041026
10	6	0	0.710781	6.722106	-0.289320
11	1	0	1.414837	6.703079	0.562336
12	6	0	-0.710781	6.722106	0.289320
13	1	0	-1.414837	6.703079	-0.562336
14	6	0	-0.953094	7.990175	1.116289
15	1	0	-1.976867	7.967155	1.505496
16	1	0	-0.281405	7.967929	1.984426
17	6	0	-0.706816	9.254296	0.292121
18	1	0	-0.867129	10.142680	0.912060
19	1	0	-1.436139	9.302627	-0.527949
20	6	0	0.706816	9.254296	-0.292121
21	1	0	0.867129	10.142680	-0.912060
22	1	0	1.436139	9.302627	0.527949
23	6	0	0.953094	7.990175	-1.116289
24	1	0	0.281405	7.967929	-1.984426
25	1	0	1.976867	7.967155	-1.505496
26	6	0	-1.859349	4.793192	0.888871
27	1	0	-2.536763	4.975953	0.041026
28	6	0	-2.175269	3.608651	1.710862
29	6	0	-1.392104	3.277977	2.825184

30	1	0	-0.543629	3.911482	3.067485
31	6	0	-1.710862	2.175269	3.608651
32	6	0	-2.825184	1.392104	3.277977
33	1	0	-3.067485	0.543629	3.911482
34	6	0	-3.608651	1.710862	2.175269
35	6	0	-3.277977	2.825184	1.392104
36	1	0	-3.911482	3.067485	0.543629
37	6	0	-4.793192	0.888871	1.859349
38	1	0	-4.975953	0.041026	2.536763
39	6	0	-6.722106	0.289320	0.710781
40	1	0	-6.703079	-0.562336	1.414837
41	6	0	-6.722106	-0.289320	-0.710781
42	1	0	-6.703079	0.562336	-1.414837
43	6	0	-7.990175	-1.116289	-0.953094
44	1	0	-7.967155	-1.505496	-1.976867
45	1	0	-7.967929	-1.984426	-0.281405
46	6	0	-9.254296	-0.292121	-0.706816
47	1	0	-9.302627	0.527949	-1.436139
48	1	0	-10.142680	-0.912060	-0.867129
49	6	0	-9.254296	0.292121	0.706816
50	1	0	-9.302627	-0.527949	1.436139
51	1	0	-10.142680	0.912060	0.867129
52	6	0	-7.990175	1.116289	0.953094
53	1	0	-7.967929	1.984426	0.281405
54	1	0	-7.967155	1.505496	1.976867
55	6	0	-4.793192	-0.888871	-1.859349
56	1	0	-4.975953	-0.041026	-2.536763
57	7	0	5.561970	1.143318	-0.883652
58	7	0	5.561970	-1.143318	0.883652
59	7	0	1.143318	-0.883652	5.561970
60	7	0	-1.143318	0.883652	5.561970
61	6	0	3.277977	2.825184	-1.392104
62	1	0	3.911482	3.067485	-0.543629
63	6	0	3.608651	1.710862	-2.175269
64	6	0	4.793192	0.888871	-1.859349
65	1	0	4.975953	0.041026	-2.536763
66	6	0	6.722106	0.289320	-0.710781
67	1	0	6.703079	-0.562336	-1.414837
68	6	0	6.722106	-0.289320	0.710781
69	1	0	6.703079	0.562336	1.414837
70	6	0	7.990175	-1.116289	0.953094
71	1	0	7.967155	-1.505496	1.976867
72	1	0	7.967929	-1.984426	0.281405
73	6	0	9.254296	-0.292121	0.706816
74	1	0	10.142680	-0.912060	0.867129
75	1	0	9.302627	0.527949	1.436139
76	6	0	9.254296	0.292121	-0.706816
77	1	0	10.142680	0.912060	-0.867129
78	1	0	9.302627	-0.527949	-1.436139
79	6	0	7.990175	1.116289	-0.953094
80	1	0	7.967929	1.984426	-0.281405
81	1	0	7.967155	1.505496	-1.976867
82	6	0	4.793192	-0.888871	1.859349
83	1	0	4.975953	-0.041026	2.536763
84	6	0	3.608651	-1.710862	2.175269
85	6	0	3.277977	-2.825184	1.392104
86	1	0	3.911482	-3.067485	0.543629
87	6	0	2.175269	-3.608651	1.710862
88	6	0	1.392104	-3.277977	2.825184

89	1	0	0.543629	-3.911482	3.067485
90	6	0	1.710862	-2.175269	3.608651
91	6	0	2.825184	-1.392104	3.277977
92	1	0	3.067485	-0.543629	3.911482
93	6	0	0.888871	-1.859349	4.793192
94	1	0	0.041026	-2.536763	4.975953
95	6	0	0.289320	-0.710781	6.722106
96	1	0	-0.562336	-1.414837	6.703079
97	6	0	-0.289320	0.710781	6.722106
98	1	0	0.562336	1.414837	6.703079
99	6	0	-1.116289	0.953094	7.990175
100	1	0	-1.505496	1.976867	7.967155
101	1	0	-1.984426	0.281405	7.967929
102	6	0	-0.292121	0.706816	9.254296
103	1	0	0.527949	1.436139	9.302627
104	1	0	-0.912060	0.867129	10.142680
105	6	0	0.292121	-0.706816	9.254296
106	1	0	-0.527949	-1.436139	9.302627
107	1	0	0.912060	-0.867129	10.142680
108	6	0	1.116289	-0.953094	7.990175
109	1	0	1.984426	-0.281405	7.967929
110	1	0	1.505496	-1.976867	7.967155
111	6	0	-0.888871	1.859349	4.793192
112	1	0	-0.041026	2.536763	4.975953
113	7	0	1.143318	0.883652	-5.561970
114	7	0	-1.143318	-0.883652	-5.561970
115	7	0	-0.883652	-5.561970	-1.143318
116	7	0	0.883652	-5.561970	1.143318
117	6	0	2.825184	1.392104	-3.277977
118	1	0	3.067485	0.543629	-3.911482
119	6	0	1.710862	2.175269	-3.608651
120	6	0	0.888871	1.859349	-4.793192
121	1	0	0.041026	2.536763	-4.975953
122	6	0	0.289320	0.710781	-6.722106
123	1	0	-0.562336	1.414837	-6.703079
124	6	0	-0.289320	-0.710781	-6.722106
125	1	0	0.562336	-1.414837	-6.703079
126	6	0	-1.116289	-0.953094	-7.990175
127	1	0	-1.505496	-1.976867	-7.967155
128	1	0	-1.984426	-0.281405	-7.967929
129	6	0	-0.292121	-0.706816	-9.254296
130	1	0	-0.912060	-0.867129	-10.142680
131	1	0	0.527949	-1.436139	-9.302627
132	6	0	0.292121	0.706816	-9.254296
133	1	0	0.912060	0.867129	-10.142680
134	1	0	-0.527949	1.436139	-9.302627
135	6	0	1.116289	0.953094	-7.990175
136	1	0	1.984426	0.281405	-7.967929
137	1	0	1.505496	1.976867	-7.967155
138	6	0	-0.888871	-1.859349	-4.793192
139	1	0	-0.041026	-2.536763	-4.975953
140	6	0	-1.710862	-2.175269	-3.608651
141	6	0	-2.825184	-1.392104	-3.277977
142	1	0	-3.067485	-0.543629	-3.911482
143	6	0	-3.608651	-1.710862	-2.175269
144	6	0	-3.277977	-2.825184	-1.392104
145	1	0	-3.911482	-3.067485	-0.543629
146	6	0	-2.175269	-3.608651	-1.710862
147	6	0	-1.392104	-3.277977	-2.825184

148	1	0	-0.543629	-3.911482	-3.067485
149	6	0	-1.859349	-4.793192	-0.888871
150	1	0	-2.536763	-4.975953	-0.041026
151	6	0	-0.710781	-6.722106	-0.289320
152	1	0	-1.414837	-6.703079	0.562336
153	6	0	0.710781	-6.722106	0.289320
154	1	0	1.414837	-6.703079	-0.562336
155	6	0	0.953094	-7.990175	1.116289
156	1	0	1.976867	-7.967155	1.505496
157	1	0	0.281405	-7.967929	1.984426
158	6	0	0.706816	-9.254296	0.292121
159	1	0	1.436139	-9.302627	-0.527949
160	1	0	0.867129	-10.142680	0.912060
161	6	0	-0.706816	-9.254296	-0.292121
162	1	0	-1.436139	-9.302627	0.527949
163	1	0	-0.867129	-10.142680	-0.912060
164	6	0	-0.953094	-7.990175	-1.116289
165	1	0	-0.281405	-7.967929	-1.984426
166	1	0	-1.976867	-7.967155	-1.505496
167	6	0	1.859349	-4.793192	0.888871
168	1	0	2.536763	-4.975953	0.041026
169	16	0	2.327471	2.327471	2.327471
170	16	0	2.327471	-2.327471	-2.327471
171	16	0	-2.327471	2.327471	-2.327471
172	16	0	-2.327471	-2.327471	2.327471
173	9	0	-1.289012	-1.267785	2.861888
174	9	0	-1.289012	1.267785	-2.861888
175	9	0	-1.267785	2.861888	-1.289012
176	9	0	1.289012	1.267785	2.861888
177	9	0	1.267785	2.861888	1.289012
178	9	0	1.289012	-1.267785	-2.861888
179	9	0	1.267785	-2.861888	-1.289012
180	9	0	-1.267785	-2.861888	1.289012
181	9	0	1.809397	-3.375300	-3.399522
182	9	0	-1.809397	3.375300	-3.399522
183	9	0	1.809397	3.375300	3.399522
184	9	0	-1.809397	-3.375300	3.399522
185	9	0	-2.861888	1.289012	-1.267785
186	9	0	2.861888	1.289012	1.267785
187	9	0	-2.861888	-1.289012	1.267785
188	9	0	2.861888	-1.289012	-1.267785
189	9	0	-3.399522	-1.809397	3.375300
190	9	0	3.399522	1.809397	3.375300
191	9	0	-3.399522	1.809397	-3.375300
192	9	0	3.399522	-1.809397	-3.375300
193	9	0	-3.375300	3.399522	-1.809397
194	9	0	3.375300	3.399522	1.809397
195	9	0	3.375300	-3.399522	-1.809397
196	9	0	-3.375300	-3.399522	1.809397

5SF6@CC3 T cc3-rsf6bx

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	1.145020	0.864217	-5.552172
2	7	0	-1.145020	-0.864217	-5.552172

3	7	0	-0.864217	-5.552172	-1.145020
4	7	0	0.864217	-5.552172	1.145020
5	6	0	2.787035	1.343657	-3.225618
6	1	0	3.041246	0.495960	-3.856388
7	6	0	1.672246	2.123186	-3.565609
8	6	0	0.871444	1.821479	-4.767181
9	1	0	0.024497	2.499350	-4.952219
10	6	0	0.300434	0.706240	-6.720923
11	1	0	-0.540922	1.422805	-6.707843
12	6	0	-0.300434	-0.706240	-6.720923
13	1	0	0.540922	-1.422805	-6.707843
14	6	0	-1.135743	-0.931987	-7.985635
15	1	0	-1.544301	-1.948190	-7.963548
16	1	0	-1.990607	-0.243620	-7.961357
17	6	0	-0.307349	-0.700549	-9.250198
18	1	0	-0.930760	-0.846663	-10.138594
19	1	0	0.496981	-1.447109	-9.299861
20	6	0	0.307349	0.700549	-9.250198
21	1	0	0.930760	0.846663	-10.138594
22	1	0	-0.496981	1.447109	-9.299861
23	6	0	1.135743	0.931987	-7.985635
24	1	0	1.990607	0.243620	-7.961357
25	1	0	1.544301	1.948190	-7.963548
26	6	0	-0.871444	-1.821479	-4.767181
27	1	0	-0.024497	-2.499350	-4.952219
28	6	0	-1.672246	-2.123186	-3.565609
29	6	0	-2.787035	-1.343657	-3.225618
30	1	0	-3.041246	-0.495960	-3.856388
31	6	0	-3.565609	-1.672246	-2.123186
32	6	0	-3.225618	-2.787035	-1.343657
33	1	0	-3.856388	-3.041246	-0.495960
34	6	0	-2.123186	-3.565609	-1.672246
35	6	0	-1.343657	-3.225618	-2.787035
36	1	0	-0.495960	-3.856388	-3.041246
37	6	0	-1.821479	-4.767181	-0.871444
38	1	0	-2.499350	-4.952219	-0.024497
39	6	0	-0.706240	-6.720923	-0.300434
40	1	0	-1.422805	-6.707843	0.540922
41	6	0	0.706240	-6.720923	0.300434
42	1	0	1.422805	-6.707843	-0.540922
43	6	0	0.931987	-7.985635	1.135743
44	1	0	1.948190	-7.963548	1.544301
45	1	0	0.243620	-7.961357	1.990607
46	6	0	0.700549	-9.250198	0.307349
47	1	0	1.447109	-9.299861	-0.496981
48	1	0	0.846663	-10.138594	0.930760
49	6	0	-0.700549	-9.250198	-0.307349
50	1	0	-1.447109	-9.299861	0.496981
51	1	0	-0.846663	-10.138594	-0.930760
52	6	0	-0.931987	-7.985635	-1.135743
53	1	0	-0.243620	-7.961357	-1.990607
54	1	0	-1.948190	-7.963548	-1.544301
55	6	0	1.821479	-4.767181	0.871444
56	1	0	2.499350	-4.952219	0.024497
57	7	0	0.864217	5.552172	-1.145020
58	7	0	-0.864217	5.552172	1.145020
59	7	0	-5.552172	1.145020	0.864217
60	7	0	-5.552172	-1.145020	-0.864217
61	6	0	1.343657	3.225618	-2.787035

62	1	0	0.495960	3.856388	-3.041246
63	6	0	2.123186	3.565609	-1.672246
64	6	0	1.821479	4.767181	-0.871444
65	1	0	2.499350	4.952219	-0.024497
66	6	0	0.706240	6.720923	-0.300434
67	1	0	1.422805	6.707843	0.540922
68	6	0	-0.706240	6.720923	0.300434
69	1	0	-1.422805	6.707843	-0.540922
70	6	0	-0.931987	7.985635	1.135743
71	1	0	-1.948190	7.963548	1.544301
72	1	0	-0.243620	7.961357	1.990607
73	6	0	-0.700549	9.250198	0.307349
74	1	0	-0.846663	10.138594	0.930760
75	1	0	-1.447109	9.299861	-0.496981
76	6	0	0.700549	9.250198	-0.307349
77	1	0	0.846663	10.138594	-0.930760
78	1	0	1.447109	9.299861	0.496981
79	6	0	0.931987	7.985635	-1.135743
80	1	0	0.243620	7.961357	-1.990607
81	1	0	1.948190	7.963548	-1.544301
82	6	0	-1.821479	4.767181	0.871444
83	1	0	-2.499350	4.952219	0.024497
84	6	0	-2.123186	3.565609	1.672246
85	6	0	-1.343657	3.225618	2.787035
86	1	0	-0.495960	3.856388	3.041246
87	6	0	-1.672246	2.123186	3.565609
88	6	0	-2.787035	1.343657	3.225618
89	1	0	-3.041246	0.495960	3.856388
90	6	0	-3.565609	1.672246	2.123186
91	6	0	-3.225618	2.787035	1.343657
92	1	0	-3.856388	3.041246	0.495960
93	6	0	-4.767181	0.871444	1.821479
94	1	0	-4.952219	0.024497	2.499350
95	6	0	-6.720923	0.300434	0.706240
96	1	0	-6.707843	-0.540922	1.422805
97	6	0	-6.720923	-0.300434	-0.706240
98	1	0	-6.707843	0.540922	-1.422805
99	6	0	-7.985635	-1.135743	-0.931987
100	1	0	-7.963548	-1.544301	-1.948190
101	1	0	-7.961357	-1.990607	-0.243620
102	6	0	-9.250198	-0.307349	-0.700549
103	1	0	-9.299861	0.496981	-1.447109
104	1	0	-10.138594	-0.930760	-0.846663
105	6	0	-9.250198	0.307349	0.700549
106	1	0	-9.299861	-0.496981	1.447109
107	1	0	-10.138594	0.930760	0.846663
108	6	0	-7.985635	1.135743	0.931987
109	1	0	-7.961357	1.990607	0.243620
110	1	0	-7.963548	1.544301	1.948190
111	6	0	-4.767181	-0.871444	-1.821479
112	1	0	-4.952219	-0.024497	-2.499350
113	7	0	5.552172	1.145020	-0.864217
114	7	0	5.552172	-1.145020	0.864217
115	7	0	1.145020	-0.864217	5.552172
116	7	0	-1.145020	0.864217	5.552172
117	6	0	3.225618	2.787035	-1.343657
118	1	0	3.856388	3.041246	-0.495960
119	6	0	3.565609	1.672246	-2.123186
120	6	0	4.767181	0.871444	-1.821479

121	1	0	4.952219	0.024497	-2.499350
122	6	0	6.720923	0.300434	-0.706240
123	1	0	6.707843	-0.540922	-1.422805
124	6	0	6.720923	-0.300434	0.706240
125	1	0	6.707843	0.540922	1.422805
126	6	0	7.985635	-1.135743	0.931987
127	1	0	7.963548	-1.544301	1.948190
128	1	0	7.961357	-1.990607	0.243620
129	6	0	9.250198	-0.307349	0.700549
130	1	0	10.138594	-0.930760	0.846663
131	1	0	9.299861	0.496981	1.447109
132	6	0	9.250198	0.307349	-0.700549
133	1	0	10.138594	0.930760	-0.846663
134	1	0	9.299861	-0.496981	-1.447109
135	6	0	7.985635	1.135743	-0.931987
136	1	0	7.961357	1.990607	-0.243620
137	1	0	7.963548	1.544301	-1.948190
138	6	0	4.767181	-0.871444	1.821479
139	1	0	4.952219	-0.024497	2.499350
140	6	0	3.565609	-1.672246	2.123186
141	6	0	3.225618	-2.787035	1.343657
142	1	0	3.856388	-3.041246	0.495960
143	6	0	2.123186	-3.565609	1.672246
144	6	0	1.343657	-3.225618	2.787035
145	1	0	0.495960	-3.856388	3.041246
146	6	0	1.672246	-2.123186	3.565609
147	6	0	2.787035	-1.343657	3.225618
148	1	0	3.041246	-0.495960	3.856388
149	6	0	0.871444	-1.821479	4.767181
150	1	0	0.024497	-2.499350	4.952219
151	6	0	0.300434	-0.706240	6.720923
152	1	0	-0.540922	-1.422805	6.707843
153	6	0	-0.300434	0.706240	6.720923
154	1	0	0.540922	1.422805	6.707843
155	6	0	-1.135743	0.931987	7.985635
156	1	0	-1.544301	1.948190	7.963548
157	1	0	-1.990607	0.243620	7.961357
158	6	0	-0.307349	0.700549	9.250198
159	1	0	0.496981	1.447109	9.299861
160	1	0	-0.930760	0.846663	10.138594
161	6	0	0.307349	-0.700549	9.250198
162	1	0	-0.496981	-1.447109	9.299861
163	1	0	0.930760	-0.846663	10.138594
164	6	0	1.135743	-0.931987	7.985635
165	1	0	1.990607	-0.243620	7.961357
166	1	0	1.544301	-1.948190	7.963548
167	6	0	-0.871444	1.821479	4.767181
168	1	0	-0.024497	2.499350	4.952219
169	16	0	-2.602447	2.602447	-2.602447
170	16	0	2.602447	2.602447	2.602447
171	16	0	2.602447	-2.602447	-2.602447
172	16	0	-2.602447	-2.602447	2.602447
173	9	0	-3.134767	-1.565538	1.539310
174	9	0	3.134767	-1.565538	-1.539310
175	9	0	1.565538	-1.539310	-3.134767
176	9	0	-3.134767	1.565538	-1.539310
177	9	0	-1.565538	1.539310	-3.134767
178	9	0	3.134767	1.565538	1.539310
179	9	0	1.565538	1.539310	3.134767

180	9	0	-1.565538	-1.539310	3.134767
181	9	0	3.675290	2.078296	3.645525
182	9	0	3.675290	-2.078296	-3.645525
183	9	0	-3.675290	2.078296	-3.645525
184	9	0	-3.675290	-2.078296	3.645525
185	9	0	1.539310	-3.134767	-1.565538
186	9	0	-1.539310	3.134767	-1.565538
187	9	0	-1.539310	-3.134767	1.565538
188	9	0	1.539310	3.134767	1.565538
189	9	0	-3.645525	-3.675290	2.078296
190	9	0	-3.645525	3.675290	-2.078296
191	9	0	3.645525	-3.675290	-2.078296
192	9	0	3.645525	3.675290	2.078296
193	9	0	2.078296	-3.645525	-3.675290
194	9	0	-2.078296	3.645525	-3.675290
195	9	0	2.078296	3.645525	3.675290
196	9	0	-2.078296	-3.645525	3.675290
197	16	0	0.000000	0.000000	0.000000
198	9	0	0.000000	1.580937	-0.000000
199	9	0	0.000000	-1.580937	-0.000000
200	9	0	0.000000	-0.000000	-1.580937
201	9	0	0.000000	0.000000	1.580937
202	9	0	-1.580937	-0.000000	0.000000
203	9	0	1.580937	0.000000	0.000000

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	16	0	0.000000	0.000000	-0.165008
2	9	0	1.266202	0.249335	-1.079099
3	9	0	0.845023	-0.976547	0.746516
4	9	0	-0.417171	-1.221231	-1.079099
5	9	0	-1.268226	-0.243538	0.746516
6	9	0	-0.849032	0.971896	-1.079099
7	9	0	0.423203	1.220085	0.746516
8	7	0	3.222833	1.852044	-4.361519
9	7	0	4.814558	2.259055	-1.999729
10	7	0	-3.215333	1.865033	-4.361519
11	7	0	-0.007499	-3.717077	-4.361519
12	6	0	-1.351981	-0.333161	-4.329444
13	1	0	-2.412981	-0.567703	-4.344816
14	6	0	0.387465	1.337430	-4.329444
15	1	0	0.714845	2.373554	-4.344816
16	6	0	-1.968186	2.092339	-4.361053
17	1	0	-1.563453	3.115283	-4.393154
18	7	0	1.620848	4.586320	3.096150
19	6	0	2.796112	0.658330	-4.361053
20	1	0	3.479641	-0.203652	-4.393154
21	7	0	-4.363678	3.040002	-1.999729
22	7	0	-4.782294	-0.889465	3.096150
23	7	0	3.161446	-3.696856	3.096150
24	7	0	-0.450880	-5.299057	-1.999729
25	6	0	-0.963142	1.013570	-4.330582
26	6	0	0.964516	-1.004270	-4.329444
27	1	0	1.698136	-1.805851	-4.344816

28	7	0	4.484987	-1.174451	3.427832
29	6	0	5.150003	-2.432789	3.708524
30	1	0	5.637319	-2.839172	2.803623
31	6	0	-0.559657	-5.056825	-4.422377
32	1	0	-1.660689	-5.042473	-4.326901
33	7	0	-1.225389	4.471338	3.427832
34	7	0	-3.259598	-3.296887	3.427832
35	6	0	-0.827925	-2.750669	-4.361053
36	1	0	-1.916188	-2.911631	-4.393154
37	6	0	2.790036	2.606061	2.367681
38	6	0	3.296383	1.370942	2.752961
39	1	0	3.146522	0.994145	3.761060
40	6	0	4.659168	2.043736	-4.422377
41	1	0	5.197254	1.083038	-4.326901
42	6	0	0.861897	-3.719272	2.367681
43	6	0	-0.396206	-1.340890	-4.330582
44	6	0	1.359348	0.327320	-4.330582
45	6	0	-2.835463	2.169280	2.752961
46	1	0	-2.434215	2.227895	3.761060
47	6	0	3.022027	3.073761	1.066516
48	1	0	2.632831	4.049475	0.789255
49	6	0	1.150941	-4.154033	1.066516
50	1	0	2.190533	-4.304836	0.789255
51	6	0	3.765216	2.316375	0.168451
52	6	0	-0.468145	5.676428	3.708524
53	1	0	-0.359865	6.301647	2.803623
54	6	0	-0.176501	-5.701591	-5.759162
55	1	0	-0.594581	-5.100557	-6.574117
56	1	0	0.915952	-5.660501	-5.860112
57	6	0	-4.099511	3.013090	-4.422377
58	1	0	-3.536565	3.959435	-4.326901
59	6	0	4.044460	0.598371	1.854311
60	6	0	0.943912	5.288607	4.170131
61	1	0	0.834220	4.645878	5.062540
62	6	0	4.275177	1.073891	0.569683
63	1	0	4.875313	0.505477	-0.135839
64	6	0	4.065923	2.859454	-1.170581
65	1	0	3.624271	3.841476	-1.394300
66	6	0	-1.504026	-3.801790	1.854311
67	6	0	-1.207572	-4.239358	0.569683
68	1	0	-1.999900	-4.474884	-0.135839
69	6	0	-0.004287	-5.879229	-3.251983
70	1	0	1.097865	-5.861683	-3.332180
71	6	0	0.123431	-4.418960	0.168451
72	6	0	-4.849472	3.003650	-5.759162
73	1	0	-5.360114	2.037013	-5.860112
74	1	0	-4.119921	3.065201	-6.574117
75	6	0	4.634325	-0.689856	2.265839
76	1	0	5.231648	-1.202318	1.496321
77	6	0	6.594154	3.237380	-3.335202
78	1	0	6.872460	3.882656	-2.494877
79	1	0	7.141863	2.294424	-3.208427
80	6	0	5.093705	2.935902	-3.251983
81	1	0	4.527434	3.881621	-3.332180
82	6	0	-0.460921	-3.540223	2.752961
83	1	0	-0.712306	-3.222040	3.761060
84	6	0	-4.509322	2.091466	-1.170581
85	1	0	-5.138951	1.217972	-1.394300
86	6	0	-5.089418	2.943327	-3.251983

87	1	0	-5.625299	1.980062	-3.332180
88	6	0	-3.651933	1.113212	2.367681
89	6	0	-0.493423	-7.329395	-3.335202
90	1	0	-1.583902	-7.332247	-3.208427
91	1	0	-0.073752	-7.893053	-2.494877
92	6	0	-4.681859	-3.243639	3.708524
93	1	0	-5.277454	-3.462476	2.803623
94	6	0	-0.659248	-7.150347	-5.841273
95	1	0	-1.757339	-7.170043	-5.817157
96	1	0	-0.354964	-7.592899	-6.795643
97	6	0	5.025973	2.697941	-5.759162
98	1	0	4.714502	2.035356	-6.574117
99	1	0	4.444162	3.623488	-5.860112
100	6	0	-3.067606	3.165466	0.569683
101	1	0	-2.875413	3.969406	-0.135839
102	6	0	-2.914595	-3.668515	2.265839
103	1	0	-3.657062	-3.929581	1.496321
104	6	0	-3.989735	0.066421	3.351170
105	1	0	-3.516497	0.178631	4.338443
106	6	0	-2.540434	3.203420	1.854311
107	6	0	-3.888648	2.102586	0.168451
108	6	0	0.443398	-4.950920	-1.170581
109	1	0	1.514681	-5.059449	-1.394300
110	6	0	4.108112	-3.461755	4.170131
111	1	0	3.606338	-3.045394	5.062540
112	6	0	6.522006	3.004248	-5.841273
113	1	0	7.088109	2.063121	-5.817157
114	1	0	6.753125	3.489042	-6.795643
115	6	0	6.207440	-2.218531	4.796668
116	1	0	6.940393	-1.487010	4.439283
117	1	0	5.715766	-1.776193	5.672923
118	6	0	2.052389	3.422001	3.351170
119	1	0	1.912947	2.956060	4.338443
120	6	0	1.744791	6.539814	4.545739
121	1	0	1.880933	7.146445	3.640916
122	1	0	2.743063	6.234989	4.878215
123	6	0	1.937345	-3.488422	3.351170
124	1	0	1.603549	-3.134691	4.338443
125	6	0	-4.172969	1.080272	1.066516
126	1	0	-4.823363	0.255361	0.789255
127	6	0	4.791250	-4.780940	4.545739
128	1	0	4.028127	-5.493057	4.878215
129	1	0	5.248536	-5.202158	3.640916
130	6	0	6.886625	-3.534032	5.180120
131	1	0	7.621932	-3.359238	5.972611
132	1	0	7.439042	-3.923699	4.314194
133	6	0	-1.719730	4.358371	2.265839
134	1	0	-1.574586	5.131899	1.496321
135	6	0	-6.536041	-1.758874	4.545739
136	1	0	-6.771191	-0.741932	4.878215
137	1	0	-7.129469	-1.944287	3.640916
138	6	0	-0.382751	7.731008	5.180120
139	1	0	-0.901781	8.280406	5.972611
140	1	0	-0.321498	8.404248	4.314194
141	6	0	-0.116426	-7.971761	-4.670437
142	1	0	0.977580	-8.032867	-4.749123
143	1	0	-0.495217	-8.998400	-4.712686
144	6	0	-6.100731	4.092015	-3.335202
145	1	0	-6.798709	4.010397	-2.494877

146	1	0	-5.557961	5.037823	-3.208427
147	6	0	-1.182415	6.485066	4.796668
148	1	0	-2.182408	6.754061	4.439283
149	1	0	-1.319655	5.838095	5.672923
150	6	0	6.961961	3.885052	-4.670437
151	1	0	6.467877	4.863043	-4.749123
152	1	0	8.040451	4.070330	-4.712686
153	6	0	-6.885751	-2.784156	5.625425
154	1	0	-7.953867	-2.730896	5.861074
155	1	0	-6.343899	-2.538260	6.548902
156	6	0	-5.052024	-1.826851	4.170131
157	1	0	-4.440558	-1.600483	5.062540
158	6	0	-5.862758	4.146099	-5.841273
159	1	0	-5.330770	5.106922	-5.817157
160	1	0	-6.398161	4.103857	-6.795643
161	6	0	1.031726	7.355314	5.625425
162	1	0	0.973752	6.763108	6.548902
163	1	0	1.611908	8.253699	5.861074
164	6	0	-6.845534	4.086709	-4.670437
165	1	0	-7.445457	3.169824	-4.749123
166	1	0	-7.545235	4.928070	-4.712686
167	6	0	-6.503874	-4.196976	5.180120
168	1	0	-6.720151	-4.921168	5.972611
169	1	0	-7.117544	-4.480550	4.314194
170	6	0	5.854026	-4.571158	5.625425
171	1	0	6.341959	-5.522803	5.861074
172	1	0	5.370147	-4.224848	6.548902
173	6	0	-5.025024	-4.266535	4.796668
174	1	0	-4.396111	-4.061902	5.672923
175	1	0	-4.757984	-5.267052	4.439283
176	16	0	0.151886	4.200641	-1.510442
177	9	0	-1.149121	3.389601	-1.880028
178	9	0	1.451928	5.036714	-1.154180
179	9	0	1.042883	2.922898	-1.767241
180	9	0	0.311289	4.622217	-3.030107
181	9	0	0.000000	3.786531	0.004540
182	9	0	-0.733882	5.487510	-1.245086
183	16	0	-3.713805	-1.968783	-1.510442
184	9	0	-2.360920	-2.689968	-1.880028
185	9	0	-3.052746	-0.558286	-1.767241
186	9	0	-4.158602	-2.041525	-3.030107
187	9	0	-3.279232	-1.893266	0.004540
188	9	0	-4.385382	-3.379315	-1.245086
189	9	0	-5.087886	-1.260951	-1.154180
190	16	0	0.000000	0.000000	4.339274
191	9	0	1.101249	-0.676647	3.434888
192	9	0	-0.032681	-1.290409	5.260731
193	9	0	1.133868	0.616902	5.260731
194	9	0	0.035369	1.292034	3.434888
195	9	0	-1.136618	-0.615386	3.434888
196	9	0	-1.101187	0.673507	5.260731
197	16	0	3.561919	-2.231858	-1.510442
198	9	0	2.009863	-2.364613	-1.767241
199	9	0	3.635958	-3.775763	-1.154180
200	9	0	3.279232	-1.893266	0.004540
201	9	0	3.510041	-0.699632	-1.880028
202	9	0	3.847313	-2.580692	-3.030107
203	9	0	5.119264	-2.108194	-1.245086

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	16	0	-2.006679	2.006679	2.006679
2	16	0	2.006679	-2.006679	2.006679
3	16	0	2.006679	2.006679	-2.006679
4	16	0	-2.006679	-2.006679	-2.006679
5	9	0	-2.532868	-0.946249	-0.960216
6	9	0	2.532868	0.946249	-0.960216
7	9	0	0.960216	2.532868	-0.946249
8	9	0	-2.532868	0.946249	0.960216
9	9	0	-0.960216	2.532868	0.946249
10	9	0	2.532868	-0.946249	0.960216
11	9	0	0.960216	-2.532868	0.946249
12	9	0	-0.960216	-2.532868	-0.946249
13	9	0	3.066762	-3.052714	1.480149
14	9	0	3.066762	3.052714	-1.480149
15	9	0	-3.066762	3.052714	1.480149
16	9	0	-3.066762	-3.052714	-1.480149
17	9	0	0.946249	0.960216	-2.532868
18	9	0	-0.946249	0.960216	2.532868
19	9	0	-0.946249	-0.960216	-2.532868
20	9	0	0.946249	-0.960216	2.532868
21	9	0	-3.052714	-1.480149	-3.066762
22	9	0	-3.052714	1.480149	3.066762
23	9	0	3.052714	1.480149	-3.066762
24	9	0	3.052714	-1.480149	3.066762
25	9	0	1.480149	3.066762	-3.052714
26	9	0	-1.480149	3.066762	3.052714
27	9	0	1.480149	-3.066762	3.052714
28	9	0	-1.480149	-3.066762	-3.052714

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	16	0	3.622621	2.201560	1.884006
2	16	0	-3.622621	2.201560	-1.884006
3	16	0	-3.622621	-2.201560	1.884006
4	16	0	3.622621	-2.201560	-1.884006
5	9	0	3.841163	-1.198712	-0.682854
6	9	0	-3.841163	-1.198712	0.682854
7	9	0	-3.815447	-1.015033	2.908621
8	9	0	3.841163	1.198712	0.682854
9	9	0	3.815447	1.015033	2.908621
10	9	0	-3.841163	1.198712	-0.682854
11	9	0	-3.815447	1.015033	-2.908621
12	9	0	3.815447	-1.015033	-2.908621
13	9	0	-5.175119	2.490417	-1.924191
14	9	0	-5.175119	-2.490417	1.924191
15	9	0	5.175119	2.490417	1.924191
16	9	0	5.175119	-2.490417	-1.924191

17	9	0	-2.067673	-1.914258	1.845203
18	9	0	2.067673	1.914258	1.845203
19	9	0	2.067673	-1.914258	-1.845203
20	9	0	-2.067673	1.914258	-1.845203
21	9	0	3.426918	-3.386920	-0.858407
22	9	0	3.426918	3.386920	0.858407
23	9	0	-3.426918	-3.386920	0.858407
24	9	0	-3.426918	3.386920	-0.858407
25	9	0	-3.405351	-3.204176	3.085192
26	9	0	3.405351	3.204176	3.085192
27	9	0	-3.405351	3.204176	-3.085192
28	9	0	3.405351	-3.204176	-3.085192
29	16	0	0.000000	0.000000	0.000000
30	9	0	0.000000	1.580680	0.000000
31	9	0	-0.000000	-1.580680	0.000000
32	9	0	0.000000	0.000000	1.580444
33	9	0	0.000000	0.000000	-1.580444
34	9	0	1.579294	-0.000000	-0.000000
35	9	0	-1.579294	0.000000	-0.000000

(SF6)5 C2 cc3-sf6bbx

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	16	0	-3.625957	2.076767	2.099756
2	16	0	3.625957	-2.076767	2.099756
3	16	0	3.530356	1.962939	-2.149457
4	16	0	-3.530356	-1.962939	-2.149457
5	9	0	-3.815098	-0.759060	-1.166413
6	9	0	3.815098	0.759060	-1.166413
7	9	0	3.767822	2.983431	-0.967333
8	9	0	-3.871791	1.116009	0.869601
9	9	0	-3.737502	3.328701	1.142648
10	9	0	3.871791	-1.116009	0.869601
11	9	0	3.737502	-3.328701	1.142648
12	9	0	-3.767822	-2.983431	-0.967333
13	9	0	5.182457	-2.137109	2.362786
14	9	0	5.065567	2.027261	-2.515357
15	9	0	-5.182457	2.137109	2.362786
16	9	0	-5.065567	-2.027261	-2.515357
17	9	0	1.992748	1.900537	-1.784697
18	9	0	-2.067247	2.017954	1.838296
19	9	0	-1.992748	-1.900537	-1.784697
20	9	0	2.067247	-2.017954	1.838296
21	9	0	-3.290367	-0.941381	-3.330140
22	9	0	-3.511652	0.824107	3.055192
23	9	0	3.290367	0.941381	-3.330140
24	9	0	3.511652	-0.824107	3.055192
25	9	0	3.245967	3.166568	-3.132280
26	9	0	-3.380997	3.037904	3.329309
27	9	0	3.380997	-3.037904	3.329309
28	9	0	-3.245967	-3.166568	-3.132280
29	16	0	0.000000	-0.000000	0.099637
30	9	0	0.000000	-0.000000	1.679985
31	9	0	-0.000000	0.000000	-1.480856
32	9	0	0.000000	1.580326	0.098673

33	9	0	-0.000000	-1.580326	0.098673
34	9	0	-1.580030	-0.000454	0.099940
35	9	0	1.580030	0.000454	0.099940

CO2@CC3-a C3 cc3-rco2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-0.334986	4.781575	3.035431
2	7	0	2.399993	3.982185	3.251635
3	7	0	5.019563	1.644147	-2.109453
4	7	0	3.602421	0.886645	-4.497716
5	6	0	-1.947582	3.667684	0.935751
6	1	0	-1.304508	4.507517	0.685642
7	6	0	-1.844286	3.104198	2.215440
8	6	0	-0.919294	3.671109	3.217269
9	1	0	-0.792503	3.084997	4.140625
10	6	0	0.530018	5.274408	4.088121
11	1	0	0.532714	4.597690	4.961493
12	6	0	1.970321	5.332384	3.551377
13	1	0	1.960349	5.966499	2.646392
14	6	0	2.908407	5.945828	4.595486
15	1	0	3.921916	5.985979	4.181860
16	1	0	2.943674	5.272219	5.461481
17	6	0	2.434573	7.334167	5.027316
18	1	0	3.111067	7.741175	5.786175
19	1	0	2.473451	8.016994	4.167609
20	6	0	1.001331	7.277796	5.559549
21	1	0	0.654201	8.278864	5.836207
22	1	0	0.979902	6.669668	6.474178
23	6	0	0.060368	6.666689	4.520637
24	1	0	0.016153	7.305215	3.628811
25	1	0	-0.960966	6.591758	4.909297
26	6	0	2.681054	3.698976	2.048492
27	1	0	2.621183	4.445905	1.241777
28	6	0	3.142241	2.353972	1.651771
29	6	0	3.101230	1.290176	2.564809
30	1	0	2.688148	1.468698	3.554489
31	6	0	3.610458	0.045100	2.215440
32	6	0	4.150098	-0.147186	0.935751
33	1	0	4.555878	-1.124022	0.685642
34	6	0	4.186766	0.898149	0.021539
35	6	0	3.674320	2.151534	0.384633
36	1	0	3.724975	2.962078	-0.337792
37	6	0	4.816888	0.691615	-1.297822
38	1	0	5.127173	-0.340905	-1.521615
39	6	0	5.697293	1.338505	-3.354321
40	1	0	5.912369	0.258229	-3.443111
41	6	0	4.785737	1.722725	-4.530530
42	1	0	4.530248	2.791734	-4.415228
43	6	0	5.512196	1.514363	-5.863739
44	1	0	4.843621	1.808317	-6.680178
45	1	0	5.707925	0.440765	-5.982953
46	6	0	6.824158	2.297644	-5.917781
47	1	0	6.608961	3.373964	-5.872454
48	1	0	7.330216	2.115297	-6.871654

49	6	0	7.731239	1.916921	-4.746381
50	1	0	8.022177	0.862034	-4.843412
51	1	0	8.655374	2.504056	-4.768253
52	6	0	7.011535	2.124760	-3.413435
53	1	0	6.781209	3.188500	-3.270195
54	1	0	7.643923	1.820133	-2.572431
55	6	0	2.476640	1.458644	-4.385533
56	1	0	2.383871	2.553411	-4.311487
57	7	0	-4.648670	0.087362	3.251635
58	7	0	-3.973472	-2.680894	3.035431
59	7	0	2.248677	-4.069547	3.251635
60	7	0	4.308458	-2.100681	3.035431
61	6	0	-2.667940	2.040657	2.564809
62	1	0	-2.616004	1.593655	3.554489
63	6	0	-3.609719	1.544274	1.651771
64	6	0	-4.543934	0.472373	2.048492
65	1	0	-5.160858	0.047058	1.241777
66	6	0	-5.603140	-0.959843	3.551377
67	1	0	-6.147314	-1.285537	2.646392
68	6	0	-4.832780	-2.178195	4.088121
69	1	0	-4.248074	-1.837501	4.961493
70	6	0	-5.803706	-3.281065	4.520637
71	1	0	-5.228147	-4.128100	4.909297
72	1	0	-6.334578	-3.638618	3.628811
73	6	0	-6.803421	-2.771720	5.559549
74	1	0	-7.496807	-3.572877	5.836207
75	1	0	-6.266053	-2.486214	6.474178
76	6	0	-7.568861	-1.558681	5.027316
77	1	0	-8.259587	-1.176324	5.786175
78	1	0	-8.179646	-1.866426	4.167609
79	6	0	-6.603442	-0.454159	4.595486
80	1	0	-6.037713	-0.086813	5.461481
81	1	0	-7.144968	0.403490	4.181860
82	6	0	-2.719627	-2.631687	3.217269
83	1	0	-2.275434	-2.228826	4.140625
84	6	0	-1.766171	-3.149298	2.215440
85	6	0	-2.202516	-3.520497	0.935751
86	1	0	-3.251371	-3.383496	0.685642
87	6	0	-1.315564	-4.074920	0.021539
88	6	0	0.026123	-4.257821	0.384633
89	1	0	0.702747	-4.706962	-0.337792
90	6	0	0.467479	-3.898246	1.651771
91	6	0	-0.433290	-3.330832	2.564809
92	1	0	-0.072144	-3.062353	3.554489
93	6	0	1.862880	-4.171349	2.048492
94	1	0	2.539675	-4.492963	1.241777
95	6	0	3.632819	-4.372540	3.551377
96	1	0	4.186965	-4.680961	2.646392
97	6	0	4.302762	-3.096213	4.088121
98	1	0	3.715360	-2.760189	4.961493
99	6	0	5.743338	-3.385624	4.520637
100	1	0	6.189113	-2.463658	4.909297
101	1	0	6.318425	-3.666597	3.628811
102	6	0	5.802091	-4.506076	5.559549
103	1	0	5.286151	-4.183454	6.474178
104	1	0	6.842606	-4.705987	5.836207
105	6	0	5.134288	-5.775486	5.027316
106	1	0	5.706195	-6.150569	4.167609
107	1	0	5.148520	-6.564850	5.786175

108	6	0	3.695034	-5.491668	4.595486
109	1	0	3.094038	-5.185406	5.461481
110	1	0	3.223052	-6.389468	4.181860
111	6	0	3.638921	-1.039423	3.217269
112	1	0	3.067937	-0.856170	4.140625
113	7	0	-3.933655	3.524996	-2.109453
114	7	0	-2.569068	2.676466	-4.497716
115	7	0	-1.033353	-3.563111	-4.497716
116	7	0	-1.085908	-5.169143	-2.109453
117	6	0	-3.700443	2.106288	0.384633
118	1	0	-4.427722	1.744884	-0.337792
119	6	0	-2.871203	3.176772	0.021539
120	6	0	-3.007400	3.825740	-1.297822
121	1	0	-2.268354	4.610715	-1.521615
122	6	0	-4.007826	4.264748	-3.354321
123	1	0	-3.179817	4.991147	-3.443111
124	6	0	-3.884792	3.283207	-4.530530
125	1	0	-4.682836	2.527443	-4.415228
126	6	0	-4.067575	4.016520	-5.863739
127	1	0	-3.987859	3.290541	-6.680178
128	1	0	-3.235676	4.722825	-5.982953
129	6	0	-5.401897	4.761072	-5.917781
130	1	0	-5.497009	5.290504	-6.871654
131	1	0	-6.226419	4.036546	-5.872454
132	6	0	-5.525722	5.736989	-4.746381
133	1	0	-6.496263	6.243746	-4.768253
134	1	0	-4.757632	6.516392	-4.843412
135	6	0	-5.345863	5.009787	-3.413435
136	1	0	-6.151926	4.278449	-3.270195
137	1	0	-5.398242	5.709765	-2.572431
138	6	0	-2.501543	1.415512	-4.385533
139	1	0	-3.403254	0.787787	-4.311487
140	6	0	-1.214963	0.692815	-4.362847
141	6	0	0.000000	1.392177	-4.361234
142	1	0	-0.026792	2.478794	-4.364807
143	6	0	1.207477	0.705781	-4.362847
144	6	0	1.205660	-0.696088	-4.361234
145	1	0	2.160094	-1.216194	-4.364807
146	6	0	0.007486	-1.398596	-4.362847
147	6	0	-1.205660	-0.696088	-4.361234
148	1	0	-2.133302	-1.262599	-4.364807
149	6	0	0.024902	-2.874155	-4.385533
150	1	0	1.019383	-3.341198	-4.311487
151	6	0	-0.900945	-5.005932	-4.530530
152	1	0	0.152588	-5.319176	-4.415228
153	6	0	-1.689468	-5.603253	-3.354321
154	1	0	-2.732552	-5.249376	-3.443111
155	6	0	-1.665671	-7.134547	-3.413435
156	1	0	-2.245680	-7.529897	-2.572431
157	1	0	-0.629283	-7.466949	-3.270195
158	6	0	-2.205517	-7.653910	-4.746381
159	1	0	-3.264545	-7.378426	-4.843412
160	1	0	-2.159111	-8.747802	-4.768253
161	6	0	-1.422261	-7.058716	-5.917781
162	1	0	-0.382542	-7.410510	-5.872454
163	1	0	-1.833207	-7.405801	-6.871654
164	6	0	-1.444621	-5.530883	-5.863739
165	1	0	-2.472248	-5.163591	-5.982953
166	1	0	-0.855762	-5.098857	-6.680178

167	6	0	-1.809488	-4.517355	-1.297822
168	1	0	-2.858819	-4.269810	-1.521615
169	6	0	0.000000	0.000000	2.033575
170	8	0	0.000000	0.000000	3.200064
171	8	0	0.000000	0.000000	0.873073

CO2@CC3-b C2 cc3-rj0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	3.752002	4.168857	-1.178335
2	7	0	4.979727	2.794518	1.046500
3	7	0	4.453011	-3.618612	0.800741
4	7	0	2.627891	-4.998660	-0.966210
5	6	0	1.669467	3.022941	-2.794177
6	1	0	2.698392	2.760739	-3.026757
7	6	0	1.422173	3.836685	-1.679375
8	6	0	2.538111	4.355410	-0.862934
9	1	0	2.249200	4.938712	0.025159
10	6	0	4.770494	4.776744	-0.344201
11	1	0	4.328031	5.275175	0.537192
12	6	0	5.719061	3.684092	0.173325
13	1	0	6.118970	3.148765	-0.706882
14	6	0	6.877763	4.305634	0.961161
15	1	0	7.541789	3.504437	1.303509
16	1	0	6.463944	4.782107	1.859434
17	6	0	7.640836	5.333287	0.125162
18	1	0	8.449357	5.772794	0.718765
19	1	0	8.111475	4.830904	-0.730957
20	6	0	6.696814	6.421911	-0.387912
21	1	0	7.239036	7.138059	-1.014317
22	1	0	6.297130	6.985108	0.466400
23	6	0	5.540877	5.807573	-1.177575
24	1	0	5.922290	5.305060	-2.076017
25	1	0	4.841666	6.579228	-1.517729
26	6	0	4.935730	1.564498	0.743494
27	1	0	5.430351	1.166366	-0.156152
28	6	0	4.231323	0.573548	1.581304
29	6	0	3.500944	0.981498	2.705757
30	1	0	3.452202	2.042335	2.937156
31	6	0	2.848380	0.045719	3.499068
32	6	0	2.922014	-1.314659	3.167177
33	1	0	2.396303	-2.031334	3.792779
34	6	0	3.645377	-1.729877	2.055571
35	6	0	4.299514	-0.777493	1.261872
36	1	0	4.861322	-1.120717	0.396843
37	6	0	3.728959	-3.169393	1.739416
38	1	0	3.131252	-3.832737	2.383507
39	6	0	4.488560	-5.055066	0.605215
40	1	0	3.808379	-5.575520	1.303467
41	6	0	4.019574	-5.379970	-0.821122
42	1	0	4.667585	-4.818075	-1.518020
43	6	0	4.153220	-6.881060	-1.102821
44	1	0	3.825295	-7.077605	-2.129388
45	1	0	3.461791	-7.416747	-0.439420
46	6	0	5.583599	-7.371832	-0.878497

47	1	0	6.254467	-6.883625	-1.598506
48	1	0	5.643991	-8.448676	-1.068277
49	6	0	6.049919	-7.048797	0.541877
50	1	0	5.436721	-7.610686	1.259565
51	1	0	7.086206	-7.370556	0.689737
52	6	0	5.921786	-5.551958	0.826176
53	1	0	6.587035	-4.983613	0.163132
54	1	0	6.221816	-5.318621	1.853568
55	6	0	2.337307	-4.170686	-1.881215
56	1	0	3.107521	-3.733513	-2.535849
57	7	0	-2.627891	4.998660	-0.966210
58	7	0	-4.453011	3.618612	0.800741
59	7	0	-1.415807	0.308395	5.400632
60	7	0	1.415807	-0.308395	5.400632
61	6	0	0.115797	4.194133	-1.368387
62	1	0	-0.102593	4.829649	-0.513998
63	6	0	-0.950030	3.754310	-2.166430
64	6	0	-2.337307	4.170686	-1.881215
65	1	0	-3.107521	3.733513	-2.535849
66	6	0	-4.019574	5.379970	-0.821122
67	1	0	-4.667585	4.818075	-1.518020
68	6	0	-4.488560	5.055066	0.605215
69	1	0	-3.808379	5.575520	1.303467
70	6	0	-5.921786	5.551958	0.826176
71	1	0	-6.221816	5.318621	1.853568
72	1	0	-6.587035	4.983613	0.163132
73	6	0	-6.049919	7.048797	0.541877
74	1	0	-7.086206	7.370556	0.689737
75	1	0	-5.436721	7.610686	1.259565
76	6	0	-5.583599	7.371832	-0.878497
77	1	0	-5.643991	8.448676	-1.068277
78	1	0	-6.254467	6.883625	-1.598506
79	6	0	-4.153220	6.881060	-1.102821
80	1	0	-3.461791	7.416747	-0.439420
81	1	0	-3.825295	7.077605	-2.129388
82	6	0	-3.728959	3.169393	1.739416
83	1	0	-3.131252	3.832737	2.383507
84	6	0	-3.645377	1.729877	2.055571
85	6	0	-4.299514	0.777493	1.261872
86	1	0	-4.861322	1.120717	0.396843
87	6	0	-4.231323	-0.573548	1.581304
88	6	0	-3.500944	-0.981498	2.705757
89	1	0	-3.452202	-2.042335	2.937156
90	6	0	-2.848380	-0.045719	3.499068
91	6	0	-2.922014	1.314659	3.167177
92	1	0	-2.396303	2.031334	3.792779
93	6	0	-2.070534	-0.496945	4.671244
94	1	0	-2.089156	-1.580151	4.867103
95	6	0	-0.728918	-0.238508	6.556301
96	1	0	-0.718664	-1.342997	6.532843
97	6	0	0.728918	0.238508	6.556301
98	1	0	0.718664	1.342997	6.532843
99	6	0	1.449058	-0.233076	7.825758
100	1	0	2.480897	0.134317	7.802099
101	1	0	1.500252	-1.329552	7.804622
102	6	0	0.727471	0.236001	9.089420
103	1	0	0.751106	1.333192	9.136882
104	1	0	1.251396	-0.131764	9.977917
105	6	0	-0.727471	-0.236001	9.089420

106	1	0	-0.751106	-1.333192	9.136882
107	1	0	-1.251396	0.131764	9.977917
108	6	0	-1.449058	0.233076	7.825758
109	1	0	-1.500252	1.329552	7.804622
110	1	0	-2.480897	-0.134317	7.802099
111	6	0	2.070534	0.496945	4.671244
112	1	0	2.089156	1.580151	4.867103
113	7	0	0.000000	1.439178	-5.615059
114	7	0	-0.000000	-1.439178	-5.615059
115	7	0	-3.752002	-4.168857	-1.178335
116	7	0	-4.979727	-2.794518	1.046500
117	6	0	-0.692996	2.949209	-3.269014
118	1	0	-1.500279	2.602357	-3.908918
119	6	0	0.620671	2.580497	-3.590325
120	6	0	0.902917	1.760550	-4.785102
121	1	0	1.953613	1.460346	-4.921261
122	6	0	0.390985	0.661683	-6.774277
123	1	0	1.466604	0.409512	-6.748931
124	6	0	-0.390985	-0.661683	-6.774277
125	1	0	-1.466604	-0.409512	-6.748931
126	6	0	-0.086968	-1.465840	-8.042998
127	1	0	-0.667602	-2.394477	-8.020355
128	1	0	0.972702	-1.751814	-8.021556
129	6	0	-0.388626	-0.658741	-9.306030
130	1	0	-0.144694	-1.249654	-10.195165
131	1	0	-1.464709	-0.442701	-9.352987
132	6	0	0.388626	0.658741	-9.306030
133	1	0	0.144694	1.249654	-10.195165
134	1	0	1.464709	0.442701	-9.352987
135	6	0	0.086968	1.465840	-8.042998
136	1	0	-0.972702	1.751814	-8.021556
137	1	0	0.667602	2.394477	-8.020355
138	6	0	-0.902917	-1.760550	-4.785102
139	1	0	-1.953613	-1.460346	-4.921261
140	6	0	-0.620671	-2.580497	-3.590325
141	6	0	0.692996	-2.949209	-3.269014
142	1	0	1.500279	-2.602357	-3.908918
143	6	0	0.950030	-3.754310	-2.166430
144	6	0	-0.115797	-4.194133	-1.368387
145	1	0	0.102593	-4.829649	-0.513998
146	6	0	-1.422173	-3.836685	-1.679375
147	6	0	-1.669467	-3.022941	-2.794177
148	1	0	-2.698392	-2.760739	-3.026757
149	6	0	-2.538111	-4.355410	-0.862934
150	1	0	-2.249200	-4.938712	0.025159
151	6	0	-4.770494	-4.776744	-0.344201
152	1	0	-4.328031	-5.275175	0.537192
153	6	0	-5.719061	-3.684092	0.173325
154	1	0	-6.118970	-3.148765	-0.706882
155	6	0	-6.877763	-4.305634	0.961161
156	1	0	-7.541789	-3.504437	1.303509
157	1	0	-6.463944	-4.782107	1.859434
158	6	0	-7.640836	-5.333287	0.125162
159	1	0	-8.111475	-4.830904	-0.730957
160	1	0	-8.449357	-5.772794	0.718765
161	6	0	-6.696814	-6.421911	-0.387912
162	1	0	-6.297130	-6.985108	0.466400
163	1	0	-7.239036	-7.138059	-1.014317
164	6	0	-5.540877	-5.807573	-1.177575

165	1	0	-5.922290	-5.305060	-2.076017
166	1	0	-4.841666	-6.579228	-1.517729
167	6	0	-4.935730	-1.564498	0.743494
168	1	0	-5.430351	-1.166366	-0.156152
169	6	0	0.000000	0.000000	2.419432
170	8	0	-0.103721	-1.158734	2.416518
171	8	0	0.103721	1.158734	2.416518

 4CO2@CC3-a C2 cc3-rjj

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	1.376803	-0.436846	-5.400067
2	7	0	-1.376803	0.436846	-5.400067
3	7	0	-3.320250	4.800984	-1.094026
4	7	0	-1.669764	5.482548	1.142275
5	6	0	3.060848	-0.173106	-3.120169
6	1	0	2.877878	0.702985	-3.737604
7	6	0	2.387063	-1.360767	-3.432191
8	6	0	1.476223	-1.410772	-4.594175
9	1	0	0.910533	-2.346120	-4.727323
10	6	0	0.507476	-0.576693	-6.550395
11	1	0	-0.063094	-1.522412	-6.517345
12	6	0	-0.507476	0.576693	-6.550395
13	1	0	0.063094	1.522412	-6.517345
14	6	0	-1.364025	0.541954	-7.821749
15	1	0	-2.063770	1.384478	-7.798422
16	1	0	-1.968080	-0.374496	-7.801882
17	6	0	-0.502814	0.576209	-9.084346
18	1	0	-1.140655	0.531023	-9.973337
19	1	0	0.040716	1.529724	-9.130558
20	6	0	0.502814	-0.576209	-9.084346
21	1	0	1.140655	-0.531023	-9.973337
22	1	0	-0.040716	-1.529724	-9.130558
23	6	0	1.364025	-0.541954	-7.821749
24	1	0	1.968080	0.374496	-7.801882
25	1	0	2.063770	-1.384478	-7.798422
26	6	0	-1.476223	1.410772	-4.594175
27	1	0	-0.910533	2.346120	-4.727323
28	6	0	-2.387063	1.360767	-3.432191
29	6	0	-3.060848	0.173106	-3.120169
30	1	0	-2.877878	-0.702985	-3.737604
31	6	0	-3.945040	0.118966	-2.051609
32	6	0	-4.165034	1.267446	-1.279382
33	1	0	-4.860541	1.208642	-0.445702
34	6	0	-3.502689	2.452847	-1.581516
35	6	0	-2.607182	2.495074	-2.660314
36	1	0	-2.095785	3.429232	-2.874606
37	6	0	-3.759381	3.657453	-0.768296
38	1	0	-4.369349	3.502437	0.135998
39	6	0	-3.631848	5.916914	-0.224384
40	1	0	-4.240165	5.598425	0.641673
41	6	0	-2.315916	6.491122	0.325637
42	1	0	-1.690602	6.770736	-0.541183
43	6	0	-2.588399	7.733925	1.179302
44	1	0	-1.634485	8.127085	1.547380

45	1	0	-3.167340	7.425525	2.059543
46	6	0	-3.353895	8.797255	0.390965
47	1	0	-2.731789	9.151625	-0.442219
48	1	0	-3.553669	9.664752	1.028765
49	6	0	-4.660296	8.226896	-0.164816
50	1	0	-5.321854	7.960655	0.670835
51	1	0	-5.187403	8.981341	-0.758245
52	6	0	-4.392932	6.984856	-1.015954
53	1	0	-3.793885	7.250950	-1.896480
54	1	0	-5.328644	6.552270	-1.386339
55	6	0	-0.512234	5.097493	0.797169
56	1	0	-0.002512	5.497936	-0.091987
57	7	0	3.320250	-4.800984	-1.094026
58	7	0	1.669764	-5.482548	1.142275
59	7	0	-4.392932	-3.329132	0.839797
60	7	0	-5.515698	-1.254795	-0.848452
61	6	0	2.607182	-2.495074	-2.660314
62	1	0	2.095785	-3.429232	-2.874606
63	6	0	3.502689	-2.452847	-1.581516
64	6	0	3.759381	-3.657453	-0.768296
65	1	0	4.369349	-3.502437	0.135998
66	6	0	3.631848	-5.916914	-0.224384
67	1	0	4.240165	-5.598425	0.641673
68	6	0	2.315916	-6.491122	0.325637
69	1	0	1.690602	-6.770736	-0.541183
70	6	0	2.588399	-7.733925	1.179302
71	1	0	1.634485	-8.127085	1.547380
72	1	0	3.167340	-7.425525	2.059543
73	6	0	3.353895	-8.797255	0.390965
74	1	0	3.553669	-9.664752	1.028765
75	1	0	2.731789	-9.151625	-0.442219
76	6	0	4.660296	-8.226896	-0.164816
77	1	0	5.187403	-8.981341	-0.758245
78	1	0	5.321854	-7.960655	0.670835
79	6	0	4.392932	-6.984856	-1.015954
80	1	0	3.793885	-7.250950	-1.896480
81	1	0	5.328644	-6.552270	-1.386339
82	6	0	0.512234	-5.097493	0.797169
83	1	0	0.002512	-5.497936	-0.091987
84	6	0	-0.248684	-4.102785	1.580172
85	6	0	0.343618	-3.438130	2.664864
86	1	0	1.380673	-3.659817	2.905517
87	6	0	-0.398623	-2.549738	3.432995
88	6	0	-1.736011	-2.294193	3.097574
89	1	0	-2.300086	-1.592001	3.705427
90	6	0	-2.331547	-2.942915	2.024846
91	6	0	-1.582103	-3.858749	1.272645
92	1	0	-2.071746	-4.384974	0.455323
93	6	0	-3.759464	-2.699566	1.739772
94	1	0	-4.249527	-1.958809	2.388860
95	6	0	-5.818748	-3.078542	0.730717
96	1	0	-6.149808	-2.312951	1.455030
97	6	0	-6.144059	-2.549734	-0.673932
98	1	0	-5.759396	-3.287758	-1.401252
99	6	0	-7.658158	-2.396782	-0.855365
100	1	0	-7.857036	-2.032621	-1.869142
101	1	0	-8.007512	-1.619309	-0.163582
102	6	0	-8.395721	-3.708585	-0.586564
103	1	0	-8.091060	-4.458595	-1.329250

104	1	0	-9.474452	-3.563100	-0.706734
105	6	0	-8.075406	-4.230138	0.815010
106	1	0	-8.462040	-3.522163	1.560713
107	1	0	-8.577725	-5.186482	0.994880
108	6	0	-6.566339	-4.390070	0.999532
109	1	0	-6.180779	-5.150831	0.308305
110	1	0	-6.326754	-4.730745	2.012704
111	6	0	-4.636766	-1.149037	-1.754577
112	1	0	-4.348055	-2.003401	-2.387468
113	7	0	5.515698	1.254795	-0.848452
114	7	0	4.392932	3.329132	0.839797
115	7	0	0.521308	1.326511	5.489422
116	7	0	-0.521308	-1.326511	5.489422
117	6	0	4.165034	-1.267446	-1.279382
118	1	0	4.860541	-1.208642	-0.445702
119	6	0	3.945040	-0.118966	-2.051609
120	6	0	4.636766	1.149037	-1.754577
121	1	0	4.348055	2.003401	-2.387468
122	6	0	6.144059	2.549734	-0.673932
123	1	0	5.759396	3.287758	-1.401252
124	6	0	5.818748	3.078542	0.730717
125	1	0	6.149808	2.312951	1.455030
126	6	0	6.566339	4.390070	0.999532
127	1	0	6.326754	4.730745	2.012704
128	1	0	6.180779	5.150831	0.308305
129	6	0	8.075406	4.230138	0.815010
130	1	0	8.577725	5.186482	0.994880
131	1	0	8.462040	3.522163	1.560713
132	6	0	8.395721	3.708585	-0.586564
133	1	0	9.474452	3.563100	-0.706734
134	1	0	8.091060	4.458595	-1.329250
135	6	0	7.658158	2.396782	-0.855365
136	1	0	8.007512	1.619309	-0.163582
137	1	0	7.857036	2.032621	-1.869142
138	6	0	3.759464	2.699566	1.739772
139	1	0	4.249527	1.958809	2.388860
140	6	0	2.331547	2.942915	2.024846
141	6	0	1.582103	3.858749	1.272645
142	1	0	2.071746	4.384974	0.455323
143	6	0	0.248684	4.102785	1.580172
144	6	0	-0.343618	3.438130	2.664864
145	1	0	-1.380673	3.659817	2.905517
146	6	0	0.398623	2.549738	3.432995
147	6	0	1.736011	2.294193	3.097574
148	1	0	2.300086	1.592001	3.705427
149	6	0	-0.195784	1.925088	4.632514
150	1	0	-1.285100	2.034441	4.750884
151	6	0	-0.126111	0.758472	6.653211
152	1	0	-1.220093	0.911855	6.626636
153	6	0	0.126111	-0.758472	6.653211
154	1	0	1.220093	-0.911855	6.626636
155	6	0	-0.449730	-1.399652	7.919679
156	1	0	-0.244001	-2.475334	7.897947
157	1	0	-1.540970	-1.282870	7.897343
158	6	0	0.123581	-0.754951	9.182293
159	1	0	1.204791	-0.943440	9.229606
160	1	0	-0.317990	-1.216749	10.071614
161	6	0	-0.123581	0.754951	9.182293
162	1	0	-1.204791	0.943440	9.229606

163	1	0	0.317990	1.216749	10.071614
164	6	0	0.449730	1.399652	7.919679
165	1	0	1.540970	1.282870	7.897343
166	1	0	0.244001	2.475334	7.897947
167	6	0	0.195784	-1.925088	4.632514
168	1	0	1.285100	-2.034441	4.750884
169	6	0	1.026366	2.340022	-1.239730
170	6	0	-1.859931	0.733215	0.757786
171	6	0	1.859931	-0.733215	0.757786
172	6	0	-1.026366	-2.340022	-1.239730
173	8	0	1.731502	1.526686	-0.800901
174	8	0	-0.975880	1.181441	0.149747
175	8	0	0.975880	-1.181441	0.149747
176	8	0	-1.731502	-1.526686	-0.800901
177	8	0	0.347865	3.166108	-1.698487
178	8	0	-2.739319	0.306999	1.388355
179	8	0	2.739319	-0.306999	1.388355
180	8	0	-0.347865	-3.166108	-1.698487

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-2.217207	2.939697	4.574225
2	7	0	-4.511941	1.786838	3.244424
3	7	0	-3.849988	-4.221817	1.040272
4	7	0	-1.368771	-5.684831	0.762159
5	6	0	0.453041	2.002307	4.133935
6	1	0	-0.166938	1.465110	4.847080
7	6	0	-0.117594	3.062497	3.414485
8	6	0	-1.519152	3.461536	3.653693
9	1	0	-1.912138	4.253284	2.997526
10	6	0	-3.567311	3.429848	4.767997
11	1	0	-3.836046	4.190159	4.012600
12	6	0	-4.551641	2.259670	4.613956
13	1	0	-4.243320	1.472238	5.325291
14	6	0	-5.980377	2.710623	4.939806
15	1	0	-6.653034	1.852158	4.837066
16	1	0	-6.286340	3.446975	4.185284
17	6	0	-6.075935	3.320923	6.338149
18	1	0	-7.102239	3.648972	6.533910
19	1	0	-5.837950	2.554871	7.088713
20	6	0	-5.099831	4.489122	6.485480
21	1	0	-5.146268	4.905144	7.497420
22	1	0	-5.392599	5.293323	5.796761
23	6	0	-3.672364	4.042828	6.169129
24	1	0	-3.342550	3.289934	6.896824
25	1	0	-2.971731	4.881935	6.240253
26	6	0	-4.202029	0.574695	3.039579
27	1	0	-3.951355	-0.112347	3.862588
28	6	0	-4.187903	-0.011881	1.684116
29	6	0	-4.412177	0.792827	0.557582
30	1	0	-4.562182	1.859831	0.701124
31	6	0	-4.449279	0.230484	-0.712470
32	6	0	-4.250356	-1.149125	-0.865045
33	1	0	-4.279906	-1.569946	-1.866733

34	6	0	-4.033535	-1.955973	0.244606
35	6	0	-3.997836	-1.379029	1.522548
36	1	0	-3.833645	-2.026408	2.380210
37	6	0	-3.900646	-3.415291	0.063281
38	1	0	-3.880993	-3.763389	-0.981116
39	6	0	-3.799968	-5.640155	0.740626
40	1	0	-3.733563	-5.822230	-0.347238
41	6	0	-2.547632	-6.252739	1.386311
42	1	0	-2.585863	-6.021236	2.466132
43	6	0	-2.529527	-7.772892	1.191016
44	1	0	-1.634218	-8.180148	1.673308
45	1	0	-2.434133	-7.978466	0.116874
46	6	0	-3.796890	-8.427728	1.740654
47	1	0	-3.844062	-8.277358	2.827846
48	1	0	-3.763394	-9.509100	1.571023
49	6	0	-5.042946	-7.819852	1.094694
50	1	0	-5.041249	-8.049830	0.020495
51	1	0	-5.950943	-8.266434	1.513460
52	6	0	-5.068195	-6.303900	1.290263
53	1	0	-5.145185	-6.062313	2.358371
54	1	0	-5.940080	-5.857483	0.799790
55	6	0	-0.554645	-5.054242	1.501143
56	1	0	-0.726206	-4.922708	2.580642
57	7	0	2.374233	5.113758	0.628146
58	7	0	2.538321	4.566790	-2.211624
59	7	0	-2.716759	1.837555	-4.699949
60	7	0	-4.761373	0.625858	-3.064485
61	6	0	0.654564	3.757454	2.492982
62	1	0	0.236774	4.579592	1.917710
63	6	0	1.999623	3.413218	2.288905
64	6	0	2.834740	4.160494	1.326537
65	1	0	3.883127	3.834318	1.251608
66	6	0	3.297771	5.804717	-0.252080
67	1	0	4.253851	5.258689	-0.341672
68	6	0	2.681723	5.898556	-1.653749
69	1	0	1.702572	6.400311	-1.552477
70	6	0	3.579998	6.723908	-2.583061
71	1	0	3.107019	6.783092	-3.569431
72	1	0	4.526255	6.183187	-2.714913
73	6	0	3.844904	8.118861	-2.016205
74	1	0	4.503506	8.677533	-2.689499
75	1	0	2.899648	8.675730	-1.960742
76	6	0	4.457446	8.027778	-0.617777
77	1	0	4.613158	9.027798	-0.199522
78	1	0	5.445964	7.553747	-0.686725
79	6	0	3.564365	7.206013	0.312014
80	1	0	2.598751	7.709668	0.451135
81	1	0	4.016690	7.105166	1.304752
82	6	0	1.393288	4.229043	-2.639901
83	1	0	0.518036	4.891396	-2.556186
84	6	0	1.150049	2.927182	-3.293366
85	6	0	2.189601	2.002127	-3.463552
86	1	0	3.182931	2.261834	-3.106927
87	6	0	1.943298	0.771054	-4.061131
88	6	0	0.651247	0.463941	-4.509897
89	1	0	0.474901	-0.504253	-4.971475
90	6	0	-0.383519	1.378624	-4.350683
91	6	0	-0.127678	2.616018	-3.744354
92	1	0	-0.948590	3.318507	-3.625771

93	6	0	-1.743549	1.031775	-4.809860
94	1	0	-1.857300	0.032255	-5.256609
95	6	0	-4.000467	1.421796	-5.232234
96	1	0	-3.980147	0.364986	-5.553827
97	6	0	-5.068556	1.550935	-4.138174
98	1	0	-5.059431	2.597546	-3.784417
99	6	0	-6.455610	1.218428	-4.700924
100	1	0	-7.196514	1.331333	-3.901894
101	1	0	-6.462544	0.160849	-4.995538
102	6	0	-6.801599	2.101790	-5.900027
103	1	0	-6.866931	3.148886	-5.574435
104	1	0	-7.786610	1.829618	-6.293590
105	6	0	-5.735063	1.979920	-6.989635
106	1	0	-5.735229	0.953798	-7.381746
107	1	0	-5.967157	2.641337	-7.830980
108	6	0	-4.349945	2.309951	-6.432294
109	1	0	-4.313100	3.357706	-6.106642
110	1	0	-3.577451	2.187432	-7.199359
111	6	0	-4.710766	1.089884	-1.885267
112	1	0	-4.860775	2.158763	-1.669864
113	7	0	3.534871	0.097071	4.483371
114	7	0	3.551198	-2.649687	3.564515
115	7	0	3.503582	-3.459611	-2.814713
116	7	0	2.861787	-1.357395	-4.701090
117	6	0	2.553707	2.356572	3.000006
118	1	0	3.586268	2.054952	2.842496
119	6	0	1.780094	1.646615	3.930947
120	6	0	2.352589	0.510996	4.682093
121	1	0	1.682659	0.038341	5.417042
122	6	0	4.009793	-1.001705	5.302675
123	1	0	3.186667	-1.458552	5.880963
124	6	0	4.600463	-2.089696	4.396675
125	1	0	5.391761	-1.620484	3.785077
126	6	0	5.213259	-3.215562	5.239289
127	1	0	5.637897	-3.968052	4.565777
128	1	0	4.404826	-3.706468	5.796754
129	6	0	6.271721	-2.683338	6.205719
130	1	0	6.676163	-3.504502	6.806797
131	1	0	7.110444	-2.264483	5.633224
132	6	0	5.685194	-1.595513	7.106739
133	1	0	6.454473	-1.191011	7.772892
134	1	0	4.909067	-2.036410	7.746965
135	6	0	5.074381	-0.470801	6.270424
136	1	0	5.854591	0.029692	5.682148
137	1	0	4.618818	0.292903	6.910319
138	6	0	3.762362	-2.712269	2.315123
139	1	0	4.680762	-2.315286	1.856397
140	6	0	2.795052	-3.327083	1.382808
141	6	0	1.598690	-3.884447	1.857039
142	1	0	1.395177	-3.848246	2.924212
143	6	0	0.692708	-4.464037	0.976518
144	6	0	0.987314	-4.499872	-0.393619
145	1	0	0.269637	-4.958342	-1.069352
146	6	0	2.174059	-3.955690	-0.872288
147	6	0	3.073651	-3.358477	0.021903
148	1	0	3.986460	-2.920907	-0.373698
149	6	0	2.469776	-4.002444	-2.319499
150	1	0	1.729423	-4.528079	-2.941471
151	6	0	3.714187	-3.596835	-4.243775

152	1	0	2.812249	-3.988214	-4.747509
153	6	0	4.021233	-2.218858	-4.844168
154	1	0	4.895368	-1.808882	-4.307333
155	6	0	4.357378	-2.345258	-6.335350
156	1	0	4.584235	-1.349096	-6.730864
157	1	0	3.461378	-2.700751	-6.860800
158	6	0	5.522215	-3.307450	-6.569775
159	1	0	6.430377	-2.900566	-6.104616
160	1	0	5.726039	-3.393703	-7.642255
161	6	0	5.220868	-4.680752	-5.967684
162	1	0	4.369592	-5.128615	-6.498121
163	1	0	6.071728	-5.356336	-6.104869
164	6	0	4.884878	-4.558875	-4.481188
165	1	0	5.755185	-4.184980	-3.926053
166	1	0	4.630132	-5.535000	-4.053900
167	6	0	3.041869	-0.207223	-4.197188
168	1	0	4.025273	0.124713	-3.830602
169	8	0	-2.017180	2.346616	-1.239525
170	8	0	0.453552	-1.132493	2.838409
171	8	0	3.083658	1.718798	-0.465551
172	8	0	0.180760	-2.127488	-2.740846
173	6	0	-1.651123	1.259500	-1.430201
174	6	0	1.926534	1.785858	-0.382950
175	6	0	1.271459	-0.716798	2.123154
176	6	0	0.866905	-1.451185	-2.089196
177	8	0	1.564032	-0.791531	-1.431344
178	8	0	-1.304945	0.165519	-1.623325
179	8	0	0.768893	1.876620	-0.294027
180	8	0	2.090015	-0.297159	1.411327

6CO2@CC3-a T cc3-rjjj

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	5.580176	0.927034	-1.138603
2	7	0	5.580176	-0.927034	1.138603
3	7	0	1.138603	-5.580176	0.927034
4	7	0	-1.138603	-5.580176	-0.927034
5	6	0	3.409767	1.516403	-2.937340
6	1	0	4.028354	0.648941	-3.153180
7	6	0	3.730613	2.309253	-1.825649
8	6	0	4.888131	1.976797	-0.966410
9	1	0	5.096078	2.688107	-0.152457
10	6	0	6.722618	0.720828	-0.264865
11	1	0	6.688881	1.397439	0.607536
12	6	0	6.722618	-0.720828	0.264865
13	1	0	6.688881	-1.397439	-0.607536
14	6	0	7.998158	-0.998050	1.072626
15	1	0	7.973563	-2.037547	1.417921
16	1	0	7.980033	-0.364416	1.969114
17	6	0	9.261227	-0.719320	0.258642
18	1	0	10.149586	-0.909951	0.869982
19	1	0	9.306491	-1.410071	-0.594265
20	6	0	9.261227	0.719320	-0.258642
21	1	0	10.149586	0.909951	-0.869982
22	1	0	9.306491	1.410071	0.594265

23	6	0	7.998158	0.998050	-1.072626
24	1	0	7.980033	0.364416	-1.969114
25	1	0	7.973563	2.037547	-1.417921
26	6	0	4.888131	-1.976797	0.966410
27	1	0	5.096078	-2.688107	0.152457
28	6	0	3.730613	-2.309253	1.825649
29	6	0	3.409767	-1.516403	2.937340
30	1	0	4.028354	-0.648941	3.153180
31	6	0	2.309253	-1.825649	3.730613
32	6	0	1.516403	-2.937340	3.409767
33	1	0	0.648941	-3.153180	4.028354
34	6	0	1.825649	-3.730613	2.309253
35	6	0	2.937340	-3.409767	1.516403
36	1	0	3.153180	-4.028354	0.648941
37	6	0	0.966410	-4.888131	1.976797
38	1	0	0.152457	-5.096078	2.688107
39	6	0	0.264865	-6.722618	0.720828
40	1	0	-0.607536	-6.688881	1.397439
41	6	0	-0.264865	-6.722618	-0.720828
42	1	0	0.607536	-6.688881	-1.397439
43	6	0	-1.072626	-7.998158	-0.998050
44	1	0	-1.417921	-7.973563	-2.037547
45	1	0	-1.969114	-7.980033	-0.364416
46	6	0	-0.258642	-9.261227	-0.719320
47	1	0	0.594265	-9.306491	-1.410071
48	1	0	-0.869982	-10.149586	-0.909951
49	6	0	0.258642	-9.261227	0.719320
50	1	0	-0.594265	-9.306491	1.410071
51	1	0	0.869982	-10.149586	0.909951
52	6	0	1.072626	-7.998158	0.998050
53	1	0	1.969114	-7.980033	0.364416
54	1	0	1.417921	-7.973563	2.037547
55	6	0	-0.966410	-4.888131	-1.976797
56	1	0	-0.152457	-5.096078	-2.688107
57	7	0	1.138603	5.580176	-0.927034
58	7	0	-1.138603	5.580176	0.927034
59	7	0	-0.927034	1.138603	5.580176
60	7	0	0.927034	-1.138603	5.580176
61	6	0	2.937340	3.409767	-1.516403
62	1	0	3.153180	4.028354	-0.648941
63	6	0	1.825649	3.730613	-2.309253
64	6	0	0.966410	4.888131	-1.976797
65	1	0	0.152457	5.096078	-2.688107
66	6	0	0.264865	6.722618	-0.720828
67	1	0	-0.607536	6.688881	-1.397439
68	6	0	-0.264865	6.722618	0.720828
69	1	0	0.607536	6.688881	1.397439
70	6	0	-1.072626	7.998158	0.998050
71	1	0	-1.417921	7.973563	2.037547
72	1	0	-1.969114	7.980033	0.364416
73	6	0	-0.258642	9.261227	0.719320
74	1	0	-0.869982	10.149586	0.909951
75	1	0	0.594265	9.306491	1.410071
76	6	0	0.258642	9.261227	-0.719320
77	1	0	0.869982	10.149586	-0.909951
78	1	0	-0.594265	9.306491	-1.410071
79	6	0	1.072626	7.998158	-0.998050
80	1	0	1.969114	7.980033	-0.364416
81	1	0	1.417921	7.973563	-2.037547

82	6	0	-0.966410	4.888131	1.976797
83	1	0	-0.152457	5.096078	2.688107
84	6	0	-1.825649	3.730613	2.309253
85	6	0	-2.937340	3.409767	1.516403
86	1	0	-3.153180	4.028354	0.648941
87	6	0	-3.730613	2.309253	1.825649
88	6	0	-3.409767	1.516403	2.937340
89	1	0	-4.028354	0.648941	3.153180
90	6	0	-2.309253	1.825649	3.730613
91	6	0	-1.516403	2.937340	3.409767
92	1	0	-0.648941	3.153180	4.028354
93	6	0	-1.976797	0.966410	4.888131
94	1	0	-2.688107	0.152457	5.096078
95	6	0	-0.720828	0.264865	6.722618
96	1	0	-1.397439	-0.607536	6.688881
97	6	0	0.720828	-0.264865	6.722618
98	1	0	1.397439	0.607536	6.688881
99	6	0	0.998050	-1.072626	7.998158
100	1	0	2.037547	-1.417921	7.973563
101	1	0	0.364416	-1.969114	7.980033
102	6	0	0.719320	-0.258642	9.261227
103	1	0	1.410071	0.594265	9.306491
104	1	0	0.909951	-0.869982	10.149586
105	6	0	-0.719320	0.258642	9.261227
106	1	0	-1.410071	-0.594265	9.306491
107	1	0	-0.909951	0.869982	10.149586
108	6	0	-0.998050	1.072626	7.998158
109	1	0	-0.364416	1.969114	7.980033
110	1	0	-2.037547	1.417921	7.973563
111	6	0	1.976797	-0.966410	4.888131
112	1	0	2.688107	-0.152457	5.096078
113	7	0	0.927034	1.138603	-5.580176
114	7	0	-0.927034	-1.138603	-5.580176
115	7	0	-5.580176	-0.927034	-1.138603
116	7	0	-5.580176	0.927034	1.138603
117	6	0	1.516403	2.937340	-3.409767
118	1	0	0.648941	3.153180	-4.028354
119	6	0	2.309253	1.825649	-3.730613
120	6	0	1.976797	0.966410	-4.888131
121	1	0	2.688107	0.152457	-5.096078
122	6	0	0.720828	0.264865	-6.722618
123	1	0	1.397439	-0.607536	-6.688881
124	6	0	-0.720828	-0.264865	-6.722618
125	1	0	-1.397439	0.607536	-6.688881
126	6	0	-0.998050	-1.072626	-7.998158
127	1	0	-2.037547	-1.417921	-7.973563
128	1	0	-0.364416	-1.969114	-7.980033
129	6	0	-0.719320	-0.258642	-9.261227
130	1	0	-0.909951	-0.869982	-10.149586
131	1	0	-1.410071	0.594265	-9.306491
132	6	0	0.719320	0.258642	-9.261227
133	1	0	0.909951	0.869982	-10.149586
134	1	0	1.410071	-0.594265	-9.306491
135	6	0	0.998050	1.072626	-7.998158
136	1	0	0.364416	1.969114	-7.980033
137	1	0	2.037547	1.417921	-7.973563
138	6	0	-1.976797	-0.966410	-4.888131
139	1	0	-2.688107	-0.152457	-5.096078
140	6	0	-2.309253	-1.825649	-3.730613

141	6	0	-1.516403	-2.937340	-3.409767
142	1	0	-0.648941	-3.153180	-4.028354
143	6	0	-1.825649	-3.730613	-2.309253
144	6	0	-2.937340	-3.409767	-1.516403
145	1	0	-3.153180	-4.028354	-0.648941
146	6	0	-3.730613	-2.309253	-1.825649
147	6	0	-3.409767	-1.516403	-2.937340
148	1	0	-4.028354	-0.648941	-3.153180
149	6	0	-4.888131	-1.976797	-0.966410
150	1	0	-5.096078	-2.688107	-0.152457
151	6	0	-6.722618	-0.720828	-0.264865
152	1	0	-6.688881	-1.397439	0.607536
153	6	0	-6.722618	0.720828	0.264865
154	1	0	-6.688881	1.397439	-0.607536
155	6	0	-7.998158	0.998050	1.072626
156	1	0	-7.973563	2.037547	1.417921
157	1	0	-7.980033	0.364416	1.969114
158	6	0	-9.261227	0.719320	0.258642
159	1	0	-9.306491	1.410071	-0.594265
160	1	0	-10.149586	0.909951	0.869982
161	6	0	-9.261227	-0.719320	-0.258642
162	1	0	-9.306491	-1.410071	0.594265
163	1	0	-10.149586	-0.909951	-0.869982
164	6	0	-7.998158	-0.998050	-1.072626
165	1	0	-7.980033	-0.364416	-1.969114
166	1	0	-7.973563	-2.037547	-1.417921
167	6	0	-4.888131	1.976797	0.966410
168	1	0	-5.096078	2.688107	0.152457
169	8	0	0.777210	0.865306	2.883686
170	8	0	0.777210	-0.865306	-2.883686
171	8	0	-0.865306	2.883686	-0.777210
172	8	0	-2.883686	-0.777210	0.865306
173	6	0	0.000000	0.000000	2.891143
174	6	0	0.000000	2.891143	-0.000000
175	6	0	-0.000000	-0.000000	-2.891143
176	6	0	-2.891143	0.000000	-0.000000
177	8	0	-2.883686	0.777210	-0.865306
178	8	0	-0.777210	-0.865306	2.883686
179	8	0	0.865306	2.883686	0.777210
180	8	0	-0.777210	0.865306	-2.883686
181	6	0	-0.000000	-2.891143	0.000000
182	6	0	2.891143	-0.000000	0.000000
183	8	0	2.883686	0.777210	0.865306
184	8	0	2.883686	-0.777210	-0.865306
185	8	0	-0.865306	-2.883686	0.777210
186	8	0	0.865306	-2.883686	-0.777210

6CO2@CC3-b C3 cc3-rtt

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-4.606572	0.953823	-3.329434
2	7	0	-3.298069	3.550327	-3.077522
3	7	0	3.129321	3.512497	-3.329434
4	7	0	4.723708	1.081048	-3.077522
5	6	0	-3.452426	-1.616314	-2.765879

6	1	0	-3.300371	-1.193748	-3.755731
7	6	0	-4.233964	-0.903722	-1.844768
8	6	0	-4.835038	0.396814	-2.212498
9	1	0	-5.474300	0.860848	-1.445802
10	6	0	-5.274403	2.213457	-3.605195
11	1	0	-5.733239	2.633502	-2.692388
12	6	0	-4.254315	3.236391	-4.124810
13	1	0	-3.755137	2.793850	-5.005160
14	6	0	-4.959445	4.534004	-4.541833
15	1	0	-4.207576	5.234358	-4.922088
16	1	0	-5.395383	4.991400	-3.643933
17	6	0	-6.048408	4.278640	-5.583676
18	1	0	-6.544236	5.219591	-5.844422
19	1	0	-5.589517	3.894161	-6.504668
20	6	0	-7.064394	3.260417	-5.064899
21	1	0	-7.823559	3.051187	-5.825881
22	1	0	-7.589973	3.683662	-4.198156
23	6	0	-6.367287	1.963932	-4.652910
24	1	0	-5.902287	1.490665	-5.527700
25	1	0	-7.085147	1.243364	-4.245776
26	6	0	-2.067032	3.553797	-3.385327
27	1	0	-1.713481	3.278359	-4.390692
28	6	0	-1.013494	3.902578	-2.407722
29	6	0	-1.351522	4.316939	-1.112344
30	1	0	-2.402954	4.374699	-0.843163
31	6	0	-0.360281	4.631492	-0.189762
32	6	0	0.987816	4.538545	-0.563767
33	1	0	1.752330	4.787362	0.168950
34	6	0	1.334336	4.118582	-1.844768
35	6	0	0.326444	3.798046	-2.765879
36	1	0	0.616369	3.455079	-3.755731
37	6	0	2.761170	3.988858	-2.212498
38	1	0	3.482666	4.310459	-1.445802
39	6	0	4.554111	3.461039	-3.605195
40	1	0	5.147299	3.648380	-2.692388
41	6	0	4.929954	2.066149	-4.124810
42	1	0	4.297114	1.855119	-5.005160
43	6	0	6.406285	2.028003	-4.541833
44	1	0	6.636875	1.026689	-4.922088
45	1	0	7.020370	2.176839	-3.643933
46	6	0	6.729615	3.098755	-5.583676
47	1	0	6.167201	2.893583	-6.504668
48	1	0	7.792416	3.057679	-5.844422
49	6	0	6.355801	4.487736	-5.064899
50	1	0	6.985132	4.731278	-4.198156
51	1	0	6.554186	5.249808	-5.825881
52	6	0	4.884459	4.532266	-4.652910
53	1	0	4.242098	4.366198	-5.527700
54	1	0	4.619358	5.514235	-4.245776
55	6	0	4.111194	0.013204	-3.385327
56	1	0	3.695883	-0.155261	-4.390692
57	7	0	-4.702757	-2.603682	2.058059
58	7	0	-3.082533	-2.075943	4.413407
59	7	0	-0.256553	3.707523	4.413407
60	7	0	0.096524	5.374548	2.058059
61	6	0	-4.424403	-1.413799	-0.563767
62	1	0	-5.022142	-0.876118	0.168950
63	6	0	-3.830849	-2.627759	-0.189762
64	6	0	-4.010490	-3.183131	1.166823

65	1	0	-3.514439	-4.148584	1.350643
66	6	0	-4.881173	-3.300625	3.319857
67	1	0	-4.234260	-4.194338	3.379152
68	6	0	-4.500011	-2.378923	4.485185
69	1	0	-5.111728	-1.462901	4.401624
70	6	0	-4.790708	-3.062158	5.827232
71	1	0	-4.521348	-2.374704	6.636678
72	1	0	-4.131341	-3.935371	5.917922
73	6	0	-6.253171	-3.493368	5.936865
74	1	0	-6.424900	-3.995074	6.895020
75	1	0	-6.897719	-2.603967	5.922812
76	6	0	-6.635349	-4.409735	4.773600
77	1	0	-7.692806	-4.688044	4.833619
78	1	0	-6.056454	-5.340789	4.842220
79	6	0	-6.349066	-3.731706	3.433580
80	1	0	-6.978674	-2.839704	3.318875
81	1	0	-6.585988	-4.398217	2.596987
82	6	0	-2.745958	-0.856286	4.493675
83	1	0	-3.488236	-0.049109	4.578666
84	6	0	-1.333614	-0.422680	4.465723
85	6	0	-0.293376	-1.362238	4.460925
86	1	0	-0.545392	-2.419821	4.459207
87	6	0	1.032859	-0.943604	4.465723
88	6	0	1.326421	0.427048	4.460925
89	1	0	2.368322	0.737587	4.459207
90	6	0	0.300756	1.366284	4.465723
91	6	0	-1.033044	0.935190	4.460925
92	1	0	-1.822930	1.682233	4.459207
93	6	0	0.631414	2.806212	4.493675
94	1	0	1.701588	3.045456	4.578666
95	6	0	0.189798	5.086585	4.485185
96	1	0	1.288955	5.158337	4.401624
97	6	0	-0.417838	5.877532	3.319857
98	1	0	-1.515274	5.764145	3.379152
99	6	0	-0.057219	7.364305	3.433580
100	1	0	-0.515974	7.902741	2.596987
101	1	0	1.030082	7.463561	3.318875
102	6	0	-0.501268	7.951248	4.773600
103	1	0	-1.597031	7.915438	4.842220
104	1	0	-0.213563	9.006188	4.833619
105	6	0	0.101240	7.162089	5.936865
106	1	0	1.193758	7.275583	5.922812
107	1	0	-0.247386	7.561664	6.895020
108	6	0	-0.256553	5.679954	5.827232
109	1	0	-1.342461	5.545532	5.917922
110	1	0	0.204120	5.102954	6.636678
111	6	0	-0.751427	5.064752	1.166823
112	1	0	-1.835560	5.117885	1.350643
113	7	0	-1.425639	-4.631375	-3.077522
114	7	0	1.477251	-4.466320	-3.329434
115	7	0	4.606233	-2.770866	2.058059
116	7	0	3.339086	-1.631580	4.413407
117	6	0	-3.062818	-3.328922	-1.112344
118	1	0	-2.587123	-4.268368	-0.843163
119	6	0	-2.872985	-2.829000	-2.407722
120	6	0	-2.044162	-3.567000	-3.385327
121	1	0	-1.982402	-3.123098	-4.390692
122	6	0	-0.675639	-5.302540	-4.124810
123	1	0	-0.541976	-4.648969	-5.005160

124	6	0	0.720292	-5.674495	-3.605195
125	1	0	0.585940	-6.281882	-2.692388
126	6	0	1.482828	-6.496198	-4.652910
127	1	0	2.465789	-6.757599	-4.245776
128	1	0	1.660190	-5.856864	-5.527700
129	6	0	0.708593	-7.748153	-5.064899
130	1	0	1.269374	-8.300995	-5.825881
131	1	0	0.604841	-8.414941	-4.198156
132	6	0	-0.681206	-7.377395	-5.583676
133	1	0	-1.248180	-8.277270	-5.844422
134	1	0	-0.577684	-6.787744	-6.504668
135	6	0	-1.446840	-6.562007	-4.541833
136	1	0	-1.624988	-7.168238	-3.643933
137	1	0	-2.429299	-6.261047	-4.922088
138	6	0	2.073868	-4.385672	-2.212498
139	1	0	1.991634	-5.171306	-1.445802
140	6	0	2.899628	-3.214860	-1.844768
141	6	0	3.125982	-2.181732	-2.765879
142	1	0	2.684002	-2.261331	-3.755731
143	6	0	3.886479	-1.073578	-2.407722
144	6	0	4.414340	-0.988017	-1.112344
145	1	0	4.990077	-0.106331	-0.843163
146	6	0	4.191131	-2.003734	-0.189762
147	6	0	3.436588	-3.124746	-0.563767
148	1	0	3.269812	-3.911243	0.168950
149	6	0	4.761918	-1.881621	1.166823
150	1	0	5.349999	-0.969301	1.350643
151	6	0	5.299011	-2.576908	3.319857
152	1	0	5.749533	-1.569807	3.379152
153	6	0	4.310213	-2.707663	4.485185
154	1	0	3.822773	-3.695436	4.401624
155	6	0	5.047261	-2.617796	5.827232
156	1	0	4.317228	-2.728250	6.636678
157	1	0	5.473802	-1.610161	5.917922
158	6	0	6.151931	-3.668721	5.936865
159	1	0	5.703961	-4.671616	5.922812
160	1	0	6.672286	-3.566590	6.895020
161	6	0	7.136617	-3.541513	4.773600
162	1	0	7.653486	-2.574649	4.842220
163	1	0	7.906368	-4.318143	4.833619
164	6	0	6.406285	-3.632600	3.433580
165	1	0	5.948593	-4.623858	3.318875
166	1	0	7.101962	-3.504524	2.596987
167	6	0	2.114544	-1.949926	4.493675
168	1	0	1.786648	-2.996347	4.578666
169	6	0	0.923229	2.128906	1.463327
170	6	0	-2.305301	-0.264913	1.463327
171	6	0	1.382072	-1.863993	1.463327
172	6	0	0.013846	-2.298664	-1.590910
173	6	0	-1.997624	1.137341	-1.590910
174	6	0	1.983779	1.161323	-1.590910
175	8	0	2.561250	1.472074	-0.627572
176	8	0	-0.005772	-2.954144	-0.627572
177	8	0	-2.555478	1.482071	-0.627572
178	8	0	-1.463477	-0.923413	1.000043
179	8	0	-0.067961	1.729115	1.000043
180	8	0	1.531438	-0.805702	1.000043
181	8	0	-3.151043	0.380510	1.931496
182	8	0	1.905053	2.538628	1.931496

183	8	0	1.245990	-2.919138	1.931496
184	8	0	-1.448554	0.790079	-2.552885
185	8	0	0.040048	-1.649524	-2.552885
186	8	0	1.408506	0.859445	-2.552885

6CO2@CC3-c C1 cc3-rt

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-2.445492	4.291524	-2.849502
2	7	0	-0.281793	5.568723	-1.388708
3	7	0	5.175797	2.176332	-1.250301
4	7	0	5.351990	-0.637468	-1.990996
5	6	0	-2.723998	1.478472	-3.388480
6	1	0	-2.091138	2.060459	-4.053065
7	6	0	-3.372152	2.132094	-2.331042
8	6	0	-3.189688	3.580718	-2.107669
9	1	0	-3.743982	4.004566	-1.255984
10	6	0	-2.399026	5.717919	-2.584334
11	1	0	-2.867054	5.962537	-1.614026
12	6	0	-0.939218	6.185124	-2.526191
13	1	0	-0.456688	5.893889	-3.476223
14	6	0	-0.867970	7.709308	-2.367105
15	1	0	0.184934	8.011342	-2.344073
16	1	0	-1.296868	7.973109	-1.391429
17	6	0	-1.621694	8.429792	-3.485100
18	1	0	-1.570122	9.513090	-3.333282
19	1	0	-1.135588	8.219198	-4.447374
20	6	0	-3.076895	7.963318	-3.544208
21	1	0	-3.605495	8.453871	-4.368326
22	1	0	-3.588349	8.257326	-2.617588
23	6	0	-3.152152	6.445015	-3.705908
24	1	0	-2.712137	6.144675	-4.665856
25	1	0	-4.192262	6.100888	-3.710952
26	6	0	0.838375	5.009642	-1.591190
27	1	0	1.289146	4.946108	-2.593056
28	6	0	1.615058	4.389367	-0.497705
29	6	0	1.161635	4.454398	0.828522
30	1	0	0.222377	4.962418	1.032189
31	6	0	1.894672	3.868271	1.852520
32	6	0	3.092368	3.200070	1.553021
33	1	0	3.643148	2.730194	2.364130
34	6	0	3.547834	3.128540	0.242548
35	6	0	2.800081	3.724452	-0.785042
36	1	0	3.160680	3.639678	-1.807145
37	6	0	4.796592	2.398387	-0.060099
38	1	0	5.362588	2.036891	0.812038
39	6	0	6.436781	1.479729	-1.433728
40	1	0	6.770934	1.000009	-0.496693
41	6	0	6.263626	0.377321	-2.487734
42	1	0	5.874138	0.854643	-3.404899
43	6	0	7.610240	-0.289688	-2.795408
44	1	0	7.454801	-1.058860	-3.559797
45	1	0	7.951817	-0.806123	-1.888836
46	6	0	8.656758	0.729292	-3.246211
47	1	0	8.338916	1.184650	-4.193990

48	1	0	9.609920	0.225971	-3.439444
49	6	0	8.830839	1.826016	-2.194733
50	1	0	9.236769	1.383506	-1.274949
51	1	0	9.554875	2.574273	-2.534009
52	6	0	7.492306	2.496822	-1.887579
53	1	0	7.112892	3.009430	-2.781337
54	1	0	7.603354	3.258083	-1.107411
55	6	0	4.362292	-0.949784	-2.721035
56	1	0	4.158594	-0.443686	-3.677203
57	7	0	-5.823717	-0.213972	0.238728
58	7	0	-4.883744	-1.411433	2.699190
59	7	0	0.217670	1.387954	5.486551
60	7	0	1.963736	3.332134	4.198159
61	6	0	-4.199959	1.407979	-1.480723
62	1	0	-4.727460	1.896821	-0.666394
63	6	0	-4.350663	0.023614	-1.645001
64	6	0	-5.188857	-0.759540	-0.714162
65	1	0	-5.228492	-1.843604	-0.901188
66	6	0	-6.657349	-1.058467	1.072076
67	1	0	-6.543803	-2.125291	0.807497
68	6	0	-6.233010	-0.901766	2.538930
69	1	0	-6.290729	0.171530	2.793123
70	6	0	-7.172563	-1.693785	3.457231
71	1	0	-6.854329	-1.548207	4.495483
72	1	0	-7.051734	-2.761831	3.233225
73	6	0	-8.631343	-1.277968	3.266250
74	1	0	-9.278298	-1.873611	3.918871
75	1	0	-8.753841	-0.228783	3.567578
76	6	0	-9.052434	-1.433312	1.804159
77	1	0	-10.086707	-1.101767	1.664386
78	1	0	-9.018885	-2.496432	1.529631
79	6	0	-8.121015	-0.641440	0.886221
80	1	0	-8.201485	0.432060	1.101185
81	1	0	-8.395703	-0.776921	-0.165541
82	6	0	-4.056665	-0.693897	3.339465
83	1	0	-4.324438	0.297632	3.734480
84	6	0	-2.668907	-1.134521	3.592239
85	6	0	-2.238899	-2.403287	3.177892
86	1	0	-2.941618	-3.040984	2.648143
87	6	0	-0.946803	-2.832945	3.451121
88	6	0	-0.066986	-1.981350	4.135448
89	1	0	0.934969	-2.337934	4.358619
90	6	0	-0.467653	-0.702980	4.506367
91	6	0	-1.780239	-0.283278	4.239704
92	1	0	-2.082717	0.715254	4.546215
93	6	0	0.499510	0.190000	5.177340
94	1	0	1.487024	-0.250733	5.384199
95	6	0	1.226251	2.150202	6.201337
96	1	0	2.202989	1.634409	6.190104
97	6	0	1.415206	3.516468	5.529933
98	1	0	0.427820	4.010340	5.493124
99	6	0	2.385956	4.384644	6.340987
100	1	0	2.486878	5.355906	5.844205
101	1	0	3.375243	3.909171	6.315330
102	6	0	1.920821	4.553218	7.787422
103	1	0	0.967456	5.098607	7.803028
104	1	0	2.643041	5.159649	8.344055
105	6	0	1.732278	3.191354	8.456791
106	1	0	2.704462	2.684609	8.525330

107	1	0	1.364446	3.313022	9.481036
108	6	0	0.762879	2.324096	7.653693
109	1	0	-0.234604	2.782631	7.643135
110	1	0	0.652632	1.333155	8.107696
111	6	0	1.396146	3.942532	3.241812
112	1	0	0.490381	4.549933	3.390928
113	7	0	-2.407642	-1.783230	-4.970366
114	7	0	0.172711	-3.089853	-4.898656
115	7	0	1.949689	-5.326151	0.836769
116	7	0	0.628591	-4.644810	3.324434
117	6	0	-3.698881	-0.617610	-2.691990
118	1	0	-3.804341	-1.688796	-2.844201
119	6	0	-2.889050	0.110950	-3.574241
120	6	0	-2.219354	-0.557096	-4.707791
121	1	0	-1.565154	0.080974	-5.321171
122	6	0	-1.767020	-2.329717	-6.150672
123	1	0	-1.094404	-1.592585	-6.624921
124	6	0	-0.913998	-3.539676	-5.746223
125	1	0	-1.574146	-4.249969	-5.216710
126	6	0	-0.321591	-4.221009	-6.985528
127	1	0	0.266799	-5.087360	-6.664133
128	1	0	0.376917	-3.519747	-7.460399
129	6	0	-1.409569	-4.631968	-7.977731
130	1	0	-0.955772	-5.097403	-8.859021
131	1	0	-2.058264	-5.388914	-7.516254
132	6	0	-2.255937	-3.424126	-8.382781
133	1	0	-3.055312	-3.725975	-9.067704
134	1	0	-1.625270	-2.707041	-8.925731
135	6	0	-2.853194	-2.745000	-7.150228
136	1	0	-3.544093	-3.428789	-6.640103
137	1	0	-3.432193	-1.858202	-7.430240
138	6	0	0.290279	-3.622744	-3.754225
139	1	0	-0.415828	-4.381812	-3.384683
140	6	0	1.406631	-3.287828	-2.846274
141	6	0	2.324535	-2.280376	-3.176328
142	1	0	2.171152	-1.717951	-4.093601
143	6	0	3.406976	-2.014005	-2.346964
144	6	0	3.581110	-2.763995	-1.172370
145	1	0	4.434639	-2.545218	-0.535160
146	6	0	2.664160	-3.750760	-0.828578
147	6	0	1.568255	-4.002232	-1.666468
148	1	0	0.855486	-4.769255	-1.374903
149	6	0	2.829856	-4.508904	0.428686
150	1	0	3.747090	-4.300432	0.999947
151	6	0	2.206388	-6.029446	2.079940
152	1	0	3.011265	-5.542756	2.658729
153	6	0	0.932249	-6.008875	2.936014
154	1	0	0.119906	-6.445128	2.327058
155	6	0	1.121169	-6.846865	4.206145
156	1	0	0.192415	-6.821903	4.786551
157	1	0	1.894314	-6.367958	4.820946
158	6	0	1.525511	-8.284018	3.877502
159	1	0	0.712185	-8.775595	3.326510
160	1	0	1.671895	-8.852620	4.801879
161	6	0	2.795655	-8.306716	3.025925
162	1	0	3.630434	-7.899118	3.612101
163	1	0	3.064678	-9.334983	2.762114
164	6	0	2.612178	-7.473544	1.757310
165	1	0	1.831645	-7.916110	1.124454

166	1	0	3.531966	-7.454969	1.162132
167	6	0	-0.518190	-4.185419	3.036964
168	1	0	-1.261679	-4.772966	2.476914
169	8	0	-0.682550	1.974971	2.401805
170	8	0	-0.343475	-0.603783	-1.911324
171	8	0	-2.038549	-0.249162	0.610278
172	8	0	2.418571	-2.211430	2.295030
173	6	0	0.270712	1.323407	2.268613
174	6	0	-2.680876	0.634486	1.013447
175	6	0	-0.907996	-1.575867	-1.612485
176	6	0	1.570408	-2.021687	1.523559
177	8	0	0.726981	-1.836513	0.741622
178	8	0	1.229760	0.675525	2.144683
179	8	0	-3.326653	1.505519	1.432918
180	8	0	-1.469564	-2.558447	-1.342582
181	6	0	2.759835	0.266015	-0.384750
182	6	0	-0.214286	2.155902	-1.620868
183	8	0	-0.630531	2.051407	-0.537606
184	8	0	0.197917	2.288143	-2.698996
185	8	0	2.131633	0.715651	-1.252974
186	8	0	3.397262	-0.180016	0.481158

(CO2)4 S4 cc3-rjjx

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.154578	1.664139	1.346603
2	6	0	1.664139	-0.154578	-1.346603
3	6	0	-1.664139	0.154578	-1.346603
4	6	0	-0.154578	-1.664139	1.346603
5	8	0	-0.872382	1.166251	1.105034
6	8	0	1.166251	0.872382	-1.105034
7	8	0	-1.166251	-0.872382	-1.105034
8	8	0	0.872382	-1.166251	1.105034
9	8	0	1.166251	2.165482	1.609008
10	8	0	2.165482	-1.166251	-1.609008
11	8	0	-2.165482	1.166251	-1.609008
12	8	0	-1.166251	-2.165482	1.609008

(CO2)6-a Th cc3-rjjjx

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-0.000000	1.162777	2.494534
2	8	0	-0.000000	-1.162777	-2.494534
3	8	0	-1.162777	2.494534	0.000000
4	8	0	-2.494534	0.000000	1.162777
5	6	0	0.000000	-0.000000	2.501470
6	6	0	0.000000	2.501470	-0.000000
7	6	0	-0.000000	-0.000000	-2.501470
8	6	0	-2.501470	0.000000	-0.000000
9	8	0	-2.494534	0.000000	-1.162777
10	8	0	-0.000000	-1.162777	2.494534

11	8	0	1.162777	2.494534	-0.000000
12	8	0	0.000000	1.162777	-2.494534
13	6	0	-0.000000	-2.501470	0.000000
14	6	0	2.501470	-0.000000	0.000000
15	8	0	2.494534	0.000000	1.162777
16	8	0	2.494534	-0.000000	-1.162777
17	8	0	-1.162777	-2.494534	0.000000
18	8	0	1.162777	-2.494534	-0.000000

(CO2) 6-b C1 cc3-rtx

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	0.768060	-1.220938	-2.733855
2	8	0	0.990496	1.138544	1.806043
3	8	0	1.362748	-1.346935	0.180221
4	8	0	-1.252292	-2.881467	0.349872
5	6	0	-0.229496	-0.930419	-2.215405
6	6	0	2.346340	-0.974972	-0.327663
7	6	0	0.897928	0.227870	2.525384
8	6	0	-1.303927	-1.825225	0.826082
9	8	0	-1.358259	-0.766154	1.310069
10	8	0	-1.237626	-0.651041	-1.704306
11	8	0	3.334374	-0.617277	-0.814034
12	8	0	0.828766	-0.673763	3.253585
13	6	0	-2.630351	1.179877	-0.154476
14	6	0	0.909439	2.319172	-0.654849
15	8	0	0.984898	1.264922	-1.149943
16	8	0	0.858861	3.377418	-0.187879
17	8	0	-1.710294	1.889851	-0.092510
18	8	0	-3.562182	0.489613	-0.216569

(CO2) 6-c S6 cc3-rtxx

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.156290	1.858643	1.311233
2	8	0	2.302820	2.010849	1.389852
3	8	0	0.000000	1.722454	1.248209
4	6	0	2.187777	-0.072055	-1.311233
5	8	0	1.491689	0.861227	-1.248209
6	8	0	2.892857	-0.988876	-1.389852
7	6	0	-2.187777	0.072055	1.311233
8	8	0	-2.892857	0.988876	1.389852
9	8	0	-1.491689	-0.861227	1.248209
10	6	0	-1.156290	-1.858643	-1.311233
11	8	0	-0.000000	-1.722454	-1.248209
12	8	0	-2.302820	-2.010849	-1.389852
13	6	0	1.031487	-1.930698	1.311233
14	8	0	0.590036	-2.999726	1.389852
15	8	0	1.491689	-0.861227	1.248209
16	6	0	-1.031487	1.930698	-1.311233
17	8	0	-0.590036	2.999726	-1.389852

18 8 0 -1.491689 0.861227 -1.248209

(C2H2)@CC3 C3 cc3-rco2cc

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-4.767424	0.681472	3.009569
2	7	0	-3.387420	3.191145	3.231521
3	7	0	-0.556827	5.302074	-2.129721
4	7	0	-0.106405	3.709431	-4.486434
5	6	0	-4.066985	-1.174481	0.929794
6	1	0	-4.751664	-0.368739	0.677597
7	6	0	-3.483612	-1.182380	2.204697
8	6	0	-3.823422	-0.143989	3.198372
9	1	0	-3.221738	-0.149047	4.119947
10	6	0	-5.054242	1.636638	4.061110
11	1	0	-4.391099	1.491586	4.933013
12	6	0	-4.799229	3.055142	3.525618
13	1	0	-5.418217	3.183241	2.619066
14	6	0	-5.198543	4.104668	4.568355
15	1	0	-5.019524	5.102305	4.152831
16	1	0	-4.533221	3.996141	5.434766
17	6	0	-6.655923	3.941683	5.000747
18	1	0	-6.907907	4.691474	5.758123
19	1	0	-7.314656	4.124407	4.140767
20	6	0	-6.907796	2.530867	5.535772
21	1	0	-7.959544	2.406970	5.814592
22	1	0	-6.316682	2.380946	6.449577
23	6	0	-6.514496	1.479626	4.497495
24	1	0	-7.149328	1.572945	3.606783
25	1	0	-6.660570	0.466298	4.887046
26	6	0	-3.050172	3.456826	2.038915
27	1	0	-3.793251	3.586373	1.236548
28	6	0	-1.639275	3.643126	1.647139
29	6	0	-0.605671	3.369664	2.554538
30	1	0	-0.863149	2.980510	3.536113
31	6	0	0.717835	3.608087	2.204697
32	6	0	1.016362	4.109352	0.929794
33	1	0	2.056494	4.299431	0.677597
34	6	0	0.000000	4.371665	0.019220
35	6	0	-1.332571	4.133572	0.384096
36	1	0	-2.115774	4.356488	-0.335956
37	6	0	0.332560	4.933542	-1.304712
38	1	0	1.407194	5.031200	-1.524588
39	6	0	-0.116758	5.878045	-3.385187
40	1	0	0.984894	5.866582	-3.471878
41	6	0	-0.677796	5.040458	-4.545084
42	1	0	-1.776780	5.014380	-4.432012
43	6	0	-0.320807	5.680334	-5.891195
44	1	0	-0.742960	5.069015	-6.696216
45	1	0	0.770500	5.649849	-6.006489
46	6	0	-0.818959	7.123380	-5.977064
47	1	0	-1.916676	7.133499	-5.935232
48	1	0	-0.534114	7.561172	-6.939565
49	6	0	-0.264458	7.958139	-4.821335
50	1	0	0.827825	8.025907	-4.916864

51	1	0	-0.650949	8.981792	-4.865711
52	6	0	-0.618143	7.323638	-3.475890
53	1	0	-1.706886	7.318044	-3.335297
54	1	0	-0.193092	7.897794	-2.645443
55	6	0	-0.902532	2.729408	-4.372643
56	1	0	-1.993088	2.868838	-4.310160
57	7	0	-1.069902	-4.529164	3.231521
58	7	0	1.793540	-4.469447	3.009569
59	7	0	4.457322	1.338019	3.231521
60	7	0	2.973885	3.787975	3.009569
61	6	0	-2.615379	-2.209359	2.554538
62	1	0	-2.149623	-2.237764	3.536113
63	6	0	-2.335402	-3.241217	1.647139
64	6	0	-1.468613	-4.369939	2.038915
65	1	0	-1.209264	-5.078239	1.236548
66	6	0	-0.246216	-5.683825	3.525618
67	1	0	-0.047659	-6.283934	2.619066
68	6	0	1.109751	-5.195421	4.061110
69	1	0	0.903798	-4.548597	4.933013
70	6	0	1.975854	-6.381532	4.497495
71	1	0	2.926459	-6.001372	4.887046
72	1	0	2.212454	-6.977972	3.606783
73	6	0	1.262103	-7.247760	5.535772
74	1	0	1.895274	-8.096652	5.814592
75	1	0	1.096382	-6.660880	6.449577
76	6	0	-0.085637	-7.735040	5.000747
77	1	0	-0.608982	-8.328160	5.758123
78	1	0	0.085487	-8.396881	4.140767
79	6	0	-0.955475	-6.554404	4.568355
80	1	0	-1.194149	-5.923955	5.434766
81	1	0	-1.908964	-6.898188	4.152831
82	6	0	2.036409	-3.239186	3.198372
83	1	0	1.739947	-2.715583	4.119947
84	6	0	2.765777	-2.425707	2.204697
85	6	0	3.050622	-2.934872	0.929794
86	1	0	2.695169	-3.930692	0.677597
87	6	0	3.785973	-2.185833	0.019220
88	6	0	4.246064	-0.912746	0.384096
89	1	0	4.830717	-0.345930	-0.335956
90	6	0	3.974678	-0.401909	1.647139
91	6	0	3.221051	-1.160305	2.554538
92	1	0	3.012772	-0.742746	3.536113
93	6	0	4.518785	0.913113	2.038915
94	1	0	5.002516	1.491866	1.236548
95	6	0	5.045445	2.628683	3.525618
96	1	0	5.465876	3.100693	2.619066
97	6	0	3.944491	3.558783	4.061110
98	1	0	3.487301	3.057010	4.933013
99	6	0	4.538642	4.901906	4.497495
100	1	0	3.734111	5.535074	4.887046
101	1	0	4.936875	5.405027	3.606783
102	6	0	5.645693	4.716893	5.535772
103	1	0	5.220301	4.279934	6.449577
104	1	0	6.064269	5.689682	5.814592
105	6	0	6.741559	3.793356	5.000747
106	1	0	7.229169	4.272475	4.140767
107	1	0	7.516889	3.636686	5.758123
108	6	0	6.154018	2.449736	4.568355
109	1	0	5.727370	1.927814	5.434766

110	1	0	6.928488	1.795883	4.152831
111	6	0	1.787013	3.383175	3.198372
112	1	0	1.481791	2.864630	4.119947
113	7	0	-4.313317	-3.133263	-2.129721
114	7	0	-3.159259	-1.946865	-4.486434
115	7	0	3.265664	-1.762566	-4.486434
116	7	0	4.870144	-2.168811	-2.129721
117	6	0	-2.913493	-3.220826	0.384096
118	1	0	-2.714943	-4.010558	-0.335956
119	6	0	-3.785973	-2.185833	0.019220
120	6	0	-4.438853	-2.178766	-1.304712
121	1	0	-5.060744	-1.296934	-1.524588
122	6	0	-5.032157	-3.040138	-3.385187
123	1	0	-5.573056	-2.080348	-3.471878
124	6	0	-4.026267	-3.107217	-4.545084
125	1	0	-3.454190	-4.045926	-4.432012
126	6	0	-4.758910	-3.117994	-5.891195
127	1	0	-4.018416	-3.177930	-6.696216
128	1	0	-5.278163	-2.157651	-6.006489
129	6	0	-5.759548	-4.270930	-5.977064
130	1	0	-6.281110	-4.243143	-6.939565
131	1	0	-5.219453	-5.226639	-5.935232
132	6	0	-6.759721	-4.208097	-4.821335
133	1	0	-7.452986	-5.054634	-4.865711
134	1	0	-7.364552	-3.296036	-4.916864
135	6	0	-6.033385	-4.197147	-3.475890
136	1	0	-5.484168	-5.137229	-3.335297
137	1	0	-6.743144	-4.116120	-2.645443
138	6	0	-1.912471	-2.146319	-4.372643
139	1	0	-1.487943	-3.160484	-4.310160
140	6	0	-0.934495	-1.040996	-4.338643
141	6	0	-1.360734	0.294646	-4.336797
142	1	0	-2.428414	0.498468	-4.344078
143	6	0	-0.434282	1.329795	-4.338643
144	6	0	0.935538	1.031107	-4.336797
145	1	0	1.645893	1.853834	-4.344078
146	6	0	1.368777	-0.288798	-4.338643
147	6	0	0.425196	-1.325753	-4.336797
148	1	0	0.782521	-2.352302	-4.344078
149	6	0	2.815002	-0.583089	-4.372643
150	1	0	3.481031	0.291645	-4.310160
151	6	0	4.704063	-1.933241	-4.545084
152	1	0	5.230970	-0.968453	-4.432012
153	6	0	5.148915	-2.837907	-3.385187
154	1	0	4.588162	-3.786234	-3.471878
155	6	0	6.651528	-3.126491	-3.475890
156	1	0	6.936236	-3.781674	-2.645443
157	1	0	7.191055	-2.180815	-3.335297
158	6	0	7.024179	-3.750042	-4.821335
159	1	0	6.536727	-4.729871	-4.916864
160	1	0	8.103935	-3.927158	-4.865711
161	6	0	6.578508	-2.852450	-5.977064
162	1	0	7.136129	-1.906860	-5.935232
163	1	0	6.815225	-3.318030	-6.939565
164	6	0	5.079717	-2.562340	-5.891195
165	1	0	4.507662	-3.492197	-6.006489
166	1	0	4.761376	-1.891085	-6.696216
167	6	0	4.106293	-2.754776	-1.304712
168	1	0	3.653549	-3.734266	-1.524588

169	6	0	0.000000	0.000000	4.612552
170	6	0	0.000000	0.000000	3.408091
171	1	0	0.000000	0.000000	5.680120
172	1	0	0.000000	0.000000	2.338835

(C2H2)4@CC3 C2 cc3-rjjcc

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-0.928410	-1.113095	-5.741579
2	7	0	0.928410	1.113095	-5.741579
3	7	0	5.503860	0.542590	-1.230947
4	7	0	5.500153	-1.092009	1.163046
5	6	0	-1.437616	-2.712021	-3.371403
6	1	0	-0.560368	-2.969043	-3.960138
7	6	0	-2.192476	-1.591595	-3.744678
8	6	0	-1.842125	-0.782499	-4.927611
9	1	0	-2.446796	0.126612	-5.070086
10	6	0	-0.723023	-0.258765	-6.896025
11	1	0	-1.388690	0.622917	-6.869744
12	6	0	0.723023	0.258765	-6.896025
13	1	0	1.388690	-0.622917	-6.869744
14	6	0	1.004353	1.069321	-8.166519
15	1	0	2.044902	1.411131	-8.143328
16	1	0	0.373672	1.967679	-8.146134
17	6	0	0.720342	0.256513	-9.429817
18	1	0	0.912340	0.866663	-10.318748
19	1	0	1.408060	-0.598911	-9.476182
20	6	0	-0.720342	-0.256513	-9.429817
21	1	0	-0.912340	-0.866663	-10.318748
22	1	0	-1.408060	0.598911	-9.476182
23	6	0	-1.004353	-1.069321	-8.166519
24	1	0	-0.373672	-1.967679	-8.146134
25	1	0	-2.044902	-1.411131	-8.143328
26	6	0	1.842125	0.782499	-4.927611
27	1	0	2.446796	-0.126612	-5.070086
28	6	0	2.192476	1.591595	-3.744678
29	6	0	1.437616	2.712021	-3.371403
30	1	0	0.560368	2.969043	-3.960138
31	6	0	1.810927	3.473898	-2.267523
32	6	0	2.949382	3.114084	-1.535011
33	1	0	3.238065	3.726041	-0.684758
34	6	0	3.688759	1.991451	-1.880756
35	6	0	3.310480	1.238845	-2.998545
36	1	0	3.907898	0.373821	-3.275816
37	6	0	4.855311	1.620760	-1.060973
38	1	0	5.136578	2.347293	-0.283312
39	6	0	6.685354	0.345567	-0.407808
40	1	0	6.741192	1.100916	0.396017
41	6	0	6.631832	-1.035030	0.257234
42	1	0	6.539678	-1.786057	-0.548927
43	6	0	7.918437	-1.300044	1.047486
44	1	0	7.854232	-2.294900	1.501385
45	1	0	7.970478	-0.576485	1.871470
46	6	0	9.158074	-1.179154	0.160700
47	1	0	9.130251	-1.958242	-0.613252

48	1	0	10.061911	-1.353336	0.753910
49	6	0	9.212098	0.194176	-0.510245
50	1	0	9.336134	0.967523	0.259981
51	1	0	10.080126	0.265078	-1.174135
52	6	0	7.929378	0.464229	-1.297449
53	1	0	7.833035	-0.254997	-2.121372
54	1	0	7.946844	1.463068	-1.747316
55	6	0	4.654139	-2.016705	0.970026
56	1	0	4.759913	-2.731802	0.137932
57	7	0	-5.503860	-0.542590	-1.230947
58	7	0	-5.500153	1.092009	1.163046
59	7	0	-0.852372	5.488189	1.068434
60	7	0	1.306651	5.344691	-0.844916
61	6	0	-3.310480	-1.238845	-2.998545
62	1	0	-3.907898	-0.373821	-3.275816
63	6	0	-3.688759	-1.991451	-1.880756
64	6	0	-4.855311	-1.620760	-1.060973
65	1	0	-5.136578	-2.347293	-0.283312
66	6	0	-6.685354	-0.345567	-0.407808
67	1	0	-6.741192	-1.100916	0.396017
68	6	0	-6.631832	1.035030	0.257234
69	1	0	-6.539678	1.786057	-0.548927
70	6	0	-7.918437	1.300044	1.047486
71	1	0	-7.854232	2.294900	1.501385
72	1	0	-7.970478	0.576485	1.871470
73	6	0	-9.158074	1.179154	0.160700
74	1	0	-10.061911	1.353336	0.753910
75	1	0	-9.130251	1.958242	-0.613252
76	6	0	-9.212098	-0.194176	-0.510245
77	1	0	-10.080126	-0.265078	-1.174135
78	1	0	-9.336134	-0.967523	0.259981
79	6	0	-7.929378	-0.464229	-1.297449
80	1	0	-7.833035	0.254997	-2.121372
81	1	0	-7.946844	-1.463068	-1.747316
82	6	0	-4.654139	2.016705	0.970026
83	1	0	-4.759913	2.731802	0.137932
84	6	0	-3.477683	2.235873	1.830204
85	6	0	-3.202886	1.414534	2.932588
86	1	0	-3.870981	0.583266	3.144888
87	6	0	-2.092076	1.665378	3.733199
88	6	0	-1.248474	2.742103	3.428243
89	1	0	-0.382464	2.917440	4.060870
90	6	0	-1.516020	3.559785	2.338105
91	6	0	-2.631834	3.298027	1.536351
92	1	0	-2.817315	3.936991	0.677252
93	6	0	-0.625477	4.694212	2.030879
94	1	0	0.250490	4.809284	2.690036
95	6	0	0.070481	6.583748	0.855322
96	1	0	0.965179	6.491934	1.498417
97	6	0	0.543637	6.556360	-0.604095
98	1	0	-0.353323	6.599533	-1.246882
99	6	0	1.437616	7.766869	-0.902538
100	1	0	1.744812	7.727535	-1.953479
101	1	0	2.350802	7.677206	-0.299603
102	6	0	0.725883	9.083049	-0.587111
103	1	0	-0.141126	9.196701	-1.251946
104	1	0	1.394061	9.926709	-0.789504
105	6	0	0.251220	9.109351	0.866629
106	1	0	1.124885	9.090217	1.532235

107	1	0	-0.288740	10.038231	1.078171
108	6	0	-0.641938	7.905321	1.165872
109	1	0	-1.556335	7.952682	0.560155
110	1	0	-0.955494	7.898108	2.215448
111	6	0	1.026357	4.661877	-1.878492
112	1	0	0.194041	4.931802	-2.546324
113	7	0	-1.306651	-5.344691	-0.844916
114	7	0	0.852372	-5.488189	1.068434
115	7	0	0.911848	-1.118765	5.748793
116	7	0	-0.911848	1.118765	5.748793
117	6	0	-2.949382	-3.114084	-1.535011
118	1	0	-3.238065	-3.726041	-0.684758
119	6	0	-1.810927	-3.473898	-2.267523
120	6	0	-1.026357	-4.661877	-1.878492
121	1	0	-0.194041	-4.931802	-2.546324
122	6	0	-0.543637	-6.556360	-0.604095
123	1	0	0.353323	-6.599533	-1.246882
124	6	0	-0.070481	-6.583748	0.855322
125	1	0	-0.965179	-6.491934	1.498417
126	6	0	0.641938	-7.905321	1.165872
127	1	0	0.955494	-7.898108	2.215448
128	1	0	1.556335	-7.952682	0.560155
129	6	0	-0.251220	-9.109351	0.866629
130	1	0	0.288740	-10.038231	1.078171
131	1	0	-1.124885	-9.090217	1.532235
132	6	0	-0.725883	-9.083049	-0.587111
133	1	0	-1.394061	-9.926709	-0.789504
134	1	0	0.141126	-9.196701	-1.251946
135	6	0	-1.437616	-7.766869	-0.902538
136	1	0	-2.350802	-7.677206	-0.299603
137	1	0	-1.744812	-7.727535	-1.953479
138	6	0	0.625477	-4.694212	2.030879
139	1	0	-0.250490	-4.809284	2.690036
140	6	0	1.516020	-3.559785	2.338105
141	6	0	2.631834	-3.298027	1.536351
142	1	0	2.817315	-3.936991	0.677252
143	6	0	3.477683	-2.235873	1.830204
144	6	0	3.202886	-1.414534	2.932588
145	1	0	3.870981	-0.583266	3.144888
146	6	0	2.092076	-1.665378	3.733199
147	6	0	1.248474	-2.742103	3.428243
148	1	0	0.382464	-2.917440	4.060870
149	6	0	1.815376	-0.818516	4.911562
150	1	0	2.449504	0.074184	5.026701
151	6	0	0.723837	-0.259091	6.899219
152	1	0	1.390651	0.621426	6.864212
153	6	0	-0.723837	0.259091	6.899219
154	1	0	-1.390651	-0.621426	6.864212
155	6	0	-1.008833	1.066034	8.171131
156	1	0	-2.050453	1.404549	8.148043
157	1	0	-0.380996	1.966395	8.152090
158	6	0	-0.721798	0.252782	9.433332
159	1	0	-1.404885	-0.606406	9.478330
160	1	0	-0.917386	0.860896	10.322886
161	6	0	0.721798	-0.252782	9.433332
162	1	0	1.404885	0.606406	9.478330
163	1	0	0.917386	-0.860896	10.322886
164	6	0	1.008833	-1.066034	8.171131
165	1	0	0.380996	-1.966395	8.152090

166	1	0	2.050453	-1.404549	8.148043
167	6	0	-1.815376	0.818516	4.911562
168	1	0	-2.449504	-0.074184	5.026701
169	6	0	-2.328841	1.128886	-1.223966
170	1	0	-3.381617	0.924084	-1.210245
171	6	0	2.328841	-1.128886	-1.223966
172	1	0	3.381617	-0.924084	-1.210245
173	6	0	-1.139892	1.329247	-1.233515
174	1	0	-0.078795	1.475966	-1.210264
175	6	0	1.139892	-1.329247	-1.233515
176	1	0	0.078795	-1.475966	-1.210264
177	6	0	-1.403337	-1.100713	1.217445
178	1	0	-1.443874	-0.040310	1.362857
179	6	0	1.403337	1.100713	1.217445
180	1	0	1.443874	0.040310	1.362857
181	6	0	-1.346314	-2.288301	1.016648
182	1	0	-1.289882	-3.337181	0.799829
183	6	0	1.346314	2.288301	1.016648
184	1	0	1.289882	3.337181	0.799829

(C2H2)6@CC3 C3 cc3-rjjcc

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	3.218875	-3.455566	-3.341548
2	7	0	0.581660	-4.895850	-3.103891
3	7	0	-4.602046	-1.059844	-3.341548
4	7	0	-4.530760	1.944193	-3.103891
5	6	0	4.014682	-0.681407	-2.864320
6	1	0	3.682422	-0.925617	-3.871017
7	6	0	4.131446	-1.717223	-1.922649
8	6	0	3.801174	-3.119375	-2.264142
9	1	0	4.077016	-3.865221	-1.501231
10	6	0	3.003354	-4.874653	-3.588170
11	1	0	3.120542	-5.462355	-2.660477
12	6	0	1.585381	-5.140915	-4.129076
13	1	0	1.433214	-4.486327	-5.006242
14	6	0	1.443457	-6.608279	-4.565874
15	1	0	0.435100	-6.748947	-4.970854
16	1	0	1.514106	-7.237135	-3.668339
17	6	0	2.505285	-7.026085	-5.580745
18	1	0	2.371979	-8.079713	-5.848514
19	1	0	2.380711	-6.443539	-6.503677
20	6	0	3.904043	-6.783244	-5.016961
21	1	0	4.671056	-7.051181	-5.751358
22	1	0	4.059340	-7.429445	-4.142373
23	6	0	4.064645	-5.321216	-4.606770
24	1	0	3.982482	-4.672920	-5.489344
25	1	0	5.054644	-5.140439	-4.173529
26	6	0	-0.490767	-4.314804	-3.455432
27	1	0	-0.642594	-3.945670	-4.482943
28	6	0	-1.584135	-4.018766	-2.504513
29	6	0	-1.540104	-4.515957	-1.195504
30	1	0	-0.728470	-5.187331	-0.925566
31	6	0	-2.482624	-4.119451	-0.253551
32	6	0	-3.492308	-3.219709	-0.625265

33	1	0	-4.209882	-2.909262	0.129895
34	6	0	-3.552882	-2.719326	-1.922649
35	6	0	-2.597457	-3.136113	-2.864320
36	1	0	-2.642819	-2.726263	-3.871017
37	6	0	-4.602045	-1.732226	-2.264142
38	1	0	-5.385888	-1.598189	-1.501231
39	6	0	-5.723250	-0.163654	-3.588170
40	1	0	-6.290809	0.028709	-2.660477
41	6	0	-5.244853	1.197477	-4.129076
42	1	0	-4.601880	1.001964	-5.006242
43	6	0	-6.444666	2.054069	-4.565874
44	1	0	-6.062310	2.997666	-4.970854
45	1	0	-7.024596	2.307313	-3.668339
46	6	0	-7.337411	1.343402	-5.580745
47	1	0	-6.770624	1.160013	-6.503677
48	1	0	-8.183226	1.985662	-5.848514
49	6	0	-7.826483	0.010622	-5.016961
50	1	0	-8.463758	0.199231	-4.142373
51	1	0	-8.442030	-0.519663	-5.751358
52	6	0	-6.640631	-0.859478	-4.606770
53	1	0	-6.038108	-1.112470	-5.489344
54	1	0	-6.979072	-1.807230	-4.173529
55	6	0	-3.491346	2.582419	-3.455432
56	1	0	-3.095753	2.529337	-4.482943
57	7	0	5.328640	-0.613216	2.049511
58	7	0	3.701586	-0.139268	4.488654
59	7	0	-1.971402	-3.136034	4.488654
60	7	0	-3.195381	-4.308129	2.049511
61	6	0	4.534504	-1.414573	-0.625265
62	1	0	4.624436	-2.191234	0.129895
63	6	0	4.808861	-0.090290	-0.253551
64	6	0	5.219163	0.248397	1.124393
65	1	0	5.445410	1.313553	1.296679
66	6	0	5.860467	-0.158348	3.323574
67	1	0	5.837173	0.943850	3.399978
68	6	0	5.034134	-0.720320	4.488674
69	1	0	4.992862	-1.817713	4.371696
70	6	0	5.693215	-0.378841	5.833556
71	1	0	5.088459	-0.813953	6.636984
72	1	0	5.657738	0.710910	5.964257
73	6	0	7.138728	-0.867402	5.908034
74	1	0	7.577618	-0.591601	6.872827
75	1	0	7.158458	-1.964163	5.850152
76	6	0	7.958744	-0.288098	4.755829
77	1	0	8.987780	-0.661656	4.786829
78	1	0	8.012429	0.803833	4.863319
79	6	0	7.317338	-0.637983	3.414415
80	1	0	7.327704	-1.725648	3.264461
81	1	0	7.879096	-0.198753	2.582638
82	6	0	2.723908	-0.922228	4.687789
83	1	0	2.857920	-2.010552	4.786942
84	6	0	1.328018	-0.441694	4.766913
85	6	0	1.037990	0.928594	4.770096
86	1	0	1.863073	1.636115	4.741668
87	6	0	-0.281491	1.370944	4.766913
88	6	0	-1.323181	0.434628	4.770096
89	1	0	-2.348453	0.795411	4.741668
90	6	0	-1.046527	-0.929250	4.766913
91	6	0	0.285191	-1.363222	4.770096

92	1	0	0.485380	-2.431526	4.741668
93	6	0	-2.160627	-1.897859	4.687789
94	1	0	-3.170150	-1.469755	4.786942
95	6	0	-3.140882	-3.999528	4.488674
96	1	0	-4.070617	-3.415089	4.371696
97	6	0	-3.067366	-4.996139	3.323574
98	1	0	-2.101189	-5.527065	3.399978
99	6	0	-4.211178	-6.018009	3.414415
100	1	0	-4.111673	-6.724121	2.582638
101	1	0	-5.158307	-5.483154	3.264461
102	6	0	-4.228872	-6.748426	4.755829
103	1	0	-3.310074	-7.340883	4.863319
104	1	0	-5.066901	-7.452818	4.786829
105	6	0	-4.320556	-5.748619	5.908034
106	1	0	-5.280244	-5.217324	5.850152
107	1	0	-4.301151	-6.266609	6.872827
108	6	0	-3.174693	-4.741048	5.833556
109	1	0	-2.213203	-5.255200	5.964257
110	1	0	-3.249134	-3.999758	6.636984
111	6	0	-2.394463	-4.644126	1.124393
112	1	0	-1.585134	-5.372640	1.296679
113	7	0	3.949101	2.951657	-3.103891
114	7	0	1.383171	4.515410	-3.341548
115	7	0	-2.133259	4.921346	2.049511
116	7	0	-1.730183	3.275301	4.488654
117	6	0	4.680986	0.924209	-1.195504
118	1	0	4.856595	1.962792	-0.925566
119	6	0	4.272421	0.637482	-2.504513
120	6	0	3.982113	1.732385	-3.455432
121	1	0	3.738347	1.416333	-4.482943
122	6	0	3.659472	3.943437	-4.129076
123	1	0	3.168666	3.484363	-5.006242
124	6	0	2.719896	5.038307	-3.588170
125	1	0	3.170267	5.433646	-2.660477
126	6	0	2.575985	6.180694	-4.606770
127	1	0	1.924429	6.947669	-4.173529
128	1	0	2.055626	5.785390	-5.489344
129	6	0	3.922440	6.772622	-5.016961
130	1	0	3.770974	7.570843	-5.751358
131	1	0	4.404418	7.230214	-4.142373
132	6	0	4.832126	5.682683	-5.580745
133	1	0	5.811247	6.094051	-5.848514
134	1	0	4.389913	5.283525	-6.503677
135	6	0	5.001209	4.554210	-4.565874
136	1	0	5.510490	4.929822	-3.668339
137	1	0	5.627210	3.751282	-4.970854
138	6	0	0.800871	4.851601	-2.264142
139	1	0	1.308871	5.463410	-1.501231
140	6	0	-0.578564	4.436549	-1.922649
141	6	0	-1.417226	3.817520	-2.864320
142	1	0	-1.039604	3.651880	-3.871017
143	6	0	-2.688286	3.381284	-2.504513
144	6	0	-3.140882	3.591748	-1.195504
145	1	0	-4.128126	3.224539	-0.925566
146	6	0	-2.326237	4.209741	-0.253551
147	6	0	-1.042196	4.634282	-0.625265
148	1	0	-0.414554	5.100496	0.129895
149	6	0	-2.824700	4.395729	1.124393
150	1	0	-3.860276	4.059087	1.296679

151	6	0	-2.793100	5.154487	3.323574
152	1	0	-3.735985	4.583215	3.399978
153	6	0	-1.893252	4.719848	4.488674
154	1	0	-0.922246	5.232802	4.371696
155	6	0	-2.518522	5.119889	5.833556
156	1	0	-1.839326	4.813711	6.636984
157	1	0	-3.444535	4.544290	5.964257
158	6	0	-2.818172	6.616021	5.908034
159	1	0	-1.878213	7.181488	5.850152
160	1	0	-3.276467	6.858210	6.872827
161	6	0	-3.729872	7.036524	4.755829
162	1	0	-4.702354	6.537050	4.863319
163	1	0	-3.920879	8.114474	4.786829
164	6	0	-3.106160	6.655992	3.414415
165	1	0	-2.169397	7.208802	3.264461
166	1	0	-3.767423	6.922874	2.582638
167	6	0	-0.563281	2.820087	4.687789
168	1	0	0.312229	3.480308	4.786942
169	6	0	1.225949	1.652112	-2.189214
170	1	0	0.954557	2.298657	-2.994388
171	6	0	-2.655330	-0.538522	1.186369
172	1	0	-3.418132	0.006651	0.674588
173	6	0	-1.755342	-1.150962	1.703151
174	1	0	-0.944914	-1.689752	2.147744
175	6	0	1.874433	-0.944690	1.703151
176	1	0	1.935825	0.026557	2.147744
177	6	0	-0.119091	2.095651	1.703151
178	1	0	-0.990911	1.663196	2.147744
179	6	0	0.861291	2.568844	1.186369
180	1	0	1.714826	2.956863	0.674588
181	6	0	1.794039	-2.030322	1.186369
182	1	0	1.703306	-2.963514	0.674588
183	6	0	1.555592	0.927486	-1.286309
184	1	0	1.811604	0.230028	-0.515686
185	6	0	0.025431	-1.810925	-1.286309
186	1	0	-0.706592	-1.683909	-0.515686
187	6	0	0.817796	-1.887759	-2.189214
188	1	0	1.513417	-1.975999	-2.994388
189	6	0	-1.581022	0.883439	-1.286309
190	1	0	-1.105012	1.453881	-0.515686
191	6	0	-2.043745	0.235647	-2.189214
192	1	0	-2.467973	-0.322658	-2.994388

(C2H2)4 S4 cc3-rjjccx

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.607582	1.814760	1.563200
2	1	0	2.627703	2.002727	1.815147
3	6	0	-1.607582	-1.814760	1.563200
4	1	0	-2.627703	-2.002727	1.815147
5	6	0	0.453632	1.607582	1.289688
6	1	0	-0.563790	1.408094	1.024559
7	6	0	-0.453632	-1.607582	1.289688
8	1	0	0.563790	-1.408094	1.024559
9	6	0	1.607582	-0.453632	-1.289688

10	1	0	1.408094	0.563790	-1.024559
11	6	0	-1.607582	0.453632	-1.289688
12	1	0	-1.408094	-0.563790	-1.024559
13	6	0	1.814760	-1.607582	-1.563200
14	1	0	2.002727	-2.627703	-1.815147
15	6	0	-1.814760	1.607582	-1.563200
16	1	0	-2.002727	2.627703	-1.815147

(C2H2)4 C1 cc3-rjjccy

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.658882	2.579814	-0.053286
2	1	0	2.604485	3.069891	-0.125239
3	6	0	-1.144301	-0.609072	2.091719
4	1	0	-2.209304	-0.545167	2.125376
5	6	0	0.584400	2.043404	0.033856
6	1	0	-0.363124	1.547990	0.104979
7	6	0	0.055642	-0.679748	2.035402
8	1	0	1.119502	-0.744576	1.969960
9	6	0	1.685313	-1.101598	-0.911129
10	1	0	1.731603	-0.030935	-0.931083
11	6	0	-1.781236	-0.358582	-1.064691
12	1	0	-0.975176	-1.039479	-0.878840
13	6	0	1.613096	-2.302682	-0.867903
14	1	0	1.557563	-3.368280	-0.833780
15	6	0	-2.671970	0.427335	-1.261088
16	1	0	-3.464506	1.117325	-1.448656

(C2H2)6 C3 cc3rjjccx

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.814865	1.994196	1.990290
2	1	0	2.656464	2.099838	2.638219
3	6	0	-0.571952	-2.560794	-1.350152
4	1	0	-0.064674	-3.334952	-0.816951
5	6	0	-1.135056	-1.663478	-1.923263
6	1	0	-1.624521	-0.846281	-2.408786
7	6	0	-0.873086	1.814726	-1.923263
8	1	0	0.079359	1.830017	-2.408786
9	6	0	2.008142	-0.151248	-1.923263
10	1	0	1.545162	-0.983736	-2.408786
11	6	0	2.503688	0.785072	-1.350152
12	1	0	2.920490	1.611467	-0.816951
13	6	0	-1.931736	1.775722	-1.350152
14	1	0	-2.855816	1.723485	-0.816951
15	6	0	0.854641	1.869223	1.274596
16	1	0	0.000000	1.749757	0.638688
17	6	0	-2.046115	-0.194471	1.274596
18	1	0	-1.515334	-0.874879	0.638688
19	6	0	-2.634457	0.574621	1.990290
20	1	0	-3.146745	1.250646	2.638219

21	6	0	1.191474	-1.674752	1.274596
22	1	0	1.515334	-0.874879	0.638688
23	6	0	0.819592	-2.568817	1.990290
24	1	0	0.490281	-3.350484	2.638219

H2O@CC3 C1 cc3-ww00

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	1.628842	5.515960	0.523040
2	7	0	3.693742	4.328758	-1.102923
3	7	0	5.565772	-1.536577	0.714973
4	7	0	4.100945	-3.195238	2.562507
5	6	0	-0.222777	3.945606	2.073894
6	1	0	0.747078	4.165679	2.512711
7	6	0	-0.479717	4.379926	0.765668
8	6	0	0.531077	5.144702	0.008999
9	1	0	0.260972	5.392765	-1.029398
10	6	0	2.525485	6.305358	-0.298617
11	1	0	2.134414	6.424025	-1.325401
12	6	0	3.878451	5.584865	-0.402578
13	1	0	4.246915	5.423605	0.626693
14	6	0	4.886529	6.443804	-1.174118
15	1	0	5.842490	5.910856	-1.220250
16	1	0	4.529035	6.547131	-2.206925
17	6	0	5.055808	7.822696	-0.535483
18	1	0	5.765611	8.420119	-1.117280
19	1	0	5.484391	7.709208	0.469619
20	6	0	3.709001	8.540108	-0.429449
21	1	0	3.828196	9.512533	0.059841
22	1	0	3.324549	8.737124	-1.439499
23	6	0	2.700307	7.687532	0.340703
24	1	0	3.037511	7.546088	1.375805
25	1	0	1.723136	8.180279	0.389101
26	6	0	4.022025	3.263293	-0.499424
27	1	0	4.423395	3.274687	0.525955
28	6	0	3.917783	1.932028	-1.128912
29	6	0	3.350790	1.780584	-2.402179
30	1	0	2.971749	2.663959	-2.909704
31	6	0	3.291416	0.529024	-3.002526
32	6	0	3.799098	-0.588021	-2.323885
33	1	0	3.751265	-1.557946	-2.812262
34	6	0	4.364090	-0.448815	-1.062434
35	6	0	4.417909	0.818646	-0.465703
36	1	0	4.869672	0.909369	0.518764
37	6	0	4.933063	-1.627848	-0.379795
38	1	0	4.790366	-2.591966	-0.892360
39	6	0	6.119532	-2.750850	1.280812
40	1	0	5.859253	-3.636302	0.672967
41	6	0	5.527159	-2.965552	2.682430
42	1	0	5.743159	-2.058327	3.275309
43	6	0	6.172639	-4.180608	3.358261
44	1	0	5.740708	-4.299394	4.357923
45	1	0	5.899825	-5.076085	2.784815
46	6	0	7.693823	-4.044362	3.428791
47	1	0	7.954675	-3.188891	4.066696

48	1	0	8.127938	-4.933680	3.897666
49	6	0	8.283543	-3.829337	2.033950
50	1	0	8.103587	-4.725104	1.423995
51	1	0	9.369137	-3.697226	2.090893
52	6	0	7.644492	-2.616525	1.356841
53	1	0	7.880129	-1.702957	1.918110
54	1	0	8.037940	-2.477902	0.343929
55	6	0	3.319702	-2.406531	3.174836
56	1	0	3.695079	-1.561783	3.773255
57	7	0	-4.331442	3.569162	-0.860019
58	7	0	-4.922330	1.220811	-2.403402
59	7	0	0.006351	-1.362309	-5.603622
60	7	0	2.749441	-0.696372	-5.002676
61	6	0	-1.714512	4.115878	0.187061
62	1	0	-1.941007	4.444590	-0.823961
63	6	0	-2.704885	3.430413	0.904977
64	6	0	-4.030189	3.171566	0.307657
65	1	0	-4.740749	2.610665	0.931983
66	6	0	-5.670956	3.282239	-1.338007
67	1	0	-6.232956	2.661383	-0.618000
68	6	0	-5.570349	2.497488	-2.654775
69	1	0	-4.981153	3.103547	-3.364677
70	6	0	-6.965921	2.244531	-3.236036
71	1	0	-6.864831	1.689095	-4.174924
72	1	0	-7.518515	1.599646	-2.540030
73	6	0	-7.722855	3.556037	-3.451687
74	1	0	-8.722873	3.348568	-3.846427
75	1	0	-7.200217	4.157058	-4.208267
76	6	0	-7.813365	4.354138	-2.149590
77	1	0	-8.321651	5.308950	-2.319946
78	1	0	-8.420086	3.794924	-1.424761
79	6	0	-6.422280	4.598783	-1.563682
80	1	0	-5.827920	5.223074	-2.243805
81	1	0	-6.485523	5.135661	-0.611179
82	6	0	-3.931989	0.892920	-3.126734
83	1	0	-3.553306	1.568083	-3.908262
84	6	0	-3.228050	-0.397201	-3.005222
85	6	0	-3.635390	-1.374620	-2.084068
86	1	0	-4.475966	-1.179721	-1.422924
87	6	0	-2.971598	-2.593301	-2.014980
88	6	0	-1.884884	-2.841171	-2.864714
89	1	0	-1.382712	-3.802945	-2.797722
90	6	0	-1.472772	-1.879892	-3.779311
91	6	0	-2.152386	-0.656136	-3.846970
92	1	0	-1.820707	0.079808	-4.574869
93	6	0	-0.342993	-2.164733	-4.686679
94	1	0	0.168783	-3.126094	-4.525345
95	6	0	1.109171	-1.751181	-6.460773
96	1	0	1.540608	-2.719986	-6.150444
97	6	0	2.221746	-0.697056	-6.353201
98	1	0	1.777971	0.280592	-6.615033
99	6	0	3.359530	-1.015606	-7.330183
100	1	0	4.128758	-0.240922	-7.239937
101	1	0	3.822284	-1.961641	-7.020280
102	6	0	2.853782	-1.123541	-8.768885
103	1	0	2.462465	-0.149415	-9.092498
104	1	0	3.683335	-1.370773	-9.439625
105	6	0	1.744968	-2.171539	-8.876004
106	1	0	2.160193	-3.161536	-8.643082

107	1	0	1.360004	-2.221940	-9.899933
108	6	0	0.606522	-1.856685	-7.904965
109	1	0	0.134160	-0.902788	-8.173608
110	1	0	-0.174904	-2.622936	-7.952124
111	6	0	2.730233	0.397335	-4.361629
112	1	0	2.311734	1.319141	-4.795237
113	7	0	-1.799687	2.301783	4.914419
114	7	0	-0.709130	-0.265503	5.660266
115	7	0	-1.951386	-5.123454	1.636829
116	7	0	-2.963502	-4.793668	-1.044311
117	6	0	-2.440853	3.006832	2.201657
118	1	0	-3.194352	2.481745	2.783658
119	6	0	-1.195210	3.262316	2.793209
120	6	0	-0.918561	2.843635	4.181763
121	1	0	0.099373	3.048677	4.548406
122	6	0	-1.437128	1.972173	6.278780
123	1	0	-0.374663	2.198722	6.481561
124	6	0	-1.636338	0.465193	6.502471
125	1	0	-2.685640	0.228644	6.249644
126	6	0	-1.372506	0.100309	7.967986
127	1	0	-1.536288	-0.974914	8.098741
128	1	0	-0.312720	0.289807	8.182950
129	6	0	-2.255184	0.910593	8.917708
130	1	0	-2.032218	0.642559	9.955817
131	1	0	-3.309356	0.656184	8.742581
132	6	0	-2.056707	2.410777	8.694934
133	1	0	-2.715155	2.988169	9.352413
134	1	0	-1.025491	2.681753	8.959541
135	6	0	-2.321103	2.780362	7.235208
136	1	0	-3.370514	2.583799	6.979999
137	1	0	-2.145991	3.847566	7.060753
138	6	0	-1.190432	-1.105340	4.841454
139	1	0	-2.274662	-1.274785	4.750083
140	6	0	-0.337578	-1.937425	3.969295
141	6	0	1.053532	-1.762719	3.947523
142	1	0	1.488833	-0.987585	4.573018
143	6	0	1.853213	-2.575577	3.154005
144	6	0	1.259304	-3.571784	2.366457
145	1	0	1.901407	-4.202767	1.757323
146	6	0	-0.117662	-3.753681	2.380422
147	6	0	-0.915644	-2.928235	3.185330
148	1	0	-1.990565	-3.090328	3.189892
149	6	0	-0.718236	-4.836114	1.576095
150	1	0	-0.020704	-5.394736	0.932513
151	6	0	-2.426679	-6.236511	0.838621
152	1	0	-1.620749	-6.658015	0.210824
153	6	0	-3.533234	-5.740296	-0.104635
154	1	0	-4.313981	-5.270281	0.519787
155	6	0	-4.141615	-6.911127	-0.884668
156	1	0	-4.935301	-6.527601	-1.534946
157	1	0	-3.365057	-7.326655	-1.540051
158	6	0	-4.674267	-7.995400	0.052653
159	1	0	-5.500733	-7.587561	0.650351
160	1	0	-5.084607	-8.826032	-0.531209
161	6	0	-3.571968	-8.489982	0.990550
162	1	0	-2.787416	-8.980804	0.398583
163	1	0	-3.964397	-9.242200	1.682926
164	6	0	-2.964672	-7.325690	1.773537
165	1	0	-3.722536	-6.873146	2.426123

166	1	0	-2.150433	-7.668128	2.421437
167	6	0	-3.446987	-3.622007	-1.067390
168	1	0	-4.262434	-3.310296	-0.396568
169	8	0	-5.422682	0.213702	0.272491
170	1	0	-5.365740	0.519288	-0.656467
171	1	0	-4.498902	0.209738	0.560888

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	5.561838	-1.703164	-0.231233
2	7	0	3.891668	-3.830719	0.660922
3	7	0	-1.702228	-5.115738	-2.236811
4	7	0	-3.016957	-3.092595	-3.802126
5	6	0	4.375951	0.583268	-1.479426
6	1	0	4.536553	-0.304435	-2.085488
7	6	0	4.797461	0.571800	-0.141078
8	6	0	5.408490	-0.637179	0.439864
9	1	0	5.690844	-0.572589	1.503665
10	6	0	6.122065	-2.856997	0.442039
11	1	0	6.141592	-2.711695	1.537668
12	6	0	5.231343	-4.068488	0.145552
13	1	0	5.212245	-4.208212	-0.949474
14	6	0	5.813364	-5.328331	0.797681
15	1	0	5.164433	-6.180122	0.565456
16	1	0	5.791993	-5.197889	1.887667
17	6	0	7.244341	-5.585451	0.321432
18	1	0	7.649839	-6.473090	0.818039
19	1	0	7.233407	-5.800643	-0.755626
20	6	0	8.138185	-4.370917	0.581704
21	1	0	9.147396	-4.548666	0.196022
22	1	0	8.233969	-4.218799	1.665335
23	6	0	7.549140	-3.110685	-0.054795
24	1	0	7.522711	-3.212288	-1.147557
25	1	0	8.164620	-2.232609	0.169575
26	6	0	2.917771	-4.211496	-0.062855
27	1	0	3.078634	-4.637993	-1.065328
28	6	0	1.513805	-4.138782	0.380067
29	6	0	1.193857	-3.818420	1.707800
30	1	0	2.001437	-3.602793	2.403362
31	6	0	-0.129658	-3.794994	2.126835
32	6	0	-1.148386	-4.077280	1.206676
33	1	0	-2.178089	-4.059658	1.554301
34	6	0	-0.842900	-4.391046	-0.111452
35	6	0	0.497289	-4.427417	-0.521308
36	1	0	0.718243	-4.684293	-1.553970
37	6	0	-1.929705	-4.711905	-1.057057
38	1	0	-2.952959	-4.589774	-0.668902
39	6	0	-2.839726	-5.409920	-3.084767
40	1	0	-3.795001	-5.253585	-2.551639
41	6	0	-2.819829	-4.445942	-4.283735
42	1	0	-1.839199	-4.560984	-4.779538
43	6	0	-3.936946	-4.793512	-5.273180
44	1	0	-3.886248	-4.101904	-6.121029
45	1	0	-4.899919	-4.617993	-4.776173

46	6	0	-3.844467	-6.246288	-5.740987
47	1	0	-2.910257	-6.391635	-6.300437
48	1	0	-4.665080	-6.470480	-6.430618
49	6	0	-3.868922	-7.202081	-4.547088
50	1	0	-4.840548	-7.122452	-4.040623
51	1	0	-3.770280	-8.239944	-4.882321
52	6	0	-2.751399	-6.863630	-3.560178
53	1	0	-1.772293	-7.008642	-4.034941
54	1	0	-2.782663	-7.524303	-2.686959
55	6	0	-2.070697	-2.263343	-3.962500
56	1	0	-1.121112	-2.543916	-4.442416
57	7	0	3.508827	3.798725	2.287929
58	7	0	0.963850	4.113239	3.593832
59	7	0	-2.295467	-1.181626	5.142850
60	7	0	-1.596174	-3.755677	4.025588
61	6	0	4.558971	1.677389	0.662992
62	1	0	4.842482	1.677183	1.712805
63	6	0	3.901725	2.800987	0.141681
64	6	0	3.530337	3.921616	1.023177
65	1	0	3.248147	4.861620	0.525290
66	6	0	3.178770	4.976840	3.072061
67	1	0	2.689384	5.745153	2.448348
68	6	0	2.201322	4.583764	4.185247
69	1	0	2.685474	3.793082	4.787747
70	6	0	1.900714	5.787264	5.085675
71	1	0	1.208736	5.474057	5.874907
72	1	0	1.379116	6.544331	4.485814
73	6	0	3.182092	6.373787	5.679261
74	1	0	2.943420	7.244417	6.298960
75	1	0	3.650326	5.631682	6.340117
76	6	0	4.168312	6.756522	4.574237
77	1	0	5.099282	7.139408	5.005243
78	1	0	3.738480	7.568514	3.972221
79	6	0	4.465409	5.559695	3.669597
80	1	0	4.970379	4.769465	4.240801
81	1	0	5.138347	5.842113	2.852273
82	6	0	0.526478	2.981825	3.967895
83	1	0	1.077768	2.359014	4.692075
84	6	0	-0.755698	2.423514	3.501894
85	6	0	-1.560380	3.119222	2.586482
86	1	0	-1.207371	4.071175	2.198263
87	6	0	-2.795430	2.606652	2.211572
88	6	0	-3.219119	1.372939	2.728951
89	1	0	-4.190167	0.990574	2.424774
90	6	0	-2.422803	0.672031	3.623120
91	6	0	-1.186779	1.205995	4.010606
92	1	0	-0.575899	0.638986	4.707357
93	6	0	-2.890416	-0.610936	4.180556
94	1	0	-3.801744	-1.029875	3.725784
95	6	0	-2.842654	-2.426522	5.641023
96	1	0	-3.750364	-2.725435	5.085798
97	6	0	-1.796705	-3.536091	5.444554
98	1	0	-0.867428	-3.200259	5.939037
99	6	0	-2.270950	-4.847024	6.081337
100	1	0	-1.496119	-5.608521	5.940431
101	1	0	-3.157568	-5.190675	5.532731
102	6	0	-2.606658	-4.669963	7.562098
103	1	0	-1.697068	-4.395612	8.113758
104	1	0	-2.958874	-5.617977	7.982378

105	6	0	-3.657093	-3.574243	7.749347
106	1	0	-4.595280	-3.888491	7.271858
107	1	0	-3.875890	-3.426959	8.812284
108	6	0	-3.182916	-2.261410	7.126444
109	1	0	-2.283561	-1.902410	7.643621
110	1	0	-3.942144	-1.478460	7.229462
111	6	0	-0.447227	-3.524770	3.543803
112	1	0	0.384474	-3.150988	4.159681
113	7	0	3.093633	2.823021	-4.013894
114	7	0	0.450859	2.117459	-5.027516
115	7	0	-4.885323	2.673343	-1.687948
116	7	0	-4.888655	3.067405	1.127384
117	6	0	3.529510	2.823041	-1.195050
118	1	0	3.010765	3.676689	-1.622377
119	6	0	3.763735	1.707907	-2.012230
120	6	0	3.372794	1.730751	-3.436151
121	1	0	3.366174	0.761814	-3.955919
122	6	0	2.757108	2.794481	-5.421961
123	1	0	2.883242	1.786060	-5.854796
124	6	0	1.276186	3.176530	-5.574447
125	1	0	1.125825	4.131639	-5.040174
126	6	0	0.906263	3.348622	-7.053099
127	1	0	-0.144887	3.649842	-7.119053
128	1	0	0.985747	2.366578	-7.537090
129	6	0	1.814067	4.353786	-7.760676
130	1	0	1.529350	4.436613	-8.815005
131	1	0	1.679764	5.348989	-7.315154
132	6	0	3.279336	3.937369	-7.627814
133	1	0	3.934953	4.667650	-8.113953
134	1	0	3.430892	2.979450	-8.144004
135	6	0	3.660468	3.792085	-6.155328
136	1	0	3.572315	4.761864	-5.648527
137	1	0	4.702073	3.470961	-6.045398
138	6	0	-0.304205	2.388964	-4.046101
139	1	0	-0.326539	3.378000	-3.567322
140	6	0	-1.287592	1.401144	-3.551152
141	6	0	-1.173559	0.044164	-3.884718
142	1	0	-0.285325	-0.287440	-4.414065
143	6	0	-2.182493	-0.850899	-3.546659
144	6	0	-3.317409	-0.391065	-2.859177
145	1	0	-4.107160	-1.101078	-2.625153
146	6	0	-3.429648	0.951115	-2.509712
147	6	0	-2.401595	1.843483	-2.849841
148	1	0	-2.510951	2.890195	-2.578472
149	6	0	-4.641138	1.436766	-1.819743
150	1	0	-5.324004	0.661552	-1.437870
151	6	0	-6.088318	3.060088	-0.980912
152	1	0	-6.641514	2.179266	-0.607386
153	6	0	-5.675293	3.899681	0.240105
154	1	0	-5.088723	4.756650	-0.137645
155	6	0	-6.912382	4.415223	0.980604
156	1	0	-6.589317	5.016939	1.836992
157	1	0	-7.455725	3.551163	1.384661
158	6	0	-7.821342	5.222664	0.052539
159	1	0	-7.290678	6.123746	-0.284073
160	1	0	-8.708027	5.562323	0.598134
161	6	0	-8.227552	4.394132	-1.167848
162	1	0	-8.839689	3.543525	-0.838241
163	1	0	-8.849276	4.988111	-1.846026

164	6	0	-6.994707	3.874521	-1.909131
165	1	0	-6.411429	4.714090	-2.308977
166	1	0	-7.282128	3.250787	-2.762597
167	6	0	-3.674857	3.383173	1.316229
168	1	0	-3.219940	4.266025	0.841046
169	1	0	1.188671	0.651231	-1.851205
170	8	0	1.212595	-0.319879	-2.007301
171	1	0	1.767182	-0.672285	-1.280464
172	8	0	0.492466	2.189985	-1.038794
173	1	0	-0.331673	1.691856	-0.874242
174	1	0	0.963536	2.095332	-0.184158
175	8	0	-1.019792	-0.123768	-0.483795
176	1	0	-0.285133	-0.408929	-1.087222
177	1	0	-1.838284	-0.361736	-0.943406
178	1	0	2.460185	-0.238433	0.793210
179	8	0	2.270200	-1.140251	0.456588
180	1	0	3.055804	-1.693901	0.603141
181	8	0	1.644305	1.343926	1.397813
182	1	0	0.937174	0.803783	1.837613
183	1	0	2.003445	1.980664	2.037703
184	8	0	-0.002321	-0.669532	2.027436
185	1	0	0.685594	-1.215309	1.598010
186	1	0	-0.626259	-0.514188	1.285729

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-2.683837	2.996077	3.919922
2	7	0	-1.090388	1.151047	5.543500
3	7	0	4.711501	-0.034454	2.912240
4	7	0	5.736173	0.679279	0.260922
5	6	0	-2.507554	3.891957	1.175761
6	1	0	-1.858365	4.397297	1.886918
7	6	0	-3.487274	3.006655	1.650717
8	6	0	-3.610214	2.723289	3.092635
9	1	0	-4.548464	2.245378	3.414632
10	6	0	-2.936187	2.749773	5.334268
11	1	0	-3.629036	1.901632	5.465633
12	6	0	-1.620449	2.405617	6.044886
13	1	0	-0.920311	3.241310	5.859190
14	6	0	-1.845535	2.267866	7.556374
15	1	0	-0.886274	2.037259	8.032197
16	1	0	-2.500877	1.403694	7.727564
17	6	0	-2.468039	3.527794	8.156742
18	1	0	-2.633158	3.389731	9.230434
19	1	0	-1.769769	4.368630	8.047147
20	6	0	-3.780701	3.868712	7.451021
21	1	0	-4.209004	4.791935	7.855237
22	1	0	-4.510298	3.069287	7.638818
23	6	0	-3.563070	4.011850	5.944889
24	1	0	-2.896781	4.860291	5.739038
25	1	0	-4.508147	4.218561	5.429633
26	6	0	0.120423	1.135977	5.162027
27	1	0	0.738532	2.048041	5.158121
28	6	0	0.796647	-0.089081	4.692317

29	6	0	0.120446	-1.315625	4.663868
30	1	0	-0.911891	-1.345542	5.003858
31	6	0	0.744465	-2.456606	4.174808
32	6	0	2.075583	-2.383906	3.748632
33	1	0	2.550414	-3.286282	3.371621
34	6	0	2.755568	-1.171782	3.764553
35	6	0	2.109371	-0.021039	4.238390
36	1	0	2.646037	0.925005	4.233906
37	6	0	4.137713	-1.116803	3.255232
38	1	0	4.657425	-2.085448	3.183631
39	6	0	6.120307	-0.118675	2.541229
40	1	0	6.352001	-1.107131	2.109359
41	6	0	6.455802	0.947963	1.491649
42	1	0	6.171710	1.927979	1.918332
43	6	0	7.959083	0.951269	1.186857
44	1	0	8.162953	1.730989	0.445081
45	1	0	8.215482	-0.008000	0.718216
46	6	0	8.794981	1.160527	2.448904
47	1	0	8.585112	2.154836	2.865993
48	1	0	9.861448	1.138524	2.201177
49	6	0	8.464355	0.095822	3.495052
50	1	0	8.761405	-0.890299	3.112909
51	1	0	9.034892	0.265877	4.414247
52	6	0	6.967674	0.088213	3.805562
53	1	0	6.672489	1.041423	4.264305
54	1	0	6.720777	-0.700084	4.525953
55	6	0	5.032141	1.619216	-0.220001
56	1	0	4.931789	2.589310	0.293056
57	7	0	-5.724101	0.823570	-1.230024
58	7	0	-4.911238	-1.790218	-2.344573
59	7	0	-1.100859	-5.618018	1.174884
60	7	0	0.453070	-4.759125	3.519118
61	6	0	-4.316494	2.352435	0.748699
62	1	0	-5.066486	1.643213	1.089067
63	6	0	-4.158676	2.547204	-0.628741
64	6	0	-4.934847	1.746516	-1.594292
65	1	0	-4.769075	1.985972	-2.656511
66	6	0	-6.459608	0.114015	-2.259647
67	1	0	-6.093916	0.370154	-3.270418
68	6	0	-6.284739	-1.400837	-2.072771
69	1	0	-6.575058	-1.642955	-1.034730
70	6	0	-7.187285	-2.174445	-3.045058
71	1	0	-7.054083	-3.247025	-2.865717
72	1	0	-6.835794	-1.977182	-4.066326
73	6	0	-8.655427	-1.772846	-2.910555
74	1	0	-9.262882	-2.332480	-3.629691
75	1	0	-9.018739	-2.040938	-1.909118
76	6	0	-8.820640	-0.267608	-3.119070
77	1	0	-9.867753	0.027675	-2.993780
78	1	0	-8.538089	-0.012062	-4.149404
79	6	0	-7.938913	0.506674	-2.140842
80	1	0	-8.261127	0.311553	-1.109477
81	1	0	-8.025805	1.587016	-2.300868
82	6	0	-4.328374	-2.524570	-1.491072
83	1	0	-4.809110	-2.809621	-0.542235
84	6	0	-2.981011	-3.092215	-1.715204
85	6	0	-2.267371	-2.812638	-2.889717
86	1	0	-2.715628	-2.145284	-3.621106
87	6	0	-1.011526	-3.369695	-3.106173

88	6	0	-0.461180	-4.226749	-2.138983
89	1	0	0.522949	-4.650935	-2.322297
90	6	0	-1.154328	-4.501596	-0.961555
91	6	0	-2.421389	-3.931518	-0.758257
92	1	0	-2.944660	-4.153309	0.168121
93	6	0	-0.535202	-5.362975	0.069478
94	1	0	0.454234	-5.772452	-0.187900
95	6	0	-0.426777	-6.533369	2.079894
96	1	0	0.616339	-6.714726	1.764557
97	6	0	-0.386511	-5.943031	3.497650
98	1	0	-1.425901	-5.706603	3.789205
99	6	0	0.194907	-6.962642	4.486734
100	1	0	0.192457	-6.517101	5.487605
101	1	0	1.245405	-7.137452	4.219363
102	6	0	-0.577299	-8.281242	4.470214
103	1	0	-1.606844	-8.106566	4.811169
104	1	0	-0.125375	-8.988991	5.173181
105	6	0	-0.608080	-8.868533	3.059085
106	1	0	0.414583	-9.127592	2.752939
107	1	0	-1.190480	-9.795767	3.038931
108	6	0	-1.195630	-7.862141	2.070385
109	1	0	-2.243366	-7.653127	2.323488
110	1	0	-1.189130	-8.262594	1.050566
111	6	0	-0.021213	-3.712645	4.057455
112	1	0	-1.047945	-3.680231	4.455667
113	7	0	-1.003896	5.132871	-1.892866
114	7	0	1.724496	4.622069	-2.831200
115	7	0	2.774311	-1.315129	-5.099011
116	7	0	0.877232	-3.514755	-4.599651
117	6	0	-3.201918	3.441874	-1.087833
118	1	0	-3.072990	3.616300	-2.153757
119	6	0	-2.362654	4.115227	-0.187606
120	6	0	-1.330951	5.056010	-0.666890
121	1	0	-0.857684	5.685213	0.100665
122	6	0	-0.065578	6.180469	-2.271728
123	1	0	0.551414	6.485522	-1.409753
124	6	0	0.878723	5.670324	-3.366730
125	1	0	0.254354	5.301749	-4.201996
126	6	0	1.778610	6.804836	-3.874893
127	1	0	2.425400	6.409346	-4.665672
128	1	0	2.435775	7.113448	-3.051369
129	6	0	0.965609	7.998442	-4.374499
130	1	0	1.637409	8.794919	-4.711480
131	1	0	0.367852	7.695849	-5.245086
132	6	0	0.032559	8.510073	-3.276839
133	1	0	-0.575482	9.343908	-3.643438
134	1	0	0.633840	8.895843	-2.442483
135	6	0	-0.873028	7.387029	-2.772237
136	1	0	-1.535723	7.046438	-3.579139
137	1	0	-1.518225	7.738026	-1.958859
138	6	0	1.828775	3.544327	-3.491718
139	1	0	1.265445	3.374484	-4.423914
140	6	0	2.709115	2.439568	-3.065963
141	6	0	3.461344	2.543779	-1.887606
142	1	0	3.368358	3.447236	-1.289260
143	6	0	4.281648	1.496979	-1.483621
144	6	0	4.341921	0.327747	-2.253213
145	1	0	4.965296	-0.491998	-1.905007
146	6	0	3.572249	0.201662	-3.402663

147	6	0	2.768803	1.271823	-3.817360
148	1	0	2.167388	1.153394	-4.715228
149	6	0	3.544996	-1.088296	-4.117102
150	1	0	4.228235	-1.859369	-3.726720
151	6	0	2.861963	-2.617179	-5.734118
152	1	0	3.457173	-3.324421	-5.128481
153	6	0	1.455581	-3.213249	-5.898223
154	1	0	0.845943	-2.473485	-6.447470
155	6	0	1.511112	-4.520281	-6.701158
156	1	0	0.491695	-4.905664	-6.813640
157	1	0	2.067297	-5.260143	-6.110646
158	6	0	2.178957	-4.327815	-8.062077
159	1	0	1.575285	-3.642614	-8.672699
160	1	0	2.216806	-5.282036	-8.598215
161	6	0	3.582851	-3.747013	-7.893231
162	1	0	4.211879	-4.472185	-7.359142
163	1	0	4.050938	-3.577713	-8.868758
164	6	0	3.531244	-2.439312	-7.104341
165	1	0	2.965297	-1.683475	-7.664705
166	1	0	4.536508	-2.032102	-6.949808
167	6	0	-0.277120	-3.053973	-4.350669
168	1	0	-0.809370	-2.399971	-5.058574
169	8	0	0.567516	-0.604832	1.777580
170	8	0	-0.618301	1.770113	2.255008
171	8	0	-1.810734	0.917402	-0.129341
172	8	0	-0.492274	-1.381144	-0.543263
173	8	0	2.496740	1.055887	1.145718
174	8	0	0.939960	3.278262	0.707281
175	8	0	-0.150344	2.286821	-1.637983
176	8	0	1.455688	0.113124	-1.281544
177	1	0	-0.040520	0.083939	2.109970
178	1	0	0.125703	-1.041792	1.017301
179	1	0	-1.578870	-0.022598	-0.274953
180	1	0	-1.514979	1.149525	0.776747
181	1	0	1.689371	2.666981	0.882656
182	1	0	0.635502	3.024807	-0.194125
183	1	0	1.056367	0.932216	-1.637023
184	1	0	2.005538	0.400711	-0.523372
185	1	0	-1.121713	2.270366	2.923569
186	1	0	-0.461660	-2.281803	-0.890005
187	1	0	3.302537	0.854196	1.656080
188	1	0	-0.523834	3.064946	-2.085534
189	1	0	-0.065721	2.421445	1.737933
190	1	0	0.287042	-0.873505	-0.930652
191	1	0	-0.885644	1.816746	-1.145375
192	1	0	1.802271	0.399462	1.450158

12H2O@CC3 C3 cc3-wwc

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	3.397787	3.317239	-3.137994
2	7	0	0.859426	4.677077	-3.520945
3	7	0	-2.450218	4.591520	2.001494
4	7	0	-1.940556	3.164413	4.495605
5	6	0	4.326052	1.358917	-1.183914

6	1	0	4.394073	2.400060	-0.879940
7	6	0	3.941958	1.048334	-2.497280
8	6	0	3.596125	2.104472	-3.465226
9	1	0	3.519478	1.778895	-4.514020
10	6	0	3.162780	4.271371	-4.215334
11	1	0	2.764948	3.758209	-5.107374
12	6	0	2.133372	5.321662	-3.778981
13	1	0	2.526671	5.811653	-2.868861
14	6	0	1.951753	6.378375	-4.875104
15	1	0	1.218933	7.116635	-4.531922
16	1	0	1.520505	5.887812	-5.757742
17	6	0	3.277377	7.047753	-5.237891
18	1	0	3.121967	7.781507	-6.035721
19	1	0	3.657154	7.599535	-4.367351
20	6	0	4.312146	6.004918	-5.662870
21	1	0	5.272860	6.482038	-5.882991
22	1	0	3.976941	5.520590	-6.590100
23	6	0	4.494110	4.944243	-4.576593
24	1	0	4.908617	5.400346	-3.667746
25	1	0	5.203140	4.172468	-4.897027
26	6	0	0.315953	4.901366	-2.396177
27	1	0	0.791328	5.535335	-1.634011
28	6	0	-0.968744	4.292680	-2.001342
29	6	0	-1.705428	3.513426	-2.901091
30	1	0	-1.326571	3.392707	-3.912900
31	6	0	-2.878863	2.889669	-2.497280
32	6	0	-3.339883	3.067012	-1.183914
33	1	0	-4.275549	2.605349	-0.879940
34	6	0	-2.618029	3.839516	-0.282604
35	6	0	-1.427185	4.452772	-0.700868
36	1	0	-0.866572	5.056006	0.009053
37	6	0	-3.138604	4.043842	1.084353
38	1	0	-4.172307	3.710765	1.259419
39	6	0	-3.123921	4.887883	3.259104
40	1	0	-4.027843	4.266438	3.375813
41	6	0	-2.194967	4.588651	4.442297
42	1	0	-1.263066	5.164503	4.286869
43	6	0	-2.843924	5.026328	5.760823
44	1	0	-2.149348	4.811624	6.580063
45	1	0	-3.732782	4.403582	5.926266
46	6	0	-3.233198	6.504011	5.740907
47	1	0	-2.328597	7.120263	5.647280
48	1	0	-3.709094	6.780199	6.687761
49	6	0	-4.165802	6.797870	4.565385
50	1	0	-5.107576	6.250337	4.706355
51	1	0	-4.419083	7.862750	4.528831
52	6	0	-3.523672	6.370441	3.245594
53	1	0	-2.622095	6.967725	3.054733
54	1	0	-4.203575	6.543394	2.403608
55	6	0	-0.734113	2.775178	4.473430
56	1	0	0.108792	3.482835	4.406383
57	7	0	3.620754	-3.082823	-3.520945
58	7	0	1.173920	-4.601189	-3.137994
59	7	0	-4.480180	-1.594254	-3.520945
60	7	0	-4.571707	1.283950	-3.137994
61	6	0	3.895430	-0.279769	-2.901091
62	1	0	3.601456	-0.547509	-3.912900
63	6	0	4.201942	-1.307383	-2.001342
64	6	0	4.086731	-2.724306	-2.396177

65	1	0	4.398077	-3.452978	-1.634011
66	6	0	3.542008	-4.508385	-3.778981
67	1	0	3.769704	-5.093988	-2.868861
68	6	0	2.117726	-4.874733	-4.215334
69	1	0	1.872230	-4.273620	-5.107374
70	6	0	2.034785	-6.364135	-4.576593
71	1	0	1.011893	-6.592285	-4.897027
72	1	0	2.222528	-6.951160	-3.667746
73	6	0	3.044339	-6.736887	-5.662870
74	1	0	2.977180	-7.807450	-5.882991
75	1	0	2.792501	-6.204427	-6.590100
76	6	0	4.464845	-6.362168	-5.237891
77	1	0	5.177999	-6.594456	-6.035721
78	1	0	4.752813	-6.966956	-4.367351
79	6	0	4.547958	-4.879455	-4.875104
80	1	0	4.338742	-4.260702	-5.757742
81	1	0	5.553720	-4.613944	-4.531922
82	6	0	0.024464	-4.166572	-3.465226
83	1	0	-0.219171	-3.937405	-4.514020
84	6	0	-1.063095	-3.938003	-2.497280
85	6	0	-0.986169	-4.425929	-1.183914
86	1	0	-0.118524	-5.005409	-0.879940
87	6	0	-2.016104	-4.187038	-0.282604
88	6	0	-3.142621	-3.462364	-0.700868
89	1	0	-3.945344	-3.278476	0.009053
90	6	0	-3.233198	-2.985297	-2.001342
91	6	0	-2.190002	-3.233657	-2.901091
92	1	0	-2.274885	-2.845198	-3.912900
93	6	0	-4.402684	-2.177060	-2.396177
94	1	0	-5.189405	-2.082357	-1.634011
95	6	0	-5.675380	-0.813277	-3.778981
96	1	0	-6.296375	-0.717665	-2.868861
97	6	0	-5.280506	0.603362	-4.215334
98	1	0	-4.637178	0.515411	-5.107374
99	6	0	-6.528895	1.419892	-4.576593
100	1	0	-6.215033	2.419817	-4.897027
101	1	0	-7.131145	1.550814	-3.667746
102	6	0	-7.356485	0.731969	-5.662870
103	1	0	-6.769442	0.683837	-6.590100
104	1	0	-8.250040	1.325412	-5.882991
105	6	0	-7.742222	-0.685585	-5.237891
106	1	0	-8.409967	-0.632579	-4.367351
107	1	0	-8.299966	-1.187051	-6.035721
108	6	0	-6.499711	-1.498920	-4.875104
109	1	0	-5.859247	-1.627110	-5.757742
110	1	0	-6.772653	-2.502691	-4.531922
111	6	0	-3.620589	2.062100	-3.465226
112	1	0	-3.300307	2.158510	-4.514020
113	7	0	5.201482	-0.173809	2.001494
114	7	0	3.710740	0.098364	4.495605
115	7	0	-1.770184	-3.262777	4.495605
116	7	0	-2.751264	-4.417711	2.001494
117	6	0	4.569806	-0.990408	-0.700868
118	1	0	4.811916	-1.777530	0.009053
119	6	0	4.634133	0.347522	-0.282604
120	6	0	5.071372	0.696190	1.084353
121	1	0	5.299770	1.757941	1.259419
122	6	0	5.794991	0.261453	3.259104
123	1	0	5.708765	1.354995	3.375813

124	6	0	5.071372	-0.393428	4.442297
125	1	0	5.104124	-1.488404	4.286869
126	6	0	5.774890	-0.050254	5.760823
127	1	0	5.241663	-0.544422	6.580063
128	1	0	5.680005	1.030893	5.926266
129	6	0	7.249238	-0.451974	5.740907
130	1	0	7.726372	-0.177930	6.687761
131	1	0	7.330627	-1.543507	5.647280
132	6	0	7.970029	0.208755	4.565385
133	1	0	9.018883	-0.104337	4.528831
134	1	0	7.966739	1.298122	4.706355
135	6	0	7.278800	-0.133631	3.245594
136	1	0	7.345274	-1.213062	3.054733
137	1	0	7.768533	0.368706	2.403608
138	6	0	2.770431	-0.751828	4.473430
139	1	0	2.961828	-1.835634	4.406383
140	6	0	1.348144	-0.359248	4.514872
141	6	0	0.980297	0.992434	4.515016
142	1	0	1.762323	1.746174	4.476353
143	6	0	-0.362954	1.347151	4.514872
144	6	0	-1.349622	0.352745	4.515016
145	1	0	-2.393393	0.653129	4.476353
146	6	0	-0.985190	-0.987903	4.514872
147	6	0	0.369325	-1.345179	4.515016
148	1	0	0.631070	-2.399303	4.476353
149	6	0	-2.036318	-2.023350	4.473430
150	1	0	-3.070620	-1.647201	4.406383
151	6	0	-2.876405	-4.195223	4.442297
152	1	0	-3.841058	-3.676099	4.286869
153	6	0	-2.671070	-5.149336	3.259104
154	1	0	-1.680922	-5.621433	3.375813
155	6	0	-3.755128	-6.236810	3.245594
156	1	0	-3.564958	-6.912100	2.403608
157	1	0	-4.723179	-5.754663	3.054733
158	6	0	-3.804227	-7.006625	4.565385
159	1	0	-2.859163	-7.548459	4.706355
160	1	0	-4.599800	-7.758413	4.528831
161	6	0	-4.016040	-6.052037	5.740907
162	1	0	-5.002030	-5.576756	5.647280
163	1	0	-4.017278	-6.602269	6.687761
164	6	0	-2.930966	-4.976074	5.760823
165	1	0	-1.947223	-5.434475	5.926266
166	1	0	-3.092315	-4.267202	6.580063
167	6	0	-1.932768	-4.740032	1.084353
168	1	0	-1.127463	-5.468706	1.259419
169	8	0	-0.411828	1.522896	-0.930563
170	8	0	1.806981	3.135006	-0.668514
171	8	0	1.524781	-0.404794	-0.930563
172	8	0	1.811504	-3.132394	-0.668514
173	8	0	-1.112953	-1.118102	-0.930563
174	8	0	-3.618485	-0.002612	-0.668514
175	8	0	-0.494869	2.434756	1.591804
176	8	0	2.109834	2.006788	1.827341
177	8	0	2.355995	-0.788809	1.591804
178	8	0	0.683012	-2.830564	1.827341
179	8	0	-1.861126	-1.645947	1.591804
180	8	0	-2.792846	0.823776	1.827341
181	1	0	-0.917294	0.682246	-0.963465
182	1	0	1.049489	0.453277	-0.963465

183	1	0	-0.132195	-1.135523	-0.963465
184	1	0	2.204284	1.031473	1.851867
185	1	0	-0.208860	-2.424702	1.851867
186	1	0	-1.995424	1.393229	1.851867
187	1	0	-0.558948	1.892806	-0.027595
188	1	0	1.918692	-0.462340	-0.027595
189	1	0	-1.359744	-1.430466	-0.027595
190	1	0	2.232124	2.290826	0.894936
191	1	0	0.867852	-3.078489	0.894936
192	1	0	-3.099976	0.787663	0.894936
193	1	0	1.084362	2.618820	-1.074590
194	1	0	1.725784	-2.248495	-1.074590
195	1	0	-2.810146	-0.370325	-1.074590
196	1	0	0.469441	2.298667	1.824473
197	1	0	1.755984	-1.555881	1.824473
198	1	0	-2.225425	-0.742786	1.824473
199	1	0	2.416674	3.337958	-1.404595
200	1	0	1.682419	-3.761880	-1.404595
201	1	0	-4.099093	0.423922	-1.404595
202	1	0	-0.744610	3.349425	1.811188
203	1	0	3.272992	-1.029861	1.811188
204	1	0	-2.528382	-2.319564	1.811188

(H2O)6 C1 cc3-www1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-1.362064	-1.179423	0.711760
2	8	0	-1.279300	-0.606253	1.507624
3	1	0	-0.320624	-0.595605	1.696004
4	8	0	-1.334535	-1.335691	-1.122550
5	1	0	-1.638036	-0.418325	-1.237186
6	1	0	-0.383298	-1.294745	-1.338667
7	8	0	-1.576489	1.356480	-0.206298
8	1	0	-1.542476	0.731995	0.577080
9	1	0	-2.275012	1.997761	-0.022801
10	1	0	1.658709	-0.797754	0.556835
11	8	0	1.527184	-0.394812	1.443452
12	1	0	2.146957	-0.828020	2.044369
13	8	0	1.411114	-0.750141	-1.234081
14	1	0	1.322027	0.242870	-1.122301
15	1	0	2.076583	-0.898374	-1.918521
16	8	0	1.106411	1.707525	-0.398328
17	1	0	1.356516	1.427172	0.499446
18	1	0	0.125639	1.795576	-0.364580

(H2O)8 D2d cc3-www1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	1.948988	-0.000000	1.292765
2	8	0	0.000000	1.945448	1.316376
3	8	0	-1.948988	-0.000000	1.292765

4	8	0	-0.000000	-1.945448	1.316376
5	8	0	1.945448	-0.000000	-1.316376
6	8	0	0.000000	1.948988	-1.292765
7	8	0	-1.945448	0.000000	-1.316376
8	8	0	-0.000000	-1.948988	-1.292765
9	1	0	1.382242	0.773819	1.497221
10	1	0	1.382242	-0.773819	1.497221
11	1	0	-1.382242	-0.773819	1.497221
12	1	0	-1.382242	0.773819	1.497221
13	1	0	0.773819	1.382242	-1.497221
14	1	0	-0.773819	1.382242	-1.497221
15	1	0	-0.773819	-1.382242	-1.497221
16	1	0	0.773819	-1.382242	-1.497221
17	1	0	0.000000	2.840613	1.679595
18	1	0	-0.000000	-2.840613	1.679595
19	1	0	2.840613	-0.000000	-1.679595
20	1	0	-2.840613	0.000000	-1.679595
21	1	0	0.000000	2.040531	0.312045
22	1	0	-0.000000	-2.040531	0.312045
23	1	0	-2.040531	0.000000	-0.312045
24	1	0	2.040531	-0.000000	-0.312045

(H2O)12 D3 cc3-wwc1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-1.382727	2.328603	1.325055
2	8	0	-2.640839	0.060664	1.434194
3	8	0	-1.325266	-2.361778	1.325055
4	8	0	1.267882	-2.317366	1.434194
5	8	0	2.707993	0.033175	1.325055
6	8	0	1.372956	2.256701	1.434194
7	8	0	-1.372956	2.256701	-1.434194
8	8	0	-2.707993	0.033175	-1.325055
9	8	0	-1.267882	-2.317366	-1.434194
10	8	0	1.325266	-2.361778	-1.325055
11	8	0	2.640839	0.060664	-1.434194
12	8	0	1.382727	2.328603	-1.325055
13	1	0	-0.421465	2.287815	1.517897
14	1	0	-1.770574	-1.508907	1.517897
15	1	0	2.192039	-0.778908	1.517897
16	1	0	-2.192039	-0.778908	-1.517897
17	1	0	1.770574	-1.508907	-1.517897
18	1	0	0.421465	2.287815	-1.517897
19	1	0	-1.428912	2.510536	0.362222
20	1	0	-1.459732	-2.492742	0.362222
21	1	0	2.888644	-0.017794	0.362222
22	1	0	-2.888644	-0.017794	-0.362222
23	1	0	1.459732	-2.492742	-0.362222
24	1	0	1.428912	2.510536	-0.362222
25	1	0	-2.112157	0.920833	1.473540
26	1	0	0.258614	-2.289598	1.473540
27	1	0	1.853543	1.368765	1.473540
28	1	0	-1.853543	1.368765	-1.473540
29	1	0	-0.258614	-2.289598	-1.473540
30	1	0	2.112157	0.920833	-1.473540

31	1	0	-3.405353	0.191391	2.010304
32	1	0	1.536927	-3.044817	2.010304
33	1	0	1.868426	2.853426	2.010304
34	1	0	-1.868426	2.853426	-2.010304
35	1	0	-1.536927	-3.044817	-2.010304
36	1	0	3.405353	0.191391	-2.010304

(CC3-R)2 w-to-w D3 cc3-rdim

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-4.329975	-1.375913	1.699133
2	7	0	-4.601968	1.514348	1.769081
3	7	0	0.973412	4.437825	1.699133
4	7	0	3.612448	3.228247	1.769081
5	6	0	-1.951324	-2.749723	2.416761
6	1	0	-1.991178	-2.234154	1.459104
7	6	0	-3.042011	-2.618945	3.287378
8	6	0	-4.229497	-1.841874	2.873338
9	1	0	-5.025159	-1.723751	3.625507
10	6	0	-5.544880	-0.691432	1.304510
11	1	0	-6.222787	-0.524978	2.160859
12	6	0	-5.153536	0.674579	0.716232
13	1	0	-4.398137	0.462722	-0.057007
14	6	0	-6.343270	1.379257	0.062116
15	1	0	-5.988258	2.307677	-0.397878
16	1	0	-7.061437	1.653937	0.846216
17	6	0	-7.014239	0.495430	-0.989221
18	1	0	-7.872763	1.019252	-1.422567
19	1	0	-6.307970	0.305322	-1.809932
20	6	0	-7.444961	-0.836593	-0.376841
21	1	0	-7.907408	-1.479149	-1.133747
22	1	0	-8.205275	-0.654231	0.395479
23	6	0	-6.243685	-1.549540	0.241212
24	1	0	-5.501967	-1.785208	-0.535421
25	1	0	-6.537967	-2.501420	0.698974
26	6	0	-3.343365	1.673833	1.773620
27	1	0	-2.696869	1.201876	1.019048
28	6	0	-2.644745	2.530845	2.753455
29	6	0	-3.218954	2.847140	3.991042
30	1	0	-4.188144	2.422846	4.241186
31	6	0	-2.550664	3.679511	4.883171
32	6	0	-1.315754	4.236267	4.521023
33	1	0	-0.819989	4.899458	5.225202
34	6	0	-0.747067	3.943931	3.287378
35	6	0	-1.405668	3.064758	2.416761
36	1	0	-0.939246	2.841488	1.459104
37	6	0	0.519638	4.583789	2.873338
38	1	0	1.019768	5.213790	3.625507
39	6	0	2.173642	5.147723	1.304510
40	1	0	2.656749	5.651581	2.160859
41	6	0	3.160971	4.125804	0.716232
42	1	0	2.599798	3.577538	-0.057007
43	6	0	4.366106	4.803804	0.062116
44	1	0	4.992635	4.032145	-0.397878
45	1	0	4.963070	5.288416	0.846216

46	6	0	3.936175	5.826794	-0.989221
47	1	0	3.418401	5.310201	-1.809932
48	1	0	4.819080	6.308387	-1.422567
49	6	0	2.997970	6.865822	-0.376841
50	1	0	3.536057	7.433092	0.395479
51	1	0	2.672724	7.587591	-1.133747
52	6	0	1.779901	6.181960	0.241212
53	1	0	1.204948	5.657447	-0.535421
54	1	0	1.102690	6.912755	0.698974
55	6	0	3.121265	2.058522	1.773620
56	1	0	2.389290	1.734619	1.019048
57	7	0	-2.808729	-4.618292	7.041113
58	7	0	-1.689184	-3.307549	9.349540
59	7	0	-2.019829	3.116651	9.349540
60	7	0	-2.595194	4.741576	7.041113
61	6	0	-3.010838	-3.257610	4.521023
62	1	0	-3.833061	-3.159860	5.225202
63	6	0	-1.911218	-4.048695	4.883171
64	6	0	-1.859362	-4.703085	6.205387
65	1	0	-0.938693	-5.266234	6.423930
66	6	0	-2.652449	-5.293403	8.314066
67	1	0	-1.655455	-5.761433	8.404486
68	6	0	-2.780667	-4.258317	9.443164
69	1	0	-3.760316	-3.761049	9.323942
70	6	0	-2.725239	-4.947275	10.811326
71	1	0	-2.831811	-4.187823	11.593555
72	1	0	-1.728480	-5.391233	10.931781
73	6	0	-3.801395	-6.025601	10.941747
74	1	0	-3.725529	-6.513821	11.919041
75	1	0	-4.794167	-5.557517	10.896207
76	6	0	-3.678656	-7.054070	9.816093
77	1	0	-4.472638	-7.804419	9.892001
78	1	0	-2.724613	-7.588990	9.918395
79	6	0	-3.733762	-6.371108	8.449231
80	1	0	-4.712308	-5.895268	8.303591
81	1	0	-3.610231	-7.098929	7.639897
82	6	0	-1.985295	-2.080206	9.231700
83	1	0	-3.030226	-1.736204	9.180994
84	6	0	-0.961815	-1.016501	9.184709
85	6	0	0.404301	-1.332314	9.182757
86	1	0	0.694375	-2.379867	9.193765
87	6	0	1.361223	-0.324706	9.184709
88	6	0	0.951667	1.016291	9.182757
89	1	0	1.713838	1.791280	9.193765
90	6	0	-0.399408	1.341206	9.184709
91	6	0	-1.355968	0.316022	9.182757
92	1	0	-2.408213	0.588587	9.193765
93	6	0	-0.808864	2.759419	9.231700
94	1	0	0.011516	3.492355	9.180994
95	6	0	-2.297477	4.537287	9.443164
96	1	0	-1.377006	5.137054	9.323942
97	6	0	-3.257997	4.943790	8.314066
98	1	0	-4.161820	4.314383	8.404486
99	6	0	-3.650660	6.419087	8.449231
100	1	0	-4.342737	6.676016	7.639897
101	1	0	-2.749298	7.028613	8.303591
102	6	0	-4.269676	6.712844	9.816093
103	1	0	-5.209952	6.154079	9.918395
104	1	0	-4.522506	7.775628	9.892001

105	6	0	-3.317626	6.304905	10.941747
106	1	0	-2.415867	6.930629	10.896207
107	1	0	-3.778370	6.483313	11.919041
108	6	0	-2.921846	4.833764	10.811326
109	1	0	-3.804705	4.192524	10.931781
110	1	0	-2.210856	4.546331	11.593555
111	6	0	-3.143309	3.961797	6.205387
112	1	0	-4.091346	3.446049	6.423930
113	7	0	0.989520	-4.742595	1.769081
114	7	0	3.356563	-3.061912	1.699133
115	7	0	5.403922	-0.123285	7.041113
116	7	0	3.709013	0.190898	9.349540
117	6	0	-0.856219	-4.211266	3.991042
118	1	0	-0.004174	-4.838462	4.241186
119	6	0	-0.869403	-3.555839	2.753455
120	6	0	0.222100	-3.732356	1.773620
121	1	0	0.307579	-2.936495	1.019048
122	6	0	1.992565	-4.800383	0.716232
123	1	0	1.798340	-4.040260	-0.057007
124	6	0	3.371238	-4.456291	1.304510
125	1	0	3.566038	-5.126603	2.160859
126	6	0	4.463783	-4.632420	0.241212
127	1	0	5.435277	-4.411335	0.698974
128	1	0	4.297019	-3.872239	-0.535421
129	6	0	4.446991	-6.029229	-0.376841
130	1	0	5.234685	-6.108442	-1.133747
131	1	0	4.669218	-6.778861	0.395479
132	6	0	3.078064	-6.322224	-0.989221
133	1	0	3.053683	-7.327639	-1.422567
134	1	0	2.889569	-5.615523	-1.809932
135	6	0	1.977164	-6.183061	0.062116
136	1	0	2.098367	-6.942352	0.846216
137	1	0	0.995622	-6.339822	-0.397878
138	6	0	3.709859	-2.741915	2.873338
139	1	0	4.005391	-3.490040	3.625507
140	6	0	3.789078	-1.324987	3.287378
141	6	0	3.356992	-0.315034	2.416761
142	1	0	2.930423	-0.607333	1.459104
143	6	0	3.514149	1.024994	2.753455
144	6	0	4.075173	1.364126	3.991042
145	1	0	4.192318	2.415616	4.241186
146	6	0	4.461882	0.369184	4.883171
147	6	0	4.326592	-0.978657	4.521023
148	1	0	4.653050	-1.739598	5.225202
149	6	0	5.002672	0.741287	6.205387
150	1	0	5.030039	1.820185	6.423930
151	6	0	5.910446	0.349614	8.314066
152	1	0	5.817275	1.447051	8.404486
153	6	0	5.078144	-0.278970	9.443164
154	1	0	5.137322	-1.376005	9.323942
155	6	0	5.647085	0.113511	10.811326
156	1	0	5.042666	-0.358509	11.593555
157	1	0	5.533185	1.198709	10.931781
158	6	0	7.119021	-0.279304	10.941747
159	1	0	7.210035	-1.373112	10.896207
160	1	0	7.503899	0.030508	11.919041
161	6	0	7.948331	0.341225	9.816093
162	1	0	7.934565	1.434911	9.918395
163	1	0	8.995144	0.028791	9.892001

164	6	0	7.384423	-0.047979	8.449231
165	1	0	7.461606	-1.133344	8.303591
166	1	0	7.952968	0.422912	7.639897
167	6	0	2.794159	-0.679213	9.231700
168	1	0	3.018710	-1.756150	9.180994
169	7	0	-3.356563	-3.061912	-1.699133
170	7	0	-0.989520	-4.742595	-1.769081
171	7	0	4.329975	-1.375913	-1.699133
172	7	0	4.601968	1.514348	-1.769081
173	6	0	-3.356992	-0.315034	-2.416761
174	1	0	-2.930423	-0.607333	-1.459104
175	6	0	-3.789078	-1.324987	-3.287378
176	6	0	-3.709859	-2.741915	-2.873338
177	1	0	-4.005391	-3.490040	-3.625507
178	6	0	-3.371238	-4.456291	-1.304510
179	1	0	-3.566038	-5.126603	-2.160859
180	6	0	-1.992565	-4.800383	-0.716232
181	1	0	-1.798340	-4.040260	0.057007
182	6	0	-1.977164	-6.183061	-0.062116
183	1	0	-0.995622	-6.339822	0.397878
184	1	0	-2.098367	-6.942352	-0.846216
185	6	0	-3.078064	-6.322224	0.989221
186	1	0	-3.053683	-7.327639	1.422567
187	1	0	-2.889569	-5.615523	1.809932
188	6	0	-4.446991	-6.029229	0.376841
189	1	0	-5.234685	-6.108442	1.133747
190	1	0	-4.669218	-6.778861	-0.395479
191	6	0	-4.463783	-4.632420	-0.241212
192	1	0	-4.297019	-3.872239	0.535421
193	1	0	-5.435277	-4.411335	-0.698974
194	6	0	-0.222100	-3.732356	-1.773620
195	1	0	-0.307579	-2.936495	-1.019048
196	6	0	0.869403	-3.555839	-2.753455
197	6	0	0.856219	-4.211266	-3.991042
198	1	0	0.004174	-4.838462	-4.241186
199	6	0	1.911218	-4.048695	-4.883171
200	6	0	3.010838	-3.257610	-4.521023
201	1	0	3.833061	-3.159860	-5.225202
202	6	0	3.042011	-2.618945	-3.287378
203	6	0	1.951324	-2.749723	-2.416761
204	1	0	1.991178	-2.234154	-1.459104
205	6	0	4.229497	-1.841874	-2.873338
206	1	0	5.025159	-1.723751	-3.625507
207	6	0	5.544880	-0.691432	-1.304510
208	1	0	6.222787	-0.524978	-2.160859
209	6	0	5.153536	0.674579	-0.716232
210	1	0	4.398137	0.462722	0.057007
211	6	0	6.343270	1.379257	-0.062116
212	1	0	5.988258	2.307677	0.397878
213	1	0	7.061437	1.653937	-0.846216
214	6	0	7.014239	0.495430	0.989221
215	1	0	6.307970	0.305322	1.809932
216	1	0	7.872763	1.019252	1.422567
217	6	0	7.444961	-0.836593	0.376841
218	1	0	8.205275	-0.654231	-0.395479
219	1	0	7.907408	-1.479149	1.133747
220	6	0	6.243685	-1.549540	-0.241212
221	1	0	5.501967	-1.785208	0.535421
222	1	0	6.537967	-2.501420	-0.698974

223	6	0	3.343365	1.673833	-1.773620
224	1	0	2.696869	1.201876	-1.019048
225	7	0	-5.403922	-0.123285	-7.041113
226	7	0	-3.709013	0.190898	-9.349540
227	7	0	1.689184	-3.307549	-9.349540
228	7	0	2.808729	-4.618292	-7.041113
229	6	0	-4.326592	-0.978657	-4.521023
230	1	0	-4.653050	-1.739598	-5.225202
231	6	0	-4.461882	0.369184	-4.883171
232	6	0	-5.002672	0.741287	-6.205387
233	1	0	-5.030039	1.820185	-6.423930
234	6	0	-5.910446	0.349614	-8.314066
235	1	0	-5.817275	1.447051	-8.404486
236	6	0	-5.078144	-0.278970	-9.443164
237	1	0	-5.137322	-1.376005	-9.323942
238	6	0	-5.647085	0.113511	-10.811326
239	1	0	-5.042666	-0.358509	-11.593555
240	1	0	-5.533185	1.198709	-10.931781
241	6	0	-7.119021	-0.279304	-10.941747
242	1	0	-7.503899	0.030508	-11.919041
243	1	0	-7.210035	-1.373112	-10.896207
244	6	0	-7.948331	0.341225	-9.816093
245	1	0	-8.995144	0.028791	-9.892001
246	1	0	-7.934565	1.434911	-9.918395
247	6	0	-7.384423	-0.047979	-8.449231
248	1	0	-7.461606	-1.133344	-8.303591
249	1	0	-7.952968	0.422912	-7.639897
250	6	0	-2.794159	-0.679213	-9.231700
251	1	0	-3.018710	-1.756150	-9.180994
252	6	0	-1.361223	-0.324706	-9.184709
253	6	0	-0.951667	1.016291	-9.182757
254	1	0	-1.713838	1.791280	-9.193765
255	6	0	0.399408	1.341206	-9.184709
256	6	0	1.355968	0.316022	-9.182757
257	1	0	2.408213	0.588587	-9.193765
258	6	0	0.961815	-1.016501	-9.184709
259	6	0	-0.404301	-1.332314	-9.182757
260	1	0	-0.694375	-2.379867	-9.193765
261	6	0	1.985295	-2.080206	-9.231700
262	1	0	3.030226	-1.736204	-9.180994
263	6	0	2.780667	-4.258317	-9.443164
264	1	0	3.760316	-3.761049	-9.323942
265	6	0	2.652449	-5.293403	-8.314066
266	1	0	1.655455	-5.761433	-8.404486
267	6	0	3.733762	-6.371108	-8.449231
268	1	0	3.610231	-7.098929	-7.639897
269	1	0	4.712308	-5.895268	-8.303591
270	6	0	3.678656	-7.054070	-9.816093
271	1	0	2.724613	-7.588990	-9.918395
272	1	0	4.472638	-7.804419	-9.892001
273	6	0	3.801395	-6.025601	-10.941747
274	1	0	4.794167	-5.557517	-10.896207
275	1	0	3.725529	-6.513821	-11.919041
276	6	0	2.725239	-4.947275	-10.811326
277	1	0	1.728480	-5.391233	-10.931781
278	1	0	2.831811	-4.187823	-11.593555
279	6	0	1.859362	-4.703085	-6.205387
280	1	0	0.938693	-5.266234	-6.423930
281	7	0	-3.612448	3.228247	-1.769081

282	7	0	-0.973412	4.437825	-1.699133
283	7	0	2.595194	4.741576	-7.041113
284	7	0	2.019829	3.116651	-9.349540
285	6	0	-4.075173	1.364126	-3.991042
286	1	0	-4.192318	2.415616	-4.241186
287	6	0	-3.514149	1.024994	-2.753455
288	6	0	-3.121265	2.058522	-1.773620
289	1	0	-2.389290	1.734619	-1.019048
290	6	0	-3.160971	4.125804	-0.716232
291	1	0	-2.599798	3.577538	0.057007
292	6	0	-2.173642	5.147723	-1.304510
293	1	0	-2.656749	5.651581	-2.160859
294	6	0	-1.779901	6.181960	-0.241212
295	1	0	-1.102690	6.912755	-0.698974
296	1	0	-1.204948	5.657447	0.535421
297	6	0	-2.997970	6.865822	0.376841
298	1	0	-2.672724	7.587591	1.133747
299	1	0	-3.536057	7.433092	-0.395479
300	6	0	-3.936175	5.826794	0.989221
301	1	0	-4.819080	6.308387	1.422567
302	1	0	-3.418401	5.310201	1.809932
303	6	0	-4.366106	4.803804	-0.062116
304	1	0	-4.963070	5.288416	-0.846216
305	1	0	-4.992635	4.032145	0.397878
306	6	0	-0.519638	4.583789	-2.873338
307	1	0	-1.019768	5.213790	-3.625507
308	6	0	0.747067	3.943931	-3.287378
309	6	0	1.405668	3.064758	-2.416761
310	1	0	0.939246	2.841488	-1.459104
311	6	0	2.644745	2.530845	-2.753455
312	6	0	3.218954	2.847140	-3.991042
313	1	0	4.188144	2.422846	-4.241186
314	6	0	2.550664	3.679511	-4.883171
315	6	0	1.315754	4.236267	-4.521023
316	1	0	0.819989	4.899458	-5.225202
317	6	0	3.143309	3.961797	-6.205387
318	1	0	4.091346	3.446049	-6.423930
319	6	0	3.257997	4.943790	-8.314066
320	1	0	4.161820	4.314383	-8.404486
321	6	0	2.297477	4.537287	-9.443164
322	1	0	1.377006	5.137054	-9.323942
323	6	0	2.921846	4.833764	-10.811326
324	1	0	2.210856	4.546331	-11.593555
325	1	0	3.804705	4.192524	-10.931781
326	6	0	3.317626	6.304905	-10.941747
327	1	0	2.415867	6.930629	-10.896207
328	1	0	3.778370	6.483313	-11.919041
329	6	0	4.269676	6.712844	-9.816093
330	1	0	5.209952	6.154079	-9.918395
331	1	0	4.522506	7.775628	-9.892001
332	6	0	3.650660	6.419087	-8.449231
333	1	0	2.749298	7.028613	-8.303591
334	1	0	4.342737	6.676016	-7.639897
335	6	0	0.808864	2.759419	-9.231700
336	1	0	-0.011516	3.492355	-9.180994

(CC3-R)2 w-to-a C3 cc3-rdim6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	1.988254	4.360432	2.274098
2	7	0	-0.857197	4.552397	2.008100
3	7	0	-4.093272	3.379994	7.414868
4	7	0	-3.025928	2.148303	9.787308
5	6	0	3.199144	2.762324	4.367453
6	1	0	2.929120	3.784457	4.621135
7	6	0	2.869793	2.276454	3.095232
8	6	0	2.216528	3.127159	2.083738
9	1	0	1.971152	2.622174	1.137499
10	6	0	1.365262	5.095276	1.192068
11	1	0	1.148268	4.437829	0.329117
12	6	0	0.023038	5.658473	1.688085
13	1	0	0.237322	6.275146	2.579446
14	6	0	-0.626811	6.528631	0.609134
15	1	0	-1.577991	6.918282	0.989878
16	1	0	-0.866869	5.885942	-0.249053
17	6	0	0.300723	7.661105	0.167931
18	1	0	-0.180656	8.257238	-0.614353
19	1	0	0.482452	8.335477	1.015901
20	6	0	1.636559	7.102577	-0.327007
21	1	0	2.311713	7.916337	-0.612009
22	1	0	1.462778	6.502484	-1.230821
23	6	0	2.292223	6.229334	0.743602
24	1	0	2.542947	6.834929	1.624251
25	1	0	3.228952	5.794057	0.378324
26	6	0	-1.180477	4.385063	3.224505
27	1	0	-0.823090	5.057741	4.019057
28	6	0	-2.098293	3.309808	3.645286
29	6	0	-2.450755	2.292447	2.748676
30	1	0	-1.991103	2.273581	1.763771
31	6	0	-3.406363	1.347087	3.095232
32	6	0	-3.991815	1.389378	4.367453
33	1	0	-4.741996	0.644464	4.621135
34	6	0	-3.629073	2.377911	5.275385
35	6	0	-2.678593	3.341454	4.907453
36	1	0	-2.426361	4.120498	5.622343
37	6	0	-4.283818	2.429778	6.597266
38	1	0	-4.967479	1.596362	6.822855
39	6	0	-4.820586	3.347785	8.668572
40	1	0	-5.422574	2.425870	8.763573
41	6	0	-3.816463	3.362487	9.831904
42	1	0	-3.184855	4.261293	9.711289
43	6	0	-4.551609	3.434658	11.174663
44	1	0	-3.811759	3.455383	11.982242
45	1	0	-5.132008	2.510991	11.297715
46	6	0	-5.476218	4.650494	11.244307
47	1	0	-4.875564	5.568992	11.195032
48	1	0	-6.002103	4.666669	12.204744
49	6	0	-6.474197	4.640167	10.085040
50	1	0	-7.137177	3.770250	10.187539
51	1	0	-7.111434	5.530196	10.117697
52	6	0	-5.745430	4.567799	8.742817
53	1	0	-5.136327	5.468996	8.594408
54	1	0	-6.456240	4.523593	7.910441
55	6	0	-1.769140	2.265811	9.669233

56	1	0	-1.280243	3.249825	9.596127
57	7	0	4.371090	-1.533844	2.008100
58	7	0	2.782118	-3.902094	2.274098
59	7	0	-3.513893	-3.018553	2.008100
60	7	0	-4.770372	-0.458338	2.274098
61	6	0	3.210695	0.976193	2.748676
62	1	0	2.964530	0.587555	1.763771
63	6	0	3.915524	0.162271	3.645286
64	6	0	4.387814	-1.170208	3.224505
65	1	0	4.791677	-1.816054	4.019057
66	6	0	4.888862	-2.849188	1.688085
67	1	0	5.315775	-3.343100	2.579446
68	6	0	3.730007	-3.729990	1.192068
69	1	0	3.269139	-3.213344	0.329117
70	6	0	4.248650	-5.099790	0.743602
71	1	0	3.403325	-5.693383	0.378324
72	1	0	4.647749	-5.619721	1.624251
73	6	0	5.332733	-4.968590	-0.327007
74	1	0	5.699892	-5.960171	-0.612009
75	1	0	4.899927	-4.518045	-1.230821
76	6	0	6.484350	-4.090986	0.167931
77	1	0	7.241306	-3.972166	-0.614353
78	1	0	6.977509	-4.585554	1.015901
79	6	0	5.967366	-2.721481	0.609134
80	1	0	5.530810	-2.192240	-0.249053
81	1	0	6.780403	-2.092561	0.989878
82	6	0	1.599935	-3.483149	2.083738
83	1	0	1.285293	-3.018155	1.137499
84	6	0	0.536570	-3.623541	3.095232
85	6	0	0.792671	-4.151702	4.367453
86	1	0	1.812876	-4.428921	4.621135
87	6	0	-0.244795	-4.331825	5.275385
88	6	0	-1.554488	-3.990457	4.907453
89	1	0	-2.355275	-4.161539	5.622343
90	6	0	-1.817231	-3.472079	3.645286
91	6	0	-0.759940	-3.268640	2.748676
92	1	0	-0.973427	-2.861136	1.763771
93	6	0	-3.207337	-3.214855	3.224505
94	1	0	-3.968587	-3.241687	4.019057
95	6	0	-4.911900	-2.809285	1.688085
96	1	0	-5.553097	-2.932046	2.579446
97	6	0	-5.095269	-1.365286	1.192068
98	1	0	-4.417407	-1.224485	0.329117
99	6	0	-6.540873	-1.129544	0.743602
100	1	0	-6.632277	-0.100674	0.378324
101	1	0	-7.190696	-1.215208	1.624251
102	6	0	-6.969292	-2.133987	-0.327007
103	1	0	-6.362705	-1.984439	-1.230821
104	1	0	-8.011605	-1.956166	-0.612009
105	6	0	-6.785073	-3.570119	0.167931
106	1	0	-7.459961	-3.749923	1.015901
107	1	0	-7.060650	-4.285072	-0.614353
108	6	0	-5.340555	-3.807150	0.609134
109	1	0	-4.663941	-3.693702	-0.249053
110	1	0	-5.202412	-4.825721	0.989878
111	6	0	-3.816463	0.355990	2.083738
112	1	0	-3.256445	0.395981	1.137499
113	7	0	4.973797	1.854881	7.414868
114	7	0	3.373449	1.546379	9.787308

115	7	0	-0.347521	-3.694682	9.787308
116	7	0	-0.880525	-5.234875	7.414868
117	6	0	4.233081	0.649003	4.907453
118	1	0	4.781636	0.041041	5.622343
119	6	0	3.873868	1.953914	5.275385
120	6	0	4.246158	2.495006	6.597266
121	1	0	3.866230	3.503782	6.822855
122	6	0	5.309560	2.500857	8.668572
123	1	0	4.812152	3.483152	8.763573
124	6	0	4.820231	1.623910	9.831904
125	1	0	5.282815	0.627519	9.711289
126	6	0	5.250306	2.224480	11.174663
127	1	0	4.898329	1.573389	11.982242
128	1	0	4.740586	3.188954	11.297715
129	6	0	6.765555	2.417297	11.244307
130	1	0	7.042505	2.864639	12.204744
131	1	0	7.260671	1.437866	11.195032
132	6	0	7.255601	3.286736	10.085040
133	1	0	8.345007	3.393585	10.117697
134	1	0	6.833721	4.295852	10.187539
135	6	0	6.828545	2.691789	8.742817
136	1	0	7.304453	1.713692	8.594408
137	1	0	7.145666	3.329471	7.910441
138	6	0	2.846820	0.399215	9.669233
139	1	0	3.454552	-0.516190	9.596127
140	6	0	1.384592	0.199345	9.641209
141	6	0	0.510394	1.295327	9.639409
142	1	0	0.933561	2.296564	9.644431
143	6	0	-0.864934	1.099419	9.641209
144	6	0	-1.376983	-0.205649	9.639409
145	1	0	-2.455663	-0.339794	9.644431
146	6	0	-0.519658	-1.298764	9.641209
147	6	0	0.866589	-1.089678	9.639409
148	1	0	1.522102	-1.956770	9.644431
149	6	0	-1.077680	-2.665026	9.669233
150	1	0	-2.174309	-2.733635	9.596127
151	6	0	-1.003768	-4.986397	9.831904
152	1	0	-2.097960	-4.888812	9.711289
153	6	0	-0.488974	-5.848642	8.668572
154	1	0	0.610422	-5.909022	8.763573
155	6	0	-1.083115	-7.259588	8.742817
156	1	0	-0.689426	-7.853064	7.910441
157	1	0	-2.168126	-7.182688	8.594408
158	6	0	-0.781404	-7.926903	10.085040
159	1	0	0.303456	-8.066102	10.187539
160	1	0	-1.233573	-8.923781	10.117697
161	6	0	-1.289337	-7.067791	11.244307
162	1	0	-2.385107	-7.006858	11.195032
163	1	0	-1.040402	-7.531308	12.204744
164	6	0	-0.698697	-5.659138	11.174663
165	1	0	0.391422	-5.699945	11.297715
166	1	0	-1.086570	-5.028772	11.982242
167	6	0	0.037660	-4.924784	6.597266
168	1	0	1.101249	-5.100144	6.822855
169	7	0	2.472109	4.160172	-8.450667
170	7	0	-0.347521	4.648703	-8.719230
171	7	0	-3.643716	3.729579	-3.305179
172	7	0	-2.720247	2.528822	-0.823867
173	6	0	3.487294	2.420673	-6.392549

174	1	0	3.289586	3.456719	-6.129597
175	6	0	3.172320	1.987278	-7.688533
176	6	0	2.603641	2.920398	-8.680695
177	1	0	2.315002	2.473073	-9.644648
178	6	0	1.927506	4.988688	-9.508114
179	1	0	1.653380	4.386937	-10.393552
180	6	0	0.645840	5.666967	-8.998313
181	1	0	0.913200	6.231748	-8.086783
182	6	0	0.094054	6.633362	-10.051703
183	1	0	-0.809991	7.109171	-9.656435
184	1	0	-0.211518	6.047010	-10.928012
185	6	0	1.134744	7.678680	-10.454638
186	1	0	0.721456	8.342578	-11.221218
187	1	0	1.376149	8.306886	-9.586344
188	6	0	2.412738	7.005743	-10.958628
189	1	0	3.168358	7.756428	-11.213087
190	1	0	2.189694	6.453373	-11.881653
191	6	0	2.967133	6.040265	-9.910505
192	1	0	3.264104	6.591272	-9.008658
193	1	0	3.862622	5.528999	-10.280216
194	6	0	-0.775530	4.552857	-7.529700
195	1	0	-0.410628	5.209888	-6.724849
196	6	0	-1.812172	3.578213	-7.137039
197	6	0	-2.296436	2.634122	-8.053230
198	1	0	-1.874046	2.617991	-9.054678
199	6	0	-3.307193	1.753671	-7.688533
200	6	0	-3.840011	1.809749	-6.392549
201	1	0	-4.638399	1.120506	-6.129597
202	6	0	-3.365082	2.739259	-5.476084
203	6	0	-2.343678	3.622124	-5.854659
204	1	0	-1.993057	4.350375	-5.127989
205	6	0	-3.976497	2.831072	-4.134728
206	1	0	-4.763162	2.092644	-3.913275
207	6	0	-4.370639	3.812786	-2.052899
208	1	0	-5.039089	2.944477	-1.910267
209	6	0	-3.369378	3.827752	-0.886468
210	1	0	-2.639550	4.630273	-1.092945
211	6	0	-4.067342	4.116026	0.445672
212	1	0	-3.300073	4.192679	1.221128
213	1	0	-4.705850	3.258133	0.699377
214	6	0	-4.899712	5.396552	0.391839
215	1	0	-4.233071	6.256595	0.236116
216	1	0	-5.399738	5.552866	1.353381
217	6	0	-5.917119	5.341248	-0.746614
218	1	0	-6.631205	4.528362	-0.556286
219	1	0	-6.496652	6.269315	-0.795930
220	6	0	-5.207870	5.098251	-2.077413
221	1	0	-4.537245	5.937618	-2.303617
222	1	0	-5.924061	5.032236	-2.904021
223	6	0	-1.462305	2.482107	-0.979556
224	1	0	-0.857974	3.390270	-1.128708
225	7	0	4.199655	-2.023389	-8.719230
226	7	0	2.366760	-4.220995	-8.450667
227	7	0	-3.852134	-2.625314	-8.719230
228	7	0	-4.838869	0.060823	-8.450667
229	6	0	3.429435	0.671711	-8.053230
230	1	0	3.204270	0.313976	-9.054678
231	6	0	4.004909	-0.219719	-7.137039
232	6	0	4.330655	-1.604800	-7.529700

233	1	0	4.717209	-2.249330	-6.724849
234	6	0	4.584817	-3.392797	-8.998313
235	1	0	4.940252	-3.906728	-8.086783
236	6	0	3.356578	-4.163613	-9.508114
237	1	0	2.972509	-3.625338	-10.393552
238	6	0	3.747456	-5.589745	-9.910505
239	1	0	2.856943	-6.109628	-10.280216
240	1	0	4.076157	-6.122433	-9.008658
241	6	0	4.860782	-5.592364	-10.958628
242	1	0	5.133085	-6.622092	-11.213087
243	1	0	4.493938	-5.123017	-11.881653
244	6	0	6.082560	-4.822057	-10.454638
245	1	0	6.864156	-4.796088	-11.221218
246	1	0	6.505900	-5.345223	-9.586344
247	6	0	5.697633	-3.398134	-10.051703
248	1	0	5.342623	-2.840325	-10.928012
249	1	0	6.561718	-2.853113	-9.656435
250	6	0	1.227318	-3.715018	-8.680695
251	1	0	0.984243	-3.241387	-9.644648
252	6	0	0.134873	-3.740949	-7.688533
253	6	0	0.352717	-4.230422	-6.392549
254	1	0	1.348813	-4.577225	-6.129597
255	6	0	-0.689727	-4.283876	-5.476084
256	6	0	-1.965012	-3.840747	-5.854659
257	1	0	-2.771007	-3.901225	-5.127989
258	6	0	-2.192737	-3.358493	-7.137039
259	6	0	-1.132999	-3.305833	-8.053230
260	1	0	-1.330224	-2.931967	-9.054678
261	6	0	-3.555125	-2.948057	-7.529700
262	1	0	-4.306581	-2.960558	-6.724849
263	6	0	-5.230657	-2.274170	-8.998313
264	1	0	-5.853452	-2.325020	-8.086783
265	6	0	-5.284084	-0.825075	-9.508114
266	1	0	-4.625889	-0.761599	-10.393552
267	6	0	-6.714589	-0.450520	-9.910505
268	1	0	-6.719565	0.580629	-10.280216
269	1	0	-7.340261	-0.468839	-9.008658
270	6	0	-7.273520	-1.413379	-10.958628
271	1	0	-6.683632	-1.330356	-11.881653
272	1	0	-8.301443	-1.134335	-11.213087
273	6	0	-7.217304	-2.856623	-10.454638
274	1	0	-7.882049	-2.961663	-9.586344
275	1	0	-7.585612	-3.546490	-11.221218
276	6	0	-5.791687	-3.235228	-10.051703
277	1	0	-5.131105	-3.206685	-10.928012
278	1	0	-5.751727	-4.256058	-9.656435
279	6	0	-3.830959	0.794620	-8.680695
280	1	0	-3.299245	0.768314	-9.644648
281	7	0	5.051768	1.290761	-3.305179
282	7	0	3.550148	1.091392	-0.823867
283	7	0	-0.829901	-3.620214	-0.823867
284	7	0	-1.408052	-5.020340	-3.305179
285	6	0	4.308690	0.218623	-5.854659
286	1	0	4.764064	-0.449149	-5.127989
287	6	0	4.054809	1.544617	-5.476084
288	6	0	4.440029	2.028211	-4.134728
289	1	0	4.193864	3.078697	-3.913275
290	6	0	5.487289	1.878691	-2.052899
291	1	0	5.069536	2.891741	-1.910267

292	6	0	4.999619	1.004091	-0.886468
293	1	0	5.329709	-0.029219	-1.092945
294	6	0	5.598254	1.464409	0.445672
295	1	0	5.281003	0.761608	1.221128
296	1	0	5.174551	2.446319	0.699377
297	6	0	7.123407	1.544999	0.391839
298	1	0	7.508792	1.899877	1.353381
299	1	0	7.534906	0.537650	0.236116
300	6	0	7.584216	2.453751	-0.746614
301	1	0	8.677712	2.491608	-0.795930
302	1	0	7.237279	3.478611	-0.556286
303	6	0	7.019150	1.961022	-2.077413
304	1	0	7.410751	0.960560	-2.303617
305	1	0	7.320075	2.614269	-2.904021
306	6	0	2.880720	0.025340	-0.979556
307	1	0	3.365047	-0.952108	-1.128708
308	6	0	1.401569	0.017135	-0.960037
309	6	0	0.675106	1.217147	-0.965690
310	1	0	1.222690	2.156126	-1.001880
311	6	0	-0.715624	1.205227	-0.960037
312	6	0	-1.391633	-0.023915	-0.965690
313	1	0	-2.478605	-0.019182	-1.001880
314	6	0	-0.685945	-1.222362	-0.960037
315	6	0	0.716527	-1.193232	-0.965690
316	1	0	1.255915	-2.136944	-1.001880
317	6	0	-1.418415	-2.507447	-0.979556
318	1	0	-2.507073	-2.438162	-1.128708
319	6	0	-1.630241	-4.831843	-0.886468
320	1	0	-2.690159	-4.601054	-1.092945
321	6	0	-1.116650	-5.691477	-2.052899
322	1	0	-0.030447	-5.836218	-1.910267
323	6	0	-1.811280	-7.059273	-2.077413
324	1	0	-1.396014	-7.646505	-2.904021
325	1	0	-2.873506	-6.898178	-2.303617
326	6	0	-1.667097	-7.794999	-0.746614
327	1	0	-0.606074	-8.006973	-0.556286
328	1	0	-2.181060	-8.760923	-0.795930
329	6	0	-2.223695	-6.941551	0.391839
330	1	0	-3.301835	-6.794245	0.236116
331	1	0	-2.109054	-7.452743	1.353381
332	6	0	-1.530912	-5.580434	0.445672
333	1	0	-0.468701	-5.704452	0.699377
334	1	0	-1.980930	-4.954287	1.221128
335	6	0	-0.463532	-4.859283	-4.134728
336	1	0	0.569298	-5.171341	-3.913275

(CC3-R)2 a-to-a D3 cc3-rdim9

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-3.248500	-3.589567	8.873944
2	7	0	-0.572252	-4.633516	9.129856
3	7	0	2.952895	-4.477559	3.760726
4	7	0	2.258128	-2.942850	1.419873
5	6	0	-3.967932	-1.694562	6.833158
6	1	0	-3.975148	-2.750008	6.573303

7	6	0	-3.546750	-1.324628	8.118266
8	6	0	-3.146904	-2.347199	9.105202
9	1	0	-2.771151	-1.961917	10.065925
10	6	0	-2.866561	-4.507876	9.928666
11	1	0	-2.469955	-3.970981	10.809445
12	6	0	-1.750679	-5.429423	9.411721
13	1	0	-2.129746	-5.928569	8.501510
14	6	0	-1.397904	-6.488118	10.462523
15	1	0	-0.611316	-7.136059	10.060745
16	1	0	-0.973505	-5.975795	11.335812
17	6	0	-2.624401	-7.302360	10.875295
18	1	0	-2.346547	-8.036456	11.638955
19	1	0	-2.995122	-7.868365	10.009831
20	6	0	-3.735421	-6.385351	11.389317
21	1	0	-4.624913	-6.967633	11.652048
22	1	0	-3.397027	-5.888922	12.309030
23	6	0	-4.092701	-5.328851	10.343458
24	1	0	-4.502526	-5.809806	9.445711
25	1	0	-4.863592	-4.647127	10.718895
26	6	0	-0.108660	-4.659478	7.950157
27	1	0	-0.580820	-5.252249	7.151215
28	6	0	1.109629	-3.920583	7.563665
29	6	0	1.753153	-3.072121	8.475660
30	1	0	1.324126	-2.955564	9.467575
31	6	0	2.920537	-2.409262	8.118266
32	6	0	3.451499	-2.589049	6.833158
33	1	0	4.369151	-2.067575	6.573303
34	6	0	2.821944	-3.427445	5.921759
35	6	0	1.644272	-4.091584	6.292912
36	1	0	1.169052	-4.748703	5.569099
37	6	0	3.417692	-3.635978	4.587155
38	1	0	4.306081	-3.026016	4.360587
39	6	0	3.640042	-4.632527	2.493674
40	1	0	4.481347	-3.922141	2.399434
41	6	0	2.657291	-4.334770	1.350338
42	1	0	1.792065	-5.011092	1.474011
43	6	0	3.317431	-4.597097	-0.007922
44	1	0	2.589949	-4.389336	-0.800120
45	1	0	4.138959	-3.879811	-0.133683
46	6	0	3.848136	-6.027397	-0.109193
47	1	0	3.007969	-6.733211	-0.056544
48	1	0	4.330027	-6.179838	-1.080697
49	6	0	4.825858	-6.324225	1.028981
50	1	0	5.710116	-5.681196	0.922082
51	1	0	5.178165	-7.359669	0.974094
52	6	0	4.171062	-6.066392	2.386341
53	1	0	3.329655	-6.755371	2.536561
54	1	0	4.877135	-6.243666	3.204881
55	6	0	1.022486	-2.686762	1.541886
56	1	0	0.265585	-3.483959	1.606673
57	7	0	-3.726617	2.812343	9.129856
58	7	0	-1.484407	4.608067	8.873944
59	7	0	4.298868	1.821173	9.129856
60	7	0	4.732907	-1.018500	8.873944
61	6	0	-3.537111	0.017785	8.475660
62	1	0	-3.221656	0.331055	9.467575
63	6	0	-3.950139	0.999324	7.563665
64	6	0	-3.980896	2.423842	7.950157
65	1	0	-4.258171	3.129129	7.151215

66	6	0	-3.826679	4.230844	9.411721
67	1	0	-4.069419	4.808699	8.501510
68	6	0	-2.470654	4.736453	9.928666
69	1	0	-2.203993	4.124535	10.809445
70	6	0	-2.568569	6.208809	10.343458
71	1	0	-1.592734	6.535558	10.718895
72	1	0	-2.780177	6.804205	9.445711
73	6	0	-3.662166	6.427645	11.389317
74	1	0	-3.721691	7.489109	11.652048
75	1	0	-3.401442	5.886373	12.309030
76	6	0	-5.011829	5.923977	10.875295
77	1	0	-5.786501	6.050398	11.638955
78	1	0	-5.316643	6.528035	10.009831
79	6	0	-4.919923	4.454680	10.462523
80	1	0	-4.688438	3.830978	11.335812
81	1	0	-5.874350	4.097444	10.060745
82	6	0	-0.459282	3.898898	9.105202
83	1	0	-0.313495	3.380846	10.065925
84	6	0	0.626214	3.733890	8.118266
85	6	0	0.516433	4.283611	6.833158
86	1	0	-0.394003	4.817583	6.573303
87	6	0	1.557282	4.157597	5.921759
88	6	0	2.721280	3.469773	6.292912
89	1	0	3.527972	3.386780	5.569099
90	6	0	2.840510	2.921259	7.563665
91	6	0	1.783958	3.054336	8.475660
92	1	0	1.897530	2.624509	9.467575
93	6	0	4.089556	2.235636	7.950157
94	1	0	4.838991	2.123119	7.151215
95	6	0	5.577358	1.198579	9.411721
96	1	0	6.199165	1.119871	8.501510
97	6	0	5.337216	-0.228577	9.928666
98	1	0	4.673948	-0.153553	10.809445
99	6	0	6.661271	-0.879958	10.343458
100	1	0	6.456326	-1.888431	10.718895
101	1	0	7.282702	-0.994399	9.445711
102	6	0	7.397587	-0.042294	11.389317
103	1	0	6.798469	0.002549	12.309030
104	1	0	8.346604	-0.521476	11.652048
105	6	0	7.636229	1.378382	10.875295
106	1	0	8.311765	1.340330	10.009831
107	1	0	8.133049	1.986058	11.638955
108	6	0	6.317827	2.033439	10.462523
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112	1	0	3.084646	-1.418928	10.065925
113	7	0	-5.354128	-0.318502	3.760726
114	7	0	-3.677647	-0.484171	1.419873
115	7	0	1.419519	3.427022	1.419873
116	7	0	2.401233	4.796062	3.760726
117	6	0	-4.365552	0.621811	6.292912
118	1	0	-4.697023	1.361923	5.569099
119	6	0	-4.379226	-0.730153	5.921759
120	6	0	-4.857695	-1.141819	4.587155
121	1	0	-4.773647	-2.216167	4.360587
122	6	0	-5.831907	-0.836105	2.493674
123	1	0	-5.637347	-1.919889	2.399434
124	6	0	-5.082666	-0.133897	1.350338

125	1	0	-5.235766	0.953572	1.474011
126	6	0	-5.639918	-0.574431	-0.007922
127	1	0	-5.096251	-0.048293	-0.800120
128	1	0	-5.429494	-1.644538	-0.133683
129	6	0	-7.143947	-0.318885	-0.109193
130	1	0	-7.516910	-0.659995	-1.080697
131	1	0	-7.335117	0.761628	-0.056544
132	6	0	-7.889869	-1.017203	1.028981
133	1	0	-8.962743	-0.804588	0.974094
134	1	0	-7.775118	-2.104507	0.922082
135	6	0	-7.339180	-0.579050	2.386341
136	1	0	-7.515151	0.494119	2.536561
137	1	0	-7.845741	-1.101890	3.204881
138	6	0	-2.838047	0.457882	1.541886
139	1	0	-3.149989	1.511977	1.606673
140	6	0	-1.381821	0.218156	1.580710
141	6	0	-0.869905	-1.087097	1.582669
142	1	0	-1.569658	-1.918857	1.574423
143	6	0	0.501982	-1.305770	1.580710
144	6	0	1.376407	-0.209812	1.582669
145	1	0	2.446608	-0.399935	1.574423
146	6	0	0.879839	1.087614	1.580710
147	6	0	-0.506501	1.296909	1.582669
148	1	0	-0.876950	2.318792	1.574423
149	6	0	1.815561	2.228880	1.541886
150	1	0	2.884405	1.971983	1.606673
151	6	0	2.425375	4.468667	1.350338
152	1	0	3.443701	4.057520	1.474011
153	6	0	2.191865	5.468632	2.493674
154	1	0	1.156001	5.842031	2.399434
155	6	0	3.168118	6.645441	2.386341
156	1	0	2.968606	7.345556	3.204881
157	1	0	4.185495	6.261252	2.536561
158	6	0	3.064011	7.341429	1.028981
159	1	0	2.065002	7.785703	0.922082
160	1	0	3.784578	8.164257	0.974094
161	6	0	3.295811	6.346282	-0.109193
162	1	0	4.327147	5.971584	-0.056544
163	1	0	3.186883	6.839832	-1.080697
164	6	0	2.322487	5.171528	-0.007922
165	1	0	1.290535	5.524349	-0.133683
166	1	0	2.506302	4.437630	-0.800120
167	6	0	1.440003	4.777797	4.587155
168	1	0	0.467566	5.242183	4.360587
169	7	0	-4.732907	-1.018500	-8.873944
170	7	0	-4.298868	1.821173	-9.129856
171	7	0	-2.401233	4.796062	-3.760726
172	7	0	-1.419519	3.427022	-1.419873
173	6	0	-3.451499	-2.589049	-6.833158
174	1	0	-4.369151	-2.067575	-6.573303
175	6	0	-2.920537	-2.409262	-8.118266
176	6	0	-3.606186	-1.551699	-9.105202
177	1	0	-3.084646	-1.418928	-10.065925
178	6	0	-5.337216	-0.228577	-9.928666
179	1	0	-4.673948	-0.153553	-10.809445
180	6	0	-5.577358	1.198579	-9.411721
181	1	0	-6.199165	1.119871	-8.501510
182	6	0	-6.317827	2.033439	-10.462523
183	1	0	-6.485666	3.038614	-10.060745

184	1	0	-5.661943	2.144818	-11.335812
185	6	0	-7.636229	1.378382	-10.875295
186	1	0	-8.133049	1.986058	-11.638955
187	1	0	-8.311765	1.340330	-10.009831
188	6	0	-7.397587	-0.042294	-11.389317
189	1	0	-8.346604	-0.521476	-11.652048
190	1	0	-6.798469	0.002549	-12.309030
191	6	0	-6.661271	-0.879958	-10.343458
192	1	0	-7.282702	-0.994399	-9.445711
193	1	0	-6.456326	-1.888431	-10.718895
194	6	0	-4.089556	2.235636	-7.950157
195	1	0	-4.838991	2.123119	-7.151215
196	6	0	-2.840510	2.921259	-7.563665
197	6	0	-1.783958	3.054336	-8.475660
198	1	0	-1.897530	2.624509	-9.467575
199	6	0	-0.626214	3.733890	-8.118266
200	6	0	-0.516433	4.283611	-6.833158
201	1	0	0.394003	4.817583	-6.573303
202	6	0	-1.557282	4.157597	-5.921759
203	6	0	-2.721280	3.469773	-6.292912
204	1	0	-3.527972	3.386780	-5.569099
205	6	0	-1.440003	4.777797	-4.587155
206	1	0	-0.467566	5.242183	-4.360587
207	6	0	-2.191865	5.468632	-2.493674
208	1	0	-1.156001	5.842031	-2.399434
209	6	0	-2.425375	4.468667	-1.350338
210	1	0	-3.443701	4.057520	-1.474011
211	6	0	-2.322487	5.171528	0.007922
212	1	0	-2.506302	4.437630	0.800120
213	1	0	-1.290535	5.524349	0.133683
214	6	0	-3.295811	6.346282	0.109193
215	1	0	-4.327147	5.971584	0.056544
216	1	0	-3.186883	6.839832	1.080697
217	6	0	-3.064011	7.341429	-1.028981
218	1	0	-2.065002	7.785703	-0.922082
219	1	0	-3.784578	8.164257	-0.974094
220	6	0	-3.168118	6.645441	-2.386341
221	1	0	-4.185495	6.261252	-2.536561
222	1	0	-2.968606	7.345556	-3.204881
223	6	0	-1.815561	2.228880	-1.541886
224	1	0	-2.884405	1.971983	-1.606673
225	7	0	0.572252	-4.633516	-9.129856
226	7	0	3.248500	-3.589567	-8.873944
227	7	0	3.726617	2.812343	-9.129856
228	7	0	1.484407	4.608067	-8.873944
229	6	0	-1.753153	-3.072121	-8.475660
230	1	0	-1.324126	-2.955564	-9.467575
231	6	0	-1.109629	-3.920583	-7.563665
232	6	0	0.108660	-4.659478	-7.950157
233	1	0	0.580820	-5.252249	-7.151215
234	6	0	1.750679	-5.429423	-9.411721
235	1	0	2.129746	-5.928569	-8.501510
236	6	0	2.866561	-4.507876	-9.928666
237	1	0	2.469955	-3.970981	-10.809445
238	6	0	4.092701	-5.328851	-10.343458
239	1	0	4.863592	-4.647127	-10.718895
240	1	0	4.502526	-5.809806	-9.445711
241	6	0	3.735421	-6.385351	-11.389317
242	1	0	4.624913	-6.967633	-11.652048

243	1	0	3.397027	-5.888922	-12.309030
244	6	0	2.624401	-7.302360	-10.875295
245	1	0	2.346547	-8.036456	-11.638955
246	1	0	2.995122	-7.868365	-10.009831
247	6	0	1.397904	-6.488118	-10.462523
248	1	0	0.973505	-5.975795	-11.335812
249	1	0	0.611316	-7.136059	-10.060745
250	6	0	3.146904	-2.347199	-9.105202
251	1	0	2.771151	-1.961917	-10.065925
252	6	0	3.546750	-1.324628	-8.118266
253	6	0	3.967932	-1.694562	-6.833158
254	1	0	3.975148	-2.750008	-6.573303
255	6	0	4.379226	-0.730153	-5.921759
256	6	0	4.365552	0.621811	-6.292912
257	1	0	4.697023	1.361923	-5.569099
258	6	0	3.950139	0.999324	-7.563665
259	6	0	3.537111	0.017785	-8.475660
260	1	0	3.221656	0.331055	-9.467575
261	6	0	3.980896	2.423842	-7.950157
262	1	0	4.258171	3.129129	-7.151215
263	6	0	3.826679	4.230844	-9.411721
264	1	0	4.069419	4.808699	-8.501510
265	6	0	2.470654	4.736453	-9.928666
266	1	0	2.203993	4.124535	-10.809445
267	6	0	2.568569	6.208809	-10.343458
268	1	0	1.592734	6.535558	-10.718895
269	1	0	2.780177	6.804205	-9.445711
270	6	0	3.662166	6.427645	-11.389317
271	1	0	3.401442	5.886373	-12.309030
272	1	0	3.721691	7.489109	-11.652048
273	6	0	5.011829	5.923977	-10.875295
274	1	0	5.316643	6.528035	-10.009831
275	1	0	5.786501	6.050398	-11.638955
276	6	0	4.919923	4.454680	-10.462523
277	1	0	4.688438	3.830978	-11.335812
278	1	0	5.874350	4.097444	-10.060745
279	6	0	0.459282	3.898898	-9.105202
280	1	0	0.313495	3.380846	-10.065925
281	7	0	-2.952895	-4.477559	-3.760726
282	7	0	-2.258128	-2.942850	-1.419873
283	7	0	3.677647	-0.484171	-1.419873
284	7	0	5.354128	-0.318502	-3.760726
285	6	0	-1.644272	-4.091584	-6.292912
286	1	0	-1.169052	-4.748703	-5.569099
287	6	0	-2.821944	-3.427445	-5.921759
288	6	0	-3.417692	-3.635978	-4.587155
289	1	0	-4.306081	-3.026016	-4.360587
290	6	0	-3.640042	-4.632527	-2.493674
291	1	0	-4.481347	-3.922141	-2.399434
292	6	0	-2.657291	-4.334770	-1.350338
293	1	0	-1.792065	-5.011092	-1.474011
294	6	0	-3.317431	-4.597097	0.007922
295	1	0	-2.589949	-4.389336	0.800120
296	1	0	-4.138959	-3.879811	0.133683
297	6	0	-3.848136	-6.027397	0.109193
298	1	0	-4.330027	-6.179838	1.080697
299	1	0	-3.007969	-6.733211	0.056544
300	6	0	-4.825858	-6.324225	-1.028981
301	1	0	-5.178165	-7.359669	-0.974094

302	1	0	-5.710116	-5.681196	-0.922082
303	6	0	-4.171062	-6.066392	-2.386341
304	1	0	-3.329655	-6.755371	-2.536561
305	1	0	-4.877135	-6.243666	-3.204881
306	6	0	-1.022486	-2.686762	-1.541886
307	1	0	-0.265585	-3.483959	-1.606673
308	6	0	-0.501982	-1.305770	-1.580710
309	6	0	-1.376407	-0.209812	-1.582669
310	1	0	-2.446608	-0.399935	-1.574423
311	6	0	-0.879839	1.087614	-1.580710
312	6	0	0.506501	1.296909	-1.582669
313	1	0	0.876950	2.318792	-1.574423
314	6	0	1.381821	0.218156	-1.580710
315	6	0	0.869905	-1.087097	-1.582669
316	1	0	1.569658	-1.918857	-1.574423
317	6	0	2.838047	0.457882	-1.541886
318	1	0	3.149989	1.511977	-1.606673
319	6	0	5.082666	-0.133897	-1.350338
320	1	0	5.235766	0.953572	-1.474011
321	6	0	5.831907	-0.836105	-2.493674
322	1	0	5.637347	-1.919889	-2.399434
323	6	0	7.339180	-0.579050	-2.386341
324	1	0	7.845741	-1.101890	-3.204881
325	1	0	7.515151	0.494119	-2.536561
326	6	0	7.889869	-1.017203	-1.028981
327	1	0	7.775118	-2.104507	-0.922082
328	1	0	8.962743	-0.804588	-0.974094
329	6	0	7.143947	-0.318885	0.109193
330	1	0	7.335117	0.761628	0.056544
331	1	0	7.516910	-0.659995	1.080697
332	6	0	5.639918	-0.574431	0.007922
333	1	0	5.429494	-1.644538	0.133683
334	1	0	5.096251	-0.048293	0.800120
335	6	0	4.857695	-1.141819	-4.587155
336	1	0	4.773647	-2.216167	-4.360587

CC3-R/S w-to-w S6 cc3-rdim4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-4.507979	1.559482	1.927841
2	7	0	-2.738332	3.819290	1.642514
3	7	0	0.373631	5.382928	7.037456
4	7	0	0.534724	3.674883	9.353758
5	6	0	-4.294115	-0.473874	3.975447
6	1	0	-4.834792	0.434587	4.228753
7	6	0	-3.686264	-0.562807	2.715862
8	6	0	-3.811637	0.519926	1.718926
9	1	0	-3.305524	0.339106	0.758207
10	6	0	-4.613793	2.513477	0.838390
11	1	0	-3.963941	2.234237	-0.005001
12	6	0	-4.154764	3.895193	1.328721
13	1	0	-4.753111	4.147919	2.222407
14	6	0	-4.374880	4.955403	0.243905
15	1	0	-4.077894	5.933394	0.640141
16	1	0	-3.703173	4.733282	-0.596902
17	6	0	-5.822589	4.981625	-0.246779

18	1	0	-5.932972	5.735710	-1.033047
19	1	0	-6.485973	5.279083	0.577229
20	6	0	-6.239705	3.602496	-0.757234
21	1	0	-7.280044	3.615074	-1.099247
22	1	0	-5.619193	3.333118	-1.624016
23	6	0	-6.059964	2.550727	0.337259
24	1	0	-6.722464	2.765397	1.186520
25	1	0	-6.314599	1.553037	-0.034615
26	6	0	-2.382089	3.996754	2.847187
27	1	0	-3.107548	4.226872	3.642180
28	6	0	-0.964955	3.936281	3.259152
29	6	0	0.008046	3.443833	2.379483
30	1	0	-0.312369	3.043931	1.422063
31	6	0	1.355727	3.473802	2.715862
32	6	0	1.736671	3.955750	3.975447
33	1	0	2.793759	3.969759	4.228753
34	6	0	0.777368	4.406060	4.875739
35	6	0	-0.576637	4.403895	4.508552
36	1	0	-1.307164	4.782686	5.218697
37	6	0	1.195688	4.896690	6.203884
38	1	0	2.271513	4.816902	6.424712
39	6	0	0.893263	5.846789	8.308661
40	1	0	1.977493	5.652781	8.398466
41	6	0	0.192513	5.081400	9.442206
42	1	0	-0.894657	5.240237	9.323851
43	6	0	0.637662	5.617916	10.807188
44	1	0	0.113465	5.062870	11.592781
45	1	0	1.708076	5.405698	10.926782
46	6	0	0.381665	7.120235	10.931472
47	1	0	-0.699223	7.311114	10.885929
48	1	0	0.726400	7.479189	11.906946
49	6	0	1.074858	7.883924	9.801799
50	1	0	2.162695	7.769892	9.903714
51	1	0	0.860086	8.955366	9.873074
52	6	0	0.634002	7.352060	8.437789
53	1	0	-0.439806	7.528362	8.292575
54	1	0	1.154404	7.871045	7.625439
55	6	0	-0.416067	2.844745	9.233313
56	1	0	-1.467252	3.168527	9.178475
57	7	0	-1.938436	-4.281110	1.642514
58	7	0	0.903438	-4.683765	1.927841
59	7	0	4.676768	0.461820	1.642514
60	7	0	3.604541	3.124283	1.927841
61	6	0	-2.986470	-1.714948	2.379483
62	1	0	-2.479937	-1.792485	1.422063
63	6	0	-2.926442	-2.803816	3.259152
64	6	0	-2.270246	-4.061327	2.847187
65	1	0	-2.106805	-4.804652	3.642180
66	6	0	-1.295954	-5.545728	1.328721
67	1	0	-1.215648	-6.190274	2.222407
68	6	0	0.130162	-5.252400	0.838390
69	1	0	0.047064	-4.549992	-0.005001
70	6	0	0.820988	-6.523446	0.337259
71	1	0	1.812330	-6.245122	-0.034615
72	1	0	0.966328	-7.204523	1.186520
73	6	0	-0.000001	-7.204991	-0.757234
74	1	0	0.509276	-8.112240	-1.099247
75	1	0	-0.076968	-6.532923	-1.624016
76	6	0	-1.402919	-7.533322	-0.246779

77	1	0	-2.000785	-8.005959	-1.033047
78	1	0	-1.328833	-8.256559	0.577229
79	6	0	-2.104065	-6.266459	0.243905
80	1	0	-2.247556	-5.573683	-0.596902
81	1	0	-3.099523	-6.498257	0.640141
82	6	0	1.455549	-3.560937	1.718926
83	1	0	1.359088	-3.032221	0.758207
84	6	0	2.330537	-2.910995	2.715862
85	6	0	2.557444	-3.481876	3.975447
86	1	0	2.041033	-4.404346	4.228753
87	6	0	3.427076	-2.876250	4.875739
88	6	0	4.102203	-1.702565	4.508552
89	1	0	4.795510	-1.259306	5.218697
90	6	0	3.891397	-1.132465	3.259152
91	6	0	2.978424	-1.728885	2.379483
92	1	0	2.792306	-1.251446	1.422063
93	6	0	4.652335	0.064573	2.847187
94	1	0	5.214353	0.577780	3.642180
95	6	0	5.450718	1.650535	1.328721
96	1	0	5.968759	2.042355	2.222407
97	6	0	4.483631	2.738923	0.838390
98	1	0	3.916877	2.315755	-0.005001
99	6	0	5.238976	3.972719	0.337259
100	1	0	4.502269	4.692085	-0.034615
101	1	0	5.756136	4.439126	1.186520
102	6	0	6.239706	3.602495	-0.757234
103	1	0	5.696161	3.199805	-1.624016
104	1	0	6.770768	4.497166	-1.099247
105	6	0	7.225508	2.551697	-0.246779
106	1	0	7.814806	2.977476	0.577229
107	1	0	7.933757	2.270249	-1.033047
108	6	0	6.478945	1.311056	0.243905
109	1	0	5.950729	0.840401	-0.596902
110	1	0	7.177417	0.564863	0.640141
111	6	0	2.356088	3.041011	1.718926
112	1	0	1.946436	2.693115	0.758207
113	7	0	-4.848568	-2.367890	7.037456
114	7	0	-3.449904	-1.374357	9.353758
115	7	0	2.915180	-2.300526	9.353758
116	7	0	4.474937	-3.015038	7.037456
117	6	0	-3.525566	-2.701330	4.508552
118	1	0	-3.488346	-3.523380	5.218697
119	6	0	-4.204444	-1.529810	4.875739
120	6	0	-4.838502	-1.412849	6.203884
121	1	0	-5.307316	-0.441263	6.424712
122	6	0	-5.510099	-2.149806	8.308661
123	1	0	-5.884198	-1.113831	8.398466
124	6	0	-4.496878	-2.373979	9.442206
125	1	0	-4.090850	-3.394914	9.323851
126	6	0	-5.184089	-2.256727	10.807188
127	1	0	-4.441307	-2.433171	11.592781
128	1	0	-5.535510	-1.223612	10.926782
129	6	0	-6.357137	-3.229586	10.931472
130	1	0	-6.840368	-3.110514	11.906946
131	1	0	-5.981999	-4.261102	10.885929
132	6	0	-7.365107	-3.011108	9.801799
133	1	0	-8.185617	-3.732827	9.873074
134	1	0	-7.810271	-2.011997	9.903714
135	6	0	-6.684072	-3.126968	8.437789

136	1	0	-6.299850	-4.145064	8.292575
137	1	0	-7.393727	-2.935779	7.625439
138	6	0	-2.255588	-1.782697	9.233313
139	1	0	-2.010399	-2.854941	9.178475
140	6	0	-1.101603	-0.862734	9.187397
141	6	0	-1.288549	0.527094	9.185421
142	1	0	-2.304491	0.913491	9.196016
143	6	0	-0.196348	1.385383	9.187397
144	6	0	1.100751	0.852369	9.185421
145	1	0	1.943352	1.539002	9.196016
146	6	0	1.297951	-0.522649	9.187397
147	6	0	0.187798	-1.379463	9.185421
148	1	0	0.361139	-2.452493	9.196016
149	6	0	2.671655	-1.062048	9.233313
150	1	0	3.477651	-0.313586	9.178475
151	6	0	4.304365	-2.707421	9.442206
152	1	0	4.985507	-1.845323	9.323851
153	6	0	4.616836	-3.696983	8.308661
154	1	0	3.906705	-4.538950	8.398466
155	6	0	6.050070	-4.225092	8.437789
156	1	0	6.239323	-4.935266	7.625439
157	1	0	6.739656	-3.383298	8.292575
158	6	0	6.290249	-4.872816	9.801799
159	1	0	5.647576	-5.757895	9.903714
160	1	0	7.325531	-5.222539	9.873074
161	6	0	5.975472	-3.890649	10.931472
162	1	0	6.681222	-3.050012	10.885929
163	1	0	6.113968	-4.368675	11.906946
164	6	0	4.546427	-3.361189	10.807188
165	1	0	3.827434	-4.182086	10.926782
166	1	0	4.327842	-2.629699	11.592781
167	6	0	3.642814	-3.483841	6.203884
168	1	0	3.035803	-4.375639	6.424712
169	7	0	-0.903438	4.683765	-1.927841
170	7	0	1.938436	4.281110	-1.642514
171	7	0	4.848568	2.367890	-7.037456
172	7	0	3.449904	1.374357	-9.353758
173	6	0	-2.557444	3.481876	-3.975447
174	1	0	-2.041033	4.404346	-4.228753
175	6	0	-2.330537	2.910995	-2.715862
176	6	0	-1.455549	3.560937	-1.718926
177	1	0	-1.359088	3.032221	-0.758207
178	6	0	-0.130162	5.252400	-0.838390
179	1	0	-0.047064	4.549992	0.005001
180	6	0	1.295954	5.545728	-1.328721
181	1	0	1.215648	6.190274	-2.222407
182	6	0	2.104065	6.266459	-0.243905
183	1	0	3.099523	6.498257	-0.640141
184	1	0	2.247556	5.573683	0.596902
185	6	0	1.402919	7.533322	0.246779
186	1	0	2.000785	8.005959	1.033047
187	1	0	1.328833	8.256559	-0.577229
188	6	0	0.000001	7.204991	0.757234
189	1	0	-0.509276	8.112240	1.099247
190	1	0	0.076968	6.532923	1.624016
191	6	0	-0.820988	6.523446	-0.337259
192	1	0	-0.966328	7.204523	-1.186520
193	1	0	-1.812330	6.245122	0.034615
194	6	0	2.270246	4.061327	-2.847187

195	1	0	2.106805	4.804652	-3.642180
196	6	0	2.926442	2.803816	-3.259152
197	6	0	2.986470	1.714948	-2.379483
198	1	0	2.479937	1.792485	-1.422063
199	6	0	3.686264	0.562807	-2.715862
200	6	0	4.294115	0.473874	-3.975447
201	1	0	4.834792	-0.434587	-4.228753
202	6	0	4.204444	1.529810	-4.875739
203	6	0	3.525566	2.701330	-4.508552
204	1	0	3.488346	3.523380	-5.218697
205	6	0	4.838502	1.412849	-6.203884
206	1	0	5.307316	0.441263	-6.424712
207	6	0	5.510099	2.149806	-8.308661
208	1	0	5.884198	1.113831	-8.398466
209	6	0	4.496878	2.373979	-9.442206
210	1	0	4.090850	3.394914	-9.323851
211	6	0	5.184089	2.256727	-10.807188
212	1	0	4.441307	2.433171	-11.592781
213	1	0	5.535510	1.223612	-10.926782
214	6	0	6.357137	3.229586	-10.931472
215	1	0	5.981999	4.261102	-10.885929
216	1	0	6.840368	3.110514	-11.906946
217	6	0	7.365107	3.011108	-9.801799
218	1	0	7.810271	2.011997	-9.903714
219	1	0	8.185617	3.732827	-9.873074
220	6	0	6.684072	3.126968	-8.437789
221	1	0	6.299850	4.145064	-8.292575
222	1	0	7.393727	2.935779	-7.625439
223	6	0	2.255588	1.782697	-9.233313
224	1	0	2.010399	2.854941	-9.178475
225	7	0	-4.676768	-0.461820	-1.642514
226	7	0	-3.604541	-3.124283	-1.927841
227	7	0	2.738332	-3.819290	-1.642514
228	7	0	4.507979	-1.559482	-1.927841
229	6	0	-2.978424	1.728885	-2.379483
230	1	0	-2.792306	1.251446	-1.422063
231	6	0	-3.891397	1.132465	-3.259152
232	6	0	-4.652335	-0.064573	-2.847187
233	1	0	-5.214353	-0.577780	-3.642180
234	6	0	-5.450718	-1.650535	-1.328721
235	1	0	-5.968759	-2.042355	-2.222407
236	6	0	-4.483631	-2.738923	-0.838390
237	1	0	-3.916877	-2.315755	0.005001
238	6	0	-5.238976	-3.972719	-0.337259
239	1	0	-4.502269	-4.692085	0.034615
240	1	0	-5.756136	-4.439126	-1.186520
241	6	0	-6.239706	-3.602495	0.757234
242	1	0	-6.770768	-4.497166	1.099247
243	1	0	-5.696161	-3.199805	1.624016
244	6	0	-7.225508	-2.551697	0.246779
245	1	0	-7.933757	-2.270249	1.033047
246	1	0	-7.814806	-2.977476	-0.577229
247	6	0	-6.478945	-1.311056	-0.243905
248	1	0	-5.950729	-0.840401	0.596902
249	1	0	-7.177417	-0.564863	-0.640141
250	6	0	-2.356088	-3.041011	-1.718926
251	1	0	-1.946436	-2.693115	-0.758207
252	6	0	-1.355727	-3.473802	-2.715862
253	6	0	-1.736671	-3.955750	-3.975447

254	1	0	-2.793759	-3.969759	-4.228753
255	6	0	-0.777368	-4.406060	-4.875739
256	6	0	0.576637	-4.403895	-4.508552
257	1	0	1.307164	-4.782686	-5.218697
258	6	0	0.964955	-3.936281	-3.259152
259	6	0	-0.008046	-3.443833	-2.379483
260	1	0	0.312369	-3.043931	-1.422063
261	6	0	2.382089	-3.996754	-2.847187
262	1	0	3.107548	-4.226872	-3.642180
263	6	0	4.154764	-3.895193	-1.328721
264	1	0	4.753111	-4.147919	-2.222407
265	6	0	4.613793	-2.513477	-0.838390
266	1	0	3.963941	-2.234237	0.005001
267	6	0	6.059964	-2.550727	-0.337259
268	1	0	6.314599	-1.553037	0.034615
269	1	0	6.722464	-2.765397	-1.186520
270	6	0	6.239705	-3.602496	0.757234
271	1	0	5.619193	-3.333118	1.624016
272	1	0	7.280044	-3.615074	1.099247
273	6	0	5.822589	-4.981625	0.246779
274	1	0	6.485973	-5.279083	-0.577229
275	1	0	5.932972	-5.735710	1.033047
276	6	0	4.374880	-4.955403	-0.243905
277	1	0	3.703173	-4.733282	0.596902
278	1	0	4.077894	-5.933394	-0.640141
279	6	0	3.811637	-0.519926	-1.718926
280	1	0	3.305524	-0.339106	-0.758207
281	7	0	-4.474937	3.015038	-7.037456
282	7	0	-2.915180	2.300526	-9.353758
283	7	0	-0.534724	-3.674883	-9.353758
284	7	0	-0.373631	-5.382928	-7.037456
285	6	0	-4.102203	1.702565	-4.508552
286	1	0	-4.795510	1.259306	-5.218697
287	6	0	-3.427076	2.876250	-4.875739
288	6	0	-3.642814	3.483841	-6.203884
289	1	0	-3.035803	4.375639	-6.424712
290	6	0	-4.616836	3.696983	-8.308661
291	1	0	-3.906705	4.538950	-8.398466
292	6	0	-4.304365	2.707421	-9.442206
293	1	0	-4.985507	1.845323	-9.323851
294	6	0	-4.546427	3.361189	-10.807188
295	1	0	-4.327842	2.629699	-11.592781
296	1	0	-3.827434	4.182086	-10.926782
297	6	0	-5.975472	3.890649	-10.931472
298	1	0	-6.113968	4.368675	-11.906946
299	1	0	-6.681222	3.050012	-10.885929
300	6	0	-6.290249	4.872816	-9.801799
301	1	0	-7.325531	5.222539	-9.873074
302	1	0	-5.647576	5.757895	-9.903714
303	6	0	-6.050070	4.225092	-8.437789
304	1	0	-6.739656	3.383298	-8.292575
305	1	0	-6.239323	4.935266	-7.625439
306	6	0	-2.671655	1.062048	-9.233313
307	1	0	-3.477651	0.313586	-9.178475
308	6	0	-1.297951	0.522649	-9.187397
309	6	0	-0.187798	1.379463	-9.185421
310	1	0	-0.361139	2.452493	-9.196016
311	6	0	1.101603	0.862734	-9.187397
312	6	0	1.288549	-0.527094	-9.185421

313	1	0	2.304491	-0.913491	-9.196016
314	6	0	0.196348	-1.385383	-9.187397
315	6	0	-1.100751	-0.852369	-9.185421
316	1	0	-1.943352	-1.539002	-9.196016
317	6	0	0.416067	-2.844745	-9.233313
318	1	0	1.467252	-3.168527	-9.178475
319	6	0	-0.192513	-5.081400	-9.442206
320	1	0	0.894657	-5.240237	-9.323851
321	6	0	-0.893263	-5.846789	-8.308661
322	1	0	-1.977493	-5.652781	-8.398466
323	6	0	-0.634002	-7.352060	-8.437789
324	1	0	-1.154404	-7.871045	-7.625439
325	1	0	0.439806	-7.528362	-8.292575
326	6	0	-1.074858	-7.883924	-9.801799
327	1	0	-2.162695	-7.769892	-9.903714
328	1	0	-0.860086	-8.955366	-9.873074
329	6	0	-0.381665	-7.120235	-10.931472
330	1	0	0.699223	-7.311114	-10.885929
331	1	0	-0.726400	-7.479189	-11.906946
332	6	0	-0.637662	-5.617916	-10.807188
333	1	0	-1.708076	-5.405698	-10.926782
334	1	0	-0.113465	-5.062870	-11.592781
335	6	0	-1.195688	-4.896690	-6.203884
336	1	0	-2.271513	-4.816902	-6.424712

Xe@w-to-w-a C3 cc3-rdim33

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	0.752355	4.472377	1.494361
2	7	0	3.431098	3.384888	1.542817
3	7	0	3.497015	-2.887747	1.494361
4	7	0	1.215851	-4.663862	1.542817
5	6	0	-1.512607	2.922597	2.219051
6	1	0	-1.041375	2.737107	1.255534
7	6	0	-0.894196	3.820092	3.100803
8	6	0	0.330548	4.537321	2.687503
9	1	0	0.824383	5.151459	3.456670
10	6	0	1.914556	5.243264	1.103089
11	1	0	2.380244	5.756579	1.963496
12	6	0	2.943634	4.272403	0.498092
13	1	0	2.402988	3.709963	-0.278903
14	6	0	4.114830	5.010189	-0.151741
15	1	0	4.772838	4.272681	-0.623846
16	1	0	4.693155	5.511144	0.636084
17	6	0	3.634558	6.026440	-1.188193
18	1	0	4.493101	6.551804	-1.619588
19	1	0	3.135979	5.497373	-2.012950
20	6	0	2.654287	7.015553	-0.559177
21	1	0	2.294583	7.731689	-1.305749
22	1	0	3.170071	7.596348	0.218273
23	6	0	1.470171	6.270985	0.054390
24	1	0	0.917172	5.729727	-0.726555
25	1	0	0.762364	6.965370	0.522369
26	6	0	2.954500	2.209211	1.564812
27	1	0	2.217446	1.866353	0.823366

28	6	0	3.376101	1.196149	2.554318
29	6	0	3.902470	1.567214	3.797957
30	1	0	3.970620	2.624396	4.042311
31	6	0	4.327874	0.595835	4.698867
32	6	0	4.257572	-0.758838	4.343521
33	1	0	4.615913	-1.499989	5.053301
34	6	0	3.755395	-1.135650	3.100803
35	6	0	3.287347	-0.151342	2.219051
36	1	0	2.891092	-0.466696	1.255534
37	6	0	3.764161	-2.554923	2.687503
38	1	0	4.049103	-3.289666	3.456670
39	6	0	3.583521	-4.279686	1.103089
40	1	0	3.795222	-4.939642	1.963496
41	6	0	2.228192	-4.685463	0.498092
42	1	0	2.011428	-3.936030	-0.278903
43	6	0	2.281536	-6.068642	-0.151741
44	1	0	1.313832	-6.269739	-0.623846
45	1	0	2.426213	-6.819964	0.636084
46	6	0	3.401771	-6.160840	-1.188193
47	1	0	3.192875	-5.464524	-2.012950
48	1	0	3.427479	-7.167042	-1.619588
49	6	0	4.748503	-5.806457	-0.559177
50	1	0	4.993595	-6.543536	0.218273
51	1	0	5.548548	-5.853012	-1.305749
52	6	0	4.695747	-4.408698	0.054390
53	1	0	4.503504	-3.659158	-0.726555
54	1	0	5.651005	-4.142912	0.522369
55	6	0	0.435983	-3.663278	1.564812
56	1	0	0.507586	-2.853541	0.823366
57	7	0	-2.825402	4.561751	6.824400
58	7	0	-2.181229	3.001281	9.144487
59	7	0	3.689800	0.388359	9.144487
60	7	0	5.363293	0.165994	6.824400
61	6	0	-1.471613	4.066584	4.343521
62	1	0	-1.008928	4.747493	5.053301
63	6	0	-2.679945	3.450132	4.698867
64	6	0	-3.300422	3.714730	6.009779
65	1	0	-4.206531	3.131640	6.236308
66	6	0	-3.511185	4.743541	8.087882
67	1	0	-4.378539	4.064957	8.179375
68	6	0	-2.538619	4.403884	9.229203
69	1	0	-1.653152	5.054353	9.110716
70	6	0	-3.191319	4.677052	10.588404
71	1	0	-2.473380	4.437780	11.380386
72	1	0	-4.038047	3.988512	10.706913
73	6	0	-3.670113	6.125034	10.699410
74	1	0	-4.149112	6.287540	11.670672
75	1	0	-2.804347	6.799776	10.654987
76	6	0	-4.633091	6.467949	9.561298
77	1	0	-4.945384	7.515663	9.624030
78	1	0	-5.541685	5.858681	9.661507
79	6	0	-3.986535	6.195536	8.202678
80	1	0	-3.119156	6.852728	8.058187
81	1	0	-4.684620	6.405345	7.384984
82	6	0	-0.956647	2.713100	8.986209
83	1	0	-0.180858	3.490609	8.907396
84	6	0	-0.472033	1.319390	8.928424
85	6	0	-1.372036	0.244689	8.925092
86	1	0	-2.437582	0.459518	8.939150

87	6	0	-0.906609	-1.068487	8.928424
88	6	0	0.474111	-1.310563	8.925092
89	1	0	0.820837	-2.340767	8.939150
90	6	0	1.378642	-0.250903	8.928424
91	6	0	0.897925	1.065874	8.925092
92	1	0	1.616745	1.881249	8.939150
93	6	0	2.827937	-0.528069	8.986209
94	1	0	3.113385	-1.588677	8.907396
95	6	0	5.083184	-0.003434	9.229203
96	1	0	5.203774	-1.095505	9.110716
97	6	0	5.863620	0.669005	8.087882
98	1	0	5.709626	1.759447	8.179375
99	6	0	7.358760	0.354673	8.202678
100	1	0	7.889501	0.854328	7.384984
101	1	0	7.494214	-0.725096	8.058187
102	6	0	7.917954	0.778400	9.561298
103	1	0	7.844610	1.869900	9.661507
104	1	0	8.981448	0.524997	9.624030
105	6	0	7.139491	0.115895	10.699410
106	1	0	7.290953	-0.971252	10.654987
107	1	0	7.519725	0.449467	11.670672
108	6	0	5.646106	0.425237	10.588404
109	1	0	5.473176	1.502795	10.706913
110	1	0	5.079920	-0.076880	11.380386
111	6	0	4.867262	1.000884	6.009779
112	1	0	4.815345	2.077143	6.236308
113	7	0	-4.646948	1.278973	1.542817
114	7	0	-4.249370	-1.584630	1.494361
115	7	0	-2.537891	-4.727745	6.824400
116	7	0	-1.508571	-3.389640	9.144487
117	6	0	-3.308482	2.596031	3.797957
118	1	0	-4.258104	2.126460	4.042311
119	6	0	-2.723946	2.325715	2.554318
120	6	0	-3.390483	1.454067	1.564812
121	1	0	-2.725032	0.987188	0.823366
122	6	0	-5.171826	0.413061	0.498092
123	1	0	-4.414416	0.226067	-0.278903
124	6	0	-5.498078	-0.963577	1.103089
125	1	0	-6.175466	-0.816938	1.963496
126	6	0	-6.165918	-1.862287	0.054390
127	1	0	-6.413369	-2.822458	0.522369
128	1	0	-5.420675	-2.070570	-0.726555
129	6	0	-7.402791	-1.209096	-0.559177
130	1	0	-7.843131	-1.878677	-1.305749
131	1	0	-8.163666	-1.052812	0.218273
132	6	0	-7.036329	0.134400	-1.188193
133	1	0	-7.920580	0.615238	-1.619588
134	1	0	-6.328854	-0.032849	-2.012950
135	6	0	-6.396366	1.058453	-0.151741
136	1	0	-7.119369	1.308820	0.636084
137	1	0	-6.086669	1.997058	-0.623846
138	6	0	-4.094709	-1.982398	2.687503
139	1	0	-4.873486	-1.861793	3.456670
140	6	0	-2.861199	-2.684442	3.100803
141	6	0	-1.774739	-2.771255	2.219051
142	1	0	-1.849717	-2.270411	1.255534
143	6	0	-0.652155	-3.521864	2.554318
144	6	0	-0.593988	-4.163245	3.797957
145	1	0	0.287484	-4.750856	4.042311

146	6	0	-1.647929	-4.045967	4.698867
147	6	0	-2.785959	-3.307746	4.343521
148	1	0	-3.606985	-3.247504	5.053301
149	6	0	-1.566840	-4.715615	6.009779
150	1	0	-0.608814	-5.208782	6.236308
151	6	0	-2.352435	-5.412546	8.087882
152	1	0	-1.331087	-5.824404	8.179375
153	6	0	-2.544566	-4.400450	9.229203
154	1	0	-3.550622	-3.958848	9.110716
155	6	0	-2.454787	-5.102289	10.588404
156	1	0	-2.606540	-4.360900	11.380386
157	1	0	-1.435129	-5.491307	10.706913
158	6	0	-3.469378	-6.240928	10.699410
159	1	0	-4.486605	-5.828524	10.654987
160	1	0	-3.370613	-6.737007	11.670672
161	6	0	-3.284863	-7.246349	9.561298
162	1	0	-2.302924	-7.728581	9.661507
163	1	0	-4.036063	-8.040660	9.624030
164	6	0	-3.372224	-6.550209	8.202678
165	1	0	-4.375058	-6.127632	8.058187
166	1	0	-3.204881	-7.259672	7.384984
167	6	0	-1.871290	-2.185031	8.986209
168	1	0	-2.932527	-1.901932	8.907396
169	7	0	-1.194684	4.374769	-1.884753
170	7	0	-3.767083	3.033252	-1.942588
171	7	0	-3.191319	-3.222012	-1.884753
172	7	0	-0.743332	-4.779015	-1.942588
173	6	0	1.243324	3.122783	-2.606786
174	1	0	0.785549	2.873753	-1.651353
175	6	0	0.543555	3.969942	-3.476640
176	6	0	-0.753218	4.545368	-3.060296
177	1	0	-1.286408	5.150568	-3.810062
178	6	0	-2.426889	5.021604	-1.481317
179	1	0	-2.941094	5.501653	-2.333204
180	6	0	-3.356473	3.949165	-0.888923
181	1	0	-2.762580	3.428348	-0.120783
182	6	0	-4.589805	4.563053	-0.224604
183	1	0	-5.174608	3.759040	0.234935
184	1	0	-5.214670	5.021914	-1.002463
185	6	0	-4.202746	5.601046	0.828792
186	1	0	-5.104646	6.034611	1.273519
187	1	0	-3.651296	5.106583	1.641434
188	6	0	-3.324657	6.689621	0.213455
189	1	0	-3.030288	7.424057	0.970820
190	1	0	-3.898293	7.231569	-0.551394
191	6	0	-2.078514	6.072232	-0.418116
192	1	0	-1.469388	5.576377	0.351236
193	1	0	-1.445073	6.839095	-0.879531
194	6	0	-3.211730	1.892735	-1.957419
195	1	0	-2.458269	1.605714	-1.209071
196	6	0	-3.553770	0.844008	-2.940307
197	6	0	-4.135349	1.156259	-4.175205
198	1	0	-4.307553	2.200745	-4.422867
199	6	0	-4.472351	0.144306	-5.068872
200	6	0	-4.267636	-1.195699	-4.709912
201	1	0	-4.556825	-1.971115	-5.414559
202	6	0	-3.709849	-1.514238	-3.476640
203	6	0	-3.326071	-0.484641	-2.606786
204	1	0	-2.881518	-0.756571	-1.651353

205	6	0	-3.559795	-2.924989	-3.060296
206	1	0	-3.817318	-3.689346	-3.810062
207	6	0	-3.135392	-4.612549	-1.481317
208	1	0	-3.294025	-5.297888	-2.333204
209	6	0	-1.741840	-4.881373	-0.888923
210	1	0	-1.587746	-4.106638	-0.120783
211	6	0	-1.656818	-6.256414	-0.224604
212	1	0	-0.668120	-6.360862	0.234935
213	1	0	-1.741770	-7.026994	-1.002463
214	6	0	-2.749275	-6.440208	0.828792
215	1	0	-2.596782	-5.715406	1.641434
216	1	0	-2.673804	-7.438059	1.273519
217	6	0	-4.131053	-6.224048	0.213455
218	1	0	-4.313576	-6.991805	-0.551394
219	1	0	-4.914277	-6.336335	0.970820
220	6	0	-4.219450	-4.836162	-0.418116
221	1	0	-4.094590	-4.060716	0.351236
222	1	0	-5.200294	-4.671018	-0.879531
223	6	0	-0.033291	-3.727807	-1.957419
224	1	0	-0.161455	-2.931780	-1.209071
225	7	0	2.357920	4.861261	-7.227955
226	7	0	1.871493	3.209592	-9.538046
227	7	0	-3.715335	0.015965	-9.538046
228	7	0	-5.388935	-0.388612	-7.227955
229	6	0	1.098312	4.293730	-4.709912
230	1	0	0.571377	4.931884	-5.414559
231	6	0	2.361148	3.801017	-5.068872
232	6	0	2.943078	4.112486	-6.388854
233	1	0	3.917492	3.646812	-6.603735
234	6	0	3.014853	5.095671	-8.498467
235	1	0	3.949137	4.511853	-8.584859
236	6	0	2.080428	4.642037	-9.631404
237	1	0	1.131383	5.196434	-9.516754
238	6	0	2.695823	4.967998	-10.996890
239	1	0	2.003522	4.645533	-11.782211
240	1	0	3.609687	4.370863	-11.112705
241	6	0	3.019458	6.456702	-11.126790
242	1	0	3.475594	6.656814	-12.102040
243	1	0	2.087847	7.037414	-11.086141
244	6	0	3.944872	6.911698	-9.997041
245	1	0	4.145402	7.985600	-10.072607
246	1	0	4.911975	6.399838	-10.094393
247	6	0	3.334652	6.588507	-8.632879
248	1	0	2.403567	7.152817	-8.492010
249	1	0	4.009366	6.879817	-7.820523
250	6	0	0.678907	2.795029	-9.420243
251	1	0	-0.175310	3.488212	-9.369569
252	6	0	0.336574	1.359068	-9.373489
253	6	0	1.339166	0.379192	-9.372328
254	1	0	2.377801	0.699746	-9.383619
255	6	0	1.008700	-0.971016	-9.373489
256	6	0	-0.341193	-1.349348	-9.372328
257	1	0	-0.582903	-2.409110	-9.383619
258	6	0	-1.345274	-0.388052	-9.373489
259	6	0	-0.997973	0.970156	-9.372328
260	1	0	-1.794899	1.709363	-9.383619
261	6	0	-2.760020	-0.809564	-9.420243
262	1	0	-2.933226	-1.895929	-9.369569
263	6	0	-5.060336	-0.519315	-9.631404

264	1	0	-5.065935	-1.618411	-9.516754
265	6	0	-5.920407	0.063104	-8.498467
266	1	0	-5.881947	1.164126	-8.584859
267	6	0	-7.373140	-0.406360	-8.632879
268	1	0	-7.962779	0.032304	-7.820523
269	1	0	-7.396304	-1.494859	-8.492010
270	6	0	-7.958143	-0.039489	-9.997041
271	1	0	-7.998410	1.053976	-10.094393
272	1	0	-8.988433	-0.402777	-10.072607
273	6	0	-7.101397	-0.613424	-11.126790
274	1	0	-7.138503	-1.710578	-11.086141
275	1	0	-7.502767	-0.318454	-12.102040
276	6	0	-5.650324	-0.149348	-10.996890
277	1	0	-5.590122	0.940649	-11.112705
278	1	0	-5.024911	-0.587666	-11.782211
279	6	0	-5.033056	0.492538	-6.388854
280	1	0	-5.116977	1.569241	-6.603735
281	7	0	4.510415	1.745763	-1.942588
282	7	0	4.386003	-1.152758	-1.884753
283	7	0	3.031015	-4.472649	-7.227955
284	7	0	1.843842	-3.225557	-9.538046
285	6	0	3.069024	3.003188	-4.175205
286	1	0	4.059677	2.630078	-4.422867
287	6	0	2.507817	2.655651	-2.940307
288	6	0	3.245021	1.835072	-1.957419
289	1	0	2.619724	1.326066	-1.209071
290	6	0	5.098313	0.932209	-0.888923
291	1	0	4.350326	0.678291	-0.120783
292	6	0	5.562281	-0.409055	-1.481317
293	1	0	6.235118	-0.203765	-2.333204
294	6	0	6.297964	-1.236070	-0.418116
295	1	0	6.645367	-2.168078	-0.879531
296	1	0	5.563978	-1.515661	0.351236
297	6	0	7.455711	-0.465573	0.213455
298	1	0	7.944566	-1.087722	0.970820
299	1	0	8.211869	-0.239764	-0.551394
300	6	0	6.952021	0.839162	0.828792
301	1	0	7.778449	1.403448	1.273519
302	1	0	6.248078	0.608824	1.641434
303	6	0	6.246622	1.693361	-0.224604
304	1	0	6.956440	2.005080	-1.002463
305	1	0	5.842728	2.601822	0.234935
306	6	0	4.313013	-1.620378	-3.060296
307	1	0	5.103727	-1.461222	-3.810062
308	6	0	3.166293	-2.455704	-3.476640
309	6	0	2.082747	-2.638142	-2.606786
310	1	0	2.095969	-2.117182	-1.651353
311	6	0	1.045953	-3.499659	-2.940307
312	6	0	1.066325	-4.159447	-4.175205
313	1	0	0.247876	-4.830823	-4.422867
314	6	0	2.111203	-3.945323	-5.068872
315	6	0	3.169323	-3.098032	-4.709912
316	1	0	3.985448	-2.960769	-5.414559
317	6	0	2.089978	-4.605023	-6.388854
318	1	0	1.199486	-5.216053	-6.603735
319	6	0	2.905554	-5.158775	-8.498467
320	1	0	1.932811	-5.675979	-8.584859
321	6	0	2.979908	-4.122722	-9.631404
322	1	0	3.934552	-3.578023	-9.516754

323	6	0	2.954501	-4.818651	-10.996890
324	1	0	3.021389	-4.057868	-11.782211
325	1	0	1.980435	-5.311512	-11.112705
326	6	0	4.081939	-5.843279	-11.126790
327	1	0	5.050656	-5.326836	-11.086141
328	1	0	4.027173	-6.338359	-12.102040
329	6	0	4.013270	-6.872209	-9.997041
330	1	0	3.086435	-7.453814	-10.094393
331	1	0	4.843032	-7.582823	-10.072607
332	6	0	4.038488	-6.182146	-8.632879
333	1	0	4.992738	-5.657958	-8.492010
334	1	0	3.953413	-6.912121	-7.820523
335	6	0	2.081112	-1.985465	-9.420243
336	1	0	3.108535	-1.592283	-9.369569
337	54	0	0.000000	-0.000000	4.384123

Xe@w-to-w TS C3 cc3-rdim10

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	2.587366	3.742409	1.678239
2	7	0	4.599528	1.648849	1.803663
3	7	0	1.947339	-4.111930	1.678239
4	7	0	-0.871819	-4.807733	1.803663
5	6	0	-0.156977	3.497674	2.363984
6	1	0	0.180022	3.156178	1.387199
7	6	0	0.798774	4.014036	3.249370
8	6	0	2.214595	4.106620	2.833740
9	1	0	2.913001	4.535113	3.569590
10	6	0	3.967508	3.948245	1.283386
11	1	0	4.597123	4.259298	2.136230
12	6	0	4.520406	2.626369	0.728606
13	1	0	3.811394	2.301559	-0.051420
14	6	0	5.899113	2.809207	0.090703
15	1	0	6.212040	1.852375	-0.340702
16	1	0	6.619716	3.066985	0.878214
17	6	0	5.878566	3.891645	-0.988673
18	1	0	6.879901	4.011060	-1.415632
19	1	0	5.216772	3.575762	-1.807725
20	6	0	5.373616	5.214269	-0.413739
21	1	0	5.338060	5.985481	-1.190680
22	1	0	6.073864	5.567828	0.355927
23	6	0	3.985626	5.033535	0.197991
24	1	0	3.263321	4.741531	-0.577850
25	1	0	3.620037	5.970050	0.635605
26	6	0	3.794337	0.671135	1.734272
27	1	0	3.084240	0.574080	0.901437
28	6	0	3.746800	-0.426836	2.720177
29	6	0	4.348721	-0.316561	3.980088
30	1	0	4.847312	0.613564	4.241527
31	6	0	4.301177	-1.379735	4.876095
32	6	0	3.666662	-2.574685	4.505522
33	1	0	3.652100	-3.395617	5.217809
34	6	0	3.076871	-2.698777	3.249370
35	6	0	3.107563	-1.612891	2.363984
36	1	0	2.643319	-1.733992	1.387199

37	6	0	2.449140	-3.971206	2.833740
38	1	0	2.471022	-4.790289	3.569590
39	6	0	1.435527	-5.410086	1.283386
40	1	0	1.390098	-6.110875	2.136230
41	6	0	0.014299	-5.227971	0.728606
42	1	0	0.087511	-4.451543	-0.051420
43	6	0	-0.516712	-6.513385	0.090703
44	1	0	-1.501817	-6.305972	-0.340702
45	1	0	-0.653771	-7.266334	0.878214
46	6	0	0.430980	-7.036810	-0.988673
47	1	0	0.488315	-6.305738	-1.807725
48	1	0	0.033729	-7.963699	-1.415632
49	6	0	1.828881	-7.260823	-0.413739
50	1	0	1.784949	-8.044035	0.355927
51	1	0	2.514548	-7.615636	-1.190680
52	6	0	2.366356	-5.968421	0.197991
53	1	0	2.474626	-5.196885	-0.577850
54	1	0	3.360196	-6.120069	0.635605
55	6	0	-1.315948	-3.621560	1.734272
56	1	0	-1.044953	-2.958070	0.901437
57	7	0	-0.582570	5.390550	7.037386
58	7	0	-0.666527	3.654658	9.339681
59	7	0	3.498291	-1.250100	9.339681
60	7	0	4.959638	-2.190755	7.037386
61	6	0	0.396412	4.462765	4.505522
62	1	0	1.114640	4.860620	5.217809
63	6	0	-0.955703	4.414796	4.876095
64	6	0	-1.389681	4.883578	6.201599
65	1	0	-2.461024	4.762497	6.425362
66	6	0	-1.113733	5.820951	8.315539
67	1	0	-2.188893	5.582832	8.408029
68	6	0	-0.377528	5.072591	9.437975
69	1	0	0.702085	5.274349	9.315769
70	6	0	-0.835698	5.578296	10.810638
71	1	0	-0.285221	5.037019	11.587811
72	1	0	-1.895993	5.321915	10.933901
73	6	0	-0.639835	7.088378	10.948446
74	1	0	-0.993374	7.423733	11.929143
75	1	0	0.432170	7.323287	10.899261
76	6	0	-1.369519	7.834074	9.829868
77	1	0	-1.198378	8.912672	9.910739
78	1	0	-2.451258	7.674691	9.935729
79	6	0	-0.914252	7.333976	8.458622
80	1	0	0.150888	7.554776	8.310510
81	1	0	-1.458954	7.839679	7.653897
82	6	0	0.313978	2.859719	9.219423
83	1	0	1.353111	3.220829	9.168353
84	6	0	0.145981	1.393352	9.171250
85	6	0	-1.131531	0.815406	9.169720
86	1	0	-1.997799	1.471989	9.180291
87	6	0	-1.279668	-0.570252	9.171250
88	6	0	-0.140397	-1.387638	9.169720
89	1	0	-0.275880	-2.466139	9.180291
90	6	0	1.133687	-0.823099	9.171250
91	6	0	1.271928	0.572231	9.169720
92	1	0	2.273679	0.994150	9.180291
93	6	0	2.319600	-1.701773	9.219423
94	1	0	2.112764	-2.782243	9.168353
95	6	0	4.581756	-2.209346	9.437975

96	1	0	4.216677	-3.245198	9.315769
97	6	0	5.597958	-1.945955	8.315539
98	1	0	5.929321	-0.895780	8.408029
99	6	0	6.808535	-2.875223	8.458622
100	1	0	7.518838	-2.656349	7.653897
101	1	0	6.467184	-3.908061	8.310510
102	6	0	7.469267	-2.730999	9.829868
103	1	0	7.872106	-1.714494	9.935729
104	1	0	8.317789	-3.418510	9.910739
105	6	0	6.458633	-2.990076	10.948446
106	1	0	6.126068	-4.035913	10.899261
107	1	0	6.925829	-2.851579	11.929143
108	6	0	5.248795	-2.065412	10.810638
109	1	0	5.556910	-1.018979	10.933901
110	1	0	4.504797	-2.271501	11.587811
111	6	0	4.924143	-1.238290	6.201599
112	1	0	5.354956	-0.249940	6.425362
113	7	0	-3.727709	3.158884	1.803663
114	7	0	-4.534705	0.369520	1.678239
115	7	0	-4.377069	-3.199795	7.037386
116	7	0	-2.831763	-2.404559	9.339681
117	6	0	-1.900211	3.924383	3.980088
118	1	0	-2.955018	3.891113	4.241527
119	6	0	-1.503749	3.458242	2.720177
120	6	0	-2.478389	2.950424	1.734272
121	1	0	-2.039288	2.383991	0.901437
122	6	0	-4.534705	2.601602	0.728606
123	1	0	-3.898905	2.149984	-0.051420
124	6	0	-5.403035	1.461840	1.283386
125	1	0	-5.987222	1.851577	2.136230
126	6	0	-6.351982	0.934886	0.197991
127	1	0	-6.980233	0.150019	0.635605
128	1	0	-5.737947	0.455353	-0.577850
129	6	0	-7.202497	2.046554	-0.413739
130	1	0	-7.852609	1.630155	-1.190680
131	1	0	-7.858813	2.476206	0.355927
132	6	0	-6.309546	3.145165	-0.988673
133	1	0	-6.913630	3.952639	-1.415632
134	1	0	-5.705086	2.729976	-1.807725
135	6	0	-5.382401	3.704179	0.090703
136	1	0	-5.965945	4.199349	0.878214
137	1	0	-4.710224	4.453597	-0.340702
138	6	0	-4.663735	-0.135414	2.833740
139	1	0	-5.384023	0.255177	3.569590
140	6	0	-3.875645	-1.315260	3.249370
141	6	0	-2.950586	-1.884783	2.363984
142	1	0	-2.823341	-1.422186	1.387199
143	6	0	-2.243051	-3.031406	2.720177
144	6	0	-2.448510	-3.607822	3.980088
145	1	0	-1.892294	-4.504677	4.241527
146	6	0	-3.345474	-3.035061	4.876095
147	6	0	-4.063074	-1.888080	4.505522
148	1	0	-4.766741	-1.465003	5.217809
149	6	0	-3.534462	-3.645288	6.201599
150	1	0	-2.893932	-4.512558	6.425362
151	6	0	-4.484225	-3.874996	8.315539
152	1	0	-3.740428	-4.687053	8.408029
153	6	0	-4.204228	-2.863244	9.437975
154	1	0	-4.918763	-2.029151	9.315769

155	6	0	-4.413097	-3.512884	10.810638
156	1	0	-4.219576	-2.765518	11.587811
157	1	0	-3.660917	-4.302936	10.933901
158	6	0	-5.818799	-4.098302	10.948446
159	1	0	-6.558238	-3.287374	10.899261
160	1	0	-5.932455	-4.572154	11.929143
161	6	0	-6.099748	-5.103075	9.829868
162	1	0	-5.420848	-5.960197	9.935729
163	1	0	-7.119411	-5.494162	9.910739
164	6	0	-5.894283	-4.458753	8.458622
165	1	0	-6.618072	-3.646715	8.310510
166	1	0	-6.059885	-5.183331	7.653897
167	6	0	-2.633578	-1.157946	9.219423
168	1	0	-3.465875	-0.438586	9.168353
169	7	0	0.784208	4.470380	-1.765350
170	7	0	-2.118980	4.380335	-1.838395
171	7	0	-4.263567	-1.556046	-1.765350
172	7	0	-2.733992	-4.025258	-1.838395
173	6	0	2.469985	2.277874	-2.466961
174	1	0	1.957145	2.247751	-1.506725
175	6	0	2.194133	3.340020	-3.339952
176	6	0	1.268663	4.418185	-2.935266
177	1	0	1.055476	5.187067	-3.694455
178	6	0	-0.046661	5.599228	-1.396079
179	1	0	-0.290883	6.233886	-2.266860
180	6	0	-1.357363	5.058896	-0.801041
181	1	0	-1.057739	4.357037	-0.007890
182	6	0	-2.204369	6.172107	-0.182303
183	1	0	-3.089094	5.721422	0.280311
184	1	0	-2.556289	6.831063	-0.987154
185	6	0	-1.415925	6.972205	0.854742
186	1	0	-2.042099	7.772831	1.262255
187	1	0	-1.148410	6.316126	1.695249
188	6	0	-0.140397	7.543516	0.236872
189	1	0	0.436747	8.098434	0.984228
190	1	0	-0.406754	8.256799	-0.555575
191	6	0	0.715254	6.421326	-0.347709
192	1	0	1.033587	5.733109	0.448587
193	1	0	1.627974	6.816075	-0.809578
194	6	0	-2.088514	3.111825	-1.838331
195	1	0	-1.514851	2.541280	-1.092154
196	6	0	-2.843471	2.296591	-2.812077
197	6	0	-3.233510	2.820815	-4.050820
198	1	0	-2.943139	3.838008	-4.301572
199	6	0	-3.967864	2.046204	-4.942482
200	6	0	-4.352184	0.748280	-4.578000
201	1	0	-4.941661	0.165701	-5.281291
202	6	0	-3.989608	0.230165	-3.339952
203	6	0	-3.207689	1.000133	-2.466961
204	1	0	-2.925181	0.571062	-1.506725
205	6	0	-4.460592	-1.110398	-2.935266
206	1	0	-5.019870	-1.679464	-3.694455
207	6	0	-4.825743	-2.840024	-1.396079
208	1	0	-5.253262	-3.368855	-2.266860
209	6	0	-3.702451	-3.704959	-0.801041
210	1	0	-3.244435	-3.094547	-0.007890
211	6	0	-4.243017	-4.995093	-0.182303
212	1	0	-3.410350	-5.535945	0.280311
213	1	0	-4.637730	-5.629343	-0.987154

214	6	0	-5.330145	-4.712329	0.854742
215	1	0	-4.895721	-4.152615	1.695249
216	1	0	-5.710419	-5.654925	1.262255
217	6	0	-6.462678	-3.893345	0.236872
218	1	0	-6.947221	-4.480659	-0.555575
219	1	0	-7.231823	-3.670983	0.984228
220	6	0	-5.918658	-2.591235	-0.347709
221	1	0	-5.481812	-1.971442	0.448587
222	1	0	-6.716881	-1.998170	-0.809578
223	6	0	-1.650662	-3.364619	-1.838331
224	1	0	-1.443388	-2.582540	-1.092154
225	7	0	4.209667	3.379038	-7.094045
226	7	0	3.062179	2.103038	-9.407806
227	7	0	-3.352374	1.600405	-9.407806
228	7	0	-5.031166	1.956160	-7.094045
229	6	0	2.824122	3.394962	-4.578000
230	1	0	2.614332	4.196754	-5.281291
231	6	0	3.755996	2.413169	-4.942482
232	6	0	4.416566	2.447177	-6.259886
233	1	0	5.095651	1.608548	-6.479097
234	6	0	4.902710	3.314909	-8.365413
235	1	0	5.497473	2.387916	-8.455862
236	6	0	3.863371	3.308863	-9.497824
237	1	0	3.242676	4.215518	-9.379716
238	6	0	4.558580	3.345121	-10.863489
239	1	0	3.794650	3.352434	-11.648564
240	1	0	5.129253	2.414917	-10.982625
241	6	0	5.487793	4.552927	-10.989304
242	1	0	5.985196	4.542456	-11.964846
243	1	0	4.894022	5.476098	-10.944791
244	6	0	6.519463	4.564251	-9.859952
245	1	0	7.159953	5.449507	-9.932567
246	1	0	7.174660	3.688293	-9.960873
247	6	0	5.830182	4.528075	-8.495604
248	1	0	5.229816	5.435777	-8.351246
249	1	0	6.564904	4.499924	-7.683577
250	6	0	1.806721	2.237355	-9.290815
251	1	0	1.330052	3.228801	-9.239590
252	6	0	0.884584	1.084713	-9.245249
253	6	0	1.374108	-0.229022	-9.242230
254	1	0	2.450350	-0.381581	-9.251943
255	6	0	0.497097	-1.308429	-9.245249
256	6	0	-0.885393	-1.075501	-9.242230
257	1	0	-1.555634	-1.931275	-9.251943
258	6	0	-1.381681	0.223715	-9.245249
259	6	0	-0.488715	1.304523	-9.242230
260	1	0	-0.894716	2.312856	-9.251943
261	6	0	-2.840967	0.445989	-9.290815
262	1	0	-3.461250	-0.462541	-9.239590
263	6	0	-4.797245	1.691346	-9.497824
264	1	0	-5.272084	0.700481	-9.379716
265	6	0	-5.322151	2.588417	-8.365413
266	1	0	-4.816732	3.566993	-8.455862
267	6	0	-6.836520	2.785048	-8.495604
268	1	0	-7.179500	3.435412	-7.683577
269	1	0	-7.322428	1.811265	-8.351246
270	6	0	-7.212489	3.363895	-9.859952
271	1	0	-6.781486	4.369292	-9.960873
272	1	0	-8.299389	3.475948	-9.932567

273	6	0	-6.686847	2.476105	-10.989304
274	1	0	-7.189451	1.500299	-10.944791
275	1	0	-6.926481	2.912104	-11.964846
276	6	0	-5.176250	2.275285	-10.863489
277	1	0	-4.656006	3.234605	-10.982625
278	1	0	-4.800618	1.610047	-11.648564
279	6	0	-4.327600	2.601270	-6.259886
280	1	0	-3.940869	3.608689	-6.479097
281	7	0	4.852972	-0.355077	-1.838395
282	7	0	3.479358	-2.914334	-1.765350
283	7	0	0.821499	-5.335198	-7.094045
284	7	0	0.290195	-3.703444	-9.407806
285	6	0	4.059652	1.389894	-4.050820
286	1	0	4.795382	0.629829	-4.301572
287	6	0	3.410642	1.314223	-2.812077
288	6	0	3.739176	0.252794	-1.838331
289	1	0	2.958239	0.041260	-1.092154
290	6	0	5.059814	-1.353937	-0.801041
291	1	0	4.302174	-1.262489	-0.007890
292	6	0	4.872405	-2.759204	-1.396079
293	1	0	5.544145	-2.865031	-2.266860
294	6	0	5.203404	-3.830091	-0.347709
295	1	0	5.088907	-4.817905	-0.809578
296	1	0	4.448225	-3.761668	0.448587
297	6	0	6.603075	-3.650171	0.236872
298	1	0	6.795076	-4.427451	0.984228
299	1	0	7.353975	-3.776140	-0.555575
300	6	0	6.746069	-2.259876	0.854742
301	1	0	7.752519	-2.117906	1.262255
302	1	0	6.044131	-2.163511	1.695249
303	6	0	6.447386	-1.177014	-0.182303
304	1	0	7.194019	-1.201720	-0.987154
305	1	0	6.499443	-0.185477	0.280311
306	6	0	3.191929	-3.307787	-2.935266
307	1	0	3.964394	-3.507602	-3.694455
308	6	0	1.795475	-3.570185	-3.339952
309	6	0	0.737704	-3.278006	-2.466961
310	1	0	0.968037	-2.818812	-1.506725
311	6	0	-0.567171	-3.610814	-2.812077
312	6	0	-0.826142	-4.210709	-4.050820
313	1	0	-1.852244	-4.467837	-4.301572
314	6	0	0.211867	-4.459373	-4.942482
315	6	0	1.528062	-4.143242	-4.578000
316	1	0	2.327329	-4.362454	-5.281291
317	6	0	-0.088965	-5.048447	-6.259886
318	1	0	-1.154782	-5.217238	-6.479097
319	6	0	0.419441	-5.903326	-8.365413
320	1	0	-0.680741	-5.954909	-8.455862
321	6	0	0.933874	-5.000209	-9.497824
322	1	0	2.029407	-4.915999	-9.379716
323	6	0	0.617670	-5.620407	-10.863489
324	1	0	1.005967	-4.962480	-11.648564
325	1	0	-0.473247	-5.649521	-10.982625
326	6	0	1.199053	-7.029032	-10.989304
327	1	0	2.295428	-6.976396	-10.944791
328	1	0	0.941284	-7.454560	-11.964846
329	6	0	0.693026	-7.928146	-9.859952
330	1	0	-0.393175	-8.057585	-9.960873
331	1	0	1.139435	-8.925455	-9.932567

332	6	0	1.006337	-7.313124	-8.495604
333	1	0	2.092613	-7.247042	-8.351246
334	1	0	0.614596	-7.935335	-7.683577
335	6	0	1.034246	-2.683344	-9.290815
336	1	0	2.131198	-2.766260	-9.239590
337	54	0	0.000000	-0.000000	0.896856

Xe@w-to-w D3 cc3-rdim2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	4.331789	1.361362	1.717847
2	7	0	4.635140	-1.527275	1.795463
3	7	0	-0.986920	-4.432121	1.717847
4	7	0	-3.640229	-3.250511	1.795463
5	6	0	1.963969	2.767552	2.421475
6	1	0	2.007197	2.261828	1.458309
7	6	0	3.048910	2.623816	3.297174
8	6	0	4.234253	1.842528	2.886190
9	1	0	5.034918	1.738125	3.635091
10	6	0	5.554403	0.687223	1.327697
11	1	0	6.232102	0.532290	2.186271
12	6	0	5.182925	-0.685096	0.742494
13	1	0	4.427533	-0.484689	-0.034184
14	6	0	6.385604	-1.375464	0.096970
15	1	0	6.046721	-2.311761	-0.359080
16	1	0	7.104406	-1.635458	0.885457
17	6	0	7.048378	-0.486780	-0.955817
18	1	0	7.915593	-1.000158	-1.384278
19	1	0	6.342411	-0.309486	-1.779623
20	6	0	7.458611	0.853435	-0.347396
21	1	0	7.913970	1.499650	-1.105474
22	1	0	8.219161	0.684793	0.427768
23	6	0	6.245709	1.551532	0.264398
24	1	0	5.503878	1.775900	-0.515569
25	1	0	6.526044	2.508295	0.720695
26	6	0	3.378798	-1.704749	1.783916
27	1	0	2.738255	-1.248310	1.015479
28	6	0	2.671032	-2.552911	2.763751
29	6	0	3.233448	-2.862245	4.008400
30	1	0	4.202716	-2.441099	4.263545
31	6	0	2.554349	-3.685739	4.900541
32	6	0	1.318495	-4.237218	4.533324
33	1	0	0.813404	-4.892186	5.238586
34	6	0	0.747837	-3.952342	3.297174
35	6	0	1.414786	-3.084623	2.421475
36	1	0	0.955202	-2.869198	1.458309
37	6	0	-0.521451	-4.588235	2.886190
38	1	0	-1.012199	-5.229429	3.635091
39	6	0	-2.182049	-5.153866	1.327697
40	1	0	-2.655074	-5.663303	2.186271
41	6	0	-3.184773	-4.145996	0.742494
42	1	0	-2.633520	-3.592011	-0.034184
43	6	0	-4.383989	-4.842363	0.096970
44	1	0	-5.025405	-4.080734	-0.359080
45	1	0	-4.968552	-5.334867	0.885457

46	6	0	-3.945753	-5.860685	-0.955817
47	1	0	-3.439228	-5.337946	-1.779623
48	1	0	-4.823959	-6.355026	-1.384278
49	6	0	-2.990209	-6.886064	-0.347396
50	1	0	-3.516532	-7.460398	0.427768
51	1	0	-2.658250	-7.603524	-1.105474
52	6	0	-1.779189	-6.184709	0.264398
53	1	0	-1.213965	-5.654449	-0.515569
54	1	0	-1.090775	-6.905868	0.720695
55	6	0	-3.165755	-2.073750	1.783916
56	1	0	-2.450195	-1.747243	1.015479
57	7	0	2.816908	4.618463	7.054774
58	7	0	1.689700	3.310991	9.361574
59	7	0	2.022552	-3.118818	9.361574
60	7	0	2.591253	-4.748745	7.054774
61	6	0	3.010291	3.260459	4.533324
62	1	0	3.830056	3.150522	5.238586
63	6	0	1.914769	4.055001	4.900541
64	6	0	1.869661	4.708135	6.217158
65	1	0	0.951215	5.275478	6.434012
66	6	0	2.660716	5.294277	8.327391
67	1	0	1.665254	5.766009	8.415584
68	6	0	2.783088	4.259277	9.457126
69	1	0	3.761989	3.759727	9.341139
70	6	0	2.725445	4.949203	10.824660
71	1	0	2.826601	4.189943	11.607781
72	1	0	1.729931	5.396961	10.941416
73	6	0	3.805091	6.023574	10.958026
74	1	0	3.728112	6.512530	11.934858
75	1	0	4.796268	5.551800	10.915642
76	6	0	3.689444	7.051953	9.831471
77	1	0	4.486077	7.799288	9.909288
78	1	0	2.737120	7.590436	9.930795
79	6	0	3.745766	6.368132	8.465004
80	1	0	4.722932	5.888490	8.322454
81	1	0	3.627286	7.096033	7.654979
82	6	0	1.983621	2.082861	9.246763
83	1	0	3.027940	1.736538	9.199162
84	6	0	0.958476	1.020953	9.200574
85	6	0	-0.407181	1.338441	9.198980
86	1	0	-0.696290	2.386335	9.209111
87	6	0	-1.363409	0.319588	9.200574
88	6	0	-0.955534	-1.021850	9.198980
89	1	0	-1.718482	-1.796172	9.209111
90	6	0	0.404934	-1.340541	9.200574
91	6	0	1.362715	-0.316592	9.198980
92	1	0	2.414772	-0.590163	9.209111
93	6	0	0.812000	-2.759296	9.246763
94	1	0	-0.010084	-3.490542	9.199162
95	6	0	2.297099	-4.539863	9.457126
96	1	0	1.375025	-5.137842	9.341139
97	6	0	3.254621	-4.951386	8.327391
98	1	0	4.160883	-4.325157	8.415584
99	6	0	3.642081	-6.427994	8.465004
100	1	0	4.331702	-6.689338	7.654979
101	1	0	2.738115	-7.034424	8.322454
102	6	0	4.262449	-6.721129	9.831471
103	1	0	5.204951	-6.165633	9.930795
104	1	0	4.511343	-7.784701	9.909288

105	6	0	3.314023	-6.307093	10.958026
106	1	0	2.409866	-6.929590	10.915642
107	1	0	3.775960	-6.484904	11.934858
108	6	0	2.923413	-4.834907	10.824660
109	1	0	3.808940	-4.196645	10.941416
110	1	0	2.215297	-4.542880	11.607781
111	6	0	3.142534	-3.973241	6.217158
112	1	0	4.093091	-3.461516	6.434012
113	7	0	-0.994911	4.777786	1.795463
114	7	0	-3.344869	3.070758	1.717847
115	7	0	-5.408160	0.130282	7.054774
116	7	0	-3.712252	-0.192172	9.361574
117	6	0	0.862053	4.231370	4.008400
118	1	0	0.012696	4.860208	4.263545
119	6	0	0.875370	3.589638	2.763751
120	6	0	-0.213043	3.778499	1.783916
121	1	0	-0.288059	2.995553	1.015479
122	6	0	-1.998152	4.831093	0.742494
123	1	0	-1.794013	4.076700	-0.034184
124	6	0	-3.372354	4.466642	1.327697
125	1	0	-3.577027	5.131013	2.186271
126	6	0	-4.466521	4.633177	0.264398
127	1	0	-5.435270	4.397573	0.720695
128	1	0	-4.289914	3.878549	-0.515569
129	6	0	-4.468402	6.032629	-0.347396
130	1	0	-5.255720	6.103874	-1.105474
131	1	0	-4.702628	6.775606	0.427768
132	6	0	-3.102625	6.347464	-0.955817
133	1	0	-3.091634	7.355184	-1.384278
134	1	0	-2.903183	5.647432	-1.779623
135	6	0	-2.001615	6.217827	0.096970
136	1	0	-2.135854	6.970325	0.885457
137	1	0	-1.021317	6.392495	-0.359080
138	6	0	-3.712802	2.745707	2.886190
139	1	0	-4.022719	3.491304	3.635091
140	6	0	-3.796747	1.328525	3.297174
141	6	0	-3.378755	0.317071	2.421475
142	1	0	-2.962400	0.607370	1.458309
143	6	0	-3.546402	-1.036726	2.763751
144	6	0	-4.095501	-1.369125	4.008400
145	1	0	-4.215411	-2.419109	4.263545
146	6	0	-4.469118	-0.369262	4.900541
147	6	0	-4.328786	0.976759	4.533324
148	1	0	-4.643460	1.741665	5.238586
149	6	0	-5.012195	-0.734893	6.217158
150	1	0	-5.044306	-1.813962	6.434012
151	6	0	-5.915336	-0.342891	8.327391
152	1	0	-5.826137	-1.440852	8.415584
153	6	0	-5.080186	0.280586	9.457126
154	1	0	-5.137014	1.378115	9.341139
155	6	0	-5.648858	-0.114296	10.824660
156	1	0	-5.041898	0.352936	11.607781
157	1	0	-5.538871	-1.200316	10.941416
158	6	0	-7.119114	0.283518	10.958026
159	1	0	-7.206134	1.377790	10.915642
160	1	0	-7.504072	-0.027626	11.934858
161	6	0	-7.951893	-0.330824	9.831471
162	1	0	-7.942071	-1.424803	9.930795
163	1	0	-8.997420	-0.014587	9.909288

164	6	0	-7.387847	0.059863	8.465004
165	1	0	-7.461048	1.145935	8.322454
166	1	0	-7.958988	-0.406695	7.654979
167	6	0	-2.795621	0.676436	9.246763
168	1	0	-3.017856	1.754004	9.199162
169	7	0	3.344869	3.070758	-1.717847
170	7	0	0.994911	4.777786	-1.795463
171	7	0	-4.331789	1.361362	-1.717847
172	7	0	-4.635140	-1.527275	-1.795463
173	6	0	3.378755	0.317071	-2.421475
174	1	0	2.962400	0.607370	-1.458309
175	6	0	3.796747	1.328525	-3.297174
176	6	0	3.712802	2.745707	-2.886190
177	1	0	4.022719	3.491304	-3.635091
178	6	0	3.372354	4.466642	-1.327697
179	1	0	3.577027	5.131013	-2.186271
180	6	0	1.998152	4.831093	-0.742494
181	1	0	1.794013	4.076700	0.034184
182	6	0	2.001615	6.217827	-0.096970
183	1	0	1.021317	6.392495	0.359080
184	1	0	2.135854	6.970325	-0.885457
185	6	0	3.102625	6.347464	0.955817
186	1	0	3.091634	7.355184	1.384278
187	1	0	2.903183	5.647432	1.779623
188	6	0	4.468402	6.032629	0.347396
189	1	0	5.255720	6.103874	1.105474
190	1	0	4.702628	6.775606	-0.427768
191	6	0	4.466521	4.633177	-0.264398
192	1	0	4.289914	3.878549	0.515569
193	1	0	5.435270	4.397573	-0.720695
194	6	0	0.213043	3.778499	-1.783916
195	1	0	0.288059	2.995553	-1.015479
196	6	0	-0.875370	3.589638	-2.763751
197	6	0	-0.862053	4.231370	-4.008400
198	1	0	-0.012696	4.860208	-4.263545
199	6	0	-1.914769	4.055001	-4.900541
200	6	0	-3.010291	3.260459	-4.533324
201	1	0	-3.830056	3.150522	-5.238586
202	6	0	-3.048910	2.623816	-3.297174
203	6	0	-1.963969	2.767552	-2.421475
204	1	0	-2.007197	2.261828	-1.458309
205	6	0	-4.234253	1.842528	-2.886190
206	1	0	-5.034918	1.738125	-3.635091
207	6	0	-5.554403	0.687223	-1.327697
208	1	0	-6.232102	0.532290	-2.186271
209	6	0	-5.182925	-0.685096	-0.742494
210	1	0	-4.427533	-0.484689	0.034184
211	6	0	-6.385604	-1.375464	-0.096970
212	1	0	-6.046721	-2.311761	0.359080
213	1	0	-7.104406	-1.635458	-0.885457
214	6	0	-7.048378	-0.486780	0.955817
215	1	0	-6.342411	-0.309486	1.779623
216	1	0	-7.915593	-1.000158	1.384278
217	6	0	-7.458611	0.853435	0.347396
218	1	0	-8.219161	0.684793	-0.427768
219	1	0	-7.913970	1.499650	1.105474
220	6	0	-6.245709	1.551532	-0.264398
221	1	0	-5.503878	1.775900	0.515569
222	1	0	-6.526044	2.508295	-0.720695

223	6	0	-3.378798	-1.704749	-1.783916
224	1	0	-2.738255	-1.248310	-1.015479
225	7	0	5.408160	0.130282	-7.054774
226	7	0	3.712252	-0.192172	-9.361574
227	7	0	-1.689700	3.310991	-9.361574
228	7	0	-2.816908	4.618463	-7.054774
229	6	0	4.328786	0.976759	-4.533324
230	1	0	4.643460	1.741665	-5.238586
231	6	0	4.469118	-0.369262	-4.900541
232	6	0	5.012195	-0.734893	-6.217158
233	1	0	5.044306	-1.813962	-6.434012
234	6	0	5.915336	-0.342891	-8.327391
235	1	0	5.826137	-1.440852	-8.415584
236	6	0	5.080186	0.280586	-9.457126
237	1	0	5.137014	1.378115	-9.341139
238	6	0	5.648858	-0.114296	-10.824660
239	1	0	5.041898	0.352936	-11.607781
240	1	0	5.538871	-1.200316	-10.941416
241	6	0	7.119114	0.283518	-10.958026
242	1	0	7.504072	-0.027626	-11.934858
243	1	0	7.206134	1.377790	-10.915642
244	6	0	7.951893	-0.330824	-9.831471
245	1	0	8.997420	-0.014587	-9.909288
246	1	0	7.942071	-1.424803	-9.930795
247	6	0	7.387847	0.059863	-8.465004
248	1	0	7.461048	1.145935	-8.322454
249	1	0	7.958988	-0.406695	-7.654979
250	6	0	2.795621	0.676436	-9.246763
251	1	0	3.017856	1.754004	-9.199162
252	6	0	1.363409	0.319588	-9.200574
253	6	0	0.955534	-1.021850	-9.198980
254	1	0	1.718482	-1.796172	-9.209111
255	6	0	-0.404934	-1.340541	-9.200574
256	6	0	-1.362715	-0.316592	-9.198980
257	1	0	-2.414772	-0.590163	-9.209111
258	6	0	-0.958476	1.020953	-9.200574
259	6	0	0.407181	1.338441	-9.198980
260	1	0	0.696290	2.386335	-9.209111
261	6	0	-1.983621	2.082861	-9.246763
262	1	0	-3.027940	1.736538	-9.199162
263	6	0	-2.783088	4.259277	-9.457126
264	1	0	-3.761989	3.759727	-9.341139
265	6	0	-2.660716	5.294277	-8.327391
266	1	0	-1.665254	5.766009	-8.415584
267	6	0	-3.745766	6.368132	-8.465004
268	1	0	-3.627286	7.096033	-7.654979
269	1	0	-4.722932	5.888490	-8.322454
270	6	0	-3.689444	7.051953	-9.831471
271	1	0	-2.737120	7.590436	-9.930795
272	1	0	-4.486077	7.799288	-9.909288
273	6	0	-3.805091	6.023574	-10.958026
274	1	0	-4.796268	5.551800	-10.915642
275	1	0	-3.728112	6.512530	-11.934858
276	6	0	-2.725445	4.949203	-10.824660
277	1	0	-1.729931	5.396961	-10.941416
278	1	0	-2.826601	4.189943	-11.607781
279	6	0	-1.869661	4.708135	-6.217158
280	1	0	-0.951215	5.275478	-6.434012
281	7	0	3.640229	-3.250511	-1.795463

282	7	0	0.986920	-4.432121	-1.717847
283	7	0	-2.591253	-4.748745	-7.054774
284	7	0	-2.022552	-3.118818	-9.361574
285	6	0	4.095501	-1.369125	-4.008400
286	1	0	4.215411	-2.419109	-4.263545
287	6	0	3.546402	-1.036726	-2.763751
288	6	0	3.165755	-2.073750	-1.783916
289	1	0	2.450195	-1.747243	-1.015479
290	6	0	3.184773	-4.145996	-0.742494
291	1	0	2.633520	-3.592011	0.034184
292	6	0	2.182049	-5.153866	-1.327697
293	1	0	2.655074	-5.663303	-2.186271
294	6	0	1.779189	-6.184709	-0.264398
295	1	0	1.090775	-6.905868	-0.720695
296	1	0	1.213965	-5.654449	0.515569
297	6	0	2.990209	-6.886064	0.347396
298	1	0	2.658250	-7.603524	1.105474
299	1	0	3.516532	-7.460398	-0.427768
300	6	0	3.945753	-5.860685	0.955817
301	1	0	4.823959	-6.355026	1.384278
302	1	0	3.439228	-5.337946	1.779623
303	6	0	4.383989	-4.842363	-0.096970
304	1	0	4.968552	-5.334867	-0.885457
305	1	0	5.025405	-4.080734	0.359080
306	6	0	0.521451	-4.588235	-2.886190
307	1	0	1.012199	-5.229429	-3.635091
308	6	0	-0.747837	-3.952342	-3.297174
309	6	0	-1.414786	-3.084623	-2.421475
310	1	0	-0.955202	-2.869198	-1.458309
311	6	0	-2.671032	-2.552911	-2.763751
312	6	0	-3.233448	-2.862245	-4.008400
313	1	0	-4.202716	-2.441099	-4.263545
314	6	0	-2.554349	-3.685739	-4.900541
315	6	0	-1.318495	-4.237218	-4.533324
316	1	0	-0.813404	-4.892186	-5.238586
317	6	0	-3.142534	-3.973241	-6.217158
318	1	0	-4.093091	-3.461516	-6.434012
319	6	0	-3.254621	-4.951386	-8.327391
320	1	0	-4.160883	-4.325157	-8.415584
321	6	0	-2.297099	-4.539863	-9.457126
322	1	0	-1.375025	-5.137842	-9.341139
323	6	0	-2.923413	-4.834907	-10.824660
324	1	0	-2.215297	-4.542880	-11.607781
325	1	0	-3.808940	-4.196645	-10.941416
326	6	0	-3.314023	-6.307093	-10.958026
327	1	0	-2.409866	-6.929590	-10.915642
328	1	0	-3.775960	-6.484904	-11.934858
329	6	0	-4.262449	-6.721129	-9.831471
330	1	0	-5.204951	-6.165633	-9.930795
331	1	0	-4.511343	-7.784701	-9.909288
332	6	0	-3.642081	-6.427994	-8.465004
333	1	0	-2.738115	-7.034424	-8.322454
334	1	0	-4.331702	-6.689338	-7.654979
335	6	0	-0.812000	-2.759296	-9.246763
336	1	0	0.010083	-3.490542	-9.199162
337	54	0	0.000000	0.000000	0.000000

3Xe@w-to-w D3 cc3-rdim3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	4.320279	1.367271	1.694773
2	7	0	4.605178	-1.512032	1.781285
3	7	0	-0.976048	-4.425107	1.694773
4	7	0	-3.612047	-3.232185	1.781285
5	6	0	1.936130	2.733932	2.417247
6	1	0	1.983728	2.241843	1.447070
7	6	0	3.015036	2.574186	3.297837
8	6	0	4.205322	1.804432	2.878769
9	1	0	4.992550	1.667624	3.636517
10	6	0	5.539354	0.690033	1.301193
11	1	0	6.218341	0.531144	2.158126
12	6	0	5.157564	-0.682296	0.721539
13	1	0	4.403643	-0.480916	-0.056516
14	6	0	6.354320	-1.383890	0.077906
15	1	0	6.008437	-2.319620	-0.373958
16	1	0	7.073370	-1.644759	0.865863
17	6	0	7.018800	-0.503740	-0.980589
18	1	0	7.881240	-1.024219	-1.410110
19	1	0	6.310553	-0.325985	-1.802524
20	6	0	7.439220	0.836684	-0.379206
21	1	0	7.897176	1.476296	-1.141292
22	1	0	8.200903	0.665916	0.394398
23	6	0	6.233129	1.546295	0.233601
24	1	0	5.490336	1.773557	-0.544552
25	1	0	6.522151	2.502337	0.685863
26	6	0	3.346830	-1.673621	1.775944
27	1	0	2.709131	-1.219735	1.003745
28	6	0	2.634335	-2.508777	2.763108
29	6	0	3.189987	-2.800841	4.015132
30	1	0	4.159350	-2.378781	4.268462
31	6	0	2.507335	-3.616140	4.912428
32	6	0	1.271484	-4.169645	4.546642
33	1	0	0.765704	-4.820415	5.255266
34	6	0	0.721793	-3.898191	3.297837
35	6	0	1.399590	-3.043704	2.417247
36	1	0	0.949629	-2.838880	1.447070
37	6	0	-0.539977	-4.544132	2.878769
38	1	0	-1.052070	-5.157487	3.636517
39	6	0	-2.172091	-5.142238	1.301193
40	1	0	-2.649186	-5.650813	2.158126
41	6	0	-3.169668	-4.125434	0.721539
42	1	0	-2.618307	-3.573209	-0.056516
43	6	0	-4.375644	-4.811058	0.077906
44	1	0	-5.013068	-4.043649	-0.373958
45	1	0	-4.961088	-5.303339	0.865863
46	6	0	-3.945652	-5.826589	-0.980589
47	1	0	-3.437588	-5.302107	-1.802524
48	1	0	-4.827620	-6.313245	-1.410110
49	6	0	-2.995020	-6.860896	-0.379206
50	1	0	-3.523751	-7.435148	0.394398
51	1	0	-2.670078	-7.577303	-1.141292
52	6	0	-1.777434	-6.171196	0.233601
53	1	0	-1.209222	-5.641549	-0.544552
54	1	0	-1.093988	-6.899517	0.685863

55	6	0	-3.122813	-2.061629	1.775944
56	1	0	-2.410887	-1.736309	1.003745
57	7	0	2.806216	4.588689	7.044205
58	7	0	1.707319	3.292549	9.359647
59	7	0	1.997772	-3.124856	9.359647
60	7	0	2.570813	-4.724599	7.044205
61	6	0	2.975276	3.185960	4.546642
62	1	0	3.791750	3.073327	5.255266
63	6	0	1.878002	3.979486	4.912428
64	6	0	1.834474	4.638650	6.231772
65	1	0	0.905466	5.181314	6.465732
66	6	0	2.662756	5.271510	8.314291
67	1	0	1.666414	5.739318	8.412598
68	6	0	2.800793	4.240659	9.446522
69	1	0	3.779034	3.742354	9.320287
70	6	0	2.756776	4.934573	10.812146
71	1	0	2.869917	4.178542	11.596732
72	1	0	1.761158	5.379233	10.939057
73	6	0	3.834269	6.013288	10.928475
74	1	0	3.767226	6.505612	11.904347
75	1	0	4.826523	5.544795	10.876120
76	6	0	3.701950	7.037340	9.799736
77	1	0	4.496606	7.787876	9.866061
78	1	0	2.748898	7.572818	9.908223
79	6	0	3.745191	6.349315	8.434896
80	1	0	4.722263	5.872618	8.282547
81	1	0	3.614804	7.074159	7.624000
82	6	0	1.998295	2.067901	9.207287
83	1	0	3.041038	1.721957	9.132142
84	6	0	0.969041	1.010915	9.151839
85	6	0	-0.394254	1.335277	9.149115
86	1	0	-0.678674	2.384409	9.162378
87	6	0	-1.359999	0.333757	9.151839
88	6	0	-0.959257	-1.009072	9.149115
89	1	0	-1.725622	-1.779953	9.162378
90	6	0	0.390958	-1.344672	9.151839
91	6	0	1.353511	-0.326204	9.149115
92	1	0	2.404296	-0.604456	9.162378
93	6	0	0.791707	-2.764525	9.207287
94	1	0	-0.029260	-3.494595	9.132142
95	6	0	2.272122	-4.545887	9.446522
96	1	0	1.351457	-5.143916	9.320287
97	6	0	3.233884	-4.941769	8.314291
98	1	0	4.137188	-4.312816	8.412598
99	6	0	3.626073	-6.418088	8.434896
100	1	0	4.319000	-6.667591	7.624000
101	1	0	2.724705	-7.025909	8.282547
102	6	0	4.243540	-6.724653	9.799736
103	1	0	5.183804	-6.167024	9.908223
104	1	0	4.496196	-7.788113	9.866061
105	6	0	3.290526	-6.327218	10.928475
106	1	0	2.388672	-6.952289	10.876120
107	1	0	3.750412	-6.515319	11.904347
108	6	0	2.895078	-4.854724	10.812146
109	1	0	3.777974	-4.214824	10.939057
110	1	0	2.183765	-4.574692	11.596732
111	6	0	3.099952	-3.908026	6.231772
112	1	0	4.034417	-3.374813	6.465732
113	7	0	-0.993131	4.744217	1.781285

114	7	0	-3.344231	3.057836	1.694773
115	7	0	-5.377029	0.135910	7.044205
116	7	0	-3.705091	-0.167693	9.359647
117	6	0	0.830606	4.163030	4.015132
118	1	0	-0.019590	4.791493	4.268462
119	6	0	0.855497	3.535790	2.763108
120	6	0	-0.224017	3.735250	1.775944
121	1	0	-0.298244	2.956044	1.003745
122	6	0	-1.987896	4.807729	0.721539
123	1	0	-1.785336	4.054125	-0.056516
124	6	0	-3.367263	4.452205	1.301193
125	1	0	-3.569155	5.119669	2.158126
126	6	0	-4.455695	4.624900	0.233601
127	1	0	-5.428163	4.397180	0.685863
128	1	0	-4.281113	3.867992	-0.544552
129	6	0	-4.444200	6.024211	-0.379206
130	1	0	-5.227098	6.101007	-1.141292
131	1	0	-4.677152	6.769232	0.394398
132	6	0	-3.073148	6.330329	-0.980589
133	1	0	-3.053620	7.337463	-1.410110
134	1	0	-2.872965	5.628092	-1.802524
135	6	0	-1.978676	6.194948	0.077906
136	1	0	-2.112282	6.948098	0.865863
137	1	0	-0.995369	6.363269	-0.373958
138	6	0	-3.665345	2.739700	2.878769
139	1	0	-3.940480	3.489863	3.636517
140	6	0	-3.736828	1.324005	3.297837
141	6	0	-3.335720	0.309772	2.417247
142	1	0	-2.933357	0.597037	1.447070
143	6	0	-3.489832	-1.027013	2.763108
144	6	0	-4.020593	-1.362189	4.015132
145	1	0	-4.139760	-2.412712	4.268462
146	6	0	-4.385337	-0.363346	4.912428
147	6	0	-4.246761	0.983685	4.546642
148	1	0	-4.557454	1.747088	5.255266
149	6	0	-4.934426	-0.730624	6.231772
150	1	0	-4.939882	-1.806501	6.465732
151	6	0	-5.896640	-0.329741	8.314291
152	1	0	-5.803602	-1.426502	8.412598
153	6	0	-5.072915	0.305228	9.446522
154	1	0	-5.130491	1.401562	9.320287
155	6	0	-5.651854	-0.079849	10.812146
156	1	0	-5.053682	0.396150	11.596732
157	1	0	-5.539131	-1.164409	10.939057
158	6	0	-7.124795	0.313930	10.928475
159	1	0	-7.215195	1.407494	10.876120
160	1	0	-7.517638	0.009707	11.904347
161	6	0	-7.945490	-0.312687	9.799736
162	1	0	-7.932702	-1.405794	9.908223
163	1	0	-8.992801	0.000237	9.866061
164	6	0	-7.371264	0.068773	8.434896
165	1	0	-7.446968	1.153291	8.282547
166	1	0	-7.933803	-0.406568	7.624000
167	6	0	-2.790002	0.696624	9.207287
168	1	0	-3.011778	1.772638	9.132142
169	7	0	3.344231	3.057836	-1.694773
170	7	0	0.993131	4.744217	-1.781285
171	7	0	-4.320279	1.367271	-1.694773
172	7	0	-4.605178	-1.512032	-1.781285

173	6	0	3.335720	0.309772	-2.417247
174	1	0	2.933357	0.597037	-1.447070
175	6	0	3.736828	1.324005	-3.297837
176	6	0	3.665345	2.739700	-2.878769
177	1	0	3.940480	3.489863	-3.636517
178	6	0	3.367263	4.452205	-1.301193
179	1	0	3.569155	5.119669	-2.158126
180	6	0	1.987896	4.807729	-0.721539
181	1	0	1.785336	4.054125	0.056516
182	6	0	1.978676	6.194948	-0.077906
183	1	0	0.995369	6.363269	0.373958
184	1	0	2.112282	6.948098	-0.865863
185	6	0	3.073148	6.330329	0.980589
186	1	0	3.053620	7.337463	1.410110
187	1	0	2.872965	5.628092	1.802524
188	6	0	4.444200	6.024211	0.379206
189	1	0	5.227098	6.101007	1.141292
190	1	0	4.677152	6.769232	-0.394398
191	6	0	4.455695	4.624900	-0.233601
192	1	0	4.281113	3.867992	0.544552
193	1	0	5.428163	4.397180	-0.685863
194	6	0	0.224017	3.735250	-1.775944
195	1	0	0.298244	2.956044	-1.003745
196	6	0	-0.855497	3.535790	-2.763108
197	6	0	-0.830606	4.163030	-4.015132
198	1	0	0.019590	4.791493	-4.268462
199	6	0	-1.878002	3.979486	-4.912428
200	6	0	-2.975276	3.185960	-4.546642
201	1	0	-3.791750	3.073327	-5.255266
202	6	0	-3.015036	2.574186	-3.297837
203	6	0	-1.936130	2.733932	-2.417247
204	1	0	-1.983728	2.241843	-1.447070
205	6	0	-4.205322	1.804432	-2.878769
206	1	0	-4.992550	1.667624	-3.636517
207	6	0	-5.539354	0.690033	-1.301193
208	1	0	-6.218341	0.531144	-2.158126
209	6	0	-5.157564	-0.682296	-0.721539
210	1	0	-4.403643	-0.480916	0.056516
211	6	0	-6.354320	-1.383890	-0.077906
212	1	0	-6.008437	-2.319620	0.373958
213	1	0	-7.073370	-1.644759	-0.865863
214	6	0	-7.018800	-0.503740	0.980589
215	1	0	-6.310553	-0.325985	1.802524
216	1	0	-7.881240	-1.024219	1.410110
217	6	0	-7.439220	0.836684	0.379206
218	1	0	-8.200903	0.665916	-0.394398
219	1	0	-7.897176	1.476296	1.141292
220	6	0	-6.233129	1.546295	-0.233601
221	1	0	-5.490336	1.773557	0.544552
222	1	0	-6.522151	2.502337	-0.685863
223	6	0	-3.346830	-1.673621	-1.775944
224	1	0	-2.709131	-1.219735	-1.003745
225	7	0	5.377029	0.135910	-7.044205
226	7	0	3.705091	-0.167693	-9.359647
227	7	0	-1.707319	3.292549	-9.359647
228	7	0	-2.806216	4.588689	-7.044205
229	6	0	4.246761	0.983685	-4.546642
230	1	0	4.557454	1.747088	-5.255266
231	6	0	4.385337	-0.363346	-4.912428

232	6	0	4.934426	-0.730624	-6.231772
233	1	0	4.939882	-1.806501	-6.465732
234	6	0	5.896640	-0.329741	-8.314291
235	1	0	5.803602	-1.426502	-8.412598
236	6	0	5.072915	0.305228	-9.446522
237	1	0	5.130491	1.401562	-9.320287
238	6	0	5.651854	-0.079849	-10.812146
239	1	0	5.053682	0.396150	-11.596732
240	1	0	5.539131	-1.164409	-10.939057
241	6	0	7.124795	0.313930	-10.928475
242	1	0	7.517638	0.009707	-11.904347
243	1	0	7.215195	1.407494	-10.876120
244	6	0	7.945490	-0.312687	-9.799736
245	1	0	8.992801	0.000237	-9.866061
246	1	0	7.932702	-1.405794	-9.908223
247	6	0	7.371264	0.068773	-8.434896
248	1	0	7.446968	1.153291	-8.282547
249	1	0	7.933803	-0.406568	-7.624000
250	6	0	2.790002	0.696624	-9.207287
251	1	0	3.011778	1.772638	-9.132142
252	6	0	1.359999	0.333757	-9.151839
253	6	0	0.959257	-1.009072	-9.149115
254	1	0	1.725622	-1.779953	-9.162378
255	6	0	-0.390958	-1.344672	-9.151839
256	6	0	-1.353511	-0.326204	-9.149115
257	1	0	-2.404296	-0.604456	-9.162378
258	6	0	-0.969041	1.010915	-9.151839
259	6	0	0.394254	1.335277	-9.149115
260	1	0	0.678674	2.384409	-9.162378
261	6	0	-1.998295	2.067901	-9.207287
262	1	0	-3.041038	1.721957	-9.132142
263	6	0	-2.800793	4.240659	-9.446522
264	1	0	-3.779034	3.742354	-9.320287
265	6	0	-2.662756	5.271510	-8.314291
266	1	0	-1.666414	5.739318	-8.412598
267	6	0	-3.745191	6.349315	-8.434896
268	1	0	-3.614804	7.074159	-7.624000
269	1	0	-4.722263	5.872618	-8.282547
270	6	0	-3.701950	7.037340	-9.799736
271	1	0	-2.748898	7.572818	-9.908223
272	1	0	-4.496606	7.787876	-9.866061
273	6	0	-3.834269	6.013288	-10.928475
274	1	0	-4.826523	5.544795	-10.876120
275	1	0	-3.767226	6.505612	-11.904347
276	6	0	-2.756776	4.934573	-10.812146
277	1	0	-1.761158	5.379233	-10.939057
278	1	0	-2.869917	4.178542	-11.596732
279	6	0	-1.834474	4.638650	-6.231772
280	1	0	-0.905466	5.181314	-6.465732
281	7	0	3.612047	-3.232185	-1.781285
282	7	0	0.976048	-4.425107	-1.694773
283	7	0	-2.570813	-4.724599	-7.044205
284	7	0	-1.997772	-3.124856	-9.359647
285	6	0	4.020593	-1.362189	-4.015132
286	1	0	4.139760	-2.412712	-4.268462
287	6	0	3.489832	-1.027013	-2.763108
288	6	0	3.122813	-2.061629	-1.775944
289	1	0	2.410887	-1.736309	-1.003745
290	6	0	3.169668	-4.125434	-0.721539

291	1	0	2.618307	-3.573209	0.056516
292	6	0	2.172091	-5.142238	-1.301193
293	1	0	2.649186	-5.650813	-2.158126
294	6	0	1.777434	-6.171196	-0.233601
295	1	0	1.093988	-6.899517	-0.685863
296	1	0	1.209222	-5.641549	0.544552
297	6	0	2.995020	-6.860896	0.379206
298	1	0	2.670078	-7.577303	1.141292
299	1	0	3.523751	-7.435148	-0.394398
300	6	0	3.945652	-5.826589	0.980589
301	1	0	4.827620	-6.313245	1.410110
302	1	0	3.437588	-5.302107	1.802524
303	6	0	4.375644	-4.811058	-0.077906
304	1	0	4.961088	-5.303339	-0.865863
305	1	0	5.013068	-4.043649	0.373958
306	6	0	0.539977	-4.544132	-2.878769
307	1	0	1.052070	-5.157487	-3.636517
308	6	0	-0.721793	-3.898191	-3.297837
309	6	0	-1.399590	-3.043704	-2.417247
310	1	0	-0.949629	-2.838880	-1.447070
311	6	0	-2.634335	-2.508777	-2.763108
312	6	0	-3.189987	-2.800841	-4.015132
313	1	0	-4.159350	-2.378781	-4.268462
314	6	0	-2.507335	-3.616140	-4.912428
315	6	0	-1.271484	-4.169645	-4.546642
316	1	0	-0.765704	-4.820415	-5.255266
317	6	0	-3.099952	-3.908026	-6.231772
318	1	0	-4.034417	-3.374813	-6.465732
319	6	0	-3.233884	-4.941769	-8.314291
320	1	0	-4.137188	-4.312816	-8.412598
321	6	0	-2.272122	-4.545887	-9.446522
322	1	0	-1.351457	-5.143916	-9.320287
323	6	0	-2.895078	-4.854724	-10.812146
324	1	0	-2.183765	-4.574692	-11.596732
325	1	0	-3.777974	-4.214824	-10.939057
326	6	0	-3.290526	-6.327218	-10.928475
327	1	0	-2.388672	-6.952289	-10.876120
328	1	0	-3.750412	-6.515319	-11.904347
329	6	0	-4.243540	-6.724653	-9.799736
330	1	0	-5.183804	-6.167024	-9.908223
331	1	0	-4.496196	-7.788113	-9.866061
332	6	0	-3.626073	-6.418088	-8.434896
333	1	0	-2.724705	-7.025909	-8.282547
334	1	0	-4.319000	-6.667591	-7.624000
335	6	0	-0.791707	-2.764525	-9.207287
336	1	0	0.029260	-3.494595	-9.132142
337	54	0	0.000000	-0.000000	0.000000
338	54	0	0.000000	0.000000	4.234974
339	54	0	0.000000	0.000000	-4.234974

Xe@w-to-w(R/S) S6 cc3-rdim5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-0.892505	4.680805	1.934157
2	7	0	1.945163	4.285446	1.644991

3	7	0	4.836817	2.349056	7.041404
4	7	0	3.448116	1.357058	9.361995
5	6	0	-2.545778	3.474144	3.975839
6	1	0	-2.025498	4.393746	4.231811
7	6	0	-2.322114	2.906839	2.713801
8	6	0	-1.449090	3.561383	1.718144
9	1	0	-1.364837	3.046827	0.748121
10	6	0	-0.124211	5.257691	0.845700
11	1	0	-0.040992	4.560515	-0.001989
12	6	0	1.302699	5.550577	1.334371
13	1	0	1.222993	6.192515	2.229988
14	6	0	2.108206	6.275970	0.251275
15	1	0	3.104710	6.506198	0.645758
16	1	0	2.249516	5.587492	-0.593372
17	6	0	1.405297	7.545109	-0.230609
18	1	0	1.999581	8.021526	-1.017286
19	1	0	1.335035	8.264394	0.597185
20	6	0	0.000000	7.219884	-0.737287
21	1	0	-0.510398	8.129520	-1.071345
22	1	0	0.073441	6.553798	-1.609030
23	6	0	-0.817624	6.531318	0.355174
24	1	0	-0.960502	7.206750	1.209320
25	1	0	-1.810104	6.255766	-0.015854
26	6	0	2.267364	4.059383	2.851104
27	1	0	2.099254	4.800057	3.647525
28	6	0	2.919205	2.799358	3.262098
29	6	0	2.986304	1.716568	2.375474
30	1	0	2.494569	1.805577	1.411033
31	6	0	3.678453	0.557590	2.713801
32	6	0	4.281586	0.467636	3.975839
33	1	0	4.817845	-0.442740	4.231811
34	6	0	4.186291	1.516467	4.879188
35	6	0	3.510079	2.690212	4.514589
36	1	0	3.470137	3.508926	5.228371
37	6	0	4.821038	1.395117	6.206633
38	1	0	5.288164	0.422072	6.424519
39	6	0	5.504403	2.127200	8.308865
40	1	0	5.875555	1.089843	8.394376
41	6	0	4.498405	2.352883	9.448494
42	1	0	4.095776	3.375577	9.333994
43	6	0	5.193446	2.231615	10.809198
44	1	0	4.455638	2.407101	11.599656
45	1	0	5.544133	1.197724	10.924256
46	6	0	6.368515	3.202561	10.927753
47	1	0	5.994759	4.234653	10.884271
48	1	0	6.856647	3.082631	11.900667
49	6	0	7.370080	2.982746	9.792615
50	1	0	7.814070	1.982820	9.891721
51	1	0	8.192253	3.702963	9.859779
52	6	0	6.682077	3.100457	8.432136
53	1	0	6.300340	4.119739	8.288883
54	1	0	7.386947	2.907405	7.616110
55	6	0	2.255808	1.768695	9.236901
56	1	0	2.012814	2.841942	9.179005
57	7	0	-4.683887	-0.458162	1.644991
58	7	0	-3.607444	-3.113335	1.934157
59	7	0	2.738724	-3.827284	1.644991
60	7	0	4.499949	-1.567470	1.934157
61	6	0	-2.979743	1.727931	2.375474

62	1	0	-2.810960	1.257572	1.411033
63	6	0	-3.883918	1.128427	3.262098
64	6	0	-4.649211	-0.066097	2.851104
65	1	0	-5.206598	-0.582021	3.647525
66	6	0	-5.458290	-1.647118	1.334371
67	1	0	-5.974372	-2.037114	2.229988
68	6	0	-4.491188	-2.736415	0.845700
69	1	0	-3.929026	-2.315758	-0.001989
70	6	0	-5.247475	-3.973742	0.355174
71	1	0	-4.512600	-4.695479	-0.015854
72	1	0	-5.760978	-4.435194	1.209320
73	6	0	-6.252603	-3.609942	-0.737287
74	1	0	-6.785172	-4.506778	-1.071345
75	1	0	-5.712476	-3.213297	-1.609030
76	6	0	-7.236905	-2.555532	-0.230609
77	1	0	-7.946636	-2.279075	-1.017286
78	1	0	-7.824693	-2.976023	0.597185
79	6	0	-6.489252	-1.312225	0.251275
80	1	0	-5.963668	-0.845608	-0.593372
81	1	0	-7.186888	-0.564341	0.645758
82	6	0	-2.359703	-3.035640	1.718144
83	1	0	-1.956211	-2.705397	0.748121
84	6	0	-1.356339	-3.464429	2.713801
85	6	0	-1.735808	-3.941780	3.975839
86	1	0	-2.792347	-3.951006	4.231811
87	6	0	-0.779847	-4.383668	4.879188
88	6	0	0.574752	-4.384924	4.514589
89	1	0	1.303751	-4.759690	5.228371
90	6	0	0.964713	-3.927785	3.262098
91	6	0	-0.006561	-3.444499	2.375474
92	1	0	0.316391	-3.063149	1.411033
93	6	0	2.381847	-3.993286	2.851104
94	1	0	3.107344	-4.218036	3.647525
95	6	0	4.155591	-3.903459	1.334371
96	1	0	4.751379	-4.155401	2.229988
97	6	0	4.615399	-2.521276	0.845700
98	1	0	3.970018	-2.244757	-0.001989
99	6	0	6.065099	-2.557576	0.355174
100	1	0	6.322704	-1.560287	-0.015854
101	1	0	6.721480	-2.771556	1.209320
102	6	0	6.252603	-3.609942	-0.737287
103	1	0	5.639035	-3.340501	-1.609030
104	1	0	7.295570	-3.622742	-1.071345
105	6	0	5.831608	-4.989577	-0.230609
106	1	0	6.489658	-5.288371	0.597185
107	1	0	5.947055	-5.742451	-1.017286
108	6	0	4.381046	-4.963745	0.251275
109	1	0	3.714152	-4.741884	-0.593372
110	1	0	4.082178	-5.941857	0.645758
111	6	0	3.808793	-0.525743	1.718144
112	1	0	3.321048	-0.341430	0.748121
113	7	0	-4.452751	3.014278	7.041404
114	7	0	-2.899305	2.307627	9.361995
115	7	0	-0.548811	-3.664685	9.361995
116	7	0	-0.384066	-5.363334	7.041404
117	6	0	-4.084831	1.694712	4.514589
118	1	0	-4.773888	1.250764	5.228371
119	6	0	-3.406444	2.867201	4.879188
120	6	0	-3.618726	3.477583	6.206633

121	1	0	-3.009607	4.368648	6.424519
122	6	0	-4.594411	3.703353	8.308865
123	1	0	-3.881609	4.543458	8.394376
124	6	0	-4.286859	2.719292	9.448494
125	1	0	-4.971223	1.859258	9.333994
126	6	0	-4.529358	3.381849	10.809198
127	1	0	-4.312430	2.655145	11.599656
128	1	0	-3.809326	4.202498	10.924256
129	6	0	-5.957757	3.914015	10.927753
130	1	0	-6.097960	4.396715	11.900667
131	1	0	-6.664697	3.074287	10.884271
132	6	0	-6.268174	4.891304	9.792615
133	1	0	-7.302987	5.243218	9.859779
134	1	0	-5.624207	5.775773	9.891721
135	6	0	-6.026113	4.236620	8.432136
136	1	0	-6.717969	3.396385	8.288883
137	1	0	-6.211360	4.943581	7.616110
138	6	0	-2.659639	1.069240	9.236901
139	1	0	-3.467601	0.322177	9.179005
140	6	0	-1.304443	0.505247	9.178365
141	6	0	-0.191059	1.365368	9.185449
142	1	0	-0.364975	2.438875	9.203014
143	6	0	1.089778	0.877057	9.178365
144	6	0	1.277973	-0.517222	9.185449
145	1	0	2.294615	-0.903360	9.203014
146	6	0	0.214665	-1.382304	9.178365
147	6	0	-1.086914	-0.848146	9.185449
148	1	0	-1.929640	-1.535515	9.203014
149	6	0	0.403831	-2.837935	9.236901
150	1	0	1.454787	-3.164119	9.179005
151	6	0	-0.211546	-5.072175	9.448494
152	1	0	0.875447	-5.234835	9.333994
153	6	0	-0.909992	-5.830553	8.308865
154	1	0	-1.993946	-5.633301	8.394376
155	6	0	-0.655964	-7.337077	8.432136
156	1	0	-1.175587	-7.850986	7.616110
157	1	0	0.417629	-7.516124	8.288883
158	6	0	-1.101906	-7.874050	9.792615
159	1	0	-2.189863	-7.758593	9.891721
160	1	0	-0.889266	-8.946181	9.859779
161	6	0	-0.410758	-7.116576	10.927753
162	1	0	0.669938	-7.308940	10.884271
163	1	0	-0.758687	-7.479346	11.900667
164	6	0	-0.664088	-5.613464	10.809198
165	1	0	-1.734807	-5.400222	10.924256
166	1	0	-0.143208	-5.062246	11.599656
167	6	0	-1.202312	-4.872700	6.206633
168	1	0	-2.278557	-4.790720	6.424519
169	7	0	3.607444	3.113335	-1.934157
170	7	0	4.683887	0.458162	-1.644991
171	7	0	4.452751	-3.014278	-7.041404
172	7	0	2.899305	-2.307627	-9.361995
173	6	0	1.735808	3.941780	-3.975839
174	1	0	2.792347	3.951006	-4.231811
175	6	0	1.356339	3.464429	-2.713801
176	6	0	2.359703	3.035640	-1.718144
177	1	0	1.956211	2.705397	-0.748121
178	6	0	4.491188	2.736415	-0.845700
179	1	0	3.929026	2.315758	0.001989

180	6	0	5.458290	1.647118	-1.334371
181	1	0	5.974372	2.037114	-2.229988
182	6	0	6.489252	1.312225	-0.251275
183	1	0	7.186888	0.564341	-0.645758
184	1	0	5.963668	0.845608	0.593372
185	6	0	7.236905	2.555532	0.230609
186	1	0	7.946636	2.279075	1.017286
187	1	0	7.824693	2.976023	-0.597185
188	6	0	6.252603	3.609942	0.737287
189	1	0	6.785172	4.506778	1.071345
190	1	0	5.712476	3.213297	1.609030
191	6	0	5.247475	3.973742	-0.355174
192	1	0	5.760978	4.435194	-1.209320
193	1	0	4.512600	4.695479	0.015854
194	6	0	4.649211	0.066097	-2.851104
195	1	0	5.206598	0.582021	-3.647525
196	6	0	3.883918	-1.128427	-3.262098
197	6	0	2.979743	-1.727931	-2.375474
198	1	0	2.810960	-1.257572	-1.411033
199	6	0	2.322114	-2.906839	-2.713801
200	6	0	2.545778	-3.474144	-3.975839
201	1	0	2.025498	-4.393746	-4.231811
202	6	0	3.406444	-2.867201	-4.879188
203	6	0	4.084831	-1.694712	-4.514589
204	1	0	4.773888	-1.250764	-5.228371
205	6	0	3.618726	-3.477583	-6.206633
206	1	0	3.009607	-4.368648	-6.424519
207	6	0	4.594411	-3.703353	-8.308865
208	1	0	3.881609	-4.543458	-8.394376
209	6	0	4.286859	-2.719292	-9.448494
210	1	0	4.971223	-1.859258	-9.333994
211	6	0	4.529358	-3.381849	-10.809198
212	1	0	4.312430	-2.655145	-11.599656
213	1	0	3.809326	-4.202498	-10.924256
214	6	0	5.957757	-3.914015	-10.927753
215	1	0	6.664697	-3.074287	-10.884271
216	1	0	6.097960	-4.396715	-11.900667
217	6	0	6.268174	-4.891304	-9.792615
218	1	0	5.624207	-5.775773	-9.891721
219	1	0	7.302987	-5.243218	-9.859779
220	6	0	6.026113	-4.236620	-8.432136
221	1	0	6.717969	-3.396385	-8.288883
222	1	0	6.211360	-4.943581	-7.616110
223	6	0	2.659639	-1.069240	-9.236901
224	1	0	3.467601	-0.322177	-9.179005
225	7	0	-2.738724	3.827284	-1.644991
226	7	0	-4.499949	1.567470	-1.934157
227	7	0	-1.945163	-4.285446	-1.644991
228	7	0	0.892505	-4.680805	-1.934157
229	6	0	0.006561	3.444499	-2.375474
230	1	0	-0.316391	3.063149	-1.411033
231	6	0	-0.964713	3.927785	-3.262098
232	6	0	-2.381847	3.993286	-2.851104
233	1	0	-3.107344	4.218036	-3.647525
234	6	0	-4.155591	3.903459	-1.334371
235	1	0	-4.751379	4.155401	-2.229988
236	6	0	-4.615399	2.521276	-0.845700
237	1	0	-3.970018	2.244757	0.001989
238	6	0	-6.065099	2.557576	-0.355174

239	1	0	-6.322704	1.560287	0.015854
240	1	0	-6.721480	2.771556	-1.209320
241	6	0	-6.252603	3.609942	0.737287
242	1	0	-7.295570	3.622742	1.071345
243	1	0	-5.639035	3.340501	1.609030
244	6	0	-5.831608	4.989577	0.230609
245	1	0	-5.947055	5.742451	1.017286
246	1	0	-6.489658	5.288371	-0.597185
247	6	0	-4.381046	4.963745	-0.251275
248	1	0	-3.714152	4.741884	0.593372
249	1	0	-4.082178	5.941857	-0.645758
250	6	0	-3.808793	0.525743	-1.718144
251	1	0	-3.321048	0.341430	-0.748121
252	6	0	-3.678453	-0.557590	-2.713801
253	6	0	-4.281586	-0.467636	-3.975839
254	1	0	-4.817845	0.442740	-4.231811
255	6	0	-4.186291	-1.516467	-4.879188
256	6	0	-3.510079	-2.690212	-4.514589
257	1	0	-3.470137	-3.508926	-5.228371
258	6	0	-2.919205	-2.799358	-3.262098
259	6	0	-2.986304	-1.716568	-2.375474
260	1	0	-2.494569	-1.805577	-1.411033
261	6	0	-2.267364	-4.059383	-2.851104
262	1	0	-2.099254	-4.800057	-3.647525
263	6	0	-1.302699	-5.550577	-1.334371
264	1	0	-1.222993	-6.192515	-2.229988
265	6	0	0.124211	-5.257691	-0.845700
266	1	0	0.040992	-4.560515	0.001989
267	6	0	0.817624	-6.531318	-0.355174
268	1	0	1.810104	-6.255766	0.015854
269	1	0	0.960502	-7.206750	-1.209320
270	6	0	-0.000000	-7.219884	0.737287
271	1	0	-0.073441	-6.553798	1.609030
272	1	0	0.510398	-8.129520	1.071345
273	6	0	-1.405297	-7.545109	0.230609
274	1	0	-1.335035	-8.264394	-0.597185
275	1	0	-1.999581	-8.021526	1.017286
276	6	0	-2.108206	-6.275970	-0.251275
277	1	0	-2.249516	-5.587492	0.593372
278	1	0	-3.104710	-6.506198	-0.645758
279	6	0	1.449090	-3.561383	-1.718144
280	1	0	1.364837	-3.046827	-0.748121
281	7	0	0.384066	5.363334	-7.041404
282	7	0	0.548811	3.664685	-9.361995
283	7	0	-3.448116	-1.357058	-9.361995
284	7	0	-4.836817	-2.349056	-7.041404
285	6	0	-0.574752	4.384924	-4.514589
286	1	0	-1.303751	4.759690	-5.228371
287	6	0	0.779847	4.383668	-4.879188
288	6	0	1.202312	4.872700	-6.206633
289	1	0	2.278557	4.790720	-6.424519
290	6	0	0.909992	5.830553	-8.308865
291	1	0	1.993946	5.633301	-8.394376
292	6	0	0.211546	5.072175	-9.448494
293	1	0	-0.875447	5.234835	-9.333994
294	6	0	0.664088	5.613464	-10.809198
295	1	0	0.143208	5.062246	-11.599656
296	1	0	1.734807	5.400222	-10.924256
297	6	0	0.410758	7.116576	-10.927753

298	1	0	0.758687	7.479346	-11.900667
299	1	0	-0.669938	7.308940	-10.884271
300	6	0	1.101906	7.874050	-9.792615
301	1	0	0.889266	8.946181	-9.859779
302	1	0	2.189863	7.758593	-9.891721
303	6	0	0.655964	7.337077	-8.432136
304	1	0	-0.417629	7.516124	-8.288883
305	1	0	1.175587	7.850986	-7.616110
306	6	0	-0.403831	2.837935	-9.236901
307	1	0	-1.454787	3.164119	-9.179005
308	6	0	-0.214665	1.382304	-9.178365
309	6	0	1.086914	0.848146	-9.185449
310	1	0	1.929640	1.535515	-9.203014
311	6	0	1.304443	-0.505247	-9.178365
312	6	0	0.191059	-1.365368	-9.185449
313	1	0	0.364975	-2.438875	-9.203014
314	6	0	-1.089778	-0.877057	-9.178365
315	6	0	-1.277973	0.517222	-9.185449
316	1	0	-2.294615	0.903360	-9.203014
317	6	0	-2.255808	-1.768695	-9.236901
318	1	0	-2.012814	-2.841942	-9.179005
319	6	0	-4.498405	-2.352883	-9.448494
320	1	0	-4.095776	-3.375577	-9.333994
321	6	0	-5.504403	-2.127200	-8.308865
322	1	0	-5.875555	-1.089843	-8.394376
323	6	0	-6.682077	-3.100457	-8.432136
324	1	0	-7.386947	-2.907405	-7.616110
325	1	0	-6.300340	-4.119739	-8.288883
326	6	0	-7.370080	-2.982746	-9.792615
327	1	0	-7.814070	-1.982820	-9.891721
328	1	0	-8.192253	-3.702963	-9.859779
329	6	0	-6.368515	-3.202561	-10.927753
330	1	0	-5.994759	-4.234653	-10.884271
331	1	0	-6.856647	-3.082631	-11.900667
332	6	0	-5.193446	-2.231615	-10.809198
333	1	0	-5.544133	-1.197724	-10.924256
334	1	0	-4.455638	-2.407101	-11.599656
335	6	0	-4.821038	-1.395117	-6.206633
336	1	0	-5.288164	-0.422072	-6.424519
337	54	0	0.000000	0.000000	0.000000

Diphenlyether C2 cc3-dpe

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-0.000000	0.000000	1.212603
2	6	0	-0.000000	1.188815	0.520383
3	6	0	0.752620	1.376910	-0.638128
4	6	0	-0.734914	2.235076	1.070312
5	6	0	0.754375	2.627026	-1.249138
6	1	0	1.326449	0.552418	-1.048686
7	6	0	-0.717076	3.481834	0.453310
8	1	0	-1.304962	2.052531	1.974904
9	6	0	0.022684	3.682598	-0.709602
10	1	0	1.340121	2.776038	-2.150990
11	1	0	-1.289571	4.298181	0.882627

12	1	0	0.030854	4.654853	-1.191085
13	6	0	-0.000000	-1.188815	0.520383
14	6	0	-0.752620	-1.376910	-0.638128
15	6	0	0.734914	-2.235076	1.070312
16	6	0	-0.754375	-2.627026	-1.249138
17	1	0	-1.326449	-0.552418	-1.048686
18	6	0	0.717076	-3.481834	0.453310
19	1	0	1.304962	-2.052531	1.974904
20	6	0	-0.022684	-3.682598	-0.709602
21	1	0	-1.340121	-2.776038	-2.150990
22	1	0	1.289571	-4.298181	0.882627
23	1	0	-0.030854	-4.654853	-1.191085

Dimesitylether C2 cc3-dpe2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	0.000000	0.000000	1.227059
2	6	0	-1.166747	0.284286	0.541958
3	6	0	-1.215619	1.193097	-0.517870
4	6	0	-2.317359	-0.352505	1.024625
5	6	0	-2.458679	1.409674	-1.122444
6	6	0	-3.529710	-0.093078	0.396261
7	6	0	-3.621391	0.779552	-0.690909
8	1	0	-2.511493	2.111016	-1.952918
9	1	0	-4.426751	-0.589525	0.761926
10	6	0	1.166747	-0.284286	0.541958
11	6	0	1.215619	-1.193097	-0.517870
12	6	0	2.317359	0.352505	1.024625
13	6	0	2.458679	-1.409674	-1.122444
14	6	0	3.529710	0.093078	0.396261
15	6	0	3.621391	-0.779552	-0.690909
16	1	0	2.511493	-2.111016	-1.952918
17	1	0	4.426751	0.589525	0.761926
18	6	0	-4.949448	1.040887	-1.355579
19	6	0	-0.000000	1.940405	-1.005758
20	6	0	-2.210021	-1.296108	2.191893
21	6	0	2.210021	1.296108	2.191893
22	6	0	-0.000000	-1.940405	-1.005758
23	6	0	4.949448	-1.040887	-1.355579
24	1	0	-0.309565	2.800677	-1.604748
25	1	0	0.605297	2.305435	-0.170903
26	1	0	0.651682	1.311320	-1.622253
27	1	0	-1.822958	-0.783225	3.077662
28	1	0	-3.185939	-1.723053	2.434566
29	1	0	-1.514732	-2.115058	1.978027
30	1	0	3.185939	1.723053	2.434566
31	1	0	1.514732	2.115058	1.978027
32	1	0	1.822958	0.783225	3.077662
33	1	0	-0.651682	-1.311320	-1.622253
34	1	0	0.309565	-2.800677	-1.604748
35	1	0	-0.605297	-2.305435	-0.170903
36	1	0	4.834883	-1.693280	-2.225027
37	1	0	5.414047	-0.108579	-1.692691
38	1	0	5.649860	-1.522461	-0.664936
39	1	0	-4.834883	1.693280	-2.225027

40	1	0	-5.414047	0.108579	-1.692691
41	1	0	-5.649860	1.522461	-0.664936

Octachloropropane C2v cc3-dpe4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	1.387165	-0.249343
2	6	0	0.000000	0.000000	0.557744
3	6	0	-0.000000	-1.387165	-0.249343
4	17	0	-1.457251	0.000000	1.579605
5	17	0	1.457251	-0.000000	1.579605
6	17	0	0.000000	2.723316	0.938936
7	17	0	-0.000000	-2.723316	0.938936
8	17	0	-1.441663	1.583295	-1.264481
9	17	0	1.441663	1.583295	-1.264481
10	17	0	-1.441663	-1.583295	-1.264481
11	17	0	1.441663	-1.583295	-1.264481

Hexachloropropene Cs cc3-dpe6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.345643	-0.498115	0.000000
2	6	0	0.006418	-0.619332	0.000000
3	6	0	-0.951655	0.582384	-0.000000
4	17	0	-0.684206	-2.197645	0.000000
5	17	0	-2.660504	0.094505	-0.000000
6	17	0	2.392933	-1.861747	0.000000
7	17	0	2.178870	1.002484	0.000000
8	17	0	-0.684206	1.575625	1.464751
9	17	0	-0.684206	1.575625	-1.464751

Benzylbenzoate C1 cc3-dpe8

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.218485	1.321574	0.088452
2	1	0	1.161409	1.872856	1.033516
3	1	0	1.230302	2.059895	-0.719608
4	6	0	2.427199	0.426772	0.037909
5	6	0	2.428900	-0.803382	0.698624
6	6	0	3.574693	0.839404	-0.637093
7	6	0	3.563838	-1.606926	0.682377
8	1	0	1.532138	-1.129553	1.217186
9	6	0	4.715009	0.039603	-0.646535
10	1	0	3.575643	1.791502	-1.161933
11	6	0	4.711029	-1.186093	0.012039
12	1	0	3.554373	-2.563991	1.194966
13	1	0	5.602396	0.371211	-1.176727

14	1	0	5.596560	-1.813893	0.000607
15	8	0	0.048058	0.506790	-0.031826
16	6	0	-1.120952	1.155618	0.113109
17	8	0	-1.194718	2.343841	0.319235
18	6	0	-2.294004	0.244303	-0.008780
19	6	0	-2.147754	-1.117979	-0.277388
20	6	0	-3.564342	0.798526	0.155358
21	6	0	-3.277376	-1.922899	-0.379985
22	1	0	-1.155048	-1.534879	-0.407574
23	6	0	-4.689795	-0.010059	0.053210
24	1	0	-3.645229	1.860741	0.361882
25	6	0	-4.545976	-1.370571	-0.214323
26	1	0	-3.168716	-2.982150	-0.590109
27	1	0	-5.678802	0.418100	0.181399
28	1	0	-5.425460	-2.002233	-0.294715

Tetrachloroethene D2h cc3-dpe12

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	-0.000000	0.669843
2	6	0	0.000000	-0.000000	-0.669843
3	17	0	0.000000	1.451545	-1.588960
4	17	0	-0.000000	-1.451545	-1.588960
5	17	0	-0.000000	-1.451545	1.588960
6	17	0	-0.000000	1.451545	1.588960

Mesitylene C3v cc3-mes2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.199694	0.692644	-0.011796
2	6	0	0.000000	1.404735	-0.009247
3	6	0	-1.199694	0.692644	-0.011796
4	6	0	-1.216536	-0.702367	-0.009247
5	6	0	-0.000000	-1.385288	-0.011796
6	6	0	1.216536	-0.702367	-0.009247
7	1	0	2.142466	1.236954	-0.024022
8	1	0	-2.142466	1.236954	-0.024022
9	1	0	-0.000000	-2.473907	-0.024022
10	6	0	-2.522562	-1.456402	0.012907
11	1	0	-2.848152	-1.644382	1.042255
12	1	0	-3.315643	-0.890952	-0.484710
13	1	0	-2.429409	-2.425955	-0.484710
14	6	0	0.000000	2.912803	0.012907
15	1	0	-0.886234	3.316907	-0.484710
16	1	0	0.000000	3.288763	1.042255
17	1	0	0.886234	3.316907	-0.484710
18	6	0	2.522562	-1.456402	0.012907
19	1	0	3.315643	-0.890952	-0.484710
20	1	0	2.848152	-1.644382	1.042255
21	1	0	2.429409	-2.425955	-0.484710

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-2.859179	-4.664270	1.348146
2	7	0	-4.711533	-3.293610	-0.414743
3	7	0	-1.750660	-0.496789	-5.377959
4	7	0	1.115178	-0.088588	-5.505438
5	6	0	-0.046630	-4.057972	1.551717
6	1	0	-0.359346	-4.729388	0.756342
7	6	0	-1.032151	-3.463778	2.353356
8	6	0	-2.463297	-3.775679	2.160118
9	1	0	-3.162051	-3.210753	2.796149
10	6	0	-4.280014	-4.955218	1.306157
11	1	0	-4.847643	-4.297684	1.988905
12	6	0	-4.810854	-4.708194	-0.114154
13	1	0	-4.199190	-5.315032	-0.806172
14	6	0	-6.278983	-5.136469	-0.222408
15	1	0	-6.620682	-4.964851	-1.248877
16	1	0	-6.874559	-4.479828	0.425123
17	6	0	-6.475930	-6.596048	0.187314
18	1	0	-7.535037	-6.865163	0.115880
19	1	0	-5.933920	-7.248700	-0.510614
20	6	0	-5.954541	-6.833491	1.605243
21	1	0	-6.067286	-7.885762	1.886779
22	1	0	-6.555867	-6.247960	2.313994
23	6	0	-4.487883	-6.417719	1.716844
24	1	0	-3.867268	-7.046727	1.065474
25	1	0	-4.115796	-6.553553	2.738185
26	6	0	-3.996740	-2.948705	-1.403566
27	1	0	-3.452063	-3.686304	-2.013647
28	6	0	-3.848293	-1.542670	-1.823039
29	6	0	-4.440377	-0.504048	-1.091258
30	1	0	-5.015826	-0.756310	-0.203820
31	6	0	-4.275748	0.816925	-1.487672
32	6	0	-3.519939	1.107005	-2.632415
33	1	0	-3.402445	2.146869	-2.925986
34	6	0	-2.941956	0.084479	-3.372467
35	6	0	-3.106380	-1.244426	-2.957992
36	1	0	-2.639023	-2.031985	-3.543701
37	6	0	-2.187771	0.403640	-4.599996
38	1	0	-2.048638	1.475348	-4.811223
39	6	0	-1.068133	-0.078004	-6.586033
40	1	0	-0.967815	1.021350	-6.636433
41	6	0	0.348571	-0.671447	-6.589358
42	1	0	0.247135	-1.765592	-6.471873
43	6	0	1.061185	-0.365155	-7.911909
44	1	0	2.059002	-0.816555	-7.887293
45	1	0	1.204878	0.721139	-7.978487
46	6	0	0.260565	-0.863259	-9.114931
47	1	0	0.185194	-1.958562	-9.076463
48	1	0	0.785281	-0.613532	-10.043173
49	6	0	-1.145818	-0.262380	-9.112948
50	1	0	-1.073388	0.826237	-9.241482
51	1	0	-1.729459	-0.643563	-9.957575
52	6	0	-1.863652	-0.573346	-7.799475

53	1	0	-2.005645	-1.656932	-7.695106
54	1	0	-2.860112	-0.118804	-7.776923
55	6	0	1.594800	-0.871062	-4.630973
56	1	0	1.422422	-1.958454	-4.663370
57	7	0	0.269080	-1.044200	5.597823
58	7	0	0.419393	1.811120	5.361040
59	7	0	-3.382807	4.514298	0.972975
60	7	0	-4.840263	3.115314	-1.072739
61	6	0	-0.654585	-2.602306	3.377537
62	1	0	-1.398515	-2.131402	4.014730
63	6	0	0.700035	-2.333003	3.619365
64	6	0	1.103434	-1.457494	4.738476
65	1	0	2.173381	-1.203752	4.790082
66	6	0	0.758290	-0.205424	6.673299
67	1	0	1.842669	-0.015668	6.578450
68	6	0	0.044450	1.153814	6.596931
69	1	0	-1.042277	0.957529	6.639050
70	6	0	0.448410	2.039510	7.780420
71	1	0	-0.085840	2.992898	7.706690
72	1	0	1.518598	2.266063	7.688667
73	6	0	0.168350	1.353339	9.117916
74	1	0	0.484855	1.999300	9.943567
75	1	0	-0.913645	1.200297	9.230498
76	6	0	0.877494	0.000002	9.192391
77	1	0	0.647430	-0.503808	10.137055
78	1	0	1.964128	0.160310	9.173832
79	6	0	0.474813	-0.888777	8.015077
80	1	0	-0.597849	-1.116998	8.063583
81	1	0	1.005751	-1.846505	8.044553
82	6	0	-0.500115	2.086644	4.532254
83	1	0	-1.554545	1.835285	4.726304
84	6	0	-0.232662	2.799470	3.267944
85	6	0	1.080892	3.075820	2.865832
86	1	0	1.899636	2.722397	3.487372
87	6	0	1.325317	3.806552	1.709869
88	6	0	0.246302	4.262476	0.939167
89	1	0	0.455534	4.844234	0.045053
90	6	0	-1.060378	3.996831	1.330761
91	6	0	-1.294762	3.254541	2.496517
92	1	0	-2.323417	3.065479	2.792759
93	6	0	-2.186039	4.556819	0.555895
94	1	0	-1.916364	5.046726	-0.392667
95	6	0	-4.404090	5.153953	0.166514
96	1	0	-3.982681	5.563023	-0.769597
97	6	0	-5.463370	4.112206	-0.226678
98	1	0	-5.854259	3.666700	0.706155
99	6	0	-6.611814	4.777164	-0.992910
100	1	0	-7.355137	4.013999	-1.248111
101	1	0	-6.213343	5.163354	-1.940148
102	6	0	-7.243211	5.912088	-0.185796
103	1	0	-7.703327	5.501151	0.723194
104	1	0	-8.046487	6.380984	-0.763849
105	6	0	-6.189432	6.948247	0.209047
106	1	0	-5.795841	7.426273	-0.698361
107	1	0	-6.638223	7.741491	0.816215
108	6	0	-5.041368	6.289856	0.974817
109	1	0	-5.408540	5.873013	1.921701
110	1	0	-4.266386	7.021278	1.228629
111	6	0	-4.883607	1.905025	-0.698205

112	1	0	-5.378609	1.600933	0.237614
113	7	0	3.565977	-4.340037	1.203255
114	7	0	4.684312	-3.120555	-1.142590
115	7	0	4.643344	3.312989	-1.349088
116	7	0	3.007056	4.916277	0.388513
117	6	0	1.669673	-2.922175	2.814704
118	1	0	2.727128	-2.731964	2.979269
119	6	0	1.300129	-3.791097	1.777130
120	6	0	2.330359	-4.438195	0.939046
121	1	0	1.956596	-5.021374	0.083563
122	6	0	4.502997	-5.033014	0.341637
123	1	0	3.984648	-5.552259	-0.484498
124	6	0	5.453750	-4.003329	-0.289433
125	1	0	5.939468	-3.450278	0.534967
126	6	0	6.525251	-4.709245	-1.128014
127	1	0	7.194790	-3.953957	-1.553681
128	1	0	6.028236	-5.206211	-1.971268
129	6	0	7.304758	-5.731020	-0.299339
130	1	0	8.048275	-6.232971	-0.927327
131	1	0	7.857955	-5.210959	0.494592
132	6	0	6.358554	-6.752684	0.334005
133	1	0	6.916849	-7.461115	0.954931
134	1	0	5.875260	-7.337790	-0.460235
135	6	0	5.288004	-6.053408	1.172377
136	1	0	5.753044	-5.525042	2.014783
137	1	0	4.586228	-6.778094	1.599384
138	6	0	4.733473	-1.875014	-0.909554
139	1	0	5.334670	-1.459061	-0.085825
140	6	0	4.008054	-0.891407	-1.736734
141	6	0	3.117575	-1.317971	-2.730990
142	1	0	2.964243	-2.385471	-2.866899
143	6	0	2.463048	-0.394336	-3.536403
144	6	0	2.684263	0.974211	-3.335686
145	1	0	2.166595	1.683699	-3.976103
146	6	0	3.558850	1.409123	-2.346940
147	6	0	4.223532	0.468201	-1.547590
148	1	0	4.909444	0.826700	-0.784118
149	6	0	3.788547	2.855563	-2.166188
150	1	0	3.173775	3.516787	-2.796485
151	6	0	4.788573	4.752522	-1.262548
152	1	0	4.110230	5.270813	-1.964303
153	6	0	4.409508	5.203187	0.157586
154	1	0	5.056672	4.649769	0.862028
155	6	0	4.646986	6.707837	0.324977
156	1	0	4.380871	6.996279	1.347702
157	1	0	3.959476	7.239762	-0.345437
158	6	0	6.093168	7.087201	0.004984
159	1	0	6.765164	6.607270	0.729532
160	1	0	6.229576	8.168324	0.113801
161	6	0	6.472677	6.636727	-1.406863
162	1	0	5.863735	7.187148	-2.136974
163	1	0	7.519156	6.879085	-1.619940
164	6	0	6.237995	5.135522	-1.578439
165	1	0	6.895855	4.571046	-0.904843
166	1	0	6.475130	4.813416	-2.598199
167	6	0	2.716933	4.133015	1.342531
168	1	0	3.493846	3.671922	1.972406
169	6	0	-0.023654	-0.829852	0.279392
170	1	0	0.342955	-1.431543	1.106459

171	17	0	-1.621966	-0.210060	0.723220
172	17	0	1.120759	0.491586	0.008268
173	17	0	-0.125207	-1.883013	-1.146826

Diphenlyether@CC3 C2 cc3-dpel

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	1.148652	0.876300	-5.989323
2	7	0	-1.148652	-0.876300	-5.989323
3	7	0	-5.628171	0.343791	-1.462511
4	7	0	-5.401985	1.975425	0.967614
5	6	0	1.954706	2.359209	-3.668177
6	1	0	1.099175	2.719820	-4.233413
7	6	0	2.542717	1.145808	-4.049093
8	6	0	2.034706	0.400003	-5.217718
9	1	0	2.491365	-0.586901	-5.392470
10	6	0	0.762184	0.090935	-7.144988
11	1	0	1.217105	-0.915878	-7.120962
12	6	0	-0.762184	-0.090935	-7.144988
13	1	0	-1.217105	0.915878	-7.120962
14	6	0	-1.216134	-0.821643	-8.414406
15	1	0	-2.306596	-0.924249	-8.391249
16	1	0	-0.800026	-1.837336	-8.392931
17	6	0	-0.759176	-0.092243	-9.678008
18	1	0	-1.079719	-0.646193	-10.566610
19	1	0	-1.242439	0.893119	-9.725579
20	6	0	0.759176	0.092243	-9.678008
21	1	0	1.079719	0.646193	-10.566610
22	1	0	1.242439	-0.893119	-9.725579
23	6	0	1.216134	0.821643	-8.414406
24	1	0	0.800026	1.837336	-8.392931
25	1	0	2.306596	0.924249	-8.391249
26	6	0	-2.034706	-0.400003	-5.217718
27	1	0	-2.491365	0.586901	-5.392470
28	6	0	-2.542717	-1.145808	-4.049093
29	6	0	-1.954706	-2.359209	-3.668177
30	1	0	-1.099175	-2.719820	-4.233413
31	6	0	-2.459537	-3.083918	-2.595125
32	6	0	-3.583464	-2.605336	-1.908680
33	1	0	-3.968551	-3.184937	-1.073436
34	6	0	-4.168260	-1.397010	-2.271743
35	6	0	-3.635003	-0.660694	-3.337657
36	1	0	-4.099538	0.285764	-3.603323
37	6	0	-5.311832	-0.884632	-1.490128
38	1	0	-5.851906	-1.637010	-0.892567
39	6	0	-6.772846	0.713572	-0.642291
40	1	0	-6.951231	-0.037123	0.148663
41	6	0	-6.516013	2.066433	0.038019
42	1	0	-6.306534	2.796706	-0.765040
43	6	0	-7.758821	2.519749	0.814639
44	1	0	-7.547200	3.489666	1.277553
45	1	0	-7.930993	1.808101	1.632802
46	6	0	-8.992766	2.598410	-0.083864
47	1	0	-8.837407	3.369194	-0.851001
48	1	0	-9.865266	2.905357	0.502449

49	6	0	-9.250022	1.254558	-0.766167
50	1	0	-9.500134	0.504482	-0.003602
51	1	0	-10.110424	1.321589	-1.440391
52	6	0	-8.015009	0.795749	-1.541150
53	1	0	-7.800773	1.495927	-2.359605
54	1	0	-8.181046	-0.186289	-1.998449
55	6	0	-4.454092	2.803980	0.805316
56	1	0	-4.457431	3.518833	-0.033497
57	7	0	5.628171	-0.343791	-1.462511
58	7	0	5.401985	-1.975425	0.967614
59	7	0	-0.000000	-5.467889	0.659448
60	7	0	-2.233029	-5.054482	-1.232300
61	6	0	3.635003	0.660694	-3.337657
62	1	0	4.099538	-0.285764	-3.603323
63	6	0	4.168260	1.397010	-2.271743
64	6	0	5.311832	0.884632	-1.490128
65	1	0	5.851906	1.637010	-0.892567
66	6	0	6.772846	-0.713572	-0.642291
67	1	0	6.951231	0.037123	0.148663
68	6	0	6.516013	-2.066433	0.038019
69	1	0	6.306534	-2.796706	-0.765040
70	6	0	7.758821	-2.519749	0.814639
71	1	0	7.547200	-3.489666	1.277553
72	1	0	7.930993	-1.808101	1.632802
73	6	0	8.992766	-2.598410	-0.083864
74	1	0	9.865266	-2.905357	0.502449
75	1	0	8.837407	-3.369194	-0.851001
76	6	0	9.250022	-1.254558	-0.766167
77	1	0	10.110424	-1.321589	-1.440391
78	1	0	9.500134	-0.504482	-0.003602
79	6	0	8.015009	-0.795749	-1.541150
80	1	0	7.800773	-1.495927	-2.359605
81	1	0	8.181046	0.186289	-1.998449
82	6	0	4.454092	-2.803980	0.805316
83	1	0	4.457431	-3.518833	-0.033497
84	6	0	3.269046	-2.893061	1.682534
85	6	0	3.155932	-2.150176	2.868815
86	1	0	3.968652	-1.482616	3.147156
87	6	0	1.995078	-2.222137	3.633575
88	6	0	0.946361	-3.052912	3.216836
89	1	0	0.048511	-3.099036	3.825997
90	6	0	1.048100	-3.798409	2.048970
91	6	0	2.220269	-3.716222	1.285483
92	1	0	2.287285	-4.303742	0.373105
93	6	0	-0.061898	-4.692155	1.661178
94	1	0	-0.942086	-4.664213	2.322938
95	6	0	-1.096277	-6.399864	0.461513
96	1	0	-1.953212	-6.164064	1.117738
97	6	0	-1.591938	-6.333233	-0.989872
98	1	0	-0.715886	-6.479955	-1.647212
99	6	0	-2.625177	-7.434611	-1.264967
100	1	0	-2.935560	-7.367941	-2.313540
101	1	0	-3.514714	-7.225304	-0.656445
102	6	0	-2.084396	-8.825420	-0.937493
103	1	0	-1.237408	-9.055433	-1.598175
104	1	0	-2.853303	-9.580850	-1.131200
105	6	0	-1.619425	-8.888001	0.517253
106	1	0	-2.483618	-8.741327	1.179426
107	1	0	-1.204804	-9.874811	0.749060

108	6	0	-0.575805	-7.806374	0.792092
109	1	0	0.321366	-7.987859	0.185804
110	1	0	-0.257815	-7.821832	1.840356
111	6	0	-1.821286	-4.358848	-2.208296
112	1	0	-0.971883	-4.675477	-2.833780
113	7	0	2.233029	5.054482	-1.232300
114	7	0	0.000000	5.467889	0.659448
115	7	0	-0.724194	1.283250	5.453384
116	7	0	0.724194	-1.283250	5.453384
117	6	0	3.583464	2.605336	-1.908680
118	1	0	3.968551	3.184937	-1.073436
119	6	0	2.459537	3.083918	-2.595125
120	6	0	1.821286	4.358848	-2.208296
121	1	0	0.971883	4.675477	-2.833780
122	6	0	1.591938	6.333233	-0.989872
123	1	0	0.715886	6.479955	-1.647212
124	6	0	1.096277	6.399864	0.461513
125	1	0	1.953212	6.164064	1.117738
126	6	0	0.575805	7.806374	0.792092
127	1	0	0.257815	7.821832	1.840356
128	1	0	-0.321366	7.987859	0.185804
129	6	0	1.619425	8.888001	0.517253
130	1	0	1.204804	9.874811	0.749060
131	1	0	2.483618	8.741327	1.179426
132	6	0	2.084396	8.825420	-0.937493
133	1	0	2.853303	9.580850	-1.131200
134	1	0	1.237408	9.055433	-1.598175
135	6	0	2.625177	7.434611	-1.264967
136	1	0	3.514714	7.225304	-0.656445
137	1	0	2.935560	7.367941	-2.313540
138	6	0	0.061898	4.692155	1.661178
139	1	0	0.942086	4.664213	2.322938
140	6	0	-1.048100	3.798409	2.048970
141	6	0	-2.220269	3.716222	1.285483
142	1	0	-2.287285	4.303742	0.373105
143	6	0	-3.269046	2.893061	1.682534
144	6	0	-3.155932	2.150176	2.868815
145	1	0	-3.968652	1.482616	3.147156
146	6	0	-1.995078	2.222137	3.633575
147	6	0	-0.946361	3.052912	3.216836
148	1	0	-0.048511	3.099036	3.825997
149	6	0	-1.824046	1.360246	4.824026
150	1	0	-2.699775	0.753320	5.103036
151	6	0	-0.661423	0.393141	6.600419
152	1	0	-1.486419	-0.342289	6.579002
153	6	0	0.661423	-0.393141	6.600419
154	1	0	1.486419	0.342289	6.579002
155	6	0	0.779825	-1.239014	7.876722
156	1	0	1.736642	-1.772342	7.852727
157	1	0	-0.009614	-2.002209	7.856184
158	6	0	0.657182	-0.390213	9.141521
159	1	0	1.496856	0.316506	9.189010
160	1	0	0.727767	-1.027914	10.029125
161	6	0	-0.657182	0.390213	9.141521
162	1	0	-1.496856	-0.316506	9.189010
163	1	0	-0.727767	1.027914	10.029125
164	6	0	-0.779825	1.239014	7.876722
165	1	0	0.009614	2.002209	7.856184
166	1	0	-1.736642	1.772342	7.852727

167	6	0	1.824046	-1.360246	4.824026
168	1	0	2.699775	-0.753320	5.103036
169	8	0	0.000000	0.000000	2.862838
170	6	0	1.141919	0.387383	2.227445
171	6	0	1.550357	-0.116636	0.996049
172	6	0	1.975592	1.209216	2.986214
173	6	0	2.830388	0.182458	0.543958
174	1	0	0.907256	-0.792791	0.441889
175	6	0	3.250455	1.502809	2.517324
176	1	0	1.611651	1.546258	3.953524
177	6	0	3.685557	0.979475	1.302224
178	1	0	3.180688	-0.256616	-0.384984
179	1	0	3.913628	2.121896	3.114625
180	1	0	4.700605	1.162113	0.967953
181	6	0	-1.141919	-0.387383	2.227445
182	6	0	-1.550357	0.116636	0.996049
183	6	0	-1.975592	-1.209216	2.986214
184	6	0	-2.830388	-0.182458	0.543958
185	1	0	-0.907256	0.792791	0.441889
186	6	0	-3.250455	-1.502809	2.517324
187	1	0	-1.611651	-1.546258	3.953524
188	6	0	-3.685557	-0.979475	1.302224
189	1	0	-3.180688	0.256616	-0.384984
190	1	0	-3.913628	-2.121896	3.114625
191	1	0	-4.700605	-1.162113	0.967953

Dimesitylether@CC3 C2 cc3-dpe3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-0.824690	1.138569	-6.430507
2	7	0	0.824690	-1.138569	-6.430507
3	7	0	5.510566	-1.126879	-1.886641
4	7	0	6.088391	-0.068092	0.791678
5	6	0	-0.982727	2.423564	-3.825547
6	1	0	-0.027256	2.501122	-4.338513
7	6	0	-1.953773	1.561976	-4.347187
8	6	0	-1.725602	0.816471	-5.598852
9	1	0	-2.410371	-0.026576	-5.782471
10	6	0	-0.698775	0.319622	-7.619323
11	1	0	-1.436384	-0.503554	-7.620607
12	6	0	0.698775	-0.319622	-7.619323
13	1	0	1.436384	0.503554	-7.620607
14	6	0	0.892278	-1.171489	-8.876108
15	1	0	1.893304	-1.615977	-8.856784
16	1	0	0.173469	-2.000585	-8.846763
17	6	0	0.687744	-0.335911	-10.141581
18	1	0	0.806257	-0.964990	-11.030082
19	1	0	1.465961	0.437695	-10.194396
20	6	0	-0.687744	0.335911	-10.141581
21	1	0	-0.806257	0.964990	-11.030082
22	1	0	-1.465961	-0.437695	-10.194396
23	6	0	-0.892278	1.171489	-8.876108
24	1	0	-0.173469	2.000585	-8.846763
25	1	0	-1.893304	1.615977	-8.856784
26	6	0	1.725602	-0.816471	-5.598852

27	1	0	2.410371	0.026576	-5.782471
28	6	0	1.953773	-1.561976	-4.347187
29	6	0	0.982727	-2.423564	-3.825547
30	1	0	0.027256	-2.501122	-4.338513
31	6	0	1.242870	-3.175469	-2.681726
32	6	0	2.511333	-3.104635	-2.090688
33	1	0	2.710369	-3.727249	-1.222494
34	6	0	3.481601	-2.240965	-2.598369
35	6	0	3.184043	-1.444833	-3.706994
36	1	0	3.947829	-0.772599	-4.090296
37	6	0	4.828272	-2.193296	-1.986231
38	1	0	5.204432	-3.152025	-1.603607
39	6	0	6.824547	-1.256118	-1.270717
40	1	0	6.914183	-2.210903	-0.722494
41	6	0	7.076371	-0.103838	-0.282811
42	1	0	7.038681	0.830447	-0.872284
43	6	0	8.475208	-0.239816	0.330385
44	1	0	8.631804	0.584651	1.034332
45	1	0	8.510148	-1.168819	0.914735
46	6	0	9.559704	-0.248504	-0.747946
47	1	0	9.567184	0.723087	-1.260375
48	1	0	10.546000	-0.372122	-0.288378
49	6	0	9.304112	-1.354614	-1.772938
50	1	0	9.407957	-2.332032	-1.282533
51	1	0	10.052662	-1.319293	-2.571555
52	6	0	7.899473	-1.237427	-2.366466
53	1	0	7.801686	-0.302636	-2.934167
54	1	0	7.701161	-2.057930	-3.065170
55	6	0	5.490828	1.042703	0.934238
56	1	0	5.707870	1.873542	0.243174
57	7	0	-5.510566	1.126879	-1.886641
58	7	0	-6.088391	0.068092	0.791678
59	7	0	-1.944369	-4.649731	0.878324
60	7	0	0.338894	-4.788687	-1.113896
61	6	0	-3.184043	1.444833	-3.706994
62	1	0	-3.947829	0.772599	-4.090296
63	6	0	-3.481601	2.240965	-2.598369
64	6	0	-4.828272	2.193296	-1.986231
65	1	0	-5.204432	3.152025	-1.603607
66	6	0	-6.824547	1.256118	-1.270717
67	1	0	-6.914183	2.210903	-0.722494
68	6	0	-7.076371	0.103838	-0.282811
69	1	0	-7.038681	-0.830447	-0.872284
70	6	0	-8.475208	0.239816	0.330385
71	1	0	-8.631804	-0.584651	1.034332
72	1	0	-8.510148	1.168819	0.914735
73	6	0	-9.559704	0.248504	-0.747946
74	1	0	-10.546000	0.372122	-0.288378
75	1	0	-9.567184	-0.723087	-1.260375
76	6	0	-9.304112	1.354614	-1.772938
77	1	0	-10.052662	1.319293	-2.571555
78	1	0	-9.407957	2.332032	-1.282533
79	6	0	-7.899473	1.237427	-2.366466
80	1	0	-7.801686	0.302636	-2.934167
81	1	0	-7.701161	2.057930	-3.065170
82	6	0	-5.490828	-1.042703	0.934238
83	1	0	-5.707870	-1.873542	0.243174
84	6	0	-4.456370	-1.400144	1.930208
85	6	0	-4.057279	-0.623096	3.037725

86	1	0	-4.523014	0.346394	3.200151
87	6	0	-3.030585	-1.074692	3.871204
88	6	0	-2.430551	-2.315273	3.603346
89	1	0	-1.665103	-2.665702	4.281112
90	6	0	-2.755631	-3.045313	2.470620
91	6	0	-3.792580	-2.591295	1.654764
92	1	0	-4.042861	-3.170043	0.769315
93	6	0	-1.933788	-4.204440	2.067292
94	1	0	-1.278875	-4.630067	2.844598
95	6	0	-1.130749	-5.825966	0.598488
96	1	0	-0.238013	-5.857643	1.246374
97	6	0	-0.660862	-5.818185	-0.863845
98	1	0	-1.556394	-5.669918	-1.493729
99	6	0	-0.000000	-7.156877	-1.235095
100	1	0	0.285446	-7.117115	-2.292062
101	1	0	0.931025	-7.245675	-0.659688
102	6	0	-0.900819	-8.357226	-0.955273
103	1	0	-1.797551	-8.301003	-1.587248
104	1	0	-0.381131	-9.283973	-1.220909
105	6	0	-1.319379	-8.372104	0.513305
106	1	0	-0.429363	-8.509201	1.142354
107	1	0	-1.988940	-9.214034	0.719268
108	6	0	-2.007001	-7.059370	0.879586
109	1	0	-2.936712	-6.951563	0.304523
110	1	0	-2.288935	-7.045186	1.938551
111	6	0	0.205896	-4.101704	-2.172463
112	1	0	-0.687191	-4.193876	-2.811738
113	7	0	-0.338894	4.788687	-1.113896
114	7	0	1.944369	4.649731	0.878324
115	7	0	1.391433	0.643508	5.565783
116	7	0	-1.391433	-0.643508	5.565783
117	6	0	-2.511333	3.104635	-2.090688
118	1	0	-2.710369	3.727249	-1.222494
119	6	0	-1.242870	3.175469	-2.681726
120	6	0	-0.205896	4.101704	-2.172463
121	1	0	0.687191	4.193876	-2.811738
122	6	0	0.660862	5.818185	-0.863845
123	1	0	1.556394	5.669918	-1.493729
124	6	0	1.130749	5.825966	0.598488
125	1	0	0.238013	5.857643	1.246374
126	6	0	2.007001	7.059370	0.879586
127	1	0	2.288935	7.045186	1.938551
128	1	0	2.936712	6.951563	0.304523
129	6	0	1.319379	8.372104	0.513305
130	1	0	1.988940	9.214034	0.719268
131	1	0	0.429363	8.509201	1.142354
132	6	0	0.900819	8.357226	-0.955273
133	1	0	0.381131	9.283973	-1.220909
134	1	0	1.797551	8.301003	-1.587248
135	6	0	0.000000	7.156877	-1.235095
136	1	0	-0.931025	7.245675	-0.659688
137	1	0	-0.285446	7.117115	-2.292062
138	6	0	1.933788	4.204440	2.067292
139	1	0	1.278875	4.630067	2.844598
140	6	0	2.755631	3.045313	2.470620
141	6	0	3.792580	2.591295	1.654764
142	1	0	4.042861	3.170043	0.769315
143	6	0	4.456370	1.400144	1.930208
144	6	0	4.057279	0.623096	3.037725

145	1	0	4.523014	-0.346394	3.200151
146	6	0	3.030585	1.074692	3.871204
147	6	0	2.430551	2.315273	3.603346
148	1	0	1.665103	2.665702	4.281112
149	6	0	2.442671	0.250034	4.969036
150	1	0	2.940150	-0.706693	5.193450
151	6	0	0.775627	-0.084329	6.663777
152	1	0	1.000005	-1.163478	6.624009
153	6	0	-0.775627	0.084329	6.663777
154	1	0	-1.000005	1.163478	6.624009
155	6	0	-1.369826	-0.500472	7.958690
156	1	0	-2.453980	-0.343567	7.936240
157	1	0	-1.208143	-1.586750	7.944905
158	6	0	-0.756718	0.100201	9.220713
159	1	0	-0.980542	1.174747	9.263417
160	1	0	-1.209465	-0.355593	10.107753
161	6	0	0.756718	-0.100201	9.220713
162	1	0	0.980542	-1.174747	9.263417
163	1	0	1.209465	0.355593	10.107753
164	6	0	1.369826	0.500472	7.958690
165	1	0	1.208143	1.586750	7.944905
166	1	0	2.453980	0.343567	7.936240
167	6	0	-2.442671	-0.250034	4.969036
168	1	0	-2.940150	0.706693	5.193450
169	8	0	0.000000	-0.000000	2.721316
170	6	0	-1.005828	0.732321	2.120663
171	6	0	-1.712962	0.316674	0.977719
172	6	0	-1.422676	1.867920	2.835810
173	6	0	-2.830241	1.066610	0.583476
174	6	0	-2.539605	2.564610	2.400642
175	6	0	-3.274628	2.188754	1.290073
176	1	0	-3.407770	0.703691	-0.263518
177	1	0	-2.864967	3.422657	2.987498
178	6	0	1.005828	-0.732321	2.120663
179	6	0	1.712962	-0.316674	0.977719
180	6	0	1.422676	-1.867920	2.835810
181	6	0	2.830241	-1.066610	0.583476
182	6	0	2.539605	-2.564610	2.400642
183	6	0	3.274628	-2.188754	1.290073
184	1	0	3.407770	-0.703691	-0.263518
185	1	0	2.864967	-3.422657	2.987498
186	6	0	0.787509	-2.369746	4.098182
187	6	0	-0.787509	2.369746	4.098182
188	6	0	1.382710	0.953819	0.226673
189	6	0	-1.382710	-0.953819	0.226673
190	6	0	4.526321	-2.972358	0.992123
191	6	0	-4.526321	2.972358	0.992123
192	1	0	-5.325623	2.318050	0.648255
193	1	0	-4.357301	3.764924	0.254666
194	1	0	-4.873930	3.464621	1.905841
195	1	0	-0.283758	3.325997	3.915836
196	1	0	-0.075534	1.667012	4.519580
197	1	0	-1.562324	2.572838	4.847106
198	1	0	-2.272024	-1.309901	-0.300977
199	1	0	-1.050763	-1.751824	0.893726
200	1	0	-0.592562	-0.813173	-0.517832
201	1	0	4.357301	-3.764924	0.254666
202	1	0	4.873930	-3.464621	1.905841
203	1	0	5.325623	-2.318050	0.648255

204	1	0	1.050763	1.751824	0.893726
205	1	0	0.592562	0.813173	-0.517832
206	1	0	2.272024	1.309901	-0.300977
207	1	0	0.075534	-1.667012	4.519580
208	1	0	1.562324	-2.572838	4.847106
209	1	0	0.283758	-3.325997	3.915836

 Octachloropropane@CC3 C1 cc3-dpe5
 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-0.847280	1.899475	-5.246558
2	7	0	0.058735	-0.927091	-5.584802
3	7	0	-2.376089	-5.158142	-1.441080
4	7	0	-3.820784	-4.331615	1.065707
5	6	0	-1.955525	3.372510	-3.008004
6	1	0	-2.642471	2.778945	-3.606375
7	6	0	-0.610648	3.439359	-3.401626
8	6	0	-0.130393	2.728741	-4.605603
9	1	0	0.904703	2.956146	-4.907814
10	6	0	-0.290043	1.341750	-6.469796
11	1	0	0.810406	1.432908	-6.486663
12	6	0	-0.637120	-0.148790	-6.597252
13	1	0	-1.732730	-0.247391	-6.497747
14	6	0	-0.205326	-0.688217	-7.970117
15	1	0	-0.492064	-1.743929	-8.031833
16	1	0	0.891158	-0.654518	-8.019694
17	6	0	-0.806054	0.111797	-9.124351
18	1	0	-0.460535	-0.295003	-10.080632
19	1	0	-1.899779	0.010775	-9.110522
20	6	0	-0.435317	1.588767	-8.999529
21	1	0	-0.890526	2.172544	-9.806590
22	1	0	0.652985	1.698654	-9.100214
23	6	0	-0.879955	2.137549	-7.645277
24	1	0	-1.974639	2.101311	-7.566087
25	1	0	-0.589401	3.188018	-7.532114
26	6	0	-0.592110	-1.853405	-5.010819
27	1	0	-1.663374	-2.018316	-5.209185
28	6	0	0.019252	-2.774300	-4.029209
29	6	0	1.396986	-2.737165	-3.765377
30	1	0	2.007943	-2.016313	-4.303703
31	6	0	1.958415	-3.573025	-2.806118
32	6	0	1.135125	-4.464410	-2.101803
33	1	0	1.582871	-5.085041	-1.329086
34	6	0	-0.237950	-4.490632	-2.334376
35	6	0	-0.787445	-3.655932	-3.319154
36	1	0	-1.863510	-3.675805	-3.472519
37	6	0	-1.114685	-5.296700	-1.456782
38	1	0	-0.598189	-6.004648	-0.788524
39	6	0	-3.138348	-6.047890	-0.578125
40	1	0	-2.506144	-6.471031	0.222508
41	6	0	-4.302290	-5.297962	0.089246
42	1	0	-4.882415	-4.804794	-0.710941
43	6	0	-5.216495	-6.278583	0.842010
44	1	0	-6.045450	-5.710393	1.278386
45	1	0	-4.645990	-6.700126	1.680302

46	6	0	-5.733893	-7.401384	-0.054541
47	1	0	-6.364671	-6.977007	-0.847455
48	1	0	-6.366202	-8.081482	0.526051
49	6	0	-4.566998	-8.155811	-0.689291
50	1	0	-3.984205	-8.651212	0.099130
51	1	0	-4.931116	-8.942499	-1.358605
52	6	0	-3.667255	-7.191688	-1.459386
53	1	0	-4.222882	-6.747267	-2.295918
54	1	0	-2.809081	-7.716532	-1.893792
55	6	0	-4.398296	-3.201878	1.096911
56	1	0	-5.169055	-2.923627	0.360205
57	7	0	2.117713	5.195145	-0.639062
58	7	0	3.938038	4.017251	1.452656
59	7	0	5.383209	-2.170889	0.482309
60	7	0	3.943720	-3.967390	-1.475919
61	6	0	0.297285	4.135060	-2.613675
62	1	0	1.351894	4.166741	-2.876497
63	6	0	-0.120382	4.773846	-1.436281
64	6	0	0.867878	5.397139	-0.530629
65	1	0	0.451200	6.038269	0.262964
66	6	0	2.991082	5.954251	0.249658
67	1	0	2.474924	6.206756	1.191923
68	6	0	4.254884	5.155499	0.603740
69	1	0	4.718700	4.830929	-0.345082
70	6	0	5.252422	6.033558	1.376796
71	1	0	6.146218	5.435385	1.585709
72	1	0	4.804454	6.282506	2.348054
73	6	0	5.612025	7.312693	0.624530
74	1	0	6.310626	7.912098	1.217840
75	1	0	6.125935	7.056256	-0.311837
76	6	0	4.350360	8.111852	0.304255
77	1	0	4.596065	9.015239	-0.264045
78	1	0	3.882365	8.441044	1.241939
79	6	0	3.363054	7.254255	-0.484261
80	1	0	3.795019	6.983672	-1.457167
81	1	0	2.440915	7.808713	-0.692062
82	6	0	4.526057	2.922648	1.194861
83	1	0	5.185800	2.810655	0.319290
84	6	0	4.348274	1.701803	2.010473
85	6	0	3.624804	1.735298	3.210052
86	1	0	3.225913	2.688786	3.547532
87	6	0	3.346256	0.558898	3.901468
88	6	0	3.845715	-0.659236	3.417113
89	1	0	3.596278	-1.571761	3.953298
90	6	0	4.567172	-0.706821	2.227105
91	6	0	4.822666	0.482826	1.530486
92	1	0	5.355784	0.425944	0.584433
93	6	0	4.945765	-2.020882	1.664635
94	1	0	4.802340	-2.879149	2.340773
95	6	0	5.798928	-3.511949	0.094628
96	1	0	5.342705	-4.277656	0.746493
97	6	0	5.387774	-3.823905	-1.352887
98	1	0	5.764493	-3.002764	-1.989024
99	6	0	6.009412	-5.150309	-1.821262
100	1	0	5.716481	-5.317321	-2.863752
101	1	0	5.560579	-5.961706	-1.232907
102	6	0	7.528341	-5.174103	-1.667722
103	1	0	7.975597	-4.407958	-2.315473
104	1	0	7.922129	-6.140980	-1.998712

105	6	0	7.918292	-4.897652	-0.217115
106	1	0	7.541167	-5.708978	0.420224
107	1	0	9.007448	-4.882647	-0.103133
108	6	0	7.328687	-3.567446	0.246092
109	1	0	7.757307	-2.743255	-0.339618
110	1	0	7.576905	-3.371164	1.295118
111	6	0	3.397604	-3.439951	-2.492949
112	1	0	3.973750	-2.824723	-3.204255
113	7	0	-4.150317	4.088993	-0.207395
114	7	0	-5.279978	1.908567	1.547542
115	7	0	-1.147211	-0.760036	5.660633
116	7	0	1.863174	-0.438674	5.528698
117	6	0	-1.466062	4.746733	-1.085986
118	1	0	-1.815505	5.220781	-0.171188
119	6	0	-2.385511	4.013842	-1.852685
120	6	0	-3.770237	3.798170	-1.382771
121	1	0	-4.450097	3.332699	-2.114150
122	6	0	-5.559312	3.893152	0.101312
123	1	0	-6.036875	3.209415	-0.622859
124	6	0	-5.743181	3.288790	1.501888
125	1	0	-5.187978	3.922258	2.216166
126	6	0	-7.230775	3.273182	1.893011
127	1	0	-7.314835	2.865850	2.906717
128	1	0	-7.749077	2.571019	1.226394
129	6	0	-7.878421	4.653147	1.801915
130	1	0	-8.937542	4.587064	2.072803
131	1	0	-7.404778	5.330026	2.525958
132	6	0	-7.713004	5.225210	0.395517
133	1	0	-8.147439	6.228464	0.330531
134	1	0	-8.258062	4.593775	-0.319230
135	6	0	-6.235498	5.271543	0.013132
136	1	0	-5.697181	5.957858	0.680390
137	1	0	-6.104576	5.653980	-1.005278
138	6	0	-4.673240	1.539538	2.599612
139	1	0	-4.422782	2.250487	3.403573
140	6	0	-4.236258	0.146228	2.832060
141	6	0	-4.607909	-0.883573	1.955059
142	1	0	-5.270242	-0.643964	1.126803
143	6	0	-4.086263	-2.165082	2.104458
144	6	0	-3.197427	-2.426885	3.156634
145	1	0	-2.769533	-3.423258	3.236796
146	6	0	-2.811349	-1.411302	4.028832
147	6	0	-3.357853	-0.127800	3.875717
148	1	0	-3.022630	0.661096	4.544598
149	6	0	-1.752453	-1.679310	5.028092
150	1	0	-1.503564	-2.743028	5.173737
151	6	0	-0.196371	-1.179632	6.682760
152	1	0	0.157197	-2.209790	6.500598
153	6	0	1.037445	-0.263398	6.717056
154	1	0	0.680579	0.777746	6.805959
155	6	0	1.924505	-0.596424	7.929044
156	1	0	2.773366	0.096442	7.933350
157	1	0	2.338995	-1.602487	7.779827
158	6	0	1.163029	-0.537351	9.251187
159	1	0	0.815339	0.489256	9.429548
160	1	0	1.831854	-0.795902	10.078994
161	6	0	-0.040068	-1.477091	9.211990
162	1	0	0.312409	-2.513238	9.118196
163	1	0	-0.610704	-1.417364	10.144858

164	6	0	-0.941308	-1.134772	8.028128
165	1	0	-1.357043	-0.125904	8.152727
166	1	0	-1.793008	-1.821769	7.971354
167	6	0	2.419789	0.599443	5.055073
168	1	0	2.216369	1.603473	5.461319
169	6	0	-1.209359	0.343191	-0.035094
170	6	0	0.083302	-0.146674	-0.837170
171	6	0	1.493452	0.343295	-0.289315
172	17	0	-0.025086	0.354104	-2.533099
173	17	0	0.045929	-1.916434	-0.752430
174	17	0	-2.673219	-0.013354	-1.010316
175	17	0	2.796504	-0.601999	-1.073671
176	17	0	-1.174174	2.072684	0.293700
177	17	0	-1.404002	-0.508123	1.499145
178	17	0	1.847753	2.055898	-0.619777
179	17	0	1.577019	0.068584	1.444602

Hexchloropropene@CC3 C1 cc3-dpe77

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	2.532703	0.397332	-5.137249
2	7	0	1.870662	3.190253	-4.507652
3	7	0	2.873778	4.952518	1.579947
4	7	0	3.289998	2.955814	3.681299
5	6	0	2.639983	-1.890355	-3.362434
6	1	0	3.538403	-1.285394	-3.458154
7	6	0	1.486400	-1.488610	-4.051447
8	6	0	1.497363	-0.308217	-4.940298
9	1	0	0.545539	-0.097153	-5.452664
10	6	0	2.443754	1.456816	-6.126595
11	1	0	1.411538	1.569252	-6.504868
12	6	0	2.849030	2.801991	-5.507088
13	1	0	3.854154	2.682048	-5.064696
14	6	0	2.896327	3.897539	-6.581443
15	1	0	3.208329	4.835780	-6.109345
16	1	0	1.875721	4.053560	-6.955010
17	6	0	3.826149	3.527210	-7.736373
18	1	0	3.821022	4.322046	-8.489730
19	1	0	4.856762	3.446432	-7.364831
20	6	0	3.408891	2.193256	-8.355807
21	1	0	4.093775	1.911142	-9.162438
22	1	0	2.412623	2.299887	-8.806173
23	6	0	3.373202	1.095705	-7.293024
24	1	0	4.380371	0.930175	-6.888603
25	1	0	3.043007	0.142945	-7.721094
26	6	0	2.301693	3.595690	-3.386523
27	1	0	3.376836	3.619231	-3.148305
28	6	0	1.399272	4.049576	-2.309544
29	6	0	0.009412	4.053183	-2.492402
30	1	0	-0.386853	3.757386	-3.460320
31	6	0	-0.838385	4.411142	-1.451170
32	6	0	-0.295442	4.755673	-0.204919
33	1	0	-0.974347	5.008652	0.605550
34	6	0	1.080978	4.754490	-0.011945
35	6	0	1.928718	4.419395	-1.078627

36	1	0	3.002058	4.411180	-0.905039
37	6	0	1.634716	5.042176	1.326862
38	1	0	0.900097	5.325012	2.096735
39	6	0	3.316692	5.282699	2.921268
40	1	0	2.460769	5.450055	3.599812
41	6	0	4.138891	4.119093	3.494563
42	1	0	4.960765	3.909832	2.786426
43	6	0	4.732444	4.501356	4.857678
44	1	0	5.327357	3.659189	5.228085
45	1	0	3.903856	4.640442	5.564459
46	6	0	5.573684	5.774905	4.777574
47	1	0	6.441754	5.599275	4.127674
48	1	0	5.964740	6.027556	5.768830
49	6	0	4.748570	6.931392	4.212565
50	1	0	3.932141	7.166949	4.908760
51	1	0	5.360760	7.835031	4.123348
52	6	0	4.164396	6.559485	2.850128
53	1	0	4.972924	6.393327	2.126173
54	1	0	3.544050	7.370288	2.452640
55	6	0	3.716361	1.842223	3.249166
56	1	0	4.669370	1.756303	2.703076
57	7	0	-2.031901	-3.868504	-3.540861
58	7	0	-4.386294	-3.438783	-1.831220
59	7	0	-5.223151	2.727754	-0.308423
60	7	0	-3.127618	4.753885	-0.771334
61	6	0	0.320793	-2.235888	-3.924485
62	1	0	-0.590818	-1.941629	-4.438740
63	6	0	0.297089	-3.389572	-3.129070
64	6	0	-0.935703	-4.189289	-2.987263
65	1	0	-0.839420	-5.101967	-2.377251
66	6	0	-3.135312	-4.807863	-3.422800
67	1	0	-2.969879	-5.518437	-2.593484
68	6	0	-4.444719	-4.060434	-3.141151
69	1	0	-4.578265	-3.308011	-3.939225
70	6	0	-5.634560	-5.030098	-3.158730
71	1	0	-6.551480	-4.460503	-2.971220
72	1	0	-5.518157	-5.729994	-2.320736
73	6	0	-5.724981	-5.799075	-4.476135
74	1	0	-6.571806	-6.492907	-4.447612
75	1	0	-5.916490	-5.095707	-5.297882
76	6	0	-4.421943	-6.550119	-4.750100
77	1	0	-4.472166	-7.073581	-5.710738
78	1	0	-4.277301	-7.316414	-3.976412
79	6	0	-3.233965	-5.588767	-4.741674
80	1	0	-3.328622	-4.864942	-5.561917
81	1	0	-2.292217	-6.126030	-4.900014
82	6	0	-4.748985	-2.226459	-1.740527
83	1	0	-5.047227	-1.640612	-2.624446
84	6	0	-4.773791	-1.502202	-0.455712
85	6	0	-4.475399	-2.163359	0.744995
86	1	0	-4.258818	-3.228081	0.711289
87	6	0	-4.401004	-1.454833	1.935898
88	6	0	-4.644669	-0.073545	1.937075
89	1	0	-4.549507	0.469196	2.874074
90	6	0	-4.942080	0.588163	0.754429
91	6	0	-5.011531	-0.135004	-0.445268
92	1	0	-5.214231	0.405503	-1.366325
93	6	0	-5.101428	2.054575	0.759898
94	1	0	-5.093893	2.532797	1.752255

95	6	0	-5.434923	4.157899	-0.182856
96	1	0	-5.202163	4.514332	0.836627
97	6	0	-4.519476	4.905083	-1.160646
98	1	0	-4.703032	4.492074	-2.168720
99	6	0	-4.839835	6.407166	-1.164180
100	1	0	-4.183630	6.901861	-1.888749
101	1	0	-4.585220	6.812921	-0.176242
102	6	0	-6.310132	6.679244	-1.478874
103	1	0	-6.536021	6.337324	-2.498055
104	1	0	-6.504195	7.756769	-1.454350
105	6	0	-7.214990	5.944902	-0.489694
106	1	0	-7.050945	6.348598	0.518693
107	1	0	-8.269679	6.112843	-0.732042
108	6	0	-6.910223	4.447659	-0.494936
109	1	0	-7.140996	4.020029	-1.479576
110	1	0	-7.530930	3.916164	0.234884
111	6	0	-2.297769	4.444427	-1.679951
112	1	0	-2.620509	4.216171	-2.708065
113	7	0	3.809924	-4.232778	-0.831114
114	7	0	4.409263	-3.154282	1.861983
115	7	0	-0.900962	-1.704889	5.202308
116	7	0	-3.676346	-1.499558	4.226760
117	6	0	1.450734	-3.783765	-2.461710
118	1	0	1.455300	-4.668241	-1.829386
119	6	0	2.625082	-3.025286	-2.557958
120	6	0	3.820968	-3.366830	-1.758350
121	1	0	4.723329	-2.778818	-1.991321
122	6	0	5.058441	-4.461962	-0.120632
123	1	0	5.792802	-3.664941	-0.336620
124	6	0	4.819349	-4.470918	1.398883
125	1	0	4.041495	-5.227805	1.606705
126	6	0	6.106699	-4.853520	2.142812
127	1	0	5.895328	-4.868529	3.217737
128	1	0	6.846438	-4.059394	1.975933
129	6	0	6.664835	-6.196705	1.674674
130	1	0	7.589763	-6.426285	2.214278
131	1	0	5.948763	-6.994225	1.915317
132	6	0	6.910069	-6.179406	0.166148
133	1	0	7.276997	-7.152454	-0.177297
134	1	0	7.692652	-5.443848	-0.064582
135	6	0	5.629451	-5.810931	-0.581457
136	1	0	4.863193	-6.580277	-0.417880
137	1	0	5.804536	-5.762957	-1.661956
138	6	0	3.393416	-3.096837	2.619963
139	1	0	2.814050	-3.997617	2.879598
140	6	0	2.866162	-1.833378	3.179030
141	6	0	3.547943	-0.619965	3.012838
142	1	0	4.511585	-0.630678	2.510493
143	6	0	2.988981	0.573580	3.457757
144	6	0	1.749073	0.552742	4.111003
145	1	0	1.330548	1.493474	4.459732
146	6	0	1.076446	-0.647686	4.309544
147	6	0	1.638588	-1.839892	3.833144
148	1	0	1.085792	-2.765755	3.973591
149	6	0	-0.209808	-0.653119	5.036415
150	1	0	-0.521761	0.317627	5.453524
151	6	0	-2.069436	-1.609880	6.061338
152	1	0	-2.333778	-0.556840	6.265803
153	6	0	-3.284603	-2.267695	5.393996

154	1	0	-3.003627	-3.301089	5.122844
155	6	0	-4.476657	-2.305918	6.361200
156	1	0	-5.316473	-2.798620	5.858727
157	1	0	-4.788130	-1.271995	6.560487
158	6	0	-4.129858	-3.010571	7.671676
159	1	0	-3.891834	-4.063665	7.469119
160	1	0	-4.996469	-3.003329	8.341235
161	6	0	-2.927429	-2.341864	8.337866
162	1	0	-3.195843	-1.314833	8.620471
163	1	0	-2.656100	-2.865138	9.260869
164	6	0	-1.733133	-2.312087	7.384989
165	1	0	-1.408618	-3.335671	7.155825
166	1	0	-0.877319	-1.803295	7.842206
167	6	0	-3.960725	-2.137333	3.167450
168	1	0	-3.863235	-3.232671	3.101773
169	6	0	1.497675	-1.014107	0.118664
170	6	0	0.614846	-0.004980	0.042468
171	6	0	-0.897450	-0.183938	0.214509
172	17	0	1.200972	1.585170	-0.230604
173	17	0	-1.794743	1.331705	-0.054205
174	17	0	3.179687	-0.753027	-0.128951
175	17	0	1.066488	-2.634593	0.480014
176	17	0	-1.512331	-1.377963	-0.971102
177	17	0	-1.232957	-0.731332	1.884693

Benzylbenzoate@CC3-a C1 cc3-dpe9
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	1.887212	-4.785529	2.136746
2	7	0	1.723133	-5.432500	-0.697948
3	7	0	3.324565	-0.332163	-4.310490
4	7	0	3.517979	2.447870	-3.401764
5	6	0	1.670841	-2.116754	3.295133
6	1	0	2.636962	-2.390048	2.877438
7	6	0	0.605443	-3.020311	3.180394
8	6	0	0.771058	-4.340429	2.543168
9	1	0	-0.150436	-4.940699	2.469876
10	6	0	1.914113	-6.143758	1.624960
11	1	0	0.894165	-6.557432	1.523352
12	6	0	2.560445	-6.166374	0.232199
13	1	0	3.560490	-5.705754	0.323941
14	6	0	2.708815	-7.607080	-0.271081
15	1	0	3.182665	-7.588349	-1.258691
16	1	0	1.703797	-8.027316	-0.407946
17	6	0	3.509048	-8.467546	0.706568
18	1	0	3.583157	-9.492985	0.329244
19	1	0	4.534339	-8.079935	0.779433
20	6	0	2.864706	-8.448857	2.093338
21	1	0	3.457452	-9.037181	2.801798
22	1	0	1.874450	-8.921202	2.037332
23	6	0	2.715958	-7.014623	2.600971
24	1	0	3.704700	-6.556642	2.734576
25	1	0	2.221166	-6.991915	3.578091
26	6	0	2.248395	-4.457993	-1.314661
27	1	0	3.293009	-4.153427	-1.145436

28	6	0	1.499670	-3.641967	-2.290862
29	6	0	0.152322	-3.906939	-2.577207
30	1	0	-0.323985	-4.756237	-2.093274
31	6	0	-0.556710	-3.082135	-3.442502
32	6	0	0.086473	-1.985884	-4.035912
33	1	0	-0.488166	-1.350520	-4.704943
34	6	0	1.427768	-1.726514	-3.777638
35	6	0	2.132614	-2.567851	-2.904310
36	1	0	3.182070	-2.367308	-2.710079
37	6	0	2.091715	-0.594013	-4.454984
38	1	0	1.450587	-0.003559	-5.127819
39	6	0	3.886313	0.742360	-5.110648
40	1	0	3.102659	1.253338	-5.698474
41	6	0	4.538032	1.798436	-4.207202
42	1	0	5.287363	1.291224	-3.572760
43	6	0	5.241893	2.866614	-5.056129
44	1	0	5.711516	3.591924	-4.382489
45	1	0	4.477094	3.410334	-5.626564
46	6	0	6.270051	2.254418	-6.006860
47	1	0	7.070388	1.780734	-5.422172
48	1	0	6.738454	3.040643	-6.608300
49	6	0	5.616073	1.205167	-6.906288
50	1	0	4.878693	1.695218	-7.556521
51	1	0	6.359897	0.741622	-7.562838
52	6	0	4.920957	0.134279	-6.066131
53	1	0	5.660811	-0.411939	-5.465569
54	1	0	4.421818	-0.604341	-6.702713
55	6	0	3.798350	2.665673	-2.183659
56	1	0	4.747786	2.335627	-1.734130
57	7	0	-3.211317	-1.738840	4.595955
58	7	0	-5.210556	-0.313910	3.035257
59	7	0	-4.907462	-1.386456	-3.289898
60	7	0	-2.640306	-2.685702	-4.572799
61	6	0	-0.635339	-2.682028	3.704667
62	1	0	-1.478956	-3.362585	3.620665
63	6	0	-0.830781	-1.448157	4.336925
64	6	0	-2.165640	-1.054588	4.822738
65	1	0	-2.206544	-0.106626	5.383379
66	6	0	-4.459175	-1.256706	5.160522
67	1	0	-4.357514	-0.220123	5.529875
68	6	0	-5.553981	-1.257190	4.084749
69	1	0	-5.631553	-2.285532	3.687516
70	6	0	-6.902856	-0.849920	4.691872
71	1	0	-7.663883	-0.872744	3.903970
72	1	0	-6.826633	0.191514	5.031310
73	6	0	-7.294077	-1.756622	5.859096
74	1	0	-8.248778	-1.428756	6.283787
75	1	0	-7.444241	-2.780466	5.490448
76	6	0	-6.202382	-1.763091	6.929958
77	1	0	-6.468136	-2.442737	7.746506
78	1	0	-6.118744	-0.758402	7.366207
79	6	0	-4.856525	-2.168333	6.328727
80	1	0	-4.902981	-3.201014	5.958573
81	1	0	-4.062993	-2.136757	7.083401
82	6	0	-5.314977	-0.710102	1.834236
83	1	0	-5.614242	-1.741649	1.587663
84	6	0	-5.012976	0.157146	0.679462
85	6	0	-4.724130	1.516946	0.854660
86	1	0	-4.772922	1.934487	1.857594

87	6	0	-4.369991	2.307743	-0.231459
88	6	0	-4.300381	1.734197	-1.509173
89	1	0	-4.024325	2.368038	-2.348099
90	6	0	-4.594167	0.388671	-1.694817
91	6	0	-4.954279	-0.397524	-0.591930
92	1	0	-5.168834	-1.450813	-0.753488
93	6	0	-4.561375	-0.189801	-3.053023
94	1	0	-4.242465	0.493927	-3.855442
95	6	0	-4.917444	-1.829681	-4.670519
96	1	0	-4.523502	-1.051507	-5.349255
97	6	0	-4.017778	-3.065413	-4.820910
98	1	0	-4.366154	-3.824167	-4.097306
99	6	0	-4.116587	-3.635137	-6.241961
100	1	0	-3.479378	-4.523810	-6.309096
101	1	0	-3.702409	-2.893143	-6.937094
102	6	0	-5.560062	-3.962973	-6.623292
103	1	0	-5.939522	-4.759055	-5.968303
104	1	0	-5.597456	-4.349411	-7.647279
105	6	0	-6.449868	-2.727517	-6.480372
106	1	0	-6.125762	-1.963629	-7.200244
107	1	0	-7.489660	-2.971263	-6.722647
108	6	0	-6.362280	-2.161803	-5.063187
109	1	0	-6.753406	-2.890729	-4.341451
110	1	0	-6.970641	-1.256541	-4.961313
111	6	0	-1.980100	-3.357610	-3.724863
112	1	0	-2.427930	-4.190847	-3.160847
113	7	0	2.576325	1.098639	4.750883
114	7	0	3.458609	3.239157	2.946357
115	7	0	-1.256441	5.787727	-0.641647
116	7	0	-3.861689	4.539655	-0.986682
117	6	0	0.237068	-0.568375	4.463609
118	1	0	0.117231	0.392650	4.957534
119	6	0	1.495155	-0.899704	3.943640
120	6	0	2.648557	0.004292	4.115322
121	1	0	3.592356	-0.356014	3.679305
122	6	0	3.802029	1.852059	4.931596
123	1	0	4.647175	1.391892	4.385391
124	6	0	3.624908	3.277467	4.387514
125	1	0	2.739654	3.713130	4.884935
126	6	0	4.857614	4.135863	4.700658
127	1	0	4.687495	5.147488	4.315900
128	1	0	5.709588	3.723618	4.143951
129	6	0	5.171795	4.161353	6.195754
130	1	0	6.065115	4.767501	6.380415
131	1	0	4.343986	4.640971	6.735660
132	6	0	5.362999	2.740887	6.728196
133	1	0	5.557291	2.755245	7.805958
134	1	0	6.245571	2.292533	6.251549
135	6	0	4.132418	1.885262	6.429608
136	1	0	3.258635	2.284255	6.961347
137	1	0	4.272518	0.856424	6.778759
138	6	0	2.431824	3.798030	2.456330
139	1	0	1.661532	4.261104	3.092338
140	6	0	2.194772	3.881577	1.001063
141	6	0	3.120225	3.340265	0.097598
142	1	0	4.020624	2.876855	0.494634
143	6	0	2.864313	3.350326	-1.267899
144	6	0	1.697154	3.962771	-1.747624
145	1	0	1.513297	3.964096	-2.819234

146	6	0	0.792830	4.541807	-0.864906
147	6	0	1.041588	4.487024	0.515851
148	1	0	0.311520	4.925077	1.191906
149	6	0	-0.418983	5.200815	-1.390909
150	1	0	-0.542656	5.163794	-2.484766
151	6	0	-2.376957	6.454301	-1.277502
152	1	0	-2.410378	6.242669	-2.361630
153	6	0	-3.690399	5.944823	-0.667974
154	1	0	-3.636196	6.108087	0.423607
155	6	0	-4.883895	6.723304	-1.236466
156	1	0	-5.801676	6.347943	-0.770690
157	1	0	-4.957702	6.501438	-2.309146
158	6	0	-4.733726	8.229187	-1.020230
159	1	0	-4.737840	8.445837	0.056711
160	1	0	-5.590143	8.756559	-1.453483
161	6	0	-3.425442	8.734828	-1.629562
162	1	0	-3.459741	8.602220	-2.719533
163	1	0	-3.302521	9.807042	-1.443803
164	6	0	-2.232812	7.965849	-1.061250
165	1	0	-2.143690	8.150574	0.017262
166	1	0	-1.294858	8.298576	-1.519171
167	6	0	-4.099629	3.744531	-0.027828
168	1	0	-4.141082	4.090829	1.017110
169	6	0	0.696687	0.883531	-0.795303
170	1	0	0.414315	1.029887	-1.842040
171	1	0	0.766744	1.856068	-0.302498
172	6	0	-0.289976	0.008412	-0.074248
173	6	0	-1.075054	0.534666	0.949643
174	6	0	-0.449723	-1.321632	-0.450494
175	6	0	-2.021782	-0.262420	1.580261
176	1	0	-0.930796	1.568448	1.256067
177	6	0	-1.393009	-2.124907	0.183572
178	1	0	0.180376	-1.721259	-1.236271
179	6	0	-2.184409	-1.592435	1.198436
180	1	0	-2.639396	0.143775	2.377275
181	1	0	-1.499417	-3.165799	-0.113034
182	1	0	-2.913658	-2.208619	1.721327
183	8	0	2.015310	0.318109	-0.882002
184	6	0	2.723493	0.350281	0.257641
185	8	0	2.260910	0.666655	1.328742
186	6	0	4.163016	0.023513	0.037405
187	6	0	5.048846	0.256056	1.091267
188	6	0	4.636781	-0.423654	-1.197158
189	6	0	6.406355	0.005143	0.920680
190	1	0	4.657384	0.676017	2.013993
191	6	0	5.995093	-0.680804	-1.359653
192	1	0	3.956867	-0.524011	-2.037582
193	6	0	6.878418	-0.474698	-0.300710
194	1	0	7.098171	0.192411	1.736006
195	1	0	7.938361	-0.671706	-0.431421
196	1	0	6.360502	-1.029014	-2.321927

Benzylbenzoate@CC3-b C1 cc3-dpe999

Standard orientation:

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

1	7	0	2.295255	4.643011	2.576681
2	7	0	2.159242	2.691031	4.711012
3	7	0	3.377792	-3.301019	2.705119
4	7	0	3.351252	-4.142823	-0.127177
5	6	0	1.933959	4.032262	-0.225658
6	1	0	2.926251	3.887439	0.194754
7	6	0	0.893538	4.430497	0.626282
8	6	0	1.139217	4.693793	2.057807
9	1	0	0.250247	4.968074	2.647771
10	6	0	2.419203	4.996198	3.977809
11	1	0	1.431742	5.190940	4.434612
12	6	0	3.056678	3.829581	4.747320
13	1	0	4.022593	3.598731	4.263138
14	6	0	3.302029	4.220851	6.209499
15	1	0	3.768318	3.375411	6.727271
16	1	0	2.327981	4.389114	6.687220
17	6	0	4.165870	5.477448	6.319867
18	1	0	4.308147	5.742553	7.372888
19	1	0	5.162472	5.272644	5.905537
20	6	0	3.532115	6.639257	5.553033
21	1	0	4.169955	7.527998	5.604429
22	1	0	2.576886	6.905296	6.025885
23	6	0	3.287333	6.254626	4.093864
24	1	0	4.242465	6.059329	3.589155
25	1	0	2.800252	7.069787	3.547745
26	6	0	2.614541	1.594119	4.268203
27	1	0	3.648586	1.493884	3.902148
28	6	0	1.794798	0.367891	4.205453
29	6	0	0.432928	0.391188	4.531539
30	1	0	-0.008062	1.333393	4.846942
31	6	0	-0.331354	-0.768284	4.463047
32	6	0	0.264100	-1.965681	4.040378
33	1	0	-0.352076	-2.858612	3.966970
34	6	0	1.616719	-2.000240	3.715450
35	6	0	2.381747	-0.830057	3.818658
36	1	0	3.442674	-0.873553	3.587226
37	6	0	2.220231	-3.255975	3.225575
38	1	0	1.582039	-4.150585	3.299409
39	6	0	3.864973	-4.589020	2.240918
40	1	0	3.052490	-5.338517	2.221917
41	6	0	4.416527	-4.466550	0.811122
42	1	0	5.192870	-3.680228	0.816594
43	6	0	5.051238	-5.794226	0.370693
44	1	0	5.451995	-5.667139	-0.641017
45	1	0	4.255861	-6.548554	0.304380
46	6	0	6.140005	-6.261236	1.335991
47	1	0	6.966585	-5.537756	1.331166
48	1	0	6.552941	-7.218097	0.999533
49	6	0	5.586605	-6.382395	2.755630
50	1	0	4.823941	-7.172551	2.780914
51	1	0	6.375593	-6.679740	3.454422
52	6	0	4.963691	-5.060879	3.203264
53	1	0	5.734130	-4.279308	3.252007
54	1	0	4.535747	-5.147176	4.208125
55	6	0	3.630375	-3.300999	-1.037768
56	1	0	4.605701	-2.788262	-1.071887
57	7	0	-2.896810	5.233818	-1.158299
58	7	0	-5.125519	3.394537	-1.284301
59	7	0	-4.828129	-1.158296	3.286255

60	7	0	-2.483492	-1.750259	4.935166
61	6	0	-0.378185	4.633783	0.104297
62	1	0	-1.196973	4.963821	0.738633
63	6	0	-0.625742	4.439971	-1.261949
64	6	0	-1.955228	4.722732	-1.837184
65	1	0	-2.069324	4.491524	-2.907928
66	6	0	-4.135778	5.542874	-1.844976
67	1	0	-4.117561	5.192919	-2.893091
68	6	0	-5.297966	4.826399	-1.139976
69	1	0	-5.277744	5.132094	-0.078248
70	6	0	-6.639135	5.230331	-1.762233
71	1	0	-7.445522	4.714764	-1.229334
72	1	0	-6.658466	4.866731	-2.797896
73	6	0	-6.841220	6.745418	-1.733890
74	1	0	-7.797450	7.004402	-2.200630
75	1	0	-6.892779	7.087993	-0.691377
76	6	0	-5.686778	7.457592	-2.440534
77	1	0	-5.815793	8.543957	-2.390729
78	1	0	-5.691891	7.184874	-3.504686
79	6	0	-4.346771	7.061527	-1.820364
80	1	0	-4.300917	7.395803	-0.775693
81	1	0	-3.512596	7.540957	-2.344106
82	6	0	-4.993059	2.702570	-0.230682
83	1	0	-4.998164	3.157535	0.771924
84	6	0	-4.845148	1.233894	-0.269218
85	6	0	-4.748113	0.559229	-1.495238
86	1	0	-4.755207	1.145287	-2.410619
87	6	0	-4.638202	-0.825368	-1.529360
88	6	0	-4.646068	-1.544455	-0.325695
89	1	0	-4.578238	-2.627773	-0.364458
90	6	0	-4.715418	-0.886774	0.894965
91	6	0	-4.815576	0.511273	0.918022
92	1	0	-4.877696	1.012840	1.880531
93	6	0	-4.690716	-1.680625	2.139371
94	1	0	-4.552860	-2.764866	2.003479
95	6	0	-4.856966	-2.051011	4.430378
96	1	0	-4.602681	-3.086793	4.142345
97	6	0	-3.823911	-1.589995	5.468013
98	1	0	-4.042270	-0.532157	5.701620
99	6	0	-3.933338	-2.426053	6.749445
100	1	0	-3.195768	-2.059299	7.471609
101	1	0	-3.654156	-3.459708	6.506880
102	6	0	-5.344112	-2.387949	7.335825
103	1	0	-5.586137	-1.361052	7.641944
104	1	0	-5.391628	-3.007826	8.237367
105	6	0	-6.368002	-2.859299	6.302688
106	1	0	-6.179526	-3.914659	6.062966
107	1	0	-7.382857	-2.802316	6.710295
108	6	0	-6.270053	-2.022040	5.027752
109	1	0	-6.528127	-0.976850	5.243017
110	1	0	-6.978036	-2.373886	4.269330
111	6	0	-1.746242	-0.720432	4.884018
112	1	0	-2.112733	0.272009	5.190261
113	7	0	2.674122	3.257924	-3.708644
114	7	0	3.433271	0.552354	-4.485628
115	7	0	-1.660905	-3.399497	-4.162594
116	7	0	-4.225965	-2.768178	-2.887742
117	6	0	0.409464	4.033044	-2.094326
118	1	0	0.246588	3.876173	-3.157432

119	6	0	1.697992	3.837797	-1.580546
120	6	0	2.816019	3.463073	-2.465809
121	1	0	3.798888	3.393189	-1.973020
122	6	0	3.865910	2.958656	-4.479519
123	1	0	4.732114	2.750700	-3.822417
124	6	0	3.623865	1.709615	-5.340249
125	1	0	2.728714	1.905893	-5.957570
126	6	0	4.824252	1.445911	-6.257668
127	1	0	4.613982	0.559455	-6.866056
128	1	0	5.689166	1.200751	-5.627122
129	6	0	5.142047	2.654293	-7.138101
130	1	0	6.012972	2.441383	-7.767099
131	1	0	4.298639	2.844347	-7.815866
132	6	0	5.387597	3.896561	-6.280894
133	1	0	5.580879	4.769709	-6.913131
134	1	0	6.286958	3.740916	-5.669434
135	6	0	4.192503	4.167024	-5.367057
136	1	0	3.303219	4.399654	-5.967479
137	1	0	4.376626	5.034183	-4.723263
138	6	0	2.364808	-0.116123	-4.628657
139	1	0	1.587025	0.181983	-5.348531
140	6	0	2.075582	-1.334325	-3.847233
141	6	0	2.998532	-1.822837	-2.913822
142	1	0	3.950134	-1.309176	-2.806564
143	6	0	2.682872	-2.908216	-2.101448
144	6	0	1.461176	-3.571060	-2.286155
145	1	0	1.225883	-4.427253	-1.658599
146	6	0	0.552494	-3.119126	-3.239477
147	6	0	0.858007	-1.986699	-4.007011
148	1	0	0.120953	-1.629829	-4.722220
149	6	0	-0.734886	-3.823835	-3.404583
150	1	0	-0.841923	-4.746857	-2.814474
151	6	0	-2.846100	-4.231881	-4.281691
152	1	0	-2.898184	-4.973113	-3.463154
153	6	0	-4.112276	-3.366877	-4.206339
154	1	0	-4.036436	-2.593242	-4.991133
155	6	0	-5.363873	-4.219146	-4.456737
156	1	0	-6.245562	-3.570461	-4.408984
157	1	0	-5.455946	-4.942370	-3.635473
158	6	0	-5.293280	-4.952396	-5.795837
159	1	0	-5.277121	-4.218828	-6.613284
160	1	0	-6.191074	-5.563814	-5.935074
161	6	0	-4.034742	-5.817203	-5.870613
162	1	0	-4.095465	-6.609197	-5.111789
163	1	0	-3.965673	-6.314325	-6.843960
164	6	0	-2.784504	-4.973163	-5.624724
165	1	0	-2.669151	-4.227438	-6.422463
166	1	0	-1.881871	-5.593947	-5.638114
167	6	0	-4.473970	-1.524877	-2.819670
168	1	0	-4.557896	-0.898302	-3.721126
169	6	0	-0.105930	-1.006942	-0.448460
170	1	0	-0.174704	-0.828922	-1.526927
171	1	0	-0.729943	-0.259117	0.056130
172	6	0	-0.549620	-2.407071	-0.107444
173	6	0	0.233275	-3.270014	0.655120
174	6	0	-1.759541	-2.865902	-0.625158
175	6	0	-0.200784	-4.569967	0.909509
176	1	0	1.213780	-2.947562	0.983942
177	6	0	-2.202795	-4.158537	-0.361530

178	1	0	-2.341559	-2.227684	-1.282193
179	6	0	-1.423938	-5.016589	0.414098
180	1	0	0.438131	-5.244953	1.473303
181	1	0	-3.139567	-4.493312	-0.801473
182	1	0	-1.756953	-6.031244	0.611340
183	8	0	1.246599	-0.832942	-0.031933
184	6	0	1.984458	0.058399	-0.714471
185	8	0	1.545188	0.777821	-1.579881
186	6	0	3.414794	0.018433	-0.294758
187	6	0	4.356368	0.672392	-1.091470
188	6	0	3.822507	-0.710436	0.820056
189	6	0	5.703526	0.618089	-0.750417
190	1	0	4.019956	1.156310	-2.003817
191	6	0	5.170112	-0.755249	1.166247
192	1	0	3.094178	-1.267363	1.395348
193	6	0	6.110268	-0.085399	0.385068
194	1	0	6.439241	1.113727	-1.376722
195	1	0	7.163303	-0.124597	0.648309
196	1	0	5.472194	-1.338605	2.032479

Tetrachloroethene@CC3 C1 cc3-dpel33

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	0.021525	-0.935310	-5.568524
2	7	0	2.214282	0.957789	-5.206114
3	7	0	5.884667	0.051566	0.012937
4	7	0	5.154642	-1.690581	2.227013
5	6	0	-1.255960	-2.515984	-3.527304
6	1	0	-0.345463	-2.904874	-3.977064
7	6	0	-1.708494	-1.249037	-3.921608
8	6	0	-0.994996	-0.480397	-4.962085
9	1	0	-1.421111	0.507186	-5.198824
10	6	0	0.580576	-0.136600	-6.643339
11	1	0	0.084268	0.848137	-6.715405
12	6	0	2.071522	0.121618	-6.382494
13	1	0	2.564206	-0.857755	-6.245925
14	6	0	2.709031	0.848165	-7.574273
15	1	0	3.773286	1.000428	-7.363164
16	1	0	2.253951	1.844438	-7.650456
17	6	0	2.511744	0.079957	-8.880798
18	1	0	2.962096	0.633382	-9.711594
19	1	0	3.033770	-0.884677	-8.820122
20	6	0	1.025487	-0.167962	-9.140705
21	1	0	0.885805	-0.747091	-10.059616
22	1	0	0.519466	0.795396	-9.291201
23	6	0	0.387051	-0.899500	-7.960199
24	1	0	0.835051	-1.895372	-7.847047
25	1	0	-0.685525	-1.050806	-8.123688
26	6	0	3.022838	0.582118	-4.304784
27	1	0	3.580728	-0.364555	-4.376563
28	6	0	3.262786	1.379047	-3.084668
29	6	0	2.603273	2.601452	-2.892868
30	1	0	1.944580	2.964179	-3.678144
31	6	0	2.784217	3.323880	-1.719341
32	6	0	3.632764	2.820288	-0.723755

33	1	0	3.763838	3.398448	0.187358
34	6	0	4.296962	1.612927	-0.906648
35	6	0	4.109778	0.894163	-2.095600
36	1	0	4.629639	-0.052642	-2.217671
37	6	0	5.208088	1.115673	0.144369
38	1	0	5.277992	1.742129	1.047392
39	6	0	6.799410	-0.302650	1.081658
40	1	0	6.713199	0.394588	1.934704
41	6	0	6.464170	-1.707849	1.603338
42	1	0	6.493743	-2.399938	0.742425
43	6	0	7.496299	-2.153144	2.647317
44	1	0	7.239101	-3.162577	2.986587
45	1	0	7.407440	-1.492014	3.519274
46	6	0	8.920647	-2.104906	2.094510
47	1	0	9.017643	-2.825223	1.270804
48	1	0	9.632801	-2.409853	2.868557
49	6	0	9.252552	-0.704032	1.578688
50	1	0	9.245923	0.001791	2.420444
51	1	0	10.260603	-0.679231	1.151463
52	6	0	8.230748	-0.258372	0.532894
53	1	0	8.280368	-0.913836	-0.346377
54	1	0	8.442141	0.758153	0.183527
55	6	0	4.304871	-2.548757	1.840906
56	1	0	4.528016	-3.269157	1.038035
57	7	0	-5.278279	0.220518	-2.082765
58	7	0	-5.431721	2.069268	0.163749
59	7	0	-0.250105	5.845020	0.800508
60	7	0	2.292331	5.365657	-0.540933
61	6	0	-2.853759	-0.720094	-3.337597
62	1	0	-3.218445	0.266288	-3.612938
63	6	0	-3.568359	-1.453681	-2.379758
64	6	0	-4.789734	-0.903832	-1.757643
65	1	0	-5.259668	-1.543703	-0.993770
66	6	0	-6.527350	0.613847	-1.455865
67	1	0	-6.778211	-0.048279	-0.607683
68	6	0	-6.410123	2.042856	-0.906728
69	1	0	-6.110298	2.698853	-1.743854
70	6	0	-7.758870	2.517365	-0.350995
71	1	0	-7.645292	3.542238	0.019115
72	1	0	-8.011958	1.891999	0.515193
73	6	0	-8.865443	2.432294	-1.402299
74	1	0	-9.817239	2.760266	-0.971255
75	1	0	-8.636862	3.118506	-2.229121
76	6	0	-8.983559	1.008881	-1.948652
77	1	0	-9.752410	0.957146	-2.726781
78	1	0	-9.302629	0.337126	-1.140168
79	6	0	-7.642870	0.531552	-2.506315
80	1	0	-7.350343	1.148049	-3.366408
81	1	0	-7.710830	-0.501563	-2.864526
82	6	0	-4.505973	2.933192	0.096757
83	1	0	-4.415830	3.627088	-0.753893
84	6	0	-3.467860	3.060095	1.139661
85	6	0	-3.492480	2.237613	2.276179
86	1	0	-4.310094	1.529482	2.385035
87	6	0	-2.476044	2.308560	3.219262
88	6	0	-1.425348	3.218956	3.033966
89	1	0	-0.638956	3.261957	3.783162
90	6	0	-1.396967	4.047627	1.919583
91	6	0	-2.425363	3.962825	0.969395

92	1	0	-2.382122	4.611791	0.098330
93	6	0	-0.298602	5.021989	1.763566
94	1	0	0.468763	5.003581	2.553120
95	6	0	0.837384	6.804678	0.785894
96	1	0	1.540178	6.633147	1.621244
97	6	0	1.633167	6.657949	-0.519215
98	1	0	0.921488	6.764284	-1.357764
99	6	0	2.705651	7.750232	-0.622647
100	1	0	3.240077	7.628204	-1.571154
101	1	0	3.438023	7.586649	0.178696
102	6	0	2.104231	9.150626	-0.505823
103	1	0	1.429141	9.330850	-1.353488
104	1	0	2.896804	9.904009	-0.565119
105	6	0	1.320898	9.293783	0.799631
106	1	0	2.012730	9.202434	1.648044
107	1	0	0.863431	10.286374	0.868308
108	6	0	0.243922	8.213976	0.902057
109	1	0	-0.494278	8.340964	0.099451
110	1	0	-0.301051	8.288827	1.849362
111	6	0	2.103935	4.623744	-1.551533
112	1	0	1.436632	4.920585	-2.375815
113	7	0	-1.878018	-5.180143	-1.123731
114	7	0	0.080702	-5.511839	1.042620
115	7	0	-0.253816	-1.043257	5.660597
116	7	0	-1.647560	1.497863	5.329036
117	6	0	-3.116445	-2.714461	-2.006064
118	1	0	-3.646316	-3.300062	-1.259284
119	6	0	-1.944457	-3.243962	-2.563489
120	6	0	-1.396491	-4.535734	-2.104029
121	1	0	-0.514495	-4.894743	-2.658020
122	6	0	-1.252295	-6.448843	-0.794177
123	1	0	-0.303043	-6.582900	-1.343924
124	6	0	-0.928574	-6.502732	0.705731
125	1	0	-1.869383	-6.317110	1.254769
126	6	0	-0.387332	-7.887155	1.088754
127	1	0	-0.183946	-7.897162	2.165266
128	1	0	0.576017	-8.030520	0.581784
129	6	0	-1.355318	-9.005250	0.702739
130	1	0	-0.930275	-9.977726	0.972898
131	1	0	-2.287093	-8.894825	1.273966
132	6	0	-1.672733	-8.951809	-0.791868
133	1	0	-2.393760	-9.730721	-1.061556
134	1	0	-0.756594	-9.153745	-1.363388
135	6	0	-2.219242	-7.577541	-1.176524
136	1	0	-3.175482	-7.395988	-0.668353
137	1	0	-2.415820	-7.518887	-2.252716
138	6	0	-0.152725	-4.767717	2.043199
139	1	0	-1.103099	-4.827371	2.598711
140	6	0	0.803890	-3.760431	2.543187
141	6	0	2.092535	-3.653325	2.004422
142	1	0	2.391282	-4.353593	1.227892
143	6	0	2.959720	-2.658073	2.439047
144	6	0	2.543292	-1.768709	3.439344
145	1	0	3.234974	-0.997181	3.767943
146	6	0	1.275284	-1.878637	3.997613
147	6	0	0.407113	-2.881031	3.543440
148	1	0	-0.585697	-2.944331	3.982082
149	6	0	0.866356	-0.953246	5.073440
150	1	0	1.608754	-0.188148	5.349968

151	6	0	-0.518834	-0.128488	6.754834
152	1	0	0.287603	0.619656	6.860960
153	6	0	-1.821932	0.636949	6.483828
154	1	0	-2.619461	-0.109082	6.315843
155	6	0	-2.192762	1.512486	7.688141
156	1	0	-3.133483	2.029506	7.468984
157	1	0	-1.422193	2.286754	7.798074
158	6	0	-2.301560	0.694029	8.974375
159	1	0	-3.124921	-0.027076	8.880416
160	1	0	-2.548561	1.350324	9.815553
161	6	0	-0.999788	-0.061410	9.244321
162	1	0	-0.194021	0.662106	9.428923
163	1	0	-1.089591	-0.674017	10.147626
164	6	0	-0.630185	-0.941760	8.050631
165	1	0	-1.393766	-1.716624	7.902999
166	1	0	0.319354	-1.460400	8.222238
167	6	0	-2.514876	1.431528	4.406616
168	1	0	-3.356775	0.722707	4.447392
169	6	0	-1.122974	-0.903454	-0.094510
170	6	0	-0.006940	-1.092224	-0.809594
171	17	0	0.859829	-2.575011	-0.787980
172	17	0	0.676085	0.142791	-1.784493
173	17	0	-1.965353	0.589270	-0.086240
174	17	0	-1.799413	-2.128537	0.904842

15-Crown-5@CC3 C1 cc3-crown

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	0.551022	-2.019222	-5.332609
2	7	0	-1.818560	-0.174461	-5.409004
3	7	0	-1.168663	5.200939	-2.051616
4	7	0	1.110823	5.692013	-0.084735
5	6	0	2.716696	-2.364635	-3.429138
6	1	0	2.829761	-1.588586	-4.183107
7	6	0	1.578950	-3.187517	-3.484012
8	6	0	0.540725	-2.990524	-4.516707
9	1	0	-0.257567	-3.750883	-4.530845
10	6	0	-0.474836	-2.008475	-6.364803
11	1	0	-1.317101	-2.672369	-6.099977
12	6	0	-1.041174	-0.595657	-6.564893
13	1	0	-0.188919	0.083435	-6.745851
14	6	0	-1.979836	-0.557819	-7.781939
15	1	0	-2.339314	0.469615	-7.906965
16	1	0	-2.859041	-1.174623	-7.552595
17	6	0	-1.306301	-1.062035	-9.056552
18	1	0	-2.014766	-1.031770	-9.891219
19	1	0	-0.473512	-0.395837	-9.319853
20	6	0	-0.771980	-2.478409	-8.851041
21	1	0	-0.259417	-2.834732	-9.750961
22	1	0	-1.614169	-3.160506	-8.671549
23	6	0	0.180991	-2.519100	-7.658326
24	1	0	1.062638	-1.896607	-7.861116
25	1	0	0.546810	-3.536738	-7.481371
26	6	0	-1.680420	1.030062	-5.032888
27	1	0	-0.942584	1.699994	-5.503668

28	6	0	-2.479920	1.642098	-3.952729
29	6	0	-3.522731	0.943637	-3.329737
30	1	0	-3.748712	-0.064202	-3.668494
31	6	0	-4.233457	1.521167	-2.282684
32	6	0	-3.878007	2.799406	-1.826044
33	1	0	-4.394795	3.204903	-0.960255
34	6	0	-2.835781	3.498040	-2.425609
35	6	0	-2.165609	2.924341	-3.515726
36	1	0	-1.338454	3.473244	-3.960702
37	6	0	-2.330196	4.744858	-1.805086
38	1	0	-3.004807	5.228480	-1.080808
39	6	0	-0.802582	6.479147	-1.449275
40	1	0	-1.325616	6.630445	-0.489221
41	6	0	0.712174	6.571767	-1.176678
42	1	0	1.238789	6.309991	-2.110316
43	6	0	1.102205	8.000960	-0.759000
44	1	0	2.187383	8.028948	-0.609098
45	1	0	0.643943	8.205206	0.218218
46	6	0	0.662839	9.057053	-1.769410
47	1	0	1.179420	8.890221	-2.724345
48	1	0	0.953503	10.053125	-1.418706
49	6	0	-0.845477	8.978102	-1.991690
50	1	0	-1.363185	9.224556	-1.054699
51	1	0	-1.168210	9.712405	-2.737548
52	6	0	-1.240317	7.573501	-2.439851
53	1	0	-0.784456	7.349640	-3.413867
54	1	0	-2.324877	7.496366	-2.575968
55	6	0	2.272731	5.179644	-0.122448
56	1	0	2.947690	5.314118	-0.981529
57	7	0	0.914748	-5.761094	-0.155448
58	7	0	-0.738697	-5.121885	2.257054
59	7	0	-5.510636	-0.841521	1.745041
60	7	0	-5.833795	1.079303	-0.523573
61	6	0	1.399509	-4.164527	-2.512886
62	1	0	0.514620	-4.797524	-2.516927
63	6	0	2.325118	-4.311558	-1.467859
64	6	0	2.051398	-5.224805	-0.340327
65	1	0	2.881860	-5.367497	0.370794
66	6	0	0.757062	-6.638203	0.993539
67	1	0	1.521028	-6.429333	1.763579
68	6	0	-0.624661	-6.436198	1.635275
69	1	0	-1.381875	-6.567509	0.842017
70	6	0	-0.866086	-7.481553	2.737038
71	1	0	-1.869321	-7.323749	3.148333
72	1	0	-0.155858	-7.287979	3.552027
73	6	0	-0.701869	-8.912726	2.229239
74	1	0	-0.864388	-9.620220	3.049180
75	1	0	-1.467512	-9.122299	1.469992
76	6	0	0.683146	-9.106338	1.614330
77	1	0	0.793287	-10.121531	1.218843
78	1	0	1.446476	-8.982653	2.394487
79	6	0	0.919442	-8.085631	0.503081
80	1	0	0.206454	-8.249819	-0.315915
81	1	0	1.922394	-8.194165	0.075436
82	6	0	-1.868638	-4.545228	2.179581
83	1	0	-2.693752	-4.969662	1.583486
84	6	0	-2.173544	-3.273464	2.867694
85	6	0	-1.271271	-2.725502	3.789809
86	1	0	-0.381981	-3.297414	4.043299

87	6	0	-1.493039	-1.469126	4.339310
88	6	0	-2.663122	-0.769169	4.006982
89	1	0	-2.817230	0.217759	4.436776
90	6	0	-3.592177	-1.321978	3.133073
91	6	0	-3.344697	-2.585941	2.572359
92	1	0	-4.065922	-2.986328	1.862955
93	6	0	-4.772627	-0.526246	2.728989
94	1	0	-4.959327	0.379717	3.327962
95	6	0	-6.689584	-0.019870	1.503859
96	1	0	-6.598202	0.963451	1.997870
97	6	0	-6.891193	0.230831	0.000302
98	1	0	-6.904917	-0.752894	-0.502803
99	6	0	-8.228468	0.943834	-0.252040
100	1	0	-8.345643	1.084396	-1.332243
101	1	0	-8.169306	1.945972	0.192998
102	6	0	-9.414301	0.180306	0.334266
103	1	0	-9.509833	-0.791657	-0.168616
104	1	0	-10.343198	0.728930	0.145834
105	6	0	-9.214489	-0.045138	1.832200
106	1	0	-9.206466	0.925556	2.346279
107	1	0	-10.045729	-0.621327	2.252323
108	6	0	-7.895315	-0.770159	2.092320
109	1	0	-7.923666	-1.773045	1.645771
110	1	0	-7.727313	-0.906748	3.166505
111	6	0	-5.298694	0.737730	-1.623434
112	1	0	-5.578312	-0.197992	-2.134805
113	7	0	5.466333	-1.410406	-1.243542
114	7	0	5.693785	1.271773	0.159992
115	7	0	1.746564	2.082442	5.138049
116	7	0	-0.574901	0.292202	5.711681
117	6	0	3.444643	-3.490974	-1.426979
118	1	0	4.153148	-3.550613	-0.604276
119	6	0	3.639586	-2.498798	-2.399516
120	6	0	4.745818	-1.524198	-2.282779
121	1	0	4.900628	-0.882520	-3.166249
122	6	0	6.593675	-0.490261	-1.316719
123	1	0	6.462225	0.242638	-2.132852
124	6	0	6.765229	0.300523	-0.008712
125	1	0	6.785418	-0.424751	0.823891
126	6	0	8.083410	1.093774	-0.020376
127	1	0	8.179918	1.611786	0.940366
128	1	0	8.003594	1.871464	-0.791674
129	6	0	9.300444	0.213667	-0.293821
130	1	0	10.208575	0.825736	-0.304756
131	1	0	9.416722	-0.517057	0.518113
132	6	0	9.129076	-0.527334	-1.617978
133	1	0	9.984850	-1.183160	-1.810393
134	1	0	9.093367	0.201313	-2.439156
135	6	0	7.840178	-1.345423	-1.602766
136	1	0	7.900667	-2.124218	-0.830772
137	1	0	7.689726	-1.860180	-2.558210
138	6	0	5.234111	1.442812	1.330668
139	1	0	5.562978	0.821775	2.179987
140	6	0	4.190770	2.446422	1.642002
141	6	0	3.840125	3.440677	0.714174
142	1	0	4.378784	3.484124	-0.229285
143	6	0	2.762989	4.286361	0.955189
144	6	0	2.049160	4.160963	2.155703
145	1	0	1.190405	4.808322	2.317168

146	6	0	2.385112	3.180863	3.084529
147	6	0	3.466676	2.327399	2.824242
148	1	0	3.702327	1.551445	3.548711
149	6	0	1.570935	3.026031	4.307933
150	1	0	0.794540	3.793173	4.457575
151	6	0	0.952517	2.109460	6.356034
152	1	0	0.083182	2.783475	6.256023
153	6	0	0.420259	0.707921	6.686611
154	1	0	1.283102	0.018003	6.700954
155	6	0	-0.258941	0.695554	8.064972
156	1	0	-0.600763	-0.324338	8.273459
157	1	0	-1.156635	1.325213	8.007588
158	6	0	0.664480	1.202396	9.171145
159	1	0	1.523832	0.525480	9.271169
160	1	0	0.137602	1.192042	10.131151
161	6	0	1.165859	2.608161	8.844008
162	1	0	0.314006	3.301544	8.828355
163	1	0	1.852752	2.964927	9.618755
164	6	0	1.861310	2.622783	7.484132
165	1	0	2.757513	1.988932	7.513910
166	1	0	2.197137	3.632730	7.224094
167	6	0	-0.487285	-0.886530	5.252159
168	1	0	0.351185	-1.551993	5.515711
169	8	0	2.403972	-1.230050	-0.208528
170	8	0	1.775045	2.237788	-1.106187
171	8	0	-0.220356	-1.933438	0.946920
172	8	0	-1.671962	2.116661	0.036370
173	8	0	-1.877692	-0.719395	-0.934937
174	6	0	1.714966	-0.226508	-0.934718
175	6	0	2.119904	-1.232939	1.172421
176	6	0	2.528257	1.064520	-0.885273
177	6	0	1.030259	-2.230044	1.537311
178	6	0	0.703466	2.362837	-0.188770
179	6	0	-0.404976	-2.549524	-0.316926
180	6	0	-0.598118	2.026235	-0.881332
181	6	0	-1.739720	-2.120834	-0.894626
182	6	0	-1.777566	0.966262	0.851256
183	6	0	-2.531474	-0.173929	0.205059
184	1	0	0.396242	-2.260783	-1.002010
185	1	0	-1.801918	-2.492648	-1.925372
186	1	0	1.338463	-3.250036	1.270875
187	1	0	1.830112	-0.228540	1.518573
188	1	0	-3.524064	0.176412	-0.085643
189	1	0	-0.792529	0.606381	1.179869
190	1	0	-0.589743	1.058808	-1.389631
191	1	0	1.586278	-0.586998	-1.960185
192	1	0	0.889897	1.756298	0.709736
193	1	0	3.337122	1.054471	-1.622715
194	1	0	-0.381652	-3.645407	-0.213702
195	1	0	-2.566772	-2.569232	-0.324090
196	1	0	-2.645812	-0.949819	0.960709
197	1	0	0.887967	-2.195296	2.622839
198	1	0	-2.338515	1.268189	1.745059
199	1	0	3.044557	-1.509005	1.696940
200	1	0	-0.733195	2.796653	-1.634143
201	1	0	0.716554	-0.095691	-0.510668
202	1	0	2.995859	1.101727	0.103169
203	1	0	0.621019	3.400180	0.131734

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-4.112351	-2.603183	-3.074989
2	7	0	-1.780943	-4.332564	-3.328210
3	7	0	1.708098	-5.301978	1.956445
4	7	0	1.393197	-3.444731	4.145144
5	6	0	-4.558234	-0.533082	-1.132338
6	1	0	-4.859440	-1.546149	-0.877203
7	6	0	-3.929047	-0.310716	-2.365921
8	6	0	-3.729624	-1.419163	-3.320502
9	1	0	-3.253502	-1.147064	-4.275250
10	6	0	-3.960162	-3.593478	-4.124152
11	1	0	-3.425165	-3.178164	-4.997234
12	6	0	-3.134225	-4.776621	-3.602044
13	1	0	-3.629481	-5.154903	-2.689592
14	6	0	-3.074372	-5.896586	-4.648959
15	1	0	-2.495591	-6.730693	-4.237238
16	1	0	-2.518436	-5.521956	-5.518389
17	6	0	-4.469819	-6.352226	-5.075030
18	1	0	-4.390990	-7.136757	-5.834987
19	1	0	-4.989390	-6.793878	-4.213788
20	6	0	-5.285004	-5.170823	-5.602334
21	1	0	-6.295371	-5.491368	-5.877334
22	1	0	-4.813086	-4.785594	-6.516474
23	6	0	-5.356479	-4.057129	-4.557947
24	1	0	-5.891694	-4.409958	-3.666713
25	1	0	-5.910911	-3.193006	-4.939953
26	6	0	-1.288158	-4.607290	-2.193027
27	1	0	-1.867318	-5.132314	-1.416581
28	6	0	0.102261	-4.269374	-1.831234
29	6	0	0.917914	-3.536812	-2.705717
30	1	0	0.499661	-3.209093	-3.653877
31	6	0	2.233611	-3.247297	-2.365921
32	6	0	2.740779	-3.681006	-1.132338
33	1	0	3.768724	-3.435324	-0.877203
34	6	0	1.935684	-4.392340	-0.252791
35	6	0	0.615354	-4.696601	-0.614014
36	1	0	0.000000	-5.251920	0.089600
37	6	0	2.439934	-4.735480	1.090456
38	1	0	3.477766	-4.436112	1.306116
39	6	0	2.273633	-5.551518	3.266276
40	1	0	3.284080	-5.114347	3.361375
41	6	0	1.376646	-4.885218	4.320630
42	1	0	0.358579	-5.295212	4.190418
43	6	0	1.876049	-5.213887	5.732826
44	1	0	1.210327	-4.738315	6.461247
45	1	0	2.866276	-4.757647	5.861150
46	6	0	1.957062	-6.722885	5.965691
47	1	0	0.948522	-7.155014	5.911578
48	1	0	2.335747	-6.926590	6.972883
49	6	0	2.845339	-7.387852	4.912913
50	1	0	3.875930	-7.025641	5.029034
51	1	0	2.871757	-8.472670	5.060489
52	6	0	2.349214	-7.063981	3.503521

53	1	0	1.347275	-7.485617	3.349670
54	1	0	3.001779	-7.508727	2.744170
55	6	0	0.276198	-2.859703	4.000902
56	1	0	-0.670937	-3.421458	3.963058
57	7	0	-2.861639	3.708624	-3.328210
58	7	0	-0.198247	4.862993	-3.074989
59	7	0	4.642582	0.623940	-3.328210
60	7	0	4.310599	-2.259809	-3.074989
61	6	0	-3.521926	0.973469	-2.705717
62	1	0	-3.028987	1.171828	-3.653877
63	6	0	-3.748517	2.046126	-1.831234
64	6	0	-3.345951	3.419222	-2.193027
65	1	0	-3.511055	4.183302	-1.416581
66	6	0	-2.569562	5.102629	-3.602044
67	1	0	-2.649537	5.720674	-2.689592
68	6	0	-1.131963	5.226340	-4.124152
69	1	0	-1.039788	4.555362	-4.997234
70	6	0	-0.835338	6.667412	-4.557947
71	1	0	0.190231	6.715502	-4.939953
72	1	0	-0.873289	7.307336	-3.666713
73	6	0	-1.835562	7.162359	-5.602334
74	1	0	-1.607979	8.197635	-5.877334
75	1	0	-1.737903	6.561052	-6.516474
76	6	0	-3.266280	7.047090	-5.075030
77	1	0	-3.985117	7.371087	-5.834987
78	1	0	-3.388976	7.717877	-4.213788
79	6	0	-3.569407	5.610777	-4.648959
80	1	0	-3.522936	4.942008	-5.518389
81	1	0	-4.581155	5.526592	-4.237238
82	6	0	0.635781	3.939531	-3.320502
83	1	0	0.633364	3.391147	-4.275250
84	6	0	1.695436	3.558012	-2.365921
85	6	0	1.817455	4.214087	-1.132338
86	1	0	1.090716	4.981473	-0.877203
87	6	0	2.836036	3.872522	-0.252791
88	6	0	3.759698	2.881213	-0.614014
89	1	0	4.548296	2.625960	0.089600
90	6	0	3.646255	2.223248	-1.831234
91	6	0	2.604012	2.563343	-2.705717
92	1	0	2.529326	2.037266	-3.653877
93	6	0	4.634109	1.188067	-2.193027
94	1	0	5.378373	0.949012	-1.416581
95	6	0	5.703787	-0.326009	-3.602044
96	1	0	6.279017	-0.565771	-2.689592
97	6	0	5.092125	-1.632862	-4.124152
98	1	0	4.464953	-1.377198	-4.997234
99	6	0	6.191817	-2.610282	-4.557947
100	1	0	5.720680	-3.522496	-4.939953
101	1	0	6.764983	-2.897378	-3.666713
102	6	0	7.120566	-1.991536	-5.602334
103	1	0	6.550989	-1.775458	-6.516474
104	1	0	7.903350	-2.706267	-5.877334
105	6	0	7.736099	-0.694863	-5.075030
106	1	0	8.378366	-0.924000	-4.213788
107	1	0	8.376108	-0.234331	-5.834987
108	6	0	6.643779	0.285808	-4.648959
109	1	0	6.041373	0.579949	-5.518389
110	1	0	7.076746	1.204101	-4.237238
111	6	0	3.093843	-2.520368	-3.320502

112	1	0	2.620137	-2.244083	-4.275250
113	7	0	-5.445696	1.171733	1.956445
114	7	0	-3.679823	0.515821	4.145144
115	7	0	2.286625	2.928910	4.145144
116	7	0	3.737598	4.130245	1.956445
117	6	0	-4.375053	1.815388	-0.614014
118	1	0	-4.548296	2.625960	0.089600
119	6	0	-4.771720	0.519818	-0.252791
120	6	0	-5.321013	0.254695	1.090456
121	1	0	-5.580669	-0.793778	1.306116
122	6	0	-5.944572	0.806735	3.266276
123	1	0	-6.071195	-0.286923	3.361375
124	6	0	-4.919046	1.250399	4.320630
125	1	0	-4.765078	2.337068	4.190418
126	6	0	-5.453383	0.982238	5.732826
127	1	0	-4.708665	1.320984	6.461247
128	1	0	-5.553382	-0.103445	5.861150
129	6	0	-6.800720	1.666577	5.965691
130	1	0	-7.166476	1.440478	6.972883
131	1	0	-6.670684	2.756063	5.911578
132	6	0	-7.820737	1.229790	4.912913
133	1	0	-8.773426	1.749320	5.060489
134	1	0	-8.022348	0.156167	5.029034
135	6	0	-7.292194	1.497512	3.503521
136	1	0	-7.156372	2.576034	3.349670
137	1	0	-8.003637	1.154747	2.744170
138	6	0	-2.614675	1.190657	4.000902
139	1	0	-2.627601	2.291777	3.963058
140	6	0	-1.276679	0.572106	3.931925
141	6	0	-1.123787	-0.821541	3.929940
142	1	0	-2.016209	-1.442696	3.942892
143	6	0	0.142881	-1.391689	3.931925
144	6	0	1.273369	-0.562457	3.929940
145	1	0	2.257516	-1.024740	3.942892
146	6	0	1.133797	0.819583	3.931925
147	6	0	-0.149582	1.383999	3.929940
148	1	0	-0.241307	2.467437	3.942892
149	6	0	2.338476	1.669046	4.000902
150	1	0	3.298538	1.129681	3.963058
151	6	0	3.542400	3.634820	4.320630
152	1	0	4.406499	2.958144	4.190418
153	6	0	3.670939	4.744783	3.266276
154	1	0	2.787115	5.401270	3.361375
155	6	0	4.942980	5.566469	3.503521
156	1	0	5.001859	6.353980	2.744170
157	1	0	5.809097	4.909583	3.349670
158	6	0	4.975398	6.158062	4.912913
159	1	0	4.146419	6.869474	5.029034
160	1	0	5.901669	6.723350	5.060489
161	6	0	4.843658	5.056307	5.965691
162	1	0	5.722163	4.398951	5.911578
163	1	0	4.830729	5.486111	6.972883
164	6	0	3.577334	4.231649	5.732826
165	1	0	2.687105	4.861092	5.861150
166	1	0	3.498338	3.417332	6.461247
167	6	0	2.881079	4.480784	1.090456
168	1	0	2.102902	5.229890	1.306116
169	6	0	0.428402	-1.316724	0.478193
170	6	0	-0.936895	-1.044380	0.476472

171	6	0	-1.354517	0.287355	0.478193
172	6	0	-0.436012	1.333565	0.476472
173	6	0	0.926115	1.029369	0.478193
174	6	0	1.372907	-0.289185	0.476472
175	1	0	0.763660	-2.347901	0.534546
176	1	0	-2.415172	0.512602	0.534546
177	1	0	1.651512	1.835299	0.534546
178	6	0	-0.900366	2.768296	0.503253
179	1	0	-0.912517	3.204649	-0.505147
180	1	0	-1.913921	2.844742	0.912772
181	1	0	-0.232903	3.383802	1.118088
182	6	0	-1.947232	-2.163888	0.503253
183	1	0	-2.814006	-1.893601	1.118088
184	1	0	-2.319049	-2.392587	-0.505147
185	1	0	-1.506658	-3.079875	0.912772
186	6	0	2.847597	-0.604408	0.503253
187	1	0	3.046910	-1.490201	1.118088
188	1	0	3.231566	-0.812062	-0.505147
189	1	0	3.420579	0.235134	0.912772

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-5.592959	1.716192	-0.324888
2	7	0	-5.708199	-1.201068	-0.220560
3	7	0	-1.511838	-3.980700	3.765668
4	7	0	0.855741	-2.569069	4.763034
5	6	0	-3.358209	3.432251	0.281064
6	1	0	-4.038530	3.179309	1.090618
7	6	0	-3.607180	2.904342	-0.994953
8	6	0	-4.782680	2.046259	-1.243031
9	1	0	-4.923914	1.723846	-2.286429
10	6	0	-6.762202	0.945382	-0.705573
11	1	0	-6.721714	0.650545	-1.769684
12	6	0	-6.827306	-0.343179	0.124748
13	1	0	-6.801893	-0.055452	1.191331
14	6	0	-8.127410	-1.105833	-0.163445
15	1	0	-8.149597	-2.006665	0.459657
16	1	0	-8.102159	-1.442144	-1.208248
17	6	0	-9.362308	-0.238080	0.078672
18	1	0	-10.269599	-0.805389	-0.154312
19	1	0	-9.418165	0.029633	1.142591
20	6	0	-9.295792	1.039790	-0.758413
21	1	0	-10.164424	1.676680	-0.560485
22	1	0	-9.330479	0.775816	-1.824198
23	6	0	-8.007526	1.808339	-0.465734
24	1	0	-7.996793	2.141074	0.580450
25	1	0	-7.935549	2.708379	-1.086064
26	6	0	-5.016033	-1.671167	0.732166
27	1	0	-5.220766	-1.411023	1.783193
28	6	0	-3.902795	-2.617083	0.521456
29	6	0	-3.517473	-3.013125	-0.768857
30	1	0	-4.048919	-2.596786	-1.620785
31	6	0	-2.482472	-3.922825	-0.943687
32	6	0	-1.812782	-4.433250	0.177646

33	1	0	-0.997535	-5.134495	0.019101
34	6	0	-2.168159	-4.028308	1.455206
35	6	0	-3.230396	-3.128151	1.623447
36	1	0	-3.495923	-2.820631	2.632248
37	6	0	-1.364417	-4.476041	2.607670
38	1	0	-0.600469	-5.240058	2.391832
39	6	0	-0.670595	-4.491899	4.830955
40	1	0	0.161801	-5.099604	4.432587
41	6	0	-0.065843	-3.312556	5.604041
42	1	0	-0.906415	-2.677761	5.938520
43	6	0	0.710428	-3.810160	6.830763
44	1	0	1.109675	-2.942751	7.367504
45	1	0	1.573467	-4.389094	6.476731
46	6	0	-0.159173	-4.671423	7.745870
47	1	0	-0.976974	-4.062141	8.154215
48	1	0	0.429872	-5.025054	8.598664
49	6	0	-0.748639	-5.851311	6.972643
50	1	0	0.066207	-6.508623	6.639961
51	1	0	-1.397840	-6.451851	7.618590
52	6	0	-1.533636	-5.359376	5.757146
53	1	0	-2.394257	-4.760127	6.082340
54	1	0	-1.932188	-6.200004	5.178318
55	6	0	0.660606	-1.319877	4.649388
56	1	0	-0.215786	-0.828864	5.101741
57	7	0	-0.924728	4.023707	-4.133109
58	7	0	1.353510	2.402443	-4.906508
59	7	0	0.851671	-3.898223	-3.999300
60	7	0	-1.196966	-5.245748	-2.473632
61	6	0	-2.745242	3.205545	-2.042664
62	1	0	-2.916979	2.809401	-3.040214
63	6	0	-1.630931	4.029898	-1.831305
64	6	0	-0.711232	4.371578	-2.933211
65	1	0	0.172641	4.962936	-2.646050
66	6	0	0.033472	4.445774	-5.135956
67	1	0	0.886712	4.980964	-4.681271
68	6	0	0.591617	3.203961	-5.846293
69	1	0	-0.269837	2.641678	-6.249844
70	6	0	1.515312	3.611936	-6.999844
71	1	0	1.882144	2.705948	-7.494352
72	1	0	2.390792	4.119200	-6.574009
73	6	0	0.806204	4.532312	-7.993464
74	1	0	1.495668	4.820839	-8.793884
75	1	0	-0.022471	3.989001	-8.467801
76	6	0	0.255146	5.770708	-7.285061
77	1	0	-0.281298	6.412689	-7.991709
78	1	0	1.091814	6.362517	-6.889376
79	6	0	-0.671272	5.368599	-6.137402
80	1	0	-1.549766	4.839752	-6.529543
81	1	0	-1.042963	6.249701	-5.603074
82	6	0	0.988512	1.200187	-4.733939
83	1	0	0.102384	0.784330	-5.238425
84	6	0	1.742126	0.249168	-3.893580
85	6	0	2.888014	0.649459	-3.191296
86	1	0	3.186638	1.694114	-3.234245
87	6	0	3.638868	-0.279671	-2.481773
88	6	0	3.240978	-1.625407	-2.464949
89	1	0	3.849546	-2.339950	-1.915815
90	6	0	2.107795	-2.031652	-3.158382
91	6	0	1.356854	-1.084531	-3.868507

92	1	0	0.483956	-1.424288	-4.419583
93	6	0	1.747422	-3.463121	-3.214234
94	1	0	2.331742	-4.132833	-2.563502
95	6	0	0.632207	-5.329621	-4.061696
96	1	0	1.202189	-5.863283	-3.279769
97	6	0	-0.858034	-5.624525	-3.829540
98	1	0	-1.431173	-5.039975	-4.571792
99	6	0	-1.148248	-7.117511	-4.018490
100	1	0	-2.218283	-7.292265	-3.861984
101	1	0	-0.617274	-7.670718	-3.232844
102	6	0	-0.705921	-7.609438	-5.396916
103	1	0	-1.294802	-7.101490	-6.172822
104	1	0	-0.909259	-8.681015	-5.494853
105	6	0	0.778893	-7.320123	-5.623311
106	1	0	1.373360	-7.900004	-4.904176
107	1	0	1.086498	-7.643551	-6.623323
108	6	0	1.072838	-5.831100	-5.442573
109	1	0	0.541588	-5.245890	-6.204499
110	1	0	2.140754	-5.621463	-5.568074
111	6	0	-2.080146	-4.353505	-2.297766
112	1	0	-2.593275	-3.860855	-3.137926
113	7	0	-0.839217	5.309881	2.118719
114	7	0	0.935174	3.799991	3.851543
115	7	0	5.721815	0.180929	1.523116
116	7	0	5.655800	-0.654485	-1.216892
117	6	0	-1.389247	4.539952	-0.563571
118	1	0	-0.522694	5.166661	-0.368956
119	6	0	-2.249008	4.238419	0.501564
120	6	0	-1.915802	4.689100	1.867870
121	1	0	-2.636343	4.420703	2.656782
122	6	0	-0.573444	5.693391	3.490566
123	1	0	-1.274804	5.203769	4.189946
124	6	0	0.846982	5.248672	3.864787
125	1	0	1.539441	5.701674	3.132172
126	6	0	1.211577	5.742229	5.271210
127	1	0	2.234571	5.424047	5.500130
128	1	0	0.553318	5.240625	5.992668
129	6	0	1.067955	7.259236	5.393570
130	1	0	1.314835	7.578109	6.411750
131	1	0	1.787068	7.749179	4.723062
132	6	0	-0.347588	7.700765	5.020280
133	1	0	-0.438409	8.790718	5.075193
134	1	0	-1.058986	7.284738	5.746579
135	6	0	-0.712523	7.215989	3.616992
136	1	0	-0.054280	7.683869	2.873149
137	1	0	-1.738600	7.498352	3.356528
138	6	0	1.927013	3.279810	3.254613
139	1	0	2.665734	3.893318	2.713324
140	6	0	2.203752	1.830711	3.279524
141	6	0	1.311456	0.940375	3.892404
142	1	0	0.391625	1.336073	4.315973
143	6	0	1.600215	-0.416521	3.957723
144	6	0	2.792172	-0.896137	3.397873
145	1	0	3.004694	-1.961081	3.456387
146	6	0	3.670267	-0.026283	2.764216
147	6	0	3.375432	1.343611	2.714956
148	1	0	4.078995	2.010263	2.222173
149	6	0	4.879201	-0.560843	2.113600
150	1	0	4.998545	-1.655326	2.156655

151	6	0	6.856797	-0.460788	0.892344
152	1	0	6.797083	-1.561446	0.974269
153	6	0	6.851625	-0.109035	-0.603800
154	1	0	6.876762	0.993067	-0.681462
155	6	0	8.086838	-0.694317	-1.296790
156	1	0	8.062711	-0.418830	-2.356794
157	1	0	8.020964	-1.789123	-1.250085
158	6	0	9.379226	-0.215082	-0.633801
159	1	0	9.469882	0.872778	-0.756885
160	1	0	10.244681	-0.663661	-1.132896
161	6	0	9.384619	-0.553764	0.858074
162	1	0	9.391502	-1.645545	0.979867
163	1	0	10.295386	-0.175848	1.334494
164	6	0	8.151412	0.026122	1.551508
165	1	0	8.170320	1.122710	1.503225
166	1	0	8.131954	-0.245536	2.612569
167	6	0	4.864489	0.157964	-1.784667
168	1	0	5.061916	1.241494	-1.807879
169	6	0	-0.562358	-0.968972	1.481323
170	6	0	-1.123596	0.304810	1.500297
171	6	0	-0.403569	1.358717	0.936593
172	6	0	0.835143	1.152341	0.334680
173	6	0	1.364604	-0.138981	0.313311
174	6	0	0.680816	-1.206295	0.890218
175	1	0	-1.075350	-1.786272	1.978780
176	1	0	-0.788946	2.369830	1.010579
177	1	0	2.351796	-0.303572	-0.115089
178	6	0	1.598904	2.310670	-0.254433
179	1	0	1.328145	2.469744	-1.306911
180	1	0	1.380265	3.238197	0.288558
181	1	0	2.679450	2.129531	-0.214449
182	6	0	-2.471519	0.549467	2.131346
183	1	0	-2.479125	1.491219	2.692756
184	1	0	-3.261647	0.618297	1.371259
185	1	0	-2.737717	-0.260478	2.819210
186	6	0	1.285359	-2.586202	0.925433
187	1	0	1.150433	-3.040879	1.915635
188	1	0	0.813151	-3.244738	0.185323
189	1	0	2.358224	-2.550442	0.705727

Mesitylene@CC3-TS C1 cc3-mes3tu

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-6.316287	0.267514	-0.963637
2	7	0	-5.360677	2.713889	0.280405
3	7	0	0.071907	5.633841	-1.503604
4	7	0	2.330471	4.630504	-3.048305
5	6	0	-4.535659	-1.614525	-2.179709
6	1	0	-4.761983	-0.697636	-2.717486
7	6	0	-5.045391	-1.770208	-0.882673
8	6	0	-5.910475	-0.729029	-0.293357
9	1	0	-6.189634	-0.876262	0.761771
10	6	0	-7.195653	1.216059	-0.309709
11	1	0	-7.291782	1.002872	0.770309
12	6	0	-6.609289	2.627419	-0.453323

13	1	0	-6.459045	2.816419	-1.531614
14	6	0	-7.577565	3.673657	0.113601
15	1	0	-7.137792	4.668068	-0.020244
16	1	0	-7.665908	3.507692	1.195218
17	6	0	-8.954117	3.587839	-0.545487
18	1	0	-9.626133	4.332637	-0.106246
19	1	0	-8.863927	3.830443	-1.613080
20	6	0	-9.537603	2.182114	-0.397112
21	1	0	-10.508553	2.112671	-0.898806
22	1	0	-9.713366	1.974546	0.667208
23	6	0	-8.578829	1.137265	-0.967640
24	1	0	-8.453249	1.290176	-2.047518
25	1	0	-8.974352	0.124377	-0.834146
26	6	0	-4.343409	3.157841	-0.332775
27	1	0	-4.379263	3.433097	-1.398602
28	6	0	-3.052845	3.394014	0.346490
29	6	0	-2.871383	3.021588	1.685919
30	1	0	-3.684871	2.514033	2.197867
31	6	0	-1.690381	3.329472	2.349660
32	6	0	-0.670633	4.007747	1.667256
33	1	0	0.239116	4.256610	2.207812
34	6	0	-0.836644	4.376444	0.337748
35	6	0	-2.033587	4.061572	-0.322164
36	1	0	-2.154192	4.376179	-1.355661
37	6	0	0.216091	5.165258	-0.334285
38	1	0	1.121610	5.356064	0.262632
39	6	0	1.122975	6.482838	-2.031655
40	1	0	1.974271	6.559930	-1.331515
41	6	0	1.655311	5.879302	-3.341720
42	1	0	0.786362	5.725631	-4.006751
43	6	0	2.653683	6.829323	-4.012201
44	1	0	2.995183	6.376674	-4.949403
45	1	0	3.533275	6.912099	-3.360550
46	6	0	2.050893	8.212447	-4.254877
47	1	0	1.213940	8.129568	-4.961653
48	1	0	2.794442	8.869029	-4.718902
49	6	0	1.544068	8.813829	-2.943534
50	1	0	2.395053	8.976572	-2.268126
51	1	0	1.085919	9.792978	-3.118713
52	6	0	0.535508	7.878318	-2.277588
53	1	0	-0.350785	7.765944	-2.915549
54	1	0	0.188926	8.286759	-1.322010
55	6	0	1.820593	3.558775	-3.494708
56	1	0	0.886182	3.555838	-4.076995
57	7	0	-3.055061	-4.842622	1.352543
58	7	0	-0.317218	-4.521413	2.634359
59	7	0	0.735974	1.096383	5.507405
60	7	0	-0.592884	3.430579	4.489034
61	6	0	-4.691183	-2.888153	-0.130884
62	1	0	-5.001316	-2.981604	0.907014
63	6	0	-3.900557	-3.894599	-0.696516
64	6	0	-3.281300	-4.966792	0.110759
65	1	0	-2.898758	-5.825776	-0.465488
66	6	0	-2.303401	-5.922336	1.983292
67	1	0	-1.658320	-6.433958	1.247189
68	6	0	-1.408076	-5.376764	3.106565
69	1	0	-2.068870	-4.822472	3.797175
70	6	0	-0.747684	-6.533609	3.875396
71	1	0	-0.139091	-6.107596	4.680355

72	1	0	-0.055628	-7.045161	3.193375
73	6	0	-1.766676	-7.526864	4.429718
74	1	0	-1.250868	-8.339282	4.952598
75	1	0	-2.403467	-7.024121	5.170289
76	6	0	-2.641151	-8.076873	3.304830
77	1	0	-3.399167	-8.761512	3.700076
78	1	0	-2.017019	-8.656441	2.611109
79	6	0	-3.314259	-6.933462	2.549231
80	1	0	-3.998134	-6.392786	3.217442
81	1	0	-3.919914	-7.314245	1.718945
82	6	0	-0.162863	-3.444046	3.290221
83	1	0	-0.903198	-3.148376	4.052033
84	6	0	0.981284	-2.503739	3.217054
85	6	0	2.199874	-2.772576	2.570357
86	1	0	2.307821	-3.698406	2.009456
87	6	0	3.242079	-1.842024	2.620448
88	6	0	3.068345	-0.644735	3.323681
89	1	0	3.889988	0.066912	3.344008
90	6	0	1.875163	-0.376125	3.982179
91	6	0	0.838771	-1.312111	3.925495
92	1	0	-0.083758	-1.091045	4.456230
93	6	0	1.728788	0.874645	4.750505
94	1	0	2.548278	1.602011	4.637229
95	6	0	0.710183	2.348832	6.236015
96	1	0	1.552081	3.003524	5.946099
97	6	0	-0.590549	3.092335	5.898955
98	1	0	-1.429735	2.420023	6.153867
99	6	0	-0.703736	4.378785	6.724121
100	1	0	-1.643978	4.880529	6.470620
101	1	0	0.108752	5.052812	6.422943
102	6	0	-0.621227	4.090860	8.223602
103	1	0	-1.482209	3.478759	8.525021
104	1	0	-0.684049	5.026729	8.788845
105	6	0	0.669687	3.343634	8.563144
106	1	0	1.529200	3.993767	8.350069
107	1	0	0.707838	3.107586	9.631848
108	6	0	0.787624	2.060707	7.739373
109	1	0	-0.024114	1.368539	7.998531
110	1	0	1.728549	1.541389	7.951683
111	6	0	-1.552912	2.999335	3.782239
112	1	0	-2.356912	2.378740	4.207665
113	7	0	-1.894613	-2.940702	-4.250618
114	7	0	0.682579	-1.365321	-4.790885
115	7	0	5.875686	-0.352785	-1.097576
116	7	0	5.364082	-1.136850	1.710260
117	6	0	-3.471045	-3.765356	-2.012825
118	1	0	-2.830190	-4.521104	-2.459773
119	6	0	-3.713347	-2.589263	-2.732227
120	6	0	-2.977573	-2.331188	-3.989833
121	1	0	-3.391923	-1.559232	-4.657058
122	6	0	-1.265975	-2.705803	-5.542230
123	1	0	-1.618079	-1.763772	-5.998121
124	6	0	0.264486	-2.619304	-5.412681
125	1	0	0.603365	-3.489949	-4.824977
126	6	0	0.930069	-2.652208	-6.801741
127	1	0	2.016279	-2.640457	-6.658164
128	1	0	0.672257	-1.718376	-7.319510
129	6	0	0.503817	-3.847804	-7.648603
130	1	0	0.998482	-3.807415	-8.624921

131	1	0	0.827436	-4.778727	-7.163515
132	6	0	-1.014077	-3.864056	-7.807855
133	1	0	-1.336247	-4.730956	-8.394480
134	1	0	-1.331428	-2.968283	-8.358714
135	6	0	-1.681637	-3.888249	-6.436145
136	1	0	-1.417883	-4.816087	-5.911014
137	1	0	-2.773476	-3.878428	-6.528298
138	6	0	1.784793	-1.381909	-4.159209
139	1	0	2.341768	-2.317006	-3.983083
140	6	0	2.435472	-0.158703	-3.638560
141	6	0	1.837798	1.098334	-3.794040
142	1	0	0.888040	1.160066	-4.319565
143	6	0	2.449026	2.239841	-3.286083
144	6	0	3.650760	2.122964	-2.572473
145	1	0	4.084393	3.021606	-2.140512
146	6	0	4.253435	0.881229	-2.398565
147	6	0	3.656816	-0.251993	-2.976872
148	1	0	4.142376	-1.216231	-2.856324
149	6	0	5.405011	0.765838	-1.474917
150	1	0	5.766811	1.716930	-1.052182
151	6	0	6.906095	-0.373344	-0.071814
152	1	0	6.966181	0.598282	0.450152
153	6	0	6.585634	-1.455079	0.985229
154	1	0	6.494925	-2.420629	0.455075
155	6	0	7.733792	-1.552809	2.000602
156	1	0	7.486467	-2.333456	2.728344
157	1	0	7.782356	-0.606075	2.554888
158	6	0	9.075640	-1.838073	1.327252
159	1	0	9.038578	-2.823667	0.843645
160	1	0	9.869985	-1.883009	2.079808
161	6	0	9.389602	-0.773820	0.276072
162	1	0	9.522715	0.196954	0.772575
163	1	0	10.331026	-1.001349	-0.235017
164	6	0	8.254678	-0.671104	-0.741895
165	1	0	8.159971	-1.613201	-1.298425
166	1	0	8.458057	0.113551	-1.479113
167	6	0	4.517485	-2.067401	1.896317
168	1	0	4.667996	-3.081309	1.492772
169	6	0	0.600411	-1.266928	-0.071408
170	6	0	0.477798	-2.582621	-0.517287
171	6	0	1.608606	-3.295085	-0.910177
172	6	0	2.866117	-2.703304	-0.871915
173	6	0	2.954871	-1.385855	-0.429173
174	6	0	1.843757	-0.648905	-0.026974
175	1	0	-0.291068	-0.724827	0.239531
176	1	0	1.496025	-4.321484	-1.257986
177	1	0	3.928581	-0.926731	-0.381327
178	6	0	4.098533	-3.459339	-1.306621
179	1	0	4.329512	-4.283250	-0.619554
180	1	0	3.957380	-3.908145	-2.297482
181	1	0	4.967767	-2.795515	-1.350536
182	6	0	-0.865715	-3.207000	-0.670795
183	1	0	-1.618867	-2.711662	-0.052283
184	1	0	-1.167711	-3.128315	-1.719954
185	1	0	-0.840446	-4.265164	-0.393335
186	6	0	2.006885	0.779522	0.425094
187	1	0	3.024180	0.952656	0.794904
188	1	0	1.828064	1.474775	-0.404653
189	1	0	1.301811	1.026838	1.225545

5-tBu-m-xylene@CC3 C1 cc3-dpell

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-0.566848	-5.051391	-1.962392
2	7	0	-1.604961	-5.251932	0.770368
3	7	0	-5.049361	-0.180018	2.749995
4	7	0	-4.942271	2.468012	1.468808
5	6	0	0.060421	-2.688418	-3.564883
6	1	0	-0.967069	-3.044139	-3.593965
7	6	0	1.003258	-3.415621	-2.826204
8	6	0	0.625370	-4.625639	-2.069949
9	1	0	1.466141	-5.151645	-1.588560
10	6	0	-0.747619	-6.312383	-1.258177
11	1	0	0.158234	-6.575534	-0.682105
12	6	0	-1.911087	-6.232573	-0.260191
13	1	0	-2.820964	-5.944960	-0.816043
14	6	0	-2.140504	-7.599648	0.399962
15	1	0	-2.981156	-7.514686	1.097968
16	1	0	-1.253320	-7.846908	0.998321
17	6	0	-2.398606	-8.693601	-0.636053
18	1	0	-2.538776	-9.657545	-0.135576
19	1	0	-3.332035	-8.473103	-1.171434
20	6	0	-1.248601	-8.769887	-1.640622
21	1	0	-1.455683	-9.525429	-2.405813
22	1	0	-0.334585	-9.085996	-1.119728
23	6	0	-1.012250	-7.410250	-2.297973
24	1	0	-1.888978	-7.118118	-2.891065
25	1	0	-0.161862	-7.450755	-2.987399
26	6	0	-2.573082	-4.577838	1.239539
27	1	0	-3.603840	-4.710153	0.876556
28	6	0	-2.364340	-3.517479	2.247158
29	6	0	-1.192204	-3.502239	3.012278
30	1	0	-0.477250	-4.311348	2.886099
31	6	0	-0.954957	-2.479349	3.921713
32	6	0	-1.883513	-1.438871	4.043996
33	1	0	-1.677433	-0.640093	4.751781
34	6	0	-3.045004	-1.431741	3.278857
35	6	0	-3.295485	-2.492394	2.395285
36	1	0	-4.219792	-2.485013	1.821492
37	6	0	-3.994619	-0.311832	3.442093
38	1	0	-3.728615	0.410224	4.230016
39	6	0	-5.930435	0.924134	3.093304
40	1	0	-5.483763	1.561023	3.878291
41	6	0	-6.181248	1.821080	1.873425
42	1	0	-6.581399	1.186579	1.062527
43	6	0	-7.208569	2.910628	2.213750
44	1	0	-7.379147	3.519522	1.318758
45	1	0	-6.767048	3.573568	2.969799
46	6	0	-8.519245	2.321055	2.733305
47	1	0	-8.990235	1.724516	1.940236
48	1	0	-9.218232	3.126169	2.983512
49	6	0	-8.264958	1.429752	3.948903
50	1	0	-7.880086	2.044682	4.773846
51	1	0	-9.199413	0.978169	4.298406

52	6	0	-7.250116	0.337686	3.611760
53	1	0	-7.655501	-0.328427	2.838876
54	1	0	-7.036761	-0.285129	4.487309
55	6	0	-4.740355	2.577352	0.221669
56	1	0	-5.448381	2.168700	-0.516018
57	7	0	5.007417	-1.943653	-2.774604
58	7	0	5.841581	-0.134779	-0.696699
59	7	0	2.952501	-0.404970	5.018753
60	7	0	0.466965	-1.704820	5.702635
61	6	0	2.320134	-2.972205	-2.779848
62	1	0	3.075778	-3.521211	-2.222965
63	6	0	2.698406	-1.791123	-3.432587
64	6	0	4.084559	-1.296498	-3.355649
65	1	0	4.270044	-0.321629	-3.834024
66	6	0	6.330782	-1.355722	-2.748846
67	1	0	6.350471	-0.376606	-3.261303
68	6	0	6.733198	-1.116163	-1.285019
69	1	0	6.665789	-2.087385	-0.762264
70	6	0	8.171638	-0.593104	-1.201384
71	1	0	8.433902	-0.445857	-0.148021
72	1	0	8.205148	0.394625	-1.679269
73	6	0	9.155975	-1.542315	-1.885591
74	1	0	10.170677	-1.134433	-1.827860
75	1	0	9.168204	-2.502324	-1.351658
76	6	0	8.754883	-1.782709	-3.342066
77	1	0	9.442097	-2.489624	-3.818865
78	1	0	8.833244	-0.838557	-3.898264
79	6	0	7.321153	-2.306467	-3.429186
80	1	0	7.246451	-3.286047	-2.939263
81	1	0	7.015612	-2.448246	-4.471543
82	6	0	5.177153	-0.480702	0.326362
83	1	0	5.248026	-1.494232	0.751454
84	6	0	4.306109	0.458865	1.061432
85	6	0	4.051093	1.746376	0.564975
86	1	0	4.473372	2.024727	-0.397489
87	6	0	3.309147	2.653611	1.312065
88	6	0	2.806444	2.269521	2.562862
89	1	0	2.247640	2.999714	3.142280
90	6	0	3.051806	0.997530	3.063356
91	6	0	3.798149	0.088132	2.301006
92	1	0	3.997701	-0.897141	2.714894
93	6	0	2.598415	0.658900	4.426859
94	1	0	1.964399	1.413992	4.917127
95	6	0	2.515165	-0.589625	6.389185
96	1	0	1.876934	0.247059	6.726563
97	6	0	1.675950	-1.872590	6.484430
98	1	0	2.295565	-2.702583	6.099152
99	6	0	1.292079	-2.158331	7.940513
100	1	0	0.706567	-3.083502	7.976361
101	1	0	0.633461	-1.350819	8.285863
102	6	0	2.524999	-2.252093	8.839320
103	1	0	3.138717	-3.108820	8.529171
104	1	0	2.220573	-2.438110	9.874675
105	6	0	3.361166	-0.974534	8.745512
106	1	0	2.778372	-0.132243	9.142687
107	1	0	4.261322	-1.056968	9.363700
108	6	0	3.748134	-0.685708	7.294766
109	1	0	4.393669	-1.485770	6.909685
110	1	0	4.317168	0.247058	7.216666

111	6	0	0.260037	-2.523375	4.757254
112	1	0	0.970408	-3.331121	4.519923
113	7	0	-0.440723	0.431808	-5.372779
114	7	0	-2.256771	2.534045	-4.393613
115	7	0	0.324516	6.035979	0.262695
116	7	0	2.655084	4.949614	1.573977
117	6	0	1.749169	-1.064950	-4.141723
118	1	0	2.015596	-0.139100	-4.646607
119	6	0	0.425319	-1.514638	-4.215719
120	6	0	-0.599923	-0.758125	-4.958139
121	1	0	-1.535869	-1.304246	-5.142263
122	6	0	-1.531716	0.988681	-6.159982
123	1	0	-2.468507	0.426595	-5.992884
124	6	0	-1.789497	2.448717	-5.768416
125	1	0	-0.840944	3.000356	-5.898436
126	6	0	-2.859039	3.069101	-6.678145
127	1	0	-3.009436	4.112634	-6.379986
128	1	0	-3.807770	2.546454	-6.498019
129	6	0	-2.476287	2.970645	-8.154520
130	1	0	-3.267296	3.403813	-8.775783
131	1	0	-1.568428	3.561837	-8.336061
132	6	0	-2.217031	1.516406	-8.548171
133	1	0	-1.904886	1.449904	-9.595789
134	1	0	-3.151076	0.945577	-8.456759
135	6	0	-1.152543	0.894401	-7.645002
136	1	0	-0.190628	1.404942	-7.786743
137	1	0	-0.991845	-0.159902	-7.896185
138	6	0	-1.706473	3.405830	-3.653127
139	1	0	-0.872268	4.026734	-4.017217
140	6	0	-2.096910	3.640679	-2.249792
141	6	0	-3.250843	3.068936	-1.698568
142	1	0	-3.900258	2.480219	-2.343441
143	6	0	-3.541963	3.229383	-0.346571
144	6	0	-2.679118	3.981652	0.461551
145	1	0	-2.913189	4.082664	1.518308
146	6	0	-1.555290	4.589918	-0.085949
147	6	0	-1.273578	4.420397	-1.447089
148	1	0	-0.383136	4.893309	-1.853743
149	6	0	-0.656811	5.403959	0.756875
150	1	0	-0.891328	5.431058	1.832198
151	6	0	1.157068	6.820533	1.150265
152	1	0	0.837768	6.720611	2.203481
153	6	0	2.600474	6.301737	1.054469
154	1	0	2.897136	6.341337	-0.009225
155	6	0	3.545992	7.182946	1.879750
156	1	0	4.566541	6.798689	1.775493
157	1	0	3.273213	7.079291	2.938060
158	6	0	3.464394	8.650007	1.457219
159	1	0	3.810809	8.751373	0.419666
160	1	0	4.134979	9.255226	2.076313
161	6	0	2.027422	9.163722	1.559605
162	1	0	1.712130	9.146977	2.611790
163	1	0	1.965803	10.205049	1.226316
164	6	0	1.082725	8.293037	0.731199
165	1	0	1.344632	8.359230	-0.332866
166	1	0	0.046237	8.634954	0.825337
167	6	0	3.131017	4.039206	0.830634
168	1	0	3.474584	4.241181	-0.196018
169	6	0	0.832358	-0.505787	-0.775926

170	6	0	0.225807	-1.654856	-0.272640
171	6	0	-1.101601	-1.917524	-0.610367
172	6	0	-1.841150	-1.048882	-1.418814
173	6	0	-1.210622	0.108047	-1.886074
174	6	0	0.129149	0.378707	-1.589885
175	1	0	1.882424	-0.311996	-0.556182
176	1	0	-1.533180	-2.849892	-0.268775
177	1	0	-1.741188	0.797234	-2.539536
178	6	0	-3.311509	-1.329770	-1.750979
179	6	0	-3.638297	-1.031644	-3.222336
180	6	0	-3.692244	-2.787937	-1.478097
181	6	0	-4.167525	-0.419025	-0.861591
182	1	0	-4.719020	-1.123378	-3.382789
183	1	0	-3.337851	-0.024615	-3.533151
184	1	0	-3.147638	-1.758589	-3.878438
185	1	0	-4.706070	-2.982558	-1.845874
186	1	0	-2.999417	-3.489978	-1.959136
187	1	0	-3.687306	-2.987629	-0.404398
188	1	0	-5.238487	-0.578873	-1.045122
189	1	0	-3.969687	-0.587328	0.203107
190	1	0	-3.924467	0.621402	-1.080896
191	6	0	1.010512	-2.619718	0.579179
192	6	0	0.824630	1.576236	-2.185157
193	1	0	0.487171	-3.577851	0.670954
194	1	0	2.002030	-2.800760	0.144880
195	1	0	1.166163	-2.217565	1.588220
196	1	0	0.529370	1.710337	-3.233017
197	1	0	0.578954	2.494460	-1.638622
198	1	0	1.912012	1.447703	-2.147468

CC3-R-a(+) D2 cc3-rrad

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	0.922782	5.546551	1.099266
2	7	0	-0.922782	5.546551	-1.099266
3	7	0	-5.565048	1.124357	-0.901788
4	7	0	-5.565048	-1.124357	0.901788
5	6	0	1.363463	3.240527	2.727505
6	1	0	0.517573	3.884979	2.953403
7	6	0	2.165379	3.560576	1.615294
8	6	0	1.861201	4.750147	0.795692
9	1	0	2.508494	4.909682	-0.079715
10	6	0	0.723957	6.711333	0.259423
11	1	0	1.393037	6.693773	-0.618990
12	6	0	-0.723957	6.711333	-0.259423
13	1	0	-1.393037	6.693773	0.618990
14	6	0	-0.994878	7.977287	-1.081551
15	1	0	-2.032417	7.954721	-1.431493
16	1	0	-0.355358	7.952939	-1.973210
17	6	0	-0.716998	9.240551	-0.266088
18	1	0	-0.898056	10.126980	-0.881886
19	1	0	-1.417261	9.291550	0.578360
20	6	0	0.716998	9.240551	0.266088
21	1	0	0.898056	10.126980	0.881886
22	1	0	1.417261	9.291550	-0.578360

23	6	0	0.994878	7.977287	1.081551
24	1	0	0.355358	7.952939	1.973210
25	1	0	2.032417	7.954721	1.431493
26	6	0	-1.861201	4.750147	-0.795692
27	1	0	-2.508494	4.909682	0.079715
28	6	0	-2.165379	3.560576	-1.615294
29	6	0	-1.363463	3.240527	-2.727505
30	1	0	-0.517573	3.884979	-2.953403
31	6	0	-1.658553	2.137018	-3.529002
32	6	0	-2.762442	1.340930	-3.214940
33	1	0	-2.988829	0.490067	-3.852031
34	6	0	-3.565978	1.648851	-2.115173
35	6	0	-3.259193	2.766132	-1.314865
36	1	0	-3.905712	2.992708	-0.471500
37	6	0	-4.743863	0.821683	-1.826084
38	1	0	-4.887775	-0.058998	-2.469045
39	6	0	-6.719294	0.277811	-0.723538
40	1	0	-6.704761	-0.586310	-1.410247
41	6	0	-6.719294	-0.277811	0.723538
42	1	0	-6.704761	0.586310	1.410247
43	6	0	-7.990611	-1.107252	0.962111
44	1	0	-7.966536	-1.486808	1.989043
45	1	0	-7.962133	-1.979283	0.296802
46	6	0	-9.253559	-0.285914	0.709056
47	1	0	-9.306636	0.537402	1.433648
48	1	0	-10.137964	-0.909509	0.872101
49	6	0	-9.253559	0.285914	-0.709056
50	1	0	-9.306636	-0.537402	-1.433648
51	1	0	-10.137964	0.909509	-0.872101
52	6	0	-7.990611	1.107252	-0.962111
53	1	0	-7.962133	1.979283	-0.296802
54	1	0	-7.966536	1.486808	-1.989043
55	6	0	-4.743863	-0.821683	1.826084
56	1	0	-4.887775	0.058998	2.469045
57	7	0	5.565048	1.124357	0.901788
58	7	0	5.565048	-1.124357	-0.901788
59	7	0	1.115244	-0.907561	-5.515486
60	7	0	-1.115244	0.907561	-5.515486
61	6	0	3.259193	2.766132	1.314865
62	1	0	3.905712	2.992708	0.471500
63	6	0	3.565978	1.648851	2.115173
64	6	0	4.743863	0.821683	1.826084
65	1	0	4.887775	-0.058998	2.469045
66	6	0	6.719294	0.277811	0.723538
67	1	0	6.704761	-0.586310	1.410247
68	6	0	6.719294	-0.277811	-0.723538
69	1	0	6.704761	0.586310	-1.410247
70	6	0	7.990611	-1.107252	-0.962111
71	1	0	7.966536	-1.486808	-1.989043
72	1	0	7.962133	-1.979283	-0.296802
73	6	0	9.253559	-0.285914	-0.709056
74	1	0	10.137964	-0.909509	-0.872101
75	1	0	9.306636	0.537402	-1.433648
76	6	0	9.253559	0.285914	0.709056
77	1	0	10.137964	0.909509	0.872101
78	1	0	9.306636	-0.537402	1.433648
79	6	0	7.990611	1.107252	0.962111
80	1	0	7.962133	1.979283	0.296802
81	1	0	7.966536	1.486808	1.989043

82	6	0	4.743863	-0.821683	-1.826084
83	1	0	4.887775	0.058998	-2.469045
84	6	0	3.565978	-1.648851	-2.115173
85	6	0	3.259193	-2.766132	-1.314865
86	1	0	3.905712	-2.992708	-0.471500
87	6	0	2.165379	-3.560576	-1.615294
88	6	0	1.363463	-3.240527	-2.727505
89	1	0	0.517573	-3.884979	-2.953403
90	6	0	1.658553	-2.137018	-3.529002
91	6	0	2.762442	-1.340930	-3.214940
92	1	0	2.988829	-0.490067	-3.852031
93	6	0	0.825625	-1.845117	-4.713248
94	1	0	-0.044809	-2.501160	-4.864299
95	6	0	0.268303	-0.720802	-6.676936
96	1	0	-0.601987	-1.400322	-6.655709
97	6	0	-0.268303	0.720802	-6.676936
98	1	0	0.601987	1.400322	-6.655709
99	6	0	-1.091209	0.983766	-7.944153
100	1	0	-1.451854	2.017637	-7.921362
101	1	0	-1.976338	0.335197	-7.920691
102	6	0	-0.272565	0.714503	-9.207074
103	1	0	0.565457	1.422499	-9.257376
104	1	0	-0.889647	0.890357	-10.093668
105	6	0	0.272565	-0.714503	-9.207074
106	1	0	-0.565457	-1.422499	-9.257376
107	1	0	0.889647	-0.890357	-10.093668
108	6	0	1.091209	-0.983766	-7.944153
109	1	0	1.976338	-0.335197	-7.920691
110	1	0	1.451854	-2.017637	-7.921362
111	6	0	-0.825625	1.845117	-4.713248
112	1	0	0.044809	2.501160	-4.864299
113	7	0	1.115244	0.907561	5.515486
114	7	0	-1.115244	-0.907561	5.515486
115	7	0	-0.922782	-5.546551	1.099266
116	7	0	0.922782	-5.546551	-1.099266
117	6	0	2.762442	1.340930	3.214940
118	1	0	2.988829	0.490067	3.852031
119	6	0	1.658553	2.137018	3.529002
120	6	0	0.825625	1.845117	4.713248
121	1	0	-0.044809	2.501160	4.864299
122	6	0	0.268303	0.720802	6.676936
123	1	0	-0.601987	1.400322	6.655709
124	6	0	-0.268303	-0.720802	6.676936
125	1	0	0.601987	-1.400322	6.655709
126	6	0	-1.091209	-0.983766	7.944153
127	1	0	-1.451854	-2.017637	7.921362
128	1	0	-1.976338	-0.335197	7.920691
129	6	0	-0.272565	-0.714503	9.207074
130	1	0	-0.889647	-0.890357	10.093668
131	1	0	0.565457	-1.422499	9.257376
132	6	0	0.272565	0.714503	9.207074
133	1	0	0.889647	0.890357	10.093668
134	1	0	-0.565457	1.422499	9.257376
135	6	0	1.091209	0.983766	7.944153
136	1	0	1.976338	0.335197	7.920691
137	1	0	1.451854	2.017637	7.921362
138	6	0	-0.825625	-1.845117	4.713248
139	1	0	0.044809	-2.501160	4.864299
140	6	0	-1.658553	-2.137018	3.529002

141	6	0	-2.762442	-1.340930	3.214940
142	1	0	-2.988829	-0.490067	3.852031
143	6	0	-3.565978	-1.648851	2.115173
144	6	0	-3.259193	-2.766132	1.314865
145	1	0	-3.905712	-2.992708	0.471500
146	6	0	-2.165379	-3.560576	1.615294
147	6	0	-1.363463	-3.240527	2.727505
148	1	0	-0.517573	-3.884979	2.953403
149	6	0	-1.861201	-4.750147	0.795692
150	1	0	-2.508494	-4.909682	-0.079715
151	6	0	-0.723957	-6.711333	0.259423
152	1	0	-1.393037	-6.693773	-0.618990
153	6	0	0.723957	-6.711333	-0.259423
154	1	0	1.393037	-6.693773	0.618990
155	6	0	0.994878	-7.977287	-1.081551
156	1	0	2.032417	-7.954721	-1.431493
157	1	0	0.355358	-7.952939	-1.973210
158	6	0	0.716998	-9.240551	-0.266088
159	1	0	1.417261	-9.291550	0.578360
160	1	0	0.898056	-10.126980	-0.881886
161	6	0	-0.716998	-9.240551	0.266088
162	1	0	-1.417261	-9.291550	-0.578360
163	1	0	-0.898056	-10.126980	0.881886
164	6	0	-0.994878	-7.977287	1.081551
165	1	0	-0.355358	-7.952939	1.973210
166	1	0	-2.032417	-7.954721	1.431493
167	6	0	1.861201	-4.750147	-0.795692
168	1	0	2.508494	-4.909682	0.079715

CC3-R-b(+) C2 cc3-raddx

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	2.409430	-5.097545	0.900310
2	7	0	0.298326	-5.680078	-0.944669
3	7	0	-0.577646	-1.324913	-5.565583
4	7	0	0.577646	1.324913	-5.565583
5	6	0	3.466376	-2.458851	1.355606
6	1	0	3.850601	-3.022476	0.509137
7	6	0	2.476222	-3.044518	2.157251
8	6	0	1.971041	-4.399866	1.864749
9	1	0	1.194979	-4.776202	2.549559
10	6	0	1.874039	-6.435908	0.741478
11	1	0	1.011296	-6.609623	1.409256
12	6	0	1.385882	-6.609745	-0.705642
13	1	0	2.241712	-6.402244	-1.371451
14	6	0	0.887351	-8.040223	-0.940228
15	1	0	0.550611	-8.135437	-1.978158
16	1	0	0.011250	-8.209782	-0.301270
17	6	0	1.979035	-9.062614	-0.620903
18	1	0	1.594435	-10.075535	-0.775447
19	1	0	2.817298	-8.930858	-1.318105
20	6	0	2.482509	-8.891861	0.813380
21	1	0	3.290016	-9.600267	1.022733
22	1	0	1.667954	-9.122809	1.512840
23	6	0	2.969264	-7.462300	1.054207

24	1	0	3.837644	-7.244262	0.419219
25	1	0	3.290807	-7.325279	2.092068
26	6	0	0.443814	-4.812831	-1.856246
27	1	0	1.355743	-4.736830	-2.465800
28	6	0	-0.634445	-3.852573	-2.169660
29	6	0	-1.796395	-3.814836	-1.366069
30	1	0	-1.850112	-4.497998	-0.521801
31	6	0	-2.854505	-2.942859	-1.651580
32	6	0	-2.745546	-2.089041	-2.744299
33	1	0	-3.571357	-1.418446	-2.966536
34	6	0	-1.596642	-2.114101	-3.552432
35	6	0	-0.539323	-3.006552	-3.256412
36	1	0	0.331348	-3.015580	-3.905602
37	6	0	-1.533870	-1.242893	-4.714820
38	1	0	-2.365588	-0.537164	-4.846653
39	6	0	-0.634445	-0.470801	-6.708394
40	1	0	-1.522130	0.183253	-6.706507
41	6	0	0.634445	0.470801	-6.708394
42	1	0	1.522130	-0.183253	-6.706507
43	6	0	0.605061	1.331297	-7.986347
44	1	0	1.481279	1.987513	-7.960926
45	1	0	-0.281523	1.975337	-7.946909
46	6	0	0.597151	0.476650	-9.249734
47	1	0	1.528383	-0.101455	-9.308965
48	1	0	0.570435	1.126713	-10.129350
49	6	0	-0.597151	-0.476650	-9.249734
50	1	0	-1.528383	0.101455	-9.308965
51	1	0	-0.570435	-1.126713	-10.129350
52	6	0	-0.605061	-1.331297	-7.986347
53	1	0	0.281523	-1.975337	-7.946909
54	1	0	-1.481279	-1.987513	-7.960926
55	6	0	1.533870	1.242893	-4.714820
56	1	0	2.365588	0.537164	-4.846653
57	7	0	1.149626	-0.863976	5.564214
58	7	0	-1.149626	0.863976	5.564214
59	7	0	-5.531663	-0.528059	1.065023
60	7	0	-5.099992	-2.293021	-1.156886
61	6	0	1.985396	-2.351003	3.256575
62	1	0	1.228097	-2.787228	3.903038
63	6	0	2.472549	-1.073605	3.568100
64	6	0	1.980795	-0.349208	4.758241
65	1	0	2.395969	0.659143	4.910038
66	6	0	0.763120	-0.087172	6.726892
67	1	0	1.212576	0.921782	6.704995
68	6	0	-0.763120	0.087172	6.726892
69	1	0	-1.212576	-0.921782	6.704995
70	6	0	-1.219258	0.819602	7.993787
71	1	0	-2.309783	0.919266	7.971218
72	1	0	-0.804927	1.835854	7.971583
73	6	0	-0.759397	0.090773	9.256998
74	1	0	-1.080386	0.644962	10.144739
75	1	0	-1.241599	-0.894879	9.305855
76	6	0	0.759397	-0.090773	9.256998
77	1	0	1.080386	-0.644962	10.144739
78	1	0	1.241599	0.894879	9.305855
79	6	0	1.219258	-0.819602	7.993787
80	1	0	0.804927	-1.835854	7.971583
81	1	0	2.309783	-0.919266	7.971218
82	6	0	-1.980795	0.349208	4.758241

83	1	0	-2.395969	-0.659143	4.910038
84	6	0	-2.472549	1.073605	3.568100
85	6	0	-1.985396	2.351003	3.256575
86	1	0	-1.228097	2.787228	3.903038
87	6	0	-2.476222	3.044518	2.157251
88	6	0	-3.466376	2.458851	1.355606
89	1	0	-3.850601	3.022476	0.509137
90	6	0	-3.955151	1.193290	1.654688
91	6	0	-3.450596	0.500880	2.765139
92	1	0	-3.854241	-0.482702	2.991407
93	6	0	-5.022770	0.607538	0.821098
94	1	0	-5.365273	1.229682	-0.021098
95	6	0	-6.615543	-0.979333	0.214430
96	1	0	-6.752776	-0.313539	-0.656686
97	6	0	-6.280666	-2.381587	-0.318130
98	1	0	-6.103004	-3.033453	0.554729
99	6	0	-7.443403	-2.938137	-1.147833
100	1	0	-7.178371	-3.938291	-1.507230
101	1	0	-7.571138	-2.301849	-2.033068
102	6	0	-8.736703	-2.972109	-0.332443
103	1	0	-8.620598	-3.670349	0.507155
104	1	0	-9.554759	-3.353817	-0.951283
105	6	0	-9.074902	-1.582085	0.208754
106	1	0	-9.288274	-0.908207	-0.631861
107	1	0	-9.980327	-1.619555	0.822356
108	6	0	-7.913610	-1.020041	1.029582
109	1	0	-7.742123	-1.640093	1.918837
110	1	0	-8.135259	-0.008114	1.384846
111	6	0	-4.078424	-2.962467	-0.821771
112	1	0	-4.050126	-3.598642	0.074158
113	7	0	5.531663	0.528059	1.065023
114	7	0	5.099992	2.293021	-1.156886
115	7	0	-0.298326	5.680078	-0.944669
116	7	0	-2.409430	5.097545	0.900310
117	6	0	3.450596	-0.500880	2.765139
118	1	0	3.854241	0.482702	2.991407
119	6	0	3.955151	-1.193290	1.654688
120	6	0	5.022770	-0.607538	0.821098
121	1	0	5.365273	-1.229682	-0.021098
122	6	0	6.615543	0.979333	0.214430
123	1	0	6.752776	0.313539	-0.656686
124	6	0	6.280666	2.381587	-0.318130
125	1	0	6.103004	3.033453	0.554729
126	6	0	7.443403	2.938137	-1.147833
127	1	0	7.178371	3.938291	-1.507230
128	1	0	7.571138	2.301849	-2.033068
129	6	0	8.736703	2.972109	-0.332443
130	1	0	9.554759	3.353817	-0.951283
131	1	0	8.620598	3.670349	0.507155
132	6	0	9.074902	1.582085	0.208754
133	1	0	9.980327	1.619555	0.822356
134	1	0	9.288274	0.908207	-0.631861
135	6	0	7.913610	1.020041	1.029582
136	1	0	7.742123	1.640093	1.918837
137	1	0	8.135259	0.008114	1.384846
138	6	0	4.078424	2.962467	-0.821771
139	1	0	4.050126	3.598642	0.074158
140	6	0	2.854505	2.942859	-1.651580
141	6	0	2.745546	2.089041	-2.744299

142	1	0	3.571357	1.418446	-2.966536
143	6	0	1.596642	2.114101	-3.552432
144	6	0	0.539323	3.006552	-3.256412
145	1	0	-0.331348	3.015580	-3.905602
146	6	0	0.634445	3.852573	-2.169660
147	6	0	1.796395	3.814836	-1.366069
148	1	0	1.850112	4.497998	-0.521801
149	6	0	-0.443814	4.812831	-1.856246
150	1	0	-1.355743	4.736830	-2.465800
151	6	0	-1.385882	6.609745	-0.705642
152	1	0	-2.241712	6.402244	-1.371451
153	6	0	-1.874039	6.435908	0.741478
154	1	0	-1.011296	6.609623	1.409256
155	6	0	-2.969264	7.462300	1.054207
156	1	0	-3.290807	7.325279	2.092068
157	1	0	-3.837644	7.244262	0.419219
158	6	0	-2.482509	8.891861	0.813380
159	1	0	-1.667954	9.122809	1.512840
160	1	0	-3.290016	9.600267	1.022733
161	6	0	-1.979035	9.062614	-0.620903
162	1	0	-2.817298	8.930858	-1.318105
163	1	0	-1.594435	10.075535	-0.775447
164	6	0	-0.887351	8.040223	-0.940228
165	1	0	-0.011250	8.209782	-0.301270
166	1	0	-0.550611	8.135437	-1.978158
167	6	0	-1.971041	4.399866	1.864749
168	1	0	-1.194979	4.776202	2.549559

3I@CC3-a C2 cc3-i3a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-0.666688	1.284178	5.202448
2	6	0	-0.827793	3.044594	2.937451
3	1	0	0.043461	3.121824	3.582966
4	6	0	-1.826984	2.119109	3.266944
5	6	0	-1.684622	1.242874	4.446839
6	1	0	-2.520198	0.549045	4.629953
7	6	0	-0.649364	0.409230	6.358805
8	1	0	-1.492667	-0.304380	6.336504
9	6	0	-0.743926	1.265012	7.627958
10	1	0	-1.684380	1.826404	7.604803
11	1	0	0.068649	2.002920	7.606037
12	6	0	-0.645283	0.410380	8.891800
13	1	0	-0.695460	1.048814	9.780137
14	1	0	-1.506065	-0.270374	8.939789
15	7	0	-0.000000	5.657845	0.541235
16	6	0	-2.084868	3.717282	0.992571
17	1	0	-2.165807	4.351129	0.113039
18	6	0	-0.950601	3.843124	1.806216
19	6	0	0.102763	4.830583	1.496544
20	1	0	0.978293	4.815437	2.164537
21	6	0	1.071379	6.618936	0.365023
22	1	0	1.911621	6.418375	1.054235
23	6	0	0.523388	8.026419	0.629295
24	1	0	0.157809	8.074026	1.660877

25	1	0	-0.344647	8.184447	-0.023989
26	6	0	1.579545	9.100995	0.370043
27	1	0	1.154318	10.094357	0.548021
28	1	0	2.408056	8.977398	1.080701
29	7	0	-5.292252	2.000130	0.783900
30	6	0	-2.959507	2.019815	2.466807
31	1	0	-3.756290	1.321923	2.710048
32	6	0	-3.092575	2.817052	1.321826
33	6	0	-4.304696	2.736085	0.482709
34	1	0	-4.307535	3.375316	-0.414045
35	6	0	-6.454751	2.041930	-0.081393
36	1	0	-6.289569	2.707118	-0.948267
37	6	0	-7.655595	2.548209	0.725728
38	1	0	-7.434688	3.556742	1.091825
39	1	0	-7.769371	1.906465	1.609085
40	6	0	-8.939424	2.533050	-0.104174
41	1	0	-9.781824	2.880841	0.502973
42	1	0	-8.840528	3.235202	-0.943228
43	7	0	0.666688	-1.284178	5.202448
44	6	0	0.827793	-3.044594	2.937451
45	1	0	-0.043461	-3.121824	3.582966
46	6	0	1.826984	-2.119109	3.266944
47	6	0	1.684622	-1.242874	4.446839
48	1	0	2.520198	-0.549045	4.629953
49	6	0	0.649364	-0.409230	6.358805
50	1	0	1.492667	0.304380	6.336504
51	6	0	0.743926	-1.265012	7.627958
52	1	0	1.684380	-1.826404	7.604803
53	1	0	-0.068649	-2.002920	7.606037
54	6	0	0.645283	-0.410380	8.891800
55	1	0	0.695460	-1.048814	9.780137
56	1	0	1.506065	0.270374	8.939789
57	7	0	5.292252	-2.000130	0.783900
58	6	0	2.959507	-2.019815	2.466807
59	1	0	3.756290	-1.321923	2.710048
60	6	0	3.092575	-2.817052	1.321826
61	6	0	4.304696	-2.736085	0.482709
62	1	0	4.307535	-3.375316	-0.414045
63	6	0	6.454751	-2.041930	-0.081393
64	1	0	6.289569	-2.707118	-0.948267
65	6	0	7.655595	-2.548209	0.725728
66	1	0	7.434688	-3.556742	1.091825
67	1	0	7.769371	-1.906465	1.609085
68	6	0	8.939424	-2.533050	-0.104174
69	1	0	9.781824	-2.880841	0.502973
70	1	0	8.840528	-3.235202	-0.943228
71	7	0	-0.000000	-5.657845	0.541235
72	6	0	2.084868	-3.717282	0.992571
73	1	0	2.165807	-4.351129	0.113039
74	6	0	0.950601	-3.843124	1.806216
75	6	0	-0.102763	-4.830583	1.496544
76	1	0	-0.978293	-4.815437	2.164537
77	6	0	-1.071379	-6.618936	0.365023
78	1	0	-1.911621	-6.418375	1.054235
79	6	0	-0.523388	-8.026419	0.629295
80	1	0	-0.157809	-8.074026	1.660877
81	1	0	0.344647	-8.184447	-0.023989
82	6	0	-1.579545	-9.100995	0.370043
83	1	0	-1.154318	-10.094357	0.548021

84	1	0	-2.408056	-8.977398	1.080701
85	7	0	-5.623857	0.232806	-1.479373
86	6	0	-3.414693	-0.648468	-3.105727
87	1	0	-3.856597	0.318587	-3.332078
88	6	0	-3.918238	-1.377228	-2.019846
89	6	0	-5.028572	-0.851071	-1.201421
90	1	0	-5.318313	-1.470960	-0.337590
91	6	0	-6.729165	0.634118	-0.631497
92	1	0	-6.842993	-0.044725	0.233046
93	6	0	-8.019360	0.623235	-1.459872
94	1	0	-8.195043	-0.394519	-1.825128
95	1	0	-7.864479	1.256493	-2.343169
96	6	0	-9.213311	1.131339	-0.651438
97	1	0	-10.114393	1.129855	-1.273776
98	1	0	-9.404248	0.447566	0.186854
99	7	0	2.219103	5.210116	-1.255573
100	6	0	3.379867	2.623263	-1.723531
101	1	0	3.762760	3.215141	-0.896151
102	6	0	2.329910	3.147147	-2.489608
103	6	0	1.761650	4.474267	-2.181118
104	1	0	0.921645	4.793804	-2.817462
105	6	0	1.614114	6.514178	-1.068053
106	1	0	0.762115	6.666447	-1.755135
107	6	0	2.671476	7.594210	-1.323633
108	1	0	3.029026	7.501216	-2.354915
109	1	0	3.530146	7.394656	-0.669389
110	6	0	2.121204	8.995301	-1.056417
111	1	0	2.902248	9.743424	-1.228244
112	1	0	1.311668	9.211364	-1.766886
113	7	0	5.623857	-0.232806	-1.479373
114	6	0	3.414693	0.648468	-3.105727
115	1	0	3.856597	-0.318587	-3.332078
116	6	0	3.918238	1.377228	-2.019846
117	6	0	5.028572	0.851071	-1.201421
118	1	0	5.318313	1.470960	-0.337590
119	6	0	6.729165	-0.634118	-0.631497
120	1	0	6.842993	0.044725	0.233046
121	6	0	8.019360	-0.623235	-1.459872
122	1	0	8.195043	0.394519	-1.825128
123	1	0	7.864479	-1.256493	-2.343169
124	6	0	9.213311	-1.131339	-0.651438
125	1	0	10.114393	-1.129855	-1.273776
126	1	0	9.404248	-0.447566	0.186854
127	7	0	-2.219103	-5.210116	-1.255573
128	6	0	-3.379867	-2.623263	-1.723531
129	1	0	-3.762760	-3.215141	-0.896151
130	6	0	-2.329910	-3.147147	-2.489608
131	6	0	-1.761650	-4.474267	-2.181118
132	1	0	-0.921645	-4.793804	-2.817462
133	6	0	-1.614114	-6.514178	-1.068053
134	1	0	-0.762115	-6.666447	-1.755135
135	6	0	-2.671476	-7.594210	-1.323633
136	1	0	-3.029026	-7.501216	-2.354915
137	1	0	-3.530146	-7.394656	-0.669389
138	6	0	-2.121204	-8.995301	-1.056417
139	1	0	-2.902248	-9.743424	-1.228244
140	1	0	-1.311668	-9.211364	-1.766886
141	7	0	-1.110752	-0.916617	-5.908925
142	6	0	-1.840834	-2.418596	-3.567335

143	1	0	-1.039506	-2.808504	-4.189804
144	6	0	-2.388854	-1.167976	-3.887120
145	6	0	-1.924473	-0.420875	-5.072683
146	1	0	-2.352624	0.585405	-5.201477
147	6	0	-0.759137	-0.118431	-7.066551
148	1	0	-1.247818	0.872332	-7.039524
149	6	0	-1.187590	-0.863126	-8.335688
150	1	0	-2.273646	-1.004249	-8.312950
151	1	0	-0.735782	-1.863386	-8.314477
152	6	0	-0.755711	-0.117677	-9.598755
153	1	0	-1.057696	-0.681361	-10.487723
154	1	0	-1.271756	0.850985	-9.645727
155	7	0	1.110752	0.916617	-5.908925
156	6	0	1.840834	2.418596	-3.567335
157	1	0	1.039506	2.808504	-4.189804
158	6	0	2.388854	1.167976	-3.887120
159	6	0	1.924473	0.420875	-5.072683
160	1	0	2.352624	-0.585405	-5.201477
161	6	0	0.759137	0.118431	-7.066551
162	1	0	1.247818	-0.872332	-7.039524
163	6	0	1.187590	0.863126	-8.335688
164	1	0	2.273646	1.004249	-8.312950
165	1	0	0.735782	1.863386	-8.314477
166	6	0	0.755711	0.117677	-9.598755
167	1	0	1.057696	0.681361	-10.487723
168	1	0	1.271756	-0.850985	-9.645727
169	53	0	-2.326352	-1.552904	1.622762
170	53	0	-0.000000	0.000000	0.684117
171	53	0	2.326352	1.552904	1.622762

3I@CC3-b C1 cc3-i3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	2.511559	-4.685791	1.437867
2	6	0	2.070105	-2.256350	2.898863
3	1	0	3.075514	-2.460659	2.539466
4	6	0	1.044351	-3.153741	2.569128
5	6	0	1.331453	-4.360472	1.768060
6	1	0	0.458104	-4.972053	1.492350
7	6	0	2.691657	-5.907602	0.680119
8	1	0	1.726935	-6.413677	0.494191
9	6	0	3.619708	-6.848844	1.454590
10	1	0	3.159487	-7.085301	2.420111
11	1	0	4.552151	-6.310752	1.669056
12	6	0	3.916597	-8.121300	0.660477
13	1	0	4.596433	-8.766534	1.226848
14	1	0	2.986167	-8.687583	0.517137
15	7	0	2.730281	0.785739	4.786274
16	6	0	0.497755	-0.907504	4.133125
17	1	0	0.310310	-0.032423	4.750302
18	6	0	1.801939	-1.132594	3.670500
19	6	0	2.897628	-0.203607	4.010406
20	1	0	3.873442	-0.430809	3.554516
21	6	0	3.882477	1.617843	5.071790
22	1	0	4.757861	1.317623	4.468085

23	6	0	4.228919	1.504709	6.560751
24	1	0	4.476080	0.461791	6.787297
25	1	0	3.331202	1.753340	7.141790
26	6	0	5.378713	2.437520	6.942804
27	1	0	5.591277	2.350588	8.013590
28	1	0	6.289555	2.129678	6.411509
29	7	0	-2.783507	-2.466837	4.335381
30	6	0	-0.244956	-2.922345	3.033358
31	1	0	-1.054000	-3.611797	2.805395
32	6	0	-0.521818	-1.802667	3.831755
33	6	0	-1.858897	-1.603066	4.424682
34	1	0	-1.988757	-0.671460	4.997910
35	6	0	-4.014400	-2.211500	5.059350
36	1	0	-4.008238	-1.210649	5.527767
37	6	0	-4.173789	-3.279490	6.148210
38	1	0	-3.322069	-3.212386	6.833750
39	1	0	-4.120670	-4.266206	5.670077
40	6	0	-5.497230	-3.128739	6.898590
41	1	0	-5.590492	-3.915872	7.654141
42	1	0	-5.506064	-2.170086	7.434926
43	7	0	2.341333	-4.755260	-1.426256
44	6	0	0.497367	-3.077057	-2.843898
45	1	0	0.121347	-4.001804	-2.413233
46	6	0	1.842268	-2.740831	-2.637659
47	6	0	2.729781	-3.628637	-1.859912
48	1	0	3.751092	-3.255276	-1.689397
49	6	0	3.294551	-5.561706	-0.690639
50	1	0	4.237231	-5.013485	-0.512690
51	6	0	3.590668	-6.840272	-1.482630
52	1	0	4.030798	-6.564328	-2.447136
53	1	0	2.636715	-7.339111	-1.698105
54	6	0	4.513153	-7.780853	-0.706413
55	1	0	4.691944	-8.692501	-1.286305
56	1	0	5.489397	-7.297905	-0.563583
57	7	0	3.283423	0.824178	-4.468836
58	6	0	2.347940	-1.570031	-3.189853
59	1	0	3.389438	-1.290719	-3.051650
60	6	0	1.519120	-0.722639	-3.938578
61	6	0	2.055882	0.514852	-4.538406
62	1	0	1.324812	1.147039	-5.066363
63	6	0	3.711659	2.046067	-5.119366
64	1	0	2.862935	2.568623	-5.596971
65	6	0	4.763696	1.708493	-6.181037
66	1	0	4.315243	1.039661	-6.923677
67	1	0	5.573159	1.148416	-5.695165
68	6	0	5.319175	2.970480	-6.841802
69	1	0	6.081608	2.701961	-7.580617
70	1	0	4.514025	3.481758	-7.386998
71	7	0	-2.458634	-2.082107	-4.713118
72	6	0	0.187623	-1.067243	-4.140998
73	1	0	-0.470246	-0.436059	-4.733111
74	6	0	-0.327028	-2.255308	-3.603403
75	6	0	-1.710870	-2.685328	-3.885184
76	1	0	-2.038710	-3.598230	-3.363067
77	6	0	-3.758195	-2.662174	-4.993428
78	1	0	-3.951818	-3.546826	-4.360126
79	6	0	-3.801565	-3.075255	-6.469564
80	1	0	-3.019421	-3.820842	-6.648990
81	1	0	-3.549470	-2.196926	-7.077897

82	6	0	-5.176218	-3.613166	-6.867015
83	1	0	-5.180541	-3.880376	-7.928961
84	1	0	-5.384629	-4.534410	-6.306109
85	7	0	-5.070334	-1.161987	3.144669
86	6	0	-4.699534	0.944908	1.234186
87	1	0	-4.696259	1.204923	2.289314
88	6	0	-4.846865	-0.403014	0.878566
89	6	0	-4.984853	-1.446783	1.913223
90	1	0	-5.008598	-2.485499	1.548055
91	6	0	-5.202464	-2.254977	4.086665
92	1	0	-5.178529	-3.234681	3.576485
93	6	0	-6.526409	-2.104894	4.844058
94	1	0	-7.352203	-2.151847	4.125783
95	1	0	-6.551726	-1.103903	5.294065
96	6	0	-6.678367	-3.172268	5.927889
97	1	0	-7.622894	-3.029727	6.463307
98	1	0	-6.724645	-4.164791	5.459402
99	7	0	3.313325	3.163263	3.281923
100	6	0	2.755952	3.337794	0.469996
101	1	0	3.719200	2.936643	0.775409
102	6	0	1.830091	3.689699	1.463120
103	6	0	2.165615	3.534935	2.892623
104	1	0	1.360205	3.780035	3.602430
105	6	0	3.546257	3.072914	4.709479
106	1	0	2.644589	3.353230	5.283766
107	6	0	4.702164	4.003207	5.091385
108	1	0	4.430473	5.031872	4.830576
109	1	0	5.572799	3.737936	4.477671
110	6	0	5.048587	3.885490	6.575962
111	1	0	5.888777	4.544777	6.818195
112	1	0	4.194415	4.224470	7.177956
113	7	0	3.246862	3.371369	-3.137162
114	6	0	1.198871	4.037785	-1.234131
115	1	0	0.979580	4.175594	-2.289890
116	6	0	2.444900	3.505215	-0.874394
117	6	0	3.438385	3.141805	-1.904866
118	1	0	4.360775	2.669222	-1.533597
119	6	0	4.297087	2.997348	-4.063775
120	1	0	5.116865	2.462334	-3.551429
121	6	0	4.852293	4.260797	-4.730959
122	1	0	5.273117	4.912810	-3.957729
123	1	0	4.014411	4.805046	-5.185981
124	6	0	5.898572	3.921579	-5.793145
125	1	0	6.263417	4.839649	-6.265744
126	1	0	6.764095	3.445084	-5.313038
127	7	0	-4.861276	-1.358964	-3.266864
128	6	0	-4.843724	-0.761940	-0.467932
129	1	0	-4.963726	-1.799261	-0.772801
130	6	0	-4.700920	0.218445	-1.465374
131	6	0	-4.690396	-0.160889	-2.891421
132	1	0	-4.530014	0.660653	-3.606260
133	6	0	-4.856688	-1.632907	-4.690004
134	1	0	-4.632719	-0.723926	-5.276676
135	6	0	-6.232483	-2.175323	-5.094122
136	1	0	-6.989682	-1.413605	-4.878311
137	1	0	-6.459708	-3.040205	-4.457315
138	6	0	-6.267126	-2.584224	-6.566681
139	1	0	-7.254642	-2.983563	-6.820632
140	1	0	-6.110707	-1.697582	-7.196072

141	7	0	-4.348707	4.265329	-0.212504
142	6	0	-4.555363	1.548190	-1.099883
143	1	0	-4.436250	2.325913	-1.849539
144	6	0	-4.552807	1.918010	0.254525
145	6	0	-4.401134	3.333998	0.645310
146	1	0	-4.346230	3.529963	1.727109
147	6	0	-4.225483	5.626756	0.269578
148	1	0	-4.128731	5.659866	1.369706
149	6	0	-5.466508	6.418916	-0.157314
150	1	0	-6.352228	5.957434	0.292785
151	1	0	-5.575659	6.324021	-1.245532
152	6	0	-5.355283	7.892781	0.233189
153	1	0	-6.245735	8.436078	-0.100032
154	1	0	-5.320631	7.979181	1.327739
155	7	0	-1.790280	5.552349	0.185556
156	6	0	0.598200	4.216930	1.095938
157	1	0	-0.129785	4.513660	1.846696
158	6	0	0.280101	4.403990	-0.257626
159	6	0	-0.985113	5.052850	-0.657205
160	1	0	-1.166643	5.112558	-1.741796
161	6	0	-2.954419	6.251072	-0.324982
162	1	0	-3.027720	6.166515	-1.424329
163	6	0	-2.849886	7.730526	0.064225
164	1	0	-1.944255	8.149939	-0.387260
165	1	0	-2.719844	7.789664	1.152659
166	6	0	-4.090961	8.515591	-0.360784
167	1	0	-3.995447	9.561869	-0.052095
168	1	0	-4.167697	8.512764	-1.456607
169	53	0	-1.629517	-1.048799	-0.115906
170	53	0	1.087022	0.092556	0.022739
171	53	0	4.029206	-0.368498	0.115100

5I@CC3 C2 cc3-i5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	0.325225	-5.541346	-0.758069
2	6	0	0.969730	-3.281626	-2.427976
3	1	0	0.074162	-3.850139	-2.669750
4	6	0	1.709553	-3.642359	-1.291962
5	6	0	1.312792	-4.800469	-0.466856
6	1	0	1.955643	-5.006053	0.403703
7	6	0	0.095240	-6.712717	0.065848
8	1	0	0.784016	-6.740622	0.929650
9	6	0	0.308975	-7.965141	-0.792981
10	1	0	1.340757	-7.967334	-1.160912
11	1	0	-0.342950	-7.891773	-1.673093
12	6	0	-0.000000	-9.243848	-0.014116
13	1	0	0.142328	-10.117846	-0.658360
14	1	0	0.708221	-9.344206	0.819666
15	7	0	1.017198	-1.010696	-5.270822
16	6	0	2.555636	-1.529202	-2.907874
17	1	0	2.873687	-0.715651	-3.556429
18	6	0	1.385003	-2.228071	-3.233081
19	6	0	0.606017	-1.871846	-4.435872
20	1	0	-0.345900	-2.409729	-4.568122

21	6	0	0.193425	-0.743835	-6.432256
22	1	0	-0.743563	-1.329191	-6.407491
23	6	0	0.980264	-1.093665	-7.699830
24	1	0	1.231119	-2.159791	-7.677760
25	1	0	1.929101	-0.541999	-7.677391
26	6	0	0.194921	-0.739638	-8.963136
27	1	0	0.786741	-0.981624	-9.852274
28	1	0	-0.715530	-1.352557	-9.010332
29	7	0	5.333276	-1.496293	-0.555603
30	6	0	2.864035	-2.936453	-0.972990
31	1	0	3.461592	-3.203364	-0.104851
32	6	0	3.297692	-1.879930	-1.786509
33	6	0	4.553222	-1.159359	-1.497805
34	1	0	4.786899	-0.323916	-2.176628
35	6	0	6.581054	-0.767325	-0.427500
36	1	0	6.609676	0.107164	-1.102371
37	6	0	7.739066	-1.712557	-0.771368
38	1	0	7.619436	-2.051875	-1.806030
39	1	0	7.656591	-2.601820	-0.132808
40	6	0	9.097378	-1.041744	-0.566215
41	1	0	9.901977	-1.746597	-0.800829
42	1	0	9.197841	-0.199692	-1.264380
43	7	0	-1.463261	-5.547076	1.517192
44	6	0	-1.737586	-3.236916	3.200137
45	1	0	-0.934884	-3.935122	3.422886
46	6	0	-2.582058	-3.508684	2.117766
47	6	0	-2.371248	-4.698412	1.269087
48	1	0	-3.045470	-4.794754	0.403802
49	6	0	-1.335847	-6.680205	0.621787
50	1	0	-2.025865	-6.596294	-0.236870
51	6	0	-1.641329	-7.965320	1.400061
52	1	0	-2.670806	-7.916778	1.771501
53	1	0	-0.985636	-7.997221	2.280056
54	6	0	-1.425576	-9.209757	0.538740
55	1	0	-1.633442	-10.110983	1.125094
56	1	0	-2.137420	-9.202641	-0.297795
57	7	0	-5.680914	-0.728223	1.264053
58	6	0	-3.613806	-2.624595	1.812610
59	1	0	-4.281108	-2.814485	0.974396
60	6	0	-3.802788	-1.458199	2.567069
61	6	0	-4.877923	-0.507673	2.218976
62	1	0	-4.940373	0.398353	2.841124
63	6	0	-6.722394	0.247068	1.010241
64	1	0	-6.635693	1.116100	1.687093
65	6	0	-8.086625	-0.422559	1.211629
66	1	0	-8.160229	-0.770577	2.247796
67	1	0	-8.128026	-1.313764	0.572021
68	6	0	-9.235199	0.525470	0.866779
69	1	0	-10.194667	0.015287	1.002162
70	1	0	-9.226862	1.377445	1.560253
71	7	0	-1.197711	-0.822579	5.876292
72	6	0	-2.957249	-1.192802	3.635389
73	1	0	-3.076153	-0.295278	4.237096
74	6	0	-1.921717	-2.088073	3.964123
75	6	0	-1.039386	-1.827296	5.119084
76	1	0	-0.243828	-2.569152	5.289768
77	6	0	-0.322083	-0.696292	7.026253
78	1	0	0.493070	-1.441254	6.996694
79	6	0	-1.154772	-0.905070	8.297692

80	1	0	-1.586545	-1.911578	8.273782
81	1	0	-1.993941	-0.197568	8.277853
82	6	0	-0.319440	-0.694663	9.560564
83	1	0	-0.944877	-0.831336	10.448888
84	1	0	0.470924	-1.456057	9.607117
85	7	0	5.680914	0.728223	1.264053
86	6	0	3.613806	2.624595	1.812610
87	1	0	4.281108	2.814485	0.974396
88	6	0	3.802788	1.458199	2.567069
89	6	0	4.877923	0.507673	2.218976
90	1	0	4.940373	-0.398353	2.841124
91	6	0	6.722394	-0.247068	1.010241
92	1	0	6.635693	-1.116100	1.687093
93	6	0	8.086625	0.422559	1.211629
94	1	0	8.160229	0.770577	2.247796
95	1	0	8.128026	1.313764	0.572021
96	6	0	9.235199	-0.525470	0.866779
97	1	0	10.194667	-0.015287	1.002162
98	1	0	9.226862	-1.377445	1.560253
99	7	0	-1.017198	1.010696	-5.270822
100	6	0	-2.555636	1.529202	-2.907874
101	1	0	-2.873687	0.715651	-3.556429
102	6	0	-1.385003	2.228071	-3.233081
103	6	0	-0.606017	1.871846	-4.435872
104	1	0	0.345900	2.409729	-4.568122
105	6	0	-0.193425	0.743835	-6.432256
106	1	0	0.743563	1.329191	-6.407491
107	6	0	-0.980264	1.093665	-7.699830
108	1	0	-1.231119	2.159791	-7.677760
109	1	0	-1.929101	0.541999	-7.677391
110	6	0	-0.194921	0.739638	-8.963136
111	1	0	-0.786741	0.981624	-9.852274
112	1	0	0.715530	1.352557	-9.010332
113	7	0	-5.333276	1.496293	-0.555603
114	6	0	-2.864035	2.936453	-0.972990
115	1	0	-3.461592	3.203364	-0.104851
116	6	0	-3.297692	1.879930	-1.786509
117	6	0	-4.553222	1.159359	-1.497805
118	1	0	-4.786899	0.323916	-2.176628
119	6	0	-6.581054	0.767325	-0.427500
120	1	0	-6.609676	-0.107164	-1.102371
121	6	0	-7.739066	1.712557	-0.771368
122	1	0	-7.619436	2.051875	-1.806030
123	1	0	-7.656591	2.601820	-0.132808
124	6	0	-9.097378	1.041744	-0.566215
125	1	0	-9.901977	1.746597	-0.800829
126	1	0	-9.197841	0.199692	-1.264380
127	7	0	1.197711	0.822579	5.876292
128	6	0	2.957249	1.192802	3.635389
129	1	0	3.076153	0.295278	4.237096
130	6	0	1.921717	2.088073	3.964123
131	6	0	1.039386	1.827296	5.119084
132	1	0	0.243828	2.569152	5.289768
133	6	0	0.322083	0.696292	7.026253
134	1	0	-0.493070	1.441254	6.996694
135	6	0	1.154772	0.905070	8.297692
136	1	0	1.586545	1.911578	8.273782
137	1	0	1.993941	0.197568	8.277853
138	6	0	0.319440	0.694663	9.560564

139	1	0	0.944877	0.831336	10.448888
140	1	0	-0.470924	1.456057	9.607117
141	7	0	1.463261	5.547076	1.517192
142	6	0	1.737586	3.236916	3.200137
143	1	0	0.934884	3.935122	3.422886
144	6	0	2.582058	3.508684	2.117766
145	6	0	2.371248	4.698412	1.269087
146	1	0	3.045470	4.794754	0.403802
147	6	0	1.335847	6.680205	0.621787
148	1	0	2.025865	6.596294	-0.236870
149	6	0	1.641329	7.965320	1.400061
150	1	0	2.670806	7.916778	1.771501
151	1	0	0.985636	7.997221	2.280056
152	6	0	1.425576	9.209757	0.538740
153	1	0	1.633442	10.110983	1.125094
154	1	0	2.137420	9.202641	-0.297795
155	7	0	-0.325225	5.541346	-0.758069
156	6	0	-0.969730	3.281626	-2.427976
157	1	0	-0.074162	3.850139	-2.669750
158	6	0	-1.709553	3.642359	-1.291962
159	6	0	-1.312792	4.800469	-0.466856
160	1	0	-1.955643	5.006053	0.403703
161	6	0	-0.095240	6.712717	0.065848
162	1	0	-0.784016	6.740622	0.929650
163	6	0	-0.308975	7.965141	-0.792981
164	1	0	-1.340757	7.967334	-1.160912
165	1	0	0.342950	7.891773	-1.673093
166	6	0	0.000000	9.243848	-0.014116
167	1	0	-0.142328	10.117846	-0.658360
168	1	0	-0.708221	9.344206	0.819666
169	53	0	0.000000	0.000000	2.090584
170	53	0	-1.435347	-1.214754	-0.524468
171	53	0	1.435347	1.214754	-0.524468
172	53	0	3.121137	2.656373	-2.365017
173	53	0	-3.121137	-2.656373	-2.365017

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-3.310098	0.175788	-4.617978
2	6	0	-0.586007	0.897699	-4.056050
3	1	0	-1.292109	1.697878	-4.267042
4	6	0	-1.059520	-0.421206	-4.014786
5	6	0	-2.482580	-0.719831	-4.269208
6	1	0	-2.777398	-1.774986	-4.154060
7	6	0	-4.676094	-0.231739	-4.877851
8	1	0	-4.814804	-1.314082	-4.702709
9	6	0	-5.033596	0.098132	-6.330881
10	1	0	-4.358385	-0.451947	-6.995273
11	1	0	-4.843943	1.166626	-6.496689
12	6	0	-6.495069	-0.231379	-6.636693
13	1	0	-6.729630	0.031504	-7.673602
14	1	0	-6.652751	-1.314201	-6.539522
15	7	0	2.476282	2.849490	-3.750170
16	6	0	1.647697	0.111019	-3.601725

17	1	0	2.703230	0.339576	-3.472931
18	6	0	0.761197	1.168098	-3.846648
19	6	0	1.251553	2.558825	-3.905850
20	1	0	0.489645	3.328011	-4.107609
21	6	0	2.862941	4.239959	-3.882284
22	1	0	1.979469	4.900176	-3.953529
23	6	0	3.718498	4.398594	-5.145238
24	1	0	3.121070	4.102870	-6.014562
25	1	0	4.558186	3.694077	-5.080373
26	6	0	4.239778	5.827874	-5.296823
27	1	0	4.861694	5.905992	-6.194820
28	1	0	3.391993	6.512458	-5.436085
29	7	0	1.836410	-3.518398	-3.351296
30	6	0	-0.172643	-1.462358	-3.765442
31	1	0	-0.515685	-2.494630	-3.752853
32	6	0	1.189720	-1.200562	-3.558781
33	6	0	2.162670	-2.291786	-3.362364
34	1	0	3.212228	-1.971540	-3.263229
35	6	0	2.917556	-4.486249	-3.284673
36	1	0	3.880893	-3.996870	-3.052823
37	6	0	3.023315	-5.190829	-4.643466
38	1	0	3.240012	-4.439513	-5.410570
39	1	0	2.041904	-5.619658	-4.884967
40	6	0	4.088935	-6.286951	-4.631404
41	1	0	4.125302	-6.784004	-5.606493
42	1	0	5.076280	-5.834401	-4.467295
43	7	0	-5.303223	0.100275	-2.557380
44	6	0	-4.580273	-0.641089	0.119653
45	1	0	-4.766738	-1.437414	-0.597826
46	6	0	-4.654971	0.687870	-0.319105
47	6	0	-4.977813	0.999803	-1.725453
48	1	0	-4.925101	2.064028	-2.004233
49	6	0	-5.612556	0.511085	-3.911791
50	1	0	-5.446051	1.594301	-4.053924
51	6	0	-7.075872	0.176193	-4.220685
52	1	0	-7.719402	0.726593	-3.525664
53	1	0	-7.232502	-0.892222	-4.022896
54	6	0	-7.430106	0.500834	-5.672350
55	1	0	-8.473604	0.234936	-5.871678
56	1	0	-7.340813	1.583483	-5.835856
57	7	0	-4.079784	3.754296	2.584106
58	6	0	-4.435687	1.720786	0.583739
59	1	0	-4.500273	2.760545	0.270615
60	6	0	-4.129418	1.440760	1.923115
61	6	0	-3.933291	2.533711	2.895609
62	1	0	-3.680825	2.221142	3.921111
63	6	0	-3.934344	4.742961	3.634094
64	1	0	-3.668886	4.272722	4.598308
65	6	0	-5.256691	5.503187	3.786231
66	1	0	-6.043174	4.791682	4.060236
67	1	0	-5.528203	5.916573	2.806220
68	6	0	-5.145956	6.625503	4.818331
69	1	0	-6.097904	7.161811	4.891430
70	1	0	-4.947304	6.193292	5.808615
71	7	0	-4.213219	-2.661698	3.121759
72	6	0	-4.054917	0.118893	2.348240
73	1	0	-3.837070	-0.123447	3.385502
74	6	0	-4.291863	-0.929916	1.448215
75	6	0	-4.309370	-2.335862	1.899546

76	1	0	-4.461594	-3.086356	1.106793
77	6	0	-4.373041	-4.064162	3.457271
78	1	0	-4.407556	-4.696074	2.551390
79	6	0	-5.681461	-4.227919	4.241576
80	1	0	-6.513027	-3.905527	3.605673
81	1	0	-5.653383	-3.544186	5.100053
82	6	0	-5.880500	-5.665609	4.720902
83	1	0	-6.811454	-5.743707	5.292160
84	1	0	-5.982912	-6.330054	3.852219
85	7	0	2.662059	-4.823559	-0.893868
86	6	0	2.620383	-3.483423	1.640272
87	1	0	3.523075	-3.404396	1.040516
88	6	0	1.566772	-4.276951	1.168926
89	6	0	1.646129	-4.942316	-0.145520
90	1	0	0.761479	-5.526605	-0.443203
91	6	0	2.640081	-5.506361	-2.172972
92	1	0	1.651526	-5.958167	-2.370319
93	6	0	3.711862	-6.603444	-2.164796
94	1	0	3.478419	-7.319600	-1.369237
95	1	0	4.673962	-6.141557	-1.907514
96	6	0	3.810044	-7.301208	-3.521428
97	1	0	4.593205	-8.066039	-3.491997
98	1	0	2.865516	-7.819961	-3.734407
99	7	0	2.800894	4.595534	-1.474845
100	6	0	1.156424	4.400535	0.874500
101	1	0	0.788814	4.997664	0.042679
102	6	0	2.390744	3.748383	0.736836
103	6	0	3.171241	3.859503	-0.511690
104	1	0	4.100860	3.269487	-0.548867
105	6	0	3.661132	4.661240	-2.640620
106	1	0	4.516992	3.968491	-2.547778
107	6	0	4.180131	6.095492	-2.795388
108	1	0	4.752203	6.362914	-1.900235
109	1	0	3.315650	6.771049	-2.835496
110	6	0	5.029251	6.251524	-4.057136
111	1	0	5.370150	7.287798	-4.153139
112	1	0	5.928750	5.626919	-3.970987
113	7	0	-1.547799	4.971887	3.244813
114	6	0	0.920292	3.507976	3.102910
115	1	0	0.331126	3.422602	4.012647
116	6	0	0.421640	4.285574	2.050658
117	6	0	-0.873706	4.983801	2.171307
118	1	0	-1.212608	5.522200	1.272266
119	6	0	-2.796150	5.708146	3.268143
120	1	0	-3.030439	6.139583	2.278258
121	6	0	-2.691375	6.833549	4.303917
122	1	0	-1.882828	7.511003	4.008410
123	1	0	-2.399982	6.388730	5.264374
124	6	0	-4.013384	7.586768	4.453050
125	1	0	-3.913772	8.370776	5.211090
126	1	0	-4.256743	8.088149	3.506427
127	7	0	-1.981461	-4.484185	3.486173
128	6	0	0.399888	-4.398754	1.924836
129	1	0	-0.425590	-5.016295	1.577486
130	6	0	0.254085	-3.703281	3.128322
131	6	0	-1.006893	-3.783598	3.891837
132	1	0	-1.048905	-3.198651	4.823370
133	6	0	-3.178706	-4.531606	4.300992
134	1	0	-3.102087	-3.857543	5.172862

135	6	0	-3.385763	-5.972298	4.784193
136	1	0	-2.524373	-6.267483	5.393296
137	1	0	-3.395477	-6.629460	3.904930
138	6	0	-4.690551	-6.122886	5.565989
139	1	0	-4.818320	-7.163524	5.881915
140	1	0	-4.641735	-5.515930	6.480339
141	7	0	3.536940	-1.343620	4.440125
142	6	0	1.295212	-2.895244	3.578722
143	1	0	1.218613	-2.348533	4.515536
144	6	0	2.495454	-2.796487	2.841363
145	6	0	3.610801	-1.967158	3.338150
146	1	0	4.506263	-1.932349	2.699528
147	6	0	4.704296	-0.601929	4.879316
148	1	0	5.461022	-0.530962	4.078155
149	6	0	5.312137	-1.318618	6.092070
150	1	0	5.616747	-2.326560	5.789764
151	1	0	4.527565	-1.435673	6.851030
152	6	0	6.492442	-0.538562	6.671892
153	1	0	6.892314	-1.062965	7.546029
154	1	0	7.300567	-0.494314	5.929342
155	7	0	3.818181	1.514374	4.062810
156	6	0	2.885594	2.995370	1.792484
157	1	0	3.845428	2.491343	1.718262
158	6	0	2.150965	2.867545	2.982045
159	6	0	2.682590	2.077343	4.109581
160	1	0	2.038208	2.019627	5.001032
161	6	0	4.282682	0.825203	5.251233
162	1	0	3.484927	0.749039	6.011915
163	6	0	5.468608	1.602324	5.836361
164	1	0	5.130763	2.609141	6.104889
165	1	0	6.224555	1.718788	5.048979
166	6	0	6.071814	0.884209	7.043534
167	1	0	6.927139	1.450723	7.426149
168	1	0	5.329830	0.842301	7.852491
169	53	0	0.528284	-0.142684	2.016137
170	53	0	-0.862265	1.672650	-0.380119
171	53	0	3.232922	-0.175240	-0.100008
172	53	0	-1.033555	-2.104312	-0.162821
173	53	0	-2.261588	-4.243541	-1.621030
174	53	0	-1.917271	3.933466	-1.770571
175	53	0	5.483155	-0.041787	-1.853039

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-0.021128	1.432798	-5.849707
2	6	0	-0.748723	2.890364	-3.486848
3	1	0	-1.549675	2.520858	-4.123746
4	6	0	0.574374	2.557860	-3.811754
5	6	0	0.874769	1.750476	-5.010528
6	1	0	1.929293	1.460717	-5.141707
7	6	0	0.380573	0.667170	-7.012040
8	1	0	1.459900	0.430854	-6.987871
9	6	0	0.061950	1.467506	-8.279223
10	1	0	0.627058	2.405664	-8.257068

11	1	0	-1.002373	1.735469	-8.256756
12	6	0	0.376799	0.665671	-9.542506
13	1	0	0.122274	1.252112	-10.431626
14	1	0	1.456441	0.468257	-9.589759
15	7	0	-2.708210	4.813383	-1.089099
16	6	0	0.036973	4.176347	-1.605149
17	1	0	-0.192940	4.832515	-0.769735
18	6	0	-1.021523	3.693841	-2.386011
19	6	0	-2.415094	4.060285	-2.067036
20	1	0	-3.184581	3.655803	-2.743587
21	6	0	-4.099968	5.178138	-0.912310
22	1	0	-4.757492	4.600695	-1.587388
23	6	0	-4.256710	6.675094	-1.207870
24	1	0	-3.956407	6.861904	-2.244636
25	1	0	-3.554382	7.225468	-0.567850
26	6	0	-5.686834	7.152916	-0.955344
27	1	0	-5.762998	8.226973	-1.154741
28	1	0	-6.368528	6.649972	-1.654673
29	7	0	3.666760	4.181650	-1.330025
30	6	0	1.616122	3.027421	-3.019553
31	1	0	2.650690	2.790255	-3.259080
32	6	0	1.350730	3.844374	-1.911021
33	6	0	2.441196	4.404392	-1.090121
34	1	0	2.120235	5.059307	-0.263921
35	6	0	4.642096	4.867389	-0.502628
36	1	0	4.157361	5.389394	0.342297
37	6	0	5.389822	5.889771	-1.367371
38	1	0	4.666620	6.613088	-1.759435
39	1	0	5.814802	5.362739	-2.231593
40	6	0	6.497651	6.591305	-0.581206
41	1	0	7.025493	7.298724	-1.229357
42	1	0	6.051731	7.177496	0.233731
43	7	0	0.021128	-1.432798	-5.849707
44	6	0	0.748723	-2.890364	-3.486848
45	1	0	1.549675	-2.520858	-4.123746
46	6	0	-0.574374	-2.557860	-3.811754
47	6	0	-0.874769	-1.750476	-5.010528
48	1	0	-1.929293	-1.460717	-5.141707
49	6	0	-0.380573	-0.667170	-7.012040
50	1	0	-1.459900	-0.430854	-6.987871
51	6	0	-0.061950	-1.467506	-8.279223
52	1	0	-0.627058	-2.405664	-8.257068
53	1	0	1.002373	-1.735469	-8.256756
54	6	0	-0.376799	-0.665671	-9.542506
55	1	0	-0.122274	-1.252112	-10.431626
56	1	0	-1.456441	-0.468257	-9.589759
57	7	0	-3.666760	-4.181650	-1.330025
58	6	0	-1.616122	-3.027421	-3.019553
59	1	0	-2.650690	-2.790255	-3.259080
60	6	0	-1.350730	-3.844374	-1.911021
61	6	0	-2.441196	-4.404392	-1.090121
62	1	0	-2.120235	-5.059307	-0.263921
63	6	0	-4.642096	-4.867389	-0.502628
64	1	0	-4.157361	-5.389394	0.342297
65	6	0	-5.389822	-5.889771	-1.367371
66	1	0	-4.666620	-6.613088	-1.759435
67	1	0	-5.814802	-5.362739	-2.231593
68	6	0	-6.497651	-6.591305	-0.581206
69	1	0	-7.025493	-7.298724	-1.229357

70	1	0	-6.051731	-7.177496	0.233731
71	7	0	2.708210	-4.813383	-1.089099
72	6	0	-0.036973	-4.176347	-1.605149
73	1	0	0.192940	-4.832515	-0.769735
74	6	0	1.021523	-3.693841	-2.386011
75	6	0	2.415094	-4.060285	-2.067036
76	1	0	3.184581	-3.655803	-2.743587
77	6	0	4.099968	-5.178138	-0.912310
78	1	0	4.757492	-4.600695	-1.587388
79	6	0	4.256710	-6.675094	-1.207870
80	1	0	3.956407	-6.861904	-2.244636
81	1	0	3.554382	-7.225468	-0.567850
82	6	0	5.686834	-7.152916	-0.955344
83	1	0	5.762998	-8.226973	-1.154741
84	1	0	6.368528	-6.649972	-1.654673
85	7	0	4.903423	2.960729	0.981822
86	6	0	3.486322	1.137549	2.693526
87	1	0	3.408882	2.199226	2.914325
88	6	0	4.250046	0.731748	1.593711
89	6	0	4.933996	1.718318	0.734031
90	1	0	5.473122	1.305659	-0.133230
91	6	0	5.623844	3.845141	0.086695
92	1	0	6.069511	3.287924	-0.756848
93	6	0	6.732230	4.552875	0.874676
94	1	0	7.420561	3.798995	1.272147
95	1	0	6.273590	5.053526	1.737266
96	6	0	7.473170	5.571495	0.008257
97	1	0	8.245159	6.074174	0.600278
98	1	0	7.988310	5.049370	-0.809472
99	7	0	-4.467766	3.438366	0.748797
100	6	0	-4.355177	0.626599	1.290365
101	1	0	-4.946567	0.963422	0.441121
102	6	0	-3.701440	1.588639	2.074002
103	6	0	-3.796320	3.024549	1.740401
104	1	0	-3.251793	3.709822	2.408409
105	6	0	-4.528803	4.870817	0.528418
106	1	0	-3.839777	5.410161	1.203272
107	6	0	-5.964266	5.349282	0.777298
108	1	0	-6.236034	5.125784	1.814814
109	1	0	-6.637785	4.764463	0.137193
110	6	0	-6.117452	6.840850	0.478633
111	1	0	-7.154318	7.150950	0.645841
112	1	0	-5.495544	7.417925	1.176338
113	7	0	-4.903423	-2.960729	0.981822
114	6	0	-3.486322	-1.137549	2.693526
115	1	0	-3.408882	-2.199226	2.914325
116	6	0	-4.250046	-0.731748	1.593711
117	6	0	-4.933996	-1.718318	0.734031
118	1	0	-5.473122	-1.305659	-0.133230
119	6	0	-5.623844	-3.845141	0.086695
120	1	0	-6.069511	-3.287924	-0.756848
121	6	0	-6.732230	-4.552875	0.874676
122	1	0	-7.420561	-3.798995	1.272147
123	1	0	-6.273590	-5.053526	1.737266
124	6	0	-7.473170	-5.571495	0.008257
125	1	0	-8.245159	-6.074174	0.600278
126	1	0	-7.988310	-5.049370	-0.809472
127	7	0	4.467766	-3.438366	0.748797
128	6	0	4.355177	-0.626599	1.290365

129	1	0	4.946567	-0.963422	0.441121
130	6	0	3.701440	-1.588639	2.074002
131	6	0	3.796320	-3.024549	1.740401
132	1	0	3.251793	-3.709822	2.408409
133	6	0	4.528803	-4.870817	0.528418
134	1	0	3.839777	-5.410161	1.203272
135	6	0	5.964266	-5.349282	0.777298
136	1	0	6.236034	-5.125784	1.814814
137	1	0	6.637785	-4.764463	0.137193
138	6	0	6.117452	-6.840850	0.478633
139	1	0	7.154318	-7.150950	0.645841
140	1	0	5.495544	-7.417925	1.176338
141	7	0	1.428484	-0.213910	5.381000
142	6	0	2.946546	-1.177246	3.163771
143	1	0	2.428020	-1.898409	3.790727
144	6	0	2.835058	0.191309	3.480960
145	6	0	2.032121	0.622498	4.642140
146	1	0	1.992225	1.707236	4.826263
147	6	0	0.708928	0.290275	6.535282
148	1	0	0.622244	1.390950	6.507027
149	6	0	1.462059	-0.128314	7.804507
150	1	0	2.464565	0.312730	7.780925
151	1	0	1.591607	-1.218203	7.783828
152	6	0	0.707531	0.288645	9.067262
153	1	0	1.256826	-0.040368	9.955433
154	1	0	0.651909	1.384545	9.114356
155	7	0	-1.428484	0.213910	5.381000
156	6	0	-2.946546	1.177246	3.163771
157	1	0	-2.428020	1.898409	3.790727
158	6	0	-2.835058	-0.191309	3.480960
159	6	0	-2.032121	-0.622498	4.642140
160	1	0	-1.992225	-1.707236	4.826263
161	6	0	-0.708928	-0.290275	6.535282
162	1	0	-0.622244	-1.390950	6.507027
163	6	0	-1.462059	0.128314	7.804507
164	1	0	-2.464565	-0.312730	7.780925
165	1	0	-1.591607	1.218203	7.783828
166	6	0	-0.707531	-0.288645	9.067262
167	1	0	-1.256826	0.040368	9.955433
168	1	0	-0.651909	-1.384545	9.114356
169	53	0	-0.000000	0.000000	1.621400
170	53	0	-1.865411	0.154638	-1.047023
171	53	0	0.119250	3.331211	2.085353
172	53	0	1.865411	-0.154638	-1.047023
173	53	0	-0.119250	-3.331211	2.085353
174	53	0	0.000000	-6.180529	2.227777
175	53	0	-0.000000	6.180529	2.227777
176	53	0	4.009335	-0.316701	-2.936870
177	53	0	-4.009335	0.316701	-2.936870

I2 Dih cc3-i5c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	53	0	0.000000	0.000000	1.409392
2	53	0	0.000000	0.000000	-1.409392

I3 Dih cc3-i3c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	53	0	0.000000	0.000000	0.000000
2	53	0	0.000000	0.000000	2.959416
3	53	0	0.000000	0.000000	-2.959416

I3(-) Dih cc3-i3b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	53	0	0.000000	0.000000	0.000000
2	53	0	0.000000	0.000000	3.070122
3	53	0	0.000000	0.000000	-3.070122

I5 C1 cc3-i5aa

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	53	0	0.559991	2.639329	-0.268915
2	53	0	3.722923	-2.028335	-0.316633
3	53	0	2.335239	0.364093	0.612304
4	53	0	-4.367405	-1.430755	0.075925
5	53	0	-2.250747	0.455669	-0.102680

I5(-) C2v cc3-i5b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	53	0	0.000000	0.000000	2.151418
2	53	0	0.000000	5.024827	-1.367275
3	53	0	0.000000	2.563868	0.291566
4	53	0	-0.000000	-5.024827	-1.367275
5	53	0	-0.000000	-2.563868	0.291566

I7 C1 cc3-i7c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	53	0	-0.055594	-0.938174	2.624839
2	53	0	2.487539	0.589454	0.640921
3	53	0	-1.173477	-1.727944	-0.528541

4	53	0	-1.889846	1.535483	0.764179
5	53	0	-3.319164	3.098429	-1.123930
6	53	0	4.360247	1.801310	-1.117204
7	53	0	-0.409704	-4.358559	-1.260265

I7(-) C3v cc3-i7b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	53	0	0.000000	0.000000	1.686387
2	53	0	0.000000	2.940253	0.312184
3	53	0	2.546334	-1.470127	0.312184
4	53	0	-2.546334	-1.470127	0.312184
5	53	0	-4.858044	-2.804793	-0.874313
6	53	0	0.000000	5.609587	-0.874313
7	53	0	4.858044	-2.804793	-0.874313

I9 Cs cc3-i9c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	53	0	1.276713	2.014354	-0.000000
2	53	0	-1.832903	3.821278	-0.000000
3	53	0	1.981139	-0.779239	-2.185479
4	53	0	-1.677862	0.218470	-0.000000
5	53	0	1.981139	-0.779239	2.185479
6	53	0	1.981139	-3.337772	3.400621
7	53	0	1.981139	-3.337772	-3.400621
8	53	0	-1.175703	-2.565452	0.000000
9	53	0	-4.514801	4.745373	-0.000000

I9(-) Td cc3-i9b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	53	0	0.000000	0.000000	0.000000
2	53	0	1.902858	1.902858	1.902858
3	53	0	1.902858	-1.902858	-1.902858
4	53	0	-1.902858	1.902858	-1.902858
5	53	0	-1.902858	-1.902858	1.902858
6	53	0	-3.575494	-3.575494	3.575494
7	53	0	3.575494	-3.575494	-3.575494
8	53	0	-3.575494	3.575494	-3.575494
9	53	0	3.575494	3.575494	3.575494