

## XYZ coordinates of each optimized geometry on C<sub>96</sub>H<sub>24</sub>

### propane

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.371714	-0.036415	-0.156720
2	6	0	0.628005	-1.249807	-0.150610
3	6	0	-0.794620	-1.212392	-0.138536
4	6	0	-1.473576	0.038377	-0.132545
5	6	0	-0.729833	1.251724	-0.138685
6	6	0	0.692786	1.214369	-0.150756
7	6	0	2.790494	-0.073713	-0.168769
8	6	0	1.305103	-2.497195	-0.156563
9	6	0	-1.536319	-2.422503	-0.132434
10	6	0	-2.892338	0.075669	-0.120505
11	6	0	-1.406953	2.499144	-0.132718
12	6	0	1.434471	2.424458	-0.156843
13	6	0	3.533524	1.140578	-0.174876
14	6	0	3.468705	-1.325365	-0.174736
15	6	0	2.728185	-2.533555	-0.168650
16	6	0	0.560283	-3.710392	-0.150442
17	6	0	-0.856261	-3.673157	-0.138412
18	6	0	-2.959344	-2.384051	-0.120347
19	6	0	-3.635369	-1.138626	-0.114404
20	6	0	-3.570549	1.327318	-0.114544
21	6	0	-2.830030	2.535507	-0.120631
22	6	0	-0.662127	3.712345	-0.138836
23	6	0	0.754417	3.675109	-0.150868
24	6	0	2.857500	2.386003	-0.168932
25	6	0	4.960363	1.102439	-0.186995
26	6	0	4.895577	-1.362240	-0.186853
27	6	0	3.408575	-3.788348	-0.174632
28	6	0	1.241784	-4.964582	-0.156435
29	6	0	-1.602711	-4.889810	-0.132278
30	6	0	-3.704715	-3.601366	-0.114222
31	6	0	-5.062207	-1.100486	-0.102286

32	6	0	-4.997421	1.364192	-0.102427
33	6	0	-3.510419	3.790300	-0.114648
34	6	0	-1.343629	4.966534	-0.132845
35	6	0	1.500866	4.891763	-0.157002
36	6	0	3.602871	3.603318	-0.175058
37	6	0	5.637308	-0.148546	-0.192948
38	6	0	2.663700	-5.000114	-0.168510
39	6	0	-3.024530	-4.850592	-0.120203
40	6	0	-5.739152	0.150499	-0.096332
41	6	0	-2.765545	5.002067	-0.120770
42	6	0	2.922685	4.852544	-0.169077
43	6	0	5.699650	2.314448	-0.193069
44	6	0	5.570169	-2.611415	-0.192786
45	6	0	4.827810	-3.822605	-0.186685
46	6	0	0.497301	-6.173406	-0.150316
47	6	0	-0.922762	-6.136077	-0.138256
48	6	0	-5.123790	-3.561015	-0.102170
49	6	0	-5.801494	-2.312496	-0.096211
50	6	0	-5.672014	2.613367	-0.096495
51	6	0	-4.929654	3.824558	-0.102595
52	6	0	-0.599146	6.175358	-0.138964
53	6	0	0.820917	6.138030	-0.151024
54	6	0	5.021946	3.562967	-0.187110
55	6	0	7.069562	-0.186195	-0.205111
56	6	0	3.347222	-6.259351	-0.174521
57	6	0	-3.773262	-6.072180	-0.114050
58	6	0	-7.171406	0.188147	-0.084169
59	6	0	-3.449066	6.261304	-0.114759
60	6	0	3.671417	6.074133	-0.175231
61	6	0	7.137042	2.267826	-0.205278
62	6	0	7.008026	-2.640372	-0.204995
63	6	0	5.506130	-5.090780	-0.192653
64	6	0	1.191151	-7.433149	-0.156414
65	6	0	-1.681834	-7.357629	-0.132015
66	6	0	-5.867797	-4.791801	-0.096059
67	6	0	-7.238886	-2.265873	-0.084002
68	6	0	-7.109870	2.642324	-0.084285
69	6	0	-5.607974	5.092732	-0.096628

70	6	0	-1.292995	7.435102	-0.132866
71	6	0	1.579990	7.359582	-0.157265
72	6	0	5.765953	4.793754	-0.193221
73	6	0	7.782748	1.037190	-0.210962
74	6	0	7.717492	-1.445358	-0.210819
75	6	0	4.763258	-6.265317	-0.186541
76	6	0	2.580758	-7.450079	-0.168212
77	6	0	-3.070412	-7.301531	-0.120219
78	6	0	-5.187656	-6.003745	-0.102033
79	6	0	-7.884592	-1.035237	-0.078318
80	6	0	-7.819337	1.447311	-0.078461
81	6	0	-4.865103	6.267270	-0.102739
82	6	0	-2.682603	7.452032	-0.121068
83	6	0	2.968568	7.303484	-0.169061
84	6	0	5.085812	6.005697	-0.187248
85	6	0	7.855101	3.519467	-0.211166
86	6	0	7.659339	-3.928008	-0.210737
87	6	0	6.949072	-5.086838	-0.204900
88	6	0	0.401721	-8.641043	-0.149913
89	6	0	-0.956951	-8.605329	-0.138374
90	6	0	-7.308540	-4.712058	-0.083816
91	6	0	-7.956946	-3.517514	-0.078115
92	6	0	-7.761183	3.929961	-0.078543
93	6	0	-7.050917	5.088791	-0.084380
94	6	0	-0.503565	8.642996	-0.139367
95	6	0	0.855107	8.607281	-0.150906
96	6	0	7.206696	4.714011	-0.205464
97	1	0	8.870311	1.007751	-0.220199
98	1	0	8.805100	-1.473096	-0.220056
99	1	0	5.281544	-7.221928	-0.191099
100	1	0	3.100540	-8.405878	-0.172782
101	1	0	-3.639688	-8.228702	-0.115540
102	1	0	-5.755482	-6.931805	-0.097366
103	1	0	-8.972155	-1.005798	-0.069081
104	1	0	-8.906944	1.475049	-0.069224
105	1	0	-5.383389	7.223880	-0.098181
106	1	0	-3.202384	8.407830	-0.116498
107	1	0	3.537844	8.230655	-0.173740

108	1	0	5.653638	6.933758	-0.191914
109	1	0	8.941842	3.485847	-0.220396
110	1	0	8.746345	-3.951528	-0.219968
111	1	0	7.463327	-6.044827	-0.209424
112	1	0	0.924855	-9.594212	-0.154511
113	1	0	-1.529437	-9.529698	-0.133668
114	1	0	-7.872413	-5.641707	-0.079184
115	1	0	-9.043687	-3.483894	-0.068885
116	1	0	-8.848189	3.953481	-0.069313
117	1	0	-7.565171	6.046780	-0.079857
118	1	0	-1.026699	9.596165	-0.134769
119	1	0	1.427593	9.531650	-0.155612
120	1	0	7.770568	5.643660	-0.210096
121	6	0	0.586493	-0.007505	3.325148
122	6	0	1.469818	1.244328	3.342581
123	6	0	1.401513	-1.302975	3.345479
124	1	0	-0.096226	0.014118	4.185923
125	1	0	-0.050533	0.010232	2.432954
126	1	0	0.870773	2.160705	3.291779
127	1	0	2.075806	1.286565	4.256337
128	1	0	2.157033	1.249397	2.489284
129	1	0	0.756202	-2.188402	3.297382
130	1	0	2.005463	-1.374623	4.258969
131	1	0	2.087830	-1.346851	2.492163

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***n*-pentane**

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

7	6	0	-0.229180	-2.779199	0.000000
8	6	0	-0.229180	-1.357949	2.461677
9	6	0	-0.229180	1.484551	2.461677
10	6	0	-0.229180	2.905801	0.000000
11	6	0	-0.229180	1.484551	-2.461677
12	6	0	-0.229180	-1.357949	-2.461677
13	6	0	-0.229180	-3.490091	-1.233398
14	6	0	-0.229180	-3.490091	1.233398
15	6	0	-0.229180	-2.781548	2.460629
16	6	0	-0.229180	-0.645241	3.694026
17	6	0	-0.229180	0.771843	3.694026
18	6	0	-0.229180	2.908151	2.460629
19	6	0	-0.229180	3.616693	1.233398
20	6	0	-0.229180	3.616693	-1.233398
21	6	0	-0.229180	2.908151	-2.460629
22	6	0	-0.229180	0.771843	-3.694026
23	6	0	-0.229180	-0.645241	-3.694026
24	6	0	-0.229180	-2.781548	-2.460629
25	6	0	-0.229180	-4.917490	-1.232765
26	6	0	-0.229180	-4.917490	1.232765
27	6	0	-0.229180	-3.494700	3.697110
28	6	0	-0.229180	-1.359489	4.929875
29	6	0	-0.229180	1.486091	4.929875
30	6	0	-0.229180	3.621303	3.697110
31	6	0	-0.229180	5.044093	1.232765
32	6	0	-0.229180	5.044093	-1.232765
33	6	0	-0.229180	3.621303	-3.697110
34	6	0	-0.229180	1.486091	-4.929875
35	6	0	-0.229180	-1.359489	-4.929875
36	6	0	-0.229180	-3.494700	-3.697110
37	6	0	-0.229180	-5.627099	0.000000
38	6	0	-0.229180	-2.781899	4.928031
39	6	0	-0.229180	2.908501	4.928031
40	6	0	-0.229180	5.753701	0.000000
41	6	0	-0.229180	2.908501	-4.928031
42	6	0	-0.229180	-2.781899	-4.928031
43	6	0	-0.229180	-5.624699	-2.463782
44	6	0	-0.229180	-5.624699	2.463782

45	6	0	-0.229180	-4.914397	3.694062
46	6	0	-0.229180	-0.647001	6.157844
47	6	0	-0.229180	0.773604	6.157844
48	6	0	-0.229180	5.040999	3.694062
49	6	0	-0.229180	5.751302	2.463782
50	6	0	-0.229180	5.751302	-2.463782
51	6	0	-0.229180	5.040999	-3.694062
52	6	0	-0.229180	0.773604	-6.157844
53	6	0	-0.229180	-0.647001	-6.157844
54	6	0	-0.229180	-4.914397	-3.694062
55	6	0	-0.229180	-7.059899	0.000000
56	6	0	-0.229180	-3.498299	6.168872
57	6	0	-0.229180	3.624901	6.168872
58	6	0	-0.229180	7.186501	0.000000
59	6	0	-0.229180	3.624901	-6.168872
60	6	0	-0.229180	-3.498299	-6.168872
61	6	0	-0.229180	-7.062872	-2.454947
62	6	0	-0.229180	-7.062872	2.454947
63	6	0	-0.229180	-5.625832	4.943974
64	6	0	-0.229180	-1.373739	7.398921
65	6	0	-0.229180	1.500342	7.398921
66	6	0	-0.229180	5.752434	4.943974
67	6	0	-0.229180	7.189475	2.454947
68	6	0	-0.229180	7.189475	-2.454947
69	6	0	-0.229180	5.752434	-4.943974
70	6	0	-0.229180	1.500342	-7.398921
71	6	0	-0.229180	-1.373739	-7.398921
72	6	0	-0.229180	-5.625832	-4.943974
73	6	0	-0.229180	-7.740717	-1.241703
74	6	0	-0.229180	-7.740717	1.241703
75	6	0	-0.229180	-4.914054	6.137627
76	6	0	-0.229180	-2.763362	7.379329
77	6	0	-0.229180	2.889964	7.379329
78	6	0	-0.229180	5.040656	6.137627
79	6	0	-0.229180	7.867320	1.241703
80	6	0	-0.229180	7.867320	-1.241703
81	6	0	-0.229180	5.040656	-6.137627
82	6	0	-0.229180	2.889964	-7.379329

83	6	0	-0.229180	-2.763362	-7.379329
84	6	0	-0.229180	-4.914054	-6.137627
85	6	0	-0.229180	-7.747820	-3.725024
86	6	0	-0.229180	-7.747820	3.725024
87	6	0	-0.229180	-7.068224	4.902117
88	6	0	-0.229180	-0.616294	8.627141
89	6	0	-0.229180	0.742896	8.627141
90	6	0	-0.229180	7.194827	4.902117
91	6	0	-0.229180	7.874422	3.725024
92	6	0	-0.229180	7.874422	-3.725024
93	6	0	-0.229180	7.194827	-4.902117
94	6	0	-0.229180	0.742896	-8.627141
95	6	0	-0.229180	-0.616294	-8.627141
96	6	0	-0.229180	-7.068224	-4.902117
97	1	0	-0.229180	-8.828717	-1.240852
98	1	0	-0.229180	-8.828717	1.240852
99	1	0	-0.229180	-5.457317	7.080287
100	1	0	-0.229180	-3.308098	8.321139
101	1	0	-0.229180	3.434701	8.321139
102	1	0	-0.229180	5.583920	7.080287
103	1	0	-0.229180	8.955319	1.240852
104	1	0	-0.229180	8.955319	-1.240852
105	1	0	-0.229180	5.583920	-7.080287
106	1	0	-0.229180	3.434701	-8.321139
107	1	0	-0.229180	-3.308098	-8.321139
108	1	0	-0.229180	-5.457317	-7.080287
109	1	0	-0.229180	-8.835108	-3.719972
110	1	0	-0.229180	-8.835108	3.719972
111	1	0	-0.229180	-7.607494	5.846262
112	1	0	-0.229180	-1.164313	9.566234
113	1	0	-0.229180	1.290915	9.566234
114	1	0	-0.229180	7.734096	5.846262
115	1	0	-0.229180	8.961710	3.719972
116	1	0	-0.229180	8.961710	-3.719972
117	1	0	-0.229180	7.734096	-5.846262
118	1	0	-0.229180	1.290915	-9.566234
119	1	0	-0.229180	-1.164313	-9.566234
120	1	0	-0.229180	-7.607494	-5.846262

121	6	0	3.293168	-0.590422	0.000000
122	6	0	3.267250	-1.430493	-1.281808
123	6	0	3.267250	-1.430493	1.281808
124	6	0	3.272577	-0.577498	-2.553685
125	6	0	3.272577	-0.577498	2.553685
126	1	0	4.188433	0.049806	0.000000
127	1	0	2.432559	0.092776	0.000000
128	1	0	4.130631	-2.111322	-1.288350
129	1	0	2.375926	-2.070360	-1.273646
130	1	0	2.375926	-2.070360	1.273646
131	1	0	4.130631	-2.111322	1.288350
132	1	0	4.186589	0.025802	-2.620275
133	1	0	2.420559	0.110720	-2.567112
134	1	0	3.211251	-1.197277	-3.455605
135	1	0	2.420559	0.110720	2.567112
136	1	0	4.186589	0.025802	2.620275
137	1	0	3.211251	-1.197277	3.455605

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### *n*-heptane

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.309359	-1.324755	0.000000
2	6	0	-0.309359	-0.613155	1.232527
3	6	0	-0.309359	0.810045	1.232527
4	6	0	-0.309359	1.521645	0.000000
5	6	0	-0.309359	0.810045	-1.232527
6	6	0	-0.309359	-0.613155	-1.232527
7	6	0	-0.309359	-2.744055	0.000000
8	6	0	-0.309359	-1.322805	2.461677
9	6	0	-0.309359	1.519695	2.461677
10	6	0	-0.309359	2.940945	0.000000
11	6	0	-0.309359	1.519695	-2.461677
12	6	0	-0.309359	-1.322805	-2.461677
13	6	0	-0.309359	-3.454947	-1.233398



14	6	0	-0.309359	-3.454947	1.233398
15	6	0	-0.309359	-2.746405	2.460629
16	6	0	-0.309359	-0.610097	3.694026
17	6	0	-0.309359	0.806987	3.694026
18	6	0	-0.309359	2.943295	2.460629
19	6	0	-0.309359	3.651837	1.233398
20	6	0	-0.309359	3.651837	-1.233398
21	6	0	-0.309359	2.943295	-2.460629
22	6	0	-0.309359	0.806987	-3.694026
23	6	0	-0.309359	-0.610097	-3.694026
24	6	0	-0.309359	-2.746405	-2.460629
25	6	0	-0.309359	-4.882347	-1.232765
26	6	0	-0.309359	-4.882347	1.232765
27	6	0	-0.309359	-3.459557	3.697110
28	6	0	-0.309359	-1.324345	4.929875
29	6	0	-0.309359	1.521235	4.929875
30	6	0	-0.309359	3.656446	3.697110
31	6	0	-0.309359	5.079237	1.232765
32	6	0	-0.309359	5.079237	-1.232765
33	6	0	-0.309359	3.656446	-3.697110
34	6	0	-0.309359	1.521235	-4.929875
35	6	0	-0.309359	-1.324345	-4.929875
36	6	0	-0.309359	-3.459557	-3.697110
37	6	0	-0.309359	-5.591955	0.000000
38	6	0	-0.309359	-2.746755	4.928031
39	6	0	-0.309359	2.943645	4.928031
40	6	0	-0.309359	5.788845	0.000000
41	6	0	-0.309359	2.943645	-4.928031
42	6	0	-0.309359	-2.746755	-4.928031
43	6	0	-0.309359	-5.589556	-2.463782
44	6	0	-0.309359	-5.589556	2.463782
45	6	0	-0.309359	-4.879253	3.694062
46	6	0	-0.309359	-0.611857	6.157844
47	6	0	-0.309359	0.808747	6.157844
48	6	0	-0.309359	5.076143	3.694062
49	6	0	-0.309359	5.786445	2.463782
50	6	0	-0.309359	5.786445	-2.463782
51	6	0	-0.309359	5.076143	-3.694062

52	6	0	-0.309359	0.808747	-6.157844
53	6	0	-0.309359	-0.611857	-6.157844
54	6	0	-0.309359	-4.879253	-3.694062
55	6	0	-0.309359	-7.024755	0.000000
56	6	0	-0.309359	-3.463155	6.168872
57	6	0	-0.309359	3.660045	6.168872
58	6	0	-0.309359	7.221645	0.000000
59	6	0	-0.309359	3.660045	-6.168872
60	6	0	-0.309359	-3.463155	-6.168872
61	6	0	-0.309359	-7.027729	-2.454947
62	6	0	-0.309359	-7.027729	2.454947
63	6	0	-0.309359	-5.590688	4.943974
64	6	0	-0.309359	-1.338596	7.398921
65	6	0	-0.309359	1.535485	7.398921
66	6	0	-0.309359	5.787578	4.943974
67	6	0	-0.309359	7.224618	2.454947
68	6	0	-0.309359	7.224618	-2.454947
69	6	0	-0.309359	5.787578	-4.943974
70	6	0	-0.309359	1.535485	-7.398921
71	6	0	-0.309359	-1.338596	-7.398921
72	6	0	-0.309359	-5.590688	-4.943974
73	6	0	-0.309359	-7.705573	-1.241703
74	6	0	-0.309359	-7.705573	1.241703
75	6	0	-0.309359	-4.878910	6.137627
76	6	0	-0.309359	-2.728218	7.379329
77	6	0	-0.309359	2.925108	7.379329
78	6	0	-0.309359	5.075800	6.137627
79	6	0	-0.309359	7.902463	1.241703
80	6	0	-0.309359	7.902463	-1.241703
81	6	0	-0.309359	5.075800	-6.137627
82	6	0	-0.309359	2.925108	-7.379329
83	6	0	-0.309359	-2.728218	-7.379329
84	6	0	-0.309359	-4.878910	-6.137627
85	6	0	-0.309359	-7.712676	-3.725024
86	6	0	-0.309359	-7.712676	3.725024
87	6	0	-0.309359	-7.033081	4.902117
88	6	0	-0.309359	-0.581150	8.627141
89	6	0	-0.309359	0.778040	8.627141

90	6	0	-0.309359	7.229971	4.902117
91	6	0	-0.309359	7.909566	3.725024
92	6	0	-0.309359	7.909566	-3.725024
93	6	0	-0.309359	7.229971	-4.902117
94	6	0	-0.309359	0.778040	-8.627141
95	6	0	-0.309359	-0.581150	-8.627141
96	6	0	-0.309359	-7.033081	-4.902117
97	1	0	-0.309359	-8.793573	-1.240852
98	1	0	-0.309359	-8.793573	1.240852
99	1	0	-0.309359	-5.422173	7.080287
100	1	0	-0.309359	-3.272955	8.321139
101	1	0	-0.309359	3.469845	8.321139
102	1	0	-0.309359	5.619063	7.080287
103	1	0	-0.309359	8.990463	1.240852
104	1	0	-0.309359	8.990463	-1.240852
105	1	0	-0.309359	5.619063	-7.080287
106	1	0	-0.309359	3.469845	-8.321139
107	1	0	-0.309359	-3.272955	-8.321139
108	1	0	-0.309359	-5.422173	-7.080287
109	1	0	-0.309359	-8.799964	-3.719972
110	1	0	-0.309359	-8.799964	3.719972
111	1	0	-0.309359	-7.572350	5.846262
112	1	0	-0.309359	-1.129169	9.566234
113	1	0	-0.309359	1.326059	9.566234
114	1	0	-0.309359	7.769240	5.846262
115	1	0	-0.309359	8.996854	3.719972
116	1	0	-0.309359	8.996854	-3.719972
117	1	0	-0.309359	7.769240	-5.846262
118	1	0	-0.309359	1.326059	-9.566234
119	1	0	-0.309359	-1.129169	-9.566234
120	1	0	-0.309359	-7.572350	-5.846262
121	6	0	3.212599	-0.518682	0.000000
122	6	0	3.219501	-1.360872	-1.280009
123	6	0	3.219501	-1.360872	1.280009
124	6	0	3.188457	-0.521842	-2.562227
125	6	0	3.188457	-0.521842	2.562227
126	6	0	3.189515	-1.375921	-3.833276
127	6	0	3.189515	-1.375921	3.833276

128	1	0	4.083586	0.153774	0.000000
129	1	0	2.327827	0.132142	0.000000
130	1	0	4.110193	-2.007200	-1.287756
131	1	0	2.354175	-2.037818	-1.272272
132	1	0	2.354175	-2.037818	1.272272
133	1	0	4.110193	-2.007200	1.287756
134	1	0	4.051541	0.159283	-2.572651
135	1	0	2.297064	0.117773	-2.550964
136	1	0	2.297064	0.117773	2.550964
137	1	0	4.051541	0.159283	2.572651
138	1	0	3.120630	-0.757327	-4.735469
139	1	0	2.340304	-2.067516	-3.841339
140	1	0	4.105543	-1.975769	-3.904180
141	1	0	3.120630	-0.757327	4.735469
142	1	0	4.105543	-1.975769	3.904180
143	1	0	2.340304	-2.067516	3.841339

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## fluoropropane

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.249190	0.090046	-0.575735
2	6	0	0.627841	-1.190141	-0.552360
3	6	0	-0.790951	-1.291757	-0.505441
4	6	0	-1.588394	-0.113187	-0.481897
5	6	0	-0.967046	1.167000	-0.505272
6	6	0	0.451746	1.268616	-0.552191
7	6	0	2.664094	0.191384	-0.622526
8	6	0	1.423100	-2.365481	-0.575839
9	6	0	-1.410597	-2.568436	-0.482129
10	6	0	-3.003298	-0.214525	-0.435106
11	6	0	-1.762304	2.342340	-0.481792
12	6	0	1.071392	2.545295	-0.575502
13	6	0	3.284674	1.472388	-0.645877
14	6	0	3.460894	-0.988105	-0.646046

15	6	0	2.842215	-2.262791	-0.622772
16	6	0	0.800634	-3.645569	-0.552427
17	6	0	-0.612061	-3.746749	-0.505710
18	6	0	-2.829862	-2.669035	-0.435197
19	6	0	-3.623879	-1.495529	-0.411754
20	6	0	-3.800098	0.964964	-0.411585
21	6	0	-3.181420	2.239649	-0.434860
22	6	0	-1.139838	3.622428	-0.505204
23	6	0	0.272857	3.723608	-0.551922
24	6	0	2.490658	2.645894	-0.622435
25	6	0	4.707698	1.573673	-0.692935
26	6	0	4.883827	-0.885558	-0.693104
27	6	0	3.641488	-3.445194	-0.646367
28	6	0	1.600954	-4.827263	-0.576059
29	6	0	-1.235812	-5.030437	-0.482248
30	6	0	-3.452475	-3.953276	-0.411771
31	6	0	-5.046903	-1.596814	-0.364696
32	6	0	-5.223032	0.862416	-0.364527
33	6	0	-3.980693	3.422052	-0.411264
34	6	0	-1.940159	4.804122	-0.481572
35	6	0	0.896608	5.007296	-0.575384
36	6	0	3.113271	3.930135	-0.645861
37	6	0	5.503174	0.394724	-0.716414
38	6	0	3.018827	-4.723864	-0.622952
39	6	0	-2.653949	-5.130158	-0.435354
40	6	0	-5.842378	-0.417865	-0.341218
41	6	0	-3.358032	4.700723	-0.434679
42	6	0	2.314744	5.107017	-0.622277
43	6	0	5.324777	2.852040	-0.716166
44	6	0	5.676786	-2.062935	-0.716503
45	6	0	5.056570	-3.340787	-0.693171
46	6	0	0.978395	-6.102967	-0.552654
47	6	0	-0.437809	-6.204398	-0.505821
48	6	0	-4.867993	-4.051602	-0.364967
49	6	0	-5.663982	-2.875181	-0.341466
50	6	0	-6.015990	2.039794	-0.341128
51	6	0	-5.395775	3.317646	-0.364461
52	6	0	-1.317600	6.079825	-0.504977

53	6	0	0.098605	6.181257	-0.551811
54	6	0	4.528788	4.028461	-0.692665
55	6	0	6.931536	0.497026	-0.763649
56	6	0	3.821650	-5.910384	-0.646655
57	6	0	-3.279488	-6.418980	-0.411821
58	6	0	-7.270740	-0.520167	-0.293982
59	6	0	-4.160854	5.887243	-0.410977
60	6	0	2.940284	6.395839	-0.645810
61	6	0	6.759127	2.945912	-0.763579
62	6	0	7.109873	-1.951437	-0.763915
63	6	0	5.855091	-4.536710	-0.716710
64	6	0	1.791541	-7.288983	-0.576698
65	6	0	-1.073639	-7.494193	-0.481947
66	6	0	-5.487934	-5.349117	-0.341598
67	6	0	-7.098332	-2.969054	-0.294052
68	6	0	-7.449077	1.928295	-0.293716
69	6	0	-6.194295	4.513568	-0.340921
70	6	0	-2.130745	7.265842	-0.480934
71	6	0	0.734434	7.471051	-0.575685
72	6	0	5.148730	5.325976	-0.716033
73	6	0	7.521543	1.784166	-0.786009
74	6	0	7.698948	-0.692894	-0.786179
75	6	0	5.230788	-5.778134	-0.693327
76	6	0	3.175460	-7.170223	-0.622509
77	6	0	-2.460357	-7.573871	-0.436133
78	6	0	-4.693091	-6.488900	-0.365145
79	6	0	-7.860747	-1.807308	-0.271622
80	6	0	-8.038153	0.669753	-0.271452
81	6	0	-5.569992	5.754992	-0.364305
82	6	0	-3.514664	7.147082	-0.435123
83	6	0	2.121152	7.550729	-0.621498
84	6	0	4.353886	6.465758	-0.692486
85	6	0	7.351223	4.261650	-0.786073
86	6	0	7.883429	-3.169364	-0.786583
87	6	0	7.290026	-4.391973	-0.764259
88	6	0	1.124181	-8.568147	-0.551811
89	6	0	-0.230799	-8.665194	-0.507002
90	6	0	-6.928850	-5.410354	-0.294043

91	6	0	-7.690428	-4.284791	-0.271558
92	6	0	-8.222633	3.146223	-0.271048
93	6	0	-7.629230	4.368832	-0.293372
94	6	0	-1.463386	8.545006	-0.505821
95	6	0	-0.108405	8.642052	-0.550630
96	6	0	6.589645	5.387213	-0.763588
97	1	0	8.606233	1.861001	-0.821878
98	1	0	8.783518	-0.614363	-0.822048
99	1	0	5.839709	-6.679597	-0.711301
100	1	0	3.785789	-8.070733	-0.640532
101	1	0	-2.936126	-8.552169	-0.418239
102	1	0	-5.167331	-7.467941	-0.347300
103	1	0	-8.945438	-1.884142	-0.235754
104	1	0	-9.122722	0.591221	-0.235584
105	1	0	-6.178913	6.656456	-0.346330
106	1	0	-4.124993	8.047592	-0.417100
107	1	0	2.596922	8.529027	-0.639392
108	1	0	4.828126	7.444800	-0.710332
109	1	0	8.435505	4.334244	-0.821919
110	1	0	8.966989	-3.086693	-0.822428
111	1	0	7.895072	-5.295202	-0.782102
112	1	0	1.737588	-9.465713	-0.569942
113	1	0	-0.710035	-9.641016	-0.488999
114	1	0	-7.399002	-6.390591	-0.276330
115	1	0	-8.774709	-4.357385	-0.235713
116	1	0	-9.306193	3.063551	-0.235203
117	1	0	-8.234276	5.272061	-0.275529
118	1	0	-2.076793	9.442572	-0.487689
119	1	0	0.370831	9.617875	-0.568632
120	1	0	7.059798	6.367450	-0.781302
121	6	0	0.533644	0.031648	3.522725
122	6	0	1.264297	1.394964	3.528235
123	6	0	1.462647	-1.205174	3.516672
124	9	0	-0.240531	-0.032484	4.631396
125	9	0	-0.251001	-0.023187	2.425502
126	9	0	0.358903	2.379870	3.497994
127	9	0	2.004236	1.513842	4.640046
128	9	0	2.063292	1.504230	2.460816

129	9	0	0.717480	-2.315283	3.463750
130	9	0	2.203338	-1.227435	4.634007
131	9	0	2.277369	-1.175800	2.455783

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***n*-fluoropentane**

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.770669	-1.242914	0.000000
2	6	0	-0.770669	-0.531314	1.232527
3	6	0	-0.770669	0.891886	1.232527
4	6	0	-0.770669	1.603486	0.000000
5	6	0	-0.770669	0.891886	-1.232527
6	6	0	-0.770669	-0.531314	-1.232527
7	6	0	-0.770669	-2.662214	0.000000
8	6	0	-0.770669	-1.240964	2.461677
9	6	0	-0.770669	1.601536	2.461677
10	6	0	-0.770669	3.022786	0.000000
11	6	0	-0.770669	1.601536	-2.461677
12	6	0	-0.770669	-1.240964	-2.461677
13	6	0	-0.770669	-3.373106	-1.233398
14	6	0	-0.770669	-3.373106	1.233398
15	6	0	-0.770669	-2.664564	2.460629
16	6	0	-0.770669	-0.528256	3.694026
17	6	0	-0.770669	0.888828	3.694026
18	6	0	-0.770669	3.025136	2.460629
19	6	0	-0.770669	3.733678	1.233398
20	6	0	-0.770669	3.733678	-1.233398
21	6	0	-0.770669	3.025136	-2.460629
22	6	0	-0.770669	0.888828	-3.694026
23	6	0	-0.770669	-0.528256	-3.694026
24	6	0	-0.770669	-2.664564	-2.460629
25	6	0	-0.770669	-4.800506	-1.232765
26	6	0	-0.770669	-4.800506	1.232765
27	6	0	-0.770669	-3.377716	3.697110



28	6	0	-0.770669	-1.242504	4.929875
29	6	0	-0.770669	1.603076	4.929875
30	6	0	-0.770669	3.738288	3.697110
31	6	0	-0.770669	5.161078	1.232765
32	6	0	-0.770669	5.161078	-1.232765
33	6	0	-0.770669	3.738288	-3.697110
34	6	0	-0.770669	1.603076	-4.929875
35	6	0	-0.770669	-1.242504	-4.929875
36	6	0	-0.770669	-3.377716	-3.697110
37	6	0	-0.770669	-5.510114	0.000000
38	6	0	-0.770669	-2.664914	4.928031
39	6	0	-0.770669	3.025486	4.928031
40	6	0	-0.770669	5.870686	0.000000
41	6	0	-0.770669	3.025486	-4.928031
42	6	0	-0.770669	-2.664914	-4.928031
43	6	0	-0.770669	-5.507715	-2.463782
44	6	0	-0.770669	-5.507715	2.463782
45	6	0	-0.770669	-4.797412	3.694062
46	6	0	-0.770669	-0.530016	6.157844
47	6	0	-0.770669	0.890588	6.157844
48	6	0	-0.770669	5.157984	3.694062
49	6	0	-0.770669	5.868287	2.463782
50	6	0	-0.770669	5.868287	-2.463782
51	6	0	-0.770669	5.157984	-3.694062
52	6	0	-0.770669	0.890588	-6.157844
53	6	0	-0.770669	-0.530016	-6.157844
54	6	0	-0.770669	-4.797412	-3.694062
55	6	0	-0.770669	-6.942914	0.000000
56	6	0	-0.770669	-3.381314	6.168872
57	6	0	-0.770669	3.741886	6.168872
58	6	0	-0.770669	7.303486	0.000000
59	6	0	-0.770669	3.741886	-6.168872
60	6	0	-0.770669	-3.381314	-6.168872
61	6	0	-0.770669	-6.945887	-2.454947
62	6	0	-0.770669	-6.945887	2.454947
63	6	0	-0.770669	-5.508847	4.943974
64	6	0	-0.770669	-1.256755	7.398921
65	6	0	-0.770669	1.617327	7.398921

66	6	0	-0.770669	5.869419	4.943974
67	6	0	-0.770669	7.306459	2.454947
68	6	0	-0.770669	7.306459	-2.454947
69	6	0	-0.770669	5.869419	-4.943974
70	6	0	-0.770669	1.617327	-7.398921
71	6	0	-0.770669	-1.256755	-7.398921
72	6	0	-0.770669	-5.508847	-4.943974
73	6	0	-0.770669	-7.623732	-1.241703
74	6	0	-0.770669	-7.623732	1.241703
75	6	0	-0.770669	-4.797069	6.137627
76	6	0	-0.770669	-2.646377	7.379329
77	6	0	-0.770669	3.006949	7.379329
78	6	0	-0.770669	5.157641	6.137627
79	6	0	-0.770669	7.984304	1.241703
80	6	0	-0.770669	7.984304	-1.241703
81	6	0	-0.770669	5.157641	-6.137627
82	6	0	-0.770669	3.006949	-7.379329
83	6	0	-0.770669	-2.646377	-7.379329
84	6	0	-0.770669	-4.797069	-6.137627
85	6	0	-0.770669	-7.630835	-3.725024
86	6	0	-0.770669	-7.630835	3.725024
87	6	0	-0.770669	-6.951240	4.902117
88	6	0	-0.770669	-0.499309	8.627141
89	6	0	-0.770669	0.859881	8.627141
90	6	0	-0.770669	7.311812	4.902117
91	6	0	-0.770669	7.991407	3.725024
92	6	0	-0.770669	7.991407	-3.725024
93	6	0	-0.770669	7.311812	-4.902117
94	6	0	-0.770669	0.859881	-8.627141
95	6	0	-0.770669	-0.499309	-8.627141
96	6	0	-0.770669	-6.951240	-4.902117
97	1	0	-0.770669	-8.711732	-1.240852
98	1	0	-0.770669	-8.711732	1.240852
99	1	0	-0.770669	-5.340332	7.080287
100	1	0	-0.770669	-3.191114	8.321139
101	1	0	-0.770669	3.551686	8.321139
102	1	0	-0.770669	5.700904	7.080287
103	1	0	-0.770669	9.072304	1.240852

104	1	0	-0.770669	9.072304	-1.240852
105	1	0	-0.770669	5.700904	-7.080287
106	1	0	-0.770669	3.551686	-8.321139
107	1	0	-0.770669	-3.191114	-8.321139
108	1	0	-0.770669	-5.340332	-7.080287
109	1	0	-0.770669	-8.718123	-3.719972
110	1	0	-0.770669	-8.718123	3.719972
111	1	0	-0.770669	-7.490509	5.846262
112	1	0	-0.770669	-1.047328	9.566234
113	1	0	-0.770669	1.407900	9.566234
114	1	0	-0.770669	7.851081	5.846262
115	1	0	-0.770669	9.078695	3.719972
116	1	0	-0.770669	9.078695	-3.719972
117	1	0	-0.770669	7.851081	-5.846262
118	1	0	-0.770669	1.407900	-9.566234
119	1	0	-0.770669	-1.047328	-9.566234
120	1	0	-0.770669	-7.490509	-5.846262
121	6	0	3.348612	-0.483286	0.000000
122	6	0	3.343223	-1.324657	-1.305291
123	6	0	3.343223	-1.324657	1.305291
124	6	0	3.351697	-0.481825	-2.609672
125	6	0	3.351697	-0.481825	2.609672
126	9	0	4.459256	0.294257	0.000000
127	9	0	2.252469	0.309317	0.000000
128	9	0	4.444104	-2.112319	-1.325021
129	9	0	2.237836	-2.100357	-1.323656
130	9	0	2.237836	-2.100357	1.323656
131	9	0	4.444104	-2.112319	1.325021
132	9	0	4.484991	0.227107	-2.696649
133	9	0	2.308920	0.353791	-2.645558
134	9	0	3.277768	-1.314124	-3.656014
135	9	0	2.308920	0.353791	2.645558
136	9	0	4.484991	0.227107	2.696649
137	9	0	3.277768	-1.314124	3.656014

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## *n*-fluoroheptane

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.978453	-1.162488	0.000000
2	6	0	-0.978454	-0.450863	1.232560
3	6	0	-0.978425	0.972414	1.232666
4	6	0	-0.978477	1.683955	0.000000
5	6	0	-0.978425	0.972414	-1.232666
6	6	0	-0.978454	-0.450863	-1.232560
7	6	0	-0.978438	-2.581750	0.000000
8	6	0	-0.978445	-1.160506	2.461674
9	6	0	-0.978424	1.681975	2.461692
10	6	0	-0.978460	3.103250	0.000000
11	6	0	-0.978424	1.681975	-2.461692
12	6	0	-0.978445	-1.160506	-2.461674
13	6	0	-0.978443	-3.292642	-1.233398
14	6	0	-0.978443	-3.292642	1.233398
15	6	0	-0.978439	-2.584099	2.460629
16	6	0	-0.978447	-0.447792	3.694026
17	6	0	-0.978442	0.969292	3.694026
18	6	0	-0.978441	3.105600	2.460629
19	6	0	-0.978442	3.814142	1.233398
20	6	0	-0.978442	3.814142	-1.233398
21	6	0	-0.978441	3.105600	-2.460629
22	6	0	-0.978442	0.969292	-3.694026
23	6	0	-0.978447	-0.447792	-3.694026
24	6	0	-0.978439	-2.584099	-2.460629
25	6	0	-0.978443	-4.720041	-1.232765
26	6	0	-0.978443	-4.720041	1.232765
27	6	0	-0.978443	-3.297251	3.697110
28	6	0	-0.978443	-1.162040	4.929875
29	6	0	-0.978443	1.683540	4.929875
30	6	0	-0.978443	3.818752	3.697110
31	6	0	-0.978443	5.241542	1.232765
32	6	0	-0.978443	5.241542	-1.232765
33	6	0	-0.978443	3.818752	-3.697110

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34	6	0	-0.978443	1.683540	-4.929875
35	6	0	-0.978443	-1.162040	-4.929875
36	6	0	-0.978443	-3.297251	-3.697110
37	6	0	-0.978443	-5.429650	0.000000
38	6	0	-0.978443	-2.584450	4.928031
39	6	0	-0.978443	3.105950	4.928031
40	6	0	-0.978443	5.951150	0.000000
41	6	0	-0.978443	3.105950	-4.928031
42	6	0	-0.978443	-2.584450	-4.928031
43	6	0	-0.978443	-5.427250	-2.463782
44	6	0	-0.978443	-5.427250	2.463782
45	6	0	-0.978443	-4.716948	3.694062
46	6	0	-0.978443	-0.449552	6.157844
47	6	0	-0.978443	0.971053	6.157844
48	6	0	-0.978443	5.238448	3.694062
49	6	0	-0.978443	5.948751	2.463782
50	6	0	-0.978443	5.948751	-2.463782
51	6	0	-0.978443	5.238448	-3.694062
52	6	0	-0.978443	0.971053	-6.157844
53	6	0	-0.978443	-0.449552	-6.157844
54	6	0	-0.978443	-4.716948	-3.694062
55	6	0	-0.978443	-6.862450	0.000000
56	6	0	-0.978443	-3.300850	6.168872
57	6	0	-0.978443	3.822350	6.168872
58	6	0	-0.978443	7.383950	0.000000
59	6	0	-0.978443	3.822350	-6.168872
60	6	0	-0.978443	-3.300850	-6.168872
61	6	0	-0.978443	-6.865423	-2.454947
62	6	0	-0.978443	-6.865423	2.454947
63	6	0	-0.978443	-5.428383	4.943974
64	6	0	-0.978443	-1.176290	7.398921
65	6	0	-0.978443	1.697791	7.398921
66	6	0	-0.978443	5.949883	4.943974
67	6	0	-0.978443	7.386924	2.454947
68	6	0	-0.978443	7.386924	-2.454947
69	6	0	-0.978443	5.949883	-4.943974
70	6	0	-0.978443	1.697791	-7.398921
71	6	0	-0.978443	-1.176290	-7.398921

72	6	0	-0.978443	-5.428383	-4.943974
73	6	0	-0.978443	-7.543268	-1.241703
74	6	0	-0.978443	-7.543268	1.241703
75	6	0	-0.978443	-4.716605	6.137627
76	6	0	-0.978443	-2.565913	7.379329
77	6	0	-0.978443	3.087413	7.379329
78	6	0	-0.978443	5.238105	6.137627
79	6	0	-0.978443	8.064769	1.241703
80	6	0	-0.978443	8.064769	-1.241703
81	6	0	-0.978443	5.238105	-6.137627
82	6	0	-0.978443	3.087413	-7.379329
83	6	0	-0.978443	-2.565913	-7.379329
84	6	0	-0.978443	-4.716605	-6.137627
85	6	0	-0.978443	-7.550371	-3.725024
86	6	0	-0.978443	-7.550371	3.725024
87	6	0	-0.978443	-6.870775	4.902117
88	6	0	-0.978443	-0.418845	8.627141
89	6	0	-0.978443	0.940345	8.627141
90	6	0	-0.978443	7.392276	4.902117
91	6	0	-0.978443	8.071871	3.725024
92	6	0	-0.978443	8.071871	-3.725024
93	6	0	-0.978443	7.392276	-4.902117
94	6	0	-0.978443	0.940345	-8.627141
95	6	0	-0.978443	-0.418845	-8.627141
96	6	0	-0.978443	-6.870775	-4.902117
97	1	0	-0.978443	-8.631268	-1.240852
98	1	0	-0.978443	-8.631268	1.240852
99	1	0	-0.978443	-5.259868	7.080287
100	1	0	-0.978443	-3.110649	8.321139
101	1	0	-0.978443	3.632150	8.321139
102	1	0	-0.978443	5.781369	7.080287
103	1	0	-0.978443	9.152768	1.240852
104	1	0	-0.978443	9.152768	-1.240852
105	1	0	-0.978443	5.781369	-7.080287
106	1	0	-0.978443	3.632150	-8.321139
107	1	0	-0.978443	-3.110649	-8.321139
108	1	0	-0.978443	-5.259868	-7.080287
109	1	0	-0.978443	-8.637659	-3.719972

110	1	0	-0.978443	-8.637659	3.719972
111	1	0	-0.978443	-7.410045	5.846262
112	1	0	-0.978443	-0.966864	9.566234
113	1	0	-0.978443	1.488364	9.566234
114	1	0	-0.978443	7.931545	5.846262
115	1	0	-0.978443	9.159159	3.719972
116	1	0	-0.978443	9.159159	-3.719972
117	1	0	-0.978443	7.931545	-5.846262
118	1	0	-0.978443	1.488364	-9.566234
119	1	0	-0.978443	-0.966864	-9.566234
120	1	0	-0.978443	-7.410045	-5.846262
121	6	0	3.207542	-0.332190	0.000000
122	6	0	3.146855	-1.179511	-1.307621
123	6	0	3.146855	-1.179511	1.307621
124	6	0	3.126575	-0.329969	-2.609996
125	6	0	3.126575	-0.329969	2.609996
126	6	0	3.160989	-1.169836	-3.916731
127	6	0	3.160989	-1.169836	3.916731
128	9	0	4.370789	0.359085	0.000000
129	9	0	2.169168	0.534478	0.000000
130	9	0	4.234934	-1.986708	-1.342107
131	9	0	2.029560	-1.939033	-1.290685
132	9	0	2.029560	-1.939033	1.290685
133	9	0	4.234934	-1.986708	1.342107
134	9	0	4.203910	0.489505	-2.626619
135	9	0	1.999476	0.412854	-2.630537
136	9	0	1.999476	0.412854	2.630537
137	9	0	4.203910	0.489505	2.626619
138	9	0	3.014135	-0.342605	-4.959293
139	9	0	2.170493	-2.068320	-3.932796
140	9	0	4.333485	-1.807211	-4.029689
141	9	0	3.014135	-0.342605	4.959293
142	9	0	4.333485	-1.807211	4.029689
143	9	0	2.170493	-2.068320	3.932796

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XYZ coordinates of molecules at an initial position for horizontal displacement on  $C_{96}H_{24}$

**propane**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.423200	0.000000	1.000000
2	6	0	0.711600	1.232527	1.000000
3	6	0	-0.711600	1.232527	1.000000
4	6	0	-1.423200	0.000000	1.000000
5	6	0	-0.711600	-1.232527	1.000000
6	6	0	0.711600	-1.232527	1.000000
7	6	0	2.842500	0.000000	1.000000
8	6	0	1.421250	2.461677	1.000000
9	6	0	-1.421250	2.461677	1.000000
10	6	0	-2.842500	0.000000	1.000000
11	6	0	-1.421250	-2.461677	1.000000
12	6	0	1.421250	-2.461677	1.000000
13	6	0	3.553392	-1.233398	1.000000
14	6	0	3.553392	1.233398	1.000000
15	6	0	2.844850	2.460629	1.000000
16	6	0	0.708542	3.694026	1.000000
17	6	0	-0.708542	3.694026	1.000000
18	6	0	-2.844850	2.460629	1.000000
19	6	0	-3.553392	1.233398	1.000000
20	6	0	-3.553392	-1.233398	1.000000
21	6	0	-2.844850	-2.460629	1.000000
22	6	0	-0.708542	-3.694026	1.000000
23	6	0	0.708542	-3.694026	1.000000
24	6	0	2.844850	-2.460629	1.000000
25	6	0	4.980792	-1.232765	1.000000
26	6	0	4.980792	1.232765	1.000000
27	6	0	3.558002	3.697110	1.000000
28	6	0	1.422790	4.929875	1.000000
29	6	0	-1.422790	4.929875	1.000000
30	6	0	-3.558002	3.697110	1.000000



31	6	0	-4.980792	1.232765	1.000000
32	6	0	-4.980792	-1.232765	1.000000
33	6	0	-3.558002	-3.697110	1.000000
34	6	0	-1.422790	-4.929875	1.000000
35	6	0	1.422790	-4.929875	1.000000
36	6	0	3.558002	-3.697110	1.000000
37	6	0	5.690400	0.000000	1.000000
38	6	0	2.845200	4.928031	1.000000
39	6	0	-2.845200	4.928031	1.000000
40	6	0	-5.690400	0.000000	1.000000
41	6	0	-2.845200	-4.928031	1.000000
42	6	0	2.845200	-4.928031	1.000000
43	6	0	5.688001	-2.463782	1.000000
44	6	0	5.688001	2.463782	1.000000
45	6	0	4.977698	3.694062	1.000000
46	6	0	0.710302	6.157844	1.000000
47	6	0	-0.710302	6.157844	1.000000
48	6	0	-4.977698	3.694062	1.000000
49	6	0	-5.688001	2.463782	1.000000
50	6	0	-5.688001	-2.463782	1.000000
51	6	0	-4.977698	-3.694062	1.000000
52	6	0	-0.710302	-6.157844	1.000000
53	6	0	0.710302	-6.157844	1.000000
54	6	0	4.977698	-3.694062	1.000000
55	6	0	7.123200	0.000000	1.000000
56	6	0	3.561600	6.168872	1.000000
57	6	0	-3.561600	6.168872	1.000000
58	6	0	-7.123200	0.000000	1.000000
59	6	0	-3.561600	-6.168872	1.000000
60	6	0	3.561600	-6.168872	1.000000
61	6	0	7.126173	-2.454947	1.000000
62	6	0	7.126173	2.454947	1.000000
63	6	0	5.689133	4.943974	1.000000
64	6	0	1.437041	7.398921	1.000000
65	6	0	-1.437041	7.398921	1.000000
66	6	0	-5.689133	4.943974	1.000000
67	6	0	-7.126173	2.454947	1.000000
68	6	0	-7.126173	-2.454947	1.000000

69	6	0	-5.689133	-4.943974	1.000000
70	6	0	-1.437041	-7.398921	1.000000
71	6	0	1.437041	-7.398921	1.000000
72	6	0	5.689133	-4.943974	1.000000
73	6	0	7.804018	-1.241703	1.000000
74	6	0	7.804018	1.241703	1.000000
75	6	0	4.977355	6.137627	1.000000
76	6	0	2.826663	7.379329	1.000000
77	6	0	-2.826663	7.379329	1.000000
78	6	0	-4.977355	6.137627	1.000000
79	6	0	-7.804018	1.241703	1.000000
80	6	0	-7.804018	-1.241703	1.000000
81	6	0	-4.977355	-6.137627	1.000000
82	6	0	-2.826663	-7.379329	1.000000
83	6	0	2.826663	-7.379329	1.000000
84	6	0	4.977355	-6.137627	1.000000
85	6	0	7.811121	-3.725024	1.000000
86	6	0	7.811121	3.725024	1.000000
87	6	0	7.131526	4.902117	1.000000
88	6	0	0.679595	8.627141	1.000000
89	6	0	-0.679595	8.627141	1.000000
90	6	0	-7.131526	4.902117	1.000000
91	6	0	-7.811121	3.725024	1.000000
92	6	0	-7.811121	-3.725024	1.000000
93	6	0	-7.131526	-4.902117	1.000000
94	6	0	-0.679595	-8.627141	1.000000
95	6	0	0.679595	-8.627141	1.000000
96	6	0	7.131526	-4.902117	1.000000
97	1	0	8.892018	-1.240852	1.000000
98	1	0	8.892018	1.240852	1.000000
99	1	0	5.520618	7.080287	1.000000
100	1	0	3.371400	8.321139	1.000000
101	1	0	-3.371400	8.321139	1.000000
102	1	0	-5.520618	7.080287	1.000000
103	1	0	-8.892018	1.240852	1.000000
104	1	0	-8.892018	-1.240852	1.000000
105	1	0	-5.520618	-7.080287	1.000000
106	1	0	-3.371400	-8.321139	1.000000

107	1	0	3.371400	-8.321139	1.000000
108	1	0	5.520618	-7.080287	1.000000
109	1	0	8.898409	-3.719972	1.000000
110	1	0	8.898409	3.719972	1.000000
111	1	0	7.670795	5.846262	1.000000
112	1	0	1.227614	9.566234	1.000000
113	1	0	-1.227614	9.566234	1.000000
114	1	0	-7.670795	5.846262	1.000000
115	1	0	-8.898409	3.719972	1.000000
116	1	0	-8.898409	-3.719972	1.000000
117	1	0	-7.670795	-5.846262	1.000000
118	1	0	-1.227614	-9.566234	1.000000
119	1	0	1.227614	-9.566234	1.000000
120	1	0	7.670795	-5.846262	1.000000
121	6	0	0.645200	0.000000	-2.490000
122	6	0	1.495030	-1.275162	-2.490000
123	6	0	1.495030	1.275162	-2.490000
124	1	0	-0.014533	0.000000	-3.368325
125	1	0	-0.014533	0.000000	-1.611675
126	1	0	0.870970	-2.176386	-2.490000
127	1	0	2.142732	-1.316125	-3.374800
128	1	0	2.142732	-1.316125	-1.605200
129	1	0	0.870970	2.176386	-2.490000
130	1	0	2.143359	1.245732	-3.374800
131	1	0	2.143359	1.245732	-1.605200

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***n*-pentane**

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.423200	0.000000	1.000000
2	6	0	0.711600	1.232527	1.000000
3	6	0	-0.711600	1.232527	1.000000
4	6	0	-1.423200	0.000000	1.000000
5	6	0	-0.711600	-1.232527	1.000000

6	6	0	0.711600	-1.232527	1.000000
7	6	0	2.842500	0.000000	1.000000
8	6	0	1.421250	2.461677	1.000000
9	6	0	-1.421250	2.461677	1.000000
10	6	0	-2.842500	0.000000	1.000000
11	6	0	-1.421250	-2.461677	1.000000
12	6	0	1.421250	-2.461677	1.000000
13	6	0	3.553392	-1.233398	1.000000
14	6	0	3.553392	1.233398	1.000000
15	6	0	2.844850	2.460629	1.000000
16	6	0	0.708542	3.694026	1.000000
17	6	0	-0.708542	3.694026	1.000000
18	6	0	-2.844850	2.460629	1.000000
19	6	0	-3.553392	1.233398	1.000000
20	6	0	-3.553392	-1.233398	1.000000
21	6	0	-2.844850	-2.460629	1.000000
22	6	0	-0.708542	-3.694026	1.000000
23	6	0	0.708542	-3.694026	1.000000
24	6	0	2.844850	-2.460629	1.000000
25	6	0	4.980792	-1.232765	1.000000
26	6	0	4.980792	1.232765	1.000000
27	6	0	3.558002	3.697110	1.000000
28	6	0	1.422790	4.929875	1.000000
29	6	0	-1.422790	4.929875	1.000000
30	6	0	-3.558002	3.697110	1.000000
31	6	0	-4.980792	1.232765	1.000000
32	6	0	-4.980792	-1.232765	1.000000
33	6	0	-3.558002	-3.697110	1.000000
34	6	0	-1.422790	-4.929875	1.000000
35	6	0	1.422790	-4.929875	1.000000
36	6	0	3.558002	-3.697110	1.000000
37	6	0	5.690400	0.000000	1.000000
38	6	0	2.845200	4.928031	1.000000
39	6	0	-2.845200	4.928031	1.000000
40	6	0	-5.690400	0.000000	1.000000
41	6	0	-2.845200	-4.928031	1.000000
42	6	0	2.845200	-4.928031	1.000000
43	6	0	5.688001	-2.463782	1.000000

44	6	0	5.688001	2.463782	1.000000
45	6	0	4.977698	3.694062	1.000000
46	6	0	0.710302	6.157844	1.000000
47	6	0	-0.710302	6.157844	1.000000
48	6	0	-4.977698	3.694062	1.000000
49	6	0	-5.688001	2.463782	1.000000
50	6	0	-5.688001	-2.463782	1.000000
51	6	0	-4.977698	-3.694062	1.000000
52	6	0	-0.710302	-6.157844	1.000000
53	6	0	0.710302	-6.157844	1.000000
54	6	0	4.977698	-3.694062	1.000000
55	6	0	7.123200	0.000000	1.000000
56	6	0	3.561600	6.168872	1.000000
57	6	0	-3.561600	6.168872	1.000000
58	6	0	-7.123200	0.000000	1.000000
59	6	0	-3.561600	-6.168872	1.000000
60	6	0	3.561600	-6.168872	1.000000
61	6	0	7.126173	-2.454947	1.000000
62	6	0	7.126173	2.454947	1.000000
63	6	0	5.689133	4.943974	1.000000
64	6	0	1.437041	7.398921	1.000000
65	6	0	-1.437041	7.398921	1.000000
66	6	0	-5.689133	4.943974	1.000000
67	6	0	-7.126173	2.454947	1.000000
68	6	0	-7.126173	-2.454947	1.000000
69	6	0	-5.689133	-4.943974	1.000000
70	6	0	-1.437041	-7.398921	1.000000
71	6	0	1.437041	-7.398921	1.000000
72	6	0	5.689133	-4.943974	1.000000
73	6	0	7.804018	-1.241703	1.000000
74	6	0	7.804018	1.241703	1.000000
75	6	0	4.977355	6.137627	1.000000
76	6	0	2.826663	7.379329	1.000000
77	6	0	-2.826663	7.379329	1.000000
78	6	0	-4.977355	6.137627	1.000000
79	6	0	-7.804018	1.241703	1.000000
80	6	0	-7.804018	-1.241703	1.000000
81	6	0	-4.977355	-6.137627	1.000000

82	6	0	-2.826663	-7.379329	1.000000
83	6	0	2.826663	-7.379329	1.000000
84	6	0	4.977355	-6.137627	1.000000
85	6	0	7.811121	-3.725024	1.000000
86	6	0	7.811121	3.725024	1.000000
87	6	0	7.131526	4.902117	1.000000
88	6	0	0.679595	8.627141	1.000000
89	6	0	-0.679595	8.627141	1.000000
90	6	0	-7.131526	4.902117	1.000000
91	6	0	-7.811121	3.725024	1.000000
92	6	0	-7.811121	-3.725024	1.000000
93	6	0	-7.131526	-4.902117	1.000000
94	6	0	-0.679595	-8.627141	1.000000
95	6	0	0.679595	-8.627141	1.000000
96	6	0	7.131526	-4.902117	1.000000
97	1	0	8.892018	-1.240852	1.000000
98	1	0	8.892018	1.240852	1.000000
99	1	0	5.520618	7.080287	1.000000
100	1	0	3.371400	8.321139	1.000000
101	1	0	-3.371400	8.321139	1.000000
102	1	0	-5.520618	7.080287	1.000000
103	1	0	-8.892018	1.240852	1.000000
104	1	0	-8.892018	-1.240852	1.000000
105	1	0	-5.520618	-7.080287	1.000000
106	1	0	-3.371400	-8.321139	1.000000
107	1	0	3.371400	-8.321139	1.000000
108	1	0	5.520618	-7.080287	1.000000
109	1	0	8.898409	-3.719972	1.000000
110	1	0	8.898409	3.719972	1.000000
111	1	0	7.670795	5.846262	1.000000
112	1	0	1.227614	9.566234	1.000000
113	1	0	-1.227614	9.566234	1.000000
114	1	0	-7.670795	5.846262	1.000000
115	1	0	-8.898409	3.719972	1.000000
116	1	0	-8.898409	-3.719972	1.000000
117	1	0	-7.670795	-5.846262	1.000000
118	1	0	-1.227614	-9.566234	1.000000
119	1	0	1.227614	-9.566234	1.000000

120	1	0	7.670795	-5.846262	1.000000
121	6	0	0.645200	0.000000	-2.500000
122	6	0	1.485876	-1.282292	-2.500000
123	6	0	1.485876	1.282292	-2.500000
124	6	0	0.635098	-2.556341	-2.500000
125	6	0	0.635098	2.556341	-2.500000
126	1	0	-0.017486	0.000000	-3.378731
127	1	0	-0.017486	0.000000	-1.621269
128	1	0	2.146947	-1.280706	-3.378443
129	1	0	2.146947	-1.280706	-1.621557
130	1	0	2.146947	1.280706	-1.621557
131	1	0	2.146947	1.280706	-3.378443
132	1	0	-0.012496	-2.597529	-3.384745
133	1	0	-0.012496	-2.597529	-1.615255
134	1	0	1.258772	-3.457710	-2.500000
135	1	0	-0.012496	2.597529	-1.615255
136	1	0	-0.012496	2.597529	-3.384745
137	1	0	1.258772	3.457710	-2.500000

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### *n*-heptane

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.423200	0.000000	1.000000
2	6	0	0.711600	1.232527	1.000000
3	6	0	-0.711600	1.232527	1.000000
4	6	0	-1.423200	0.000000	1.000000
5	6	0	-0.711600	-1.232527	1.000000
6	6	0	0.711600	-1.232527	1.000000
7	6	0	2.842500	0.000000	1.000000
8	6	0	1.421250	2.461677	1.000000
9	6	0	-1.421250	2.461677	1.000000
10	6	0	-2.842500	0.000000	1.000000
11	6	0	-1.421250	-2.461677	1.000000
12	6	0	1.421250	-2.461677	1.000000

13	6	0	3.553392	-1.233398	1.000000
14	6	0	3.553392	1.233398	1.000000
15	6	0	2.844850	2.460629	1.000000
16	6	0	0.708542	3.694026	1.000000
17	6	0	-0.708542	3.694026	1.000000
18	6	0	-2.844850	2.460629	1.000000
19	6	0	-3.553392	1.233398	1.000000
20	6	0	-3.553392	-1.233398	1.000000
21	6	0	-2.844850	-2.460629	1.000000
22	6	0	-0.708542	-3.694026	1.000000
23	6	0	0.708542	-3.694026	1.000000
24	6	0	2.844850	-2.460629	1.000000
25	6	0	4.980792	-1.232765	1.000000
26	6	0	4.980792	1.232765	1.000000
27	6	0	3.558002	3.697110	1.000000
28	6	0	1.422790	4.929875	1.000000
29	6	0	-1.422790	4.929875	1.000000
30	6	0	-3.558002	3.697110	1.000000
31	6	0	-4.980792	1.232765	1.000000
32	6	0	-4.980792	-1.232765	1.000000
33	6	0	-3.558002	-3.697110	1.000000
34	6	0	-1.422790	-4.929875	1.000000
35	6	0	1.422790	-4.929875	1.000000
36	6	0	3.558002	-3.697110	1.000000
37	6	0	5.690400	0.000000	1.000000
38	6	0	2.845200	4.928031	1.000000
39	6	0	-2.845200	4.928031	1.000000
40	6	0	-5.690400	0.000000	1.000000
41	6	0	-2.845200	-4.928031	1.000000
42	6	0	2.845200	-4.928031	1.000000
43	6	0	5.688001	-2.463782	1.000000
44	6	0	5.688001	2.463782	1.000000
45	6	0	4.977698	3.694062	1.000000
46	6	0	0.710302	6.157844	1.000000
47	6	0	-0.710302	6.157844	1.000000
48	6	0	-4.977698	3.694062	1.000000
49	6	0	-5.688001	2.463782	1.000000
50	6	0	-5.688001	-2.463782	1.000000



51	6	0	-4.977698	-3.694062	1.000000
52	6	0	-0.710302	-6.157844	1.000000
53	6	0	0.710302	-6.157844	1.000000
54	6	0	4.977698	-3.694062	1.000000
55	6	0	7.123200	0.000000	1.000000
56	6	0	3.561600	6.168872	1.000000
57	6	0	-3.561600	6.168872	1.000000
58	6	0	-7.123200	0.000000	1.000000
59	6	0	-3.561600	-6.168872	1.000000
60	6	0	3.561600	-6.168872	1.000000
61	6	0	7.126173	-2.454947	1.000000
62	6	0	7.126173	2.454947	1.000000
63	6	0	5.689133	4.943974	1.000000
64	6	0	1.437041	7.398921	1.000000
65	6	0	-1.437041	7.398921	1.000000
66	6	0	-5.689133	4.943974	1.000000
67	6	0	-7.126173	2.454947	1.000000
68	6	0	-7.126173	-2.454947	1.000000
69	6	0	-5.689133	-4.943974	1.000000
70	6	0	-1.437041	-7.398921	1.000000
71	6	0	1.437041	-7.398921	1.000000
72	6	0	5.689133	-4.943974	1.000000
73	6	0	7.804018	-1.241703	1.000000
74	6	0	7.804018	1.241703	1.000000
75	6	0	4.977355	6.137627	1.000000
76	6	0	2.826663	7.379329	1.000000
77	6	0	-2.826663	7.379329	1.000000
78	6	0	-4.977355	6.137627	1.000000
79	6	0	-7.804018	1.241703	1.000000
80	6	0	-7.804018	-1.241703	1.000000
81	6	0	-4.977355	-6.137627	1.000000
82	6	0	-2.826663	-7.379329	1.000000
83	6	0	2.826663	-7.379329	1.000000
84	6	0	4.977355	-6.137627	1.000000
85	6	0	7.811121	-3.725024	1.000000
86	6	0	7.811121	3.725024	1.000000
87	6	0	7.131526	4.902117	1.000000
88	6	0	0.679595	8.627141	1.000000

89	6	0	-0.679595	8.627141	1.000000
90	6	0	-7.131526	4.902117	1.000000
91	6	0	-7.811121	3.725024	1.000000
92	6	0	-7.811121	-3.725024	1.000000
93	6	0	-7.131526	-4.902117	1.000000
94	6	0	-0.679595	-8.627141	1.000000
95	6	0	0.679595	-8.627141	1.000000
96	6	0	7.131526	-4.902117	1.000000
97	1	0	8.892018	-1.240852	1.000000
98	1	0	8.892018	1.240852	1.000000
99	1	0	5.520618	7.080287	1.000000
100	1	0	3.371400	8.321139	1.000000
101	1	0	-3.371400	8.321139	1.000000
102	1	0	-5.520618	7.080287	1.000000
103	1	0	-8.892018	1.240852	1.000000
104	1	0	-8.892018	-1.240852	1.000000
105	1	0	-5.520618	-7.080287	1.000000
106	1	0	-3.371400	-8.321139	1.000000
107	1	0	3.371400	-8.321139	1.000000
108	1	0	5.520618	-7.080287	1.000000
109	1	0	8.898409	-3.719972	1.000000
110	1	0	8.898409	3.719972	1.000000
111	1	0	7.670795	5.846262	1.000000
112	1	0	1.227614	9.566234	1.000000
113	1	0	-1.227614	9.566234	1.000000
114	1	0	-7.670795	5.846262	1.000000
115	1	0	-8.898409	3.719972	1.000000
116	1	0	-8.898409	-3.719972	1.000000
117	1	0	-7.670795	-5.846262	1.000000
118	1	0	-1.227614	-9.566234	1.000000
119	1	0	1.227614	-9.566234	1.000000
120	1	0	7.670795	-5.846262	1.000000
121	6	0	0.645200	0.000000	-2.510000
122	6	0	1.486600	-1.281577	-2.510000
123	6	0	1.486600	1.281577	-2.510000
124	6	0	0.645953	-2.564008	-2.510000
125	6	0	0.645953	2.564008	-2.510000
126	6	0	1.496448	-3.838125	-2.510000

127	6	0	1.496448	3.838125	-2.510000
128	1	0	-0.017003	0.000000	-3.388719
129	1	0	-0.017003	0.000000	-1.631281
130	1	0	2.148917	-1.282124	-3.388758
131	1	0	2.148917	-1.282124	-1.631242
132	1	0	2.148917	1.282124	-1.631242
133	1	0	2.148917	1.282124	-3.388758
134	1	0	-0.015258	-2.562278	-3.388338
135	1	0	-0.015258	-2.562278	-1.631662
136	1	0	-0.015258	2.562278	-1.631662
137	1	0	-0.015258	2.562278	-3.388338
138	1	0	0.872326	-4.739183	-2.510000
139	1	0	2.144048	-3.879749	-1.625280
140	1	0	2.144048	-3.879749	-3.394720
141	1	0	0.872326	4.739183	-2.510000
142	1	0	2.144048	3.879749	-3.394720
143	1	0	2.144048	3.879749	-1.625280

---

### fluoropropane

---

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

14	6	0	3.553392	1.233398	1.000000
15	6	0	2.844850	2.460629	1.000000
16	6	0	0.708542	3.694026	1.000000
17	6	0	-0.708542	3.694026	1.000000
18	6	0	-2.844850	2.460629	1.000000
19	6	0	-3.553392	1.233398	1.000000
20	6	0	-3.553392	-1.233398	1.000000
21	6	0	-2.844850	-2.460629	1.000000
22	6	0	-0.708542	-3.694026	1.000000
23	6	0	0.708542	-3.694026	1.000000
24	6	0	2.844850	-2.460629	1.000000
25	6	0	4.980792	-1.232765	1.000000
26	6	0	4.980792	1.232765	1.000000
27	6	0	3.558002	3.697110	1.000000
28	6	0	1.422790	4.929875	1.000000
29	6	0	-1.422790	4.929875	1.000000
30	6	0	-3.558002	3.697110	1.000000
31	6	0	-4.980792	1.232765	1.000000
32	6	0	-4.980792	-1.232765	1.000000
33	6	0	-3.558002	-3.697110	1.000000
34	6	0	-1.422790	-4.929875	1.000000
35	6	0	1.422790	-4.929875	1.000000
36	6	0	3.558002	-3.697110	1.000000
37	6	0	5.690400	0.000000	1.000000
38	6	0	2.845200	4.928031	1.000000
39	6	0	-2.845200	4.928031	1.000000
40	6	0	-5.690400	0.000000	1.000000
41	6	0	-2.845200	-4.928031	1.000000
42	6	0	2.845200	-4.928031	1.000000
43	6	0	5.688001	-2.463782	1.000000
44	6	0	5.688001	2.463782	1.000000
45	6	0	4.977698	3.694062	1.000000
46	6	0	0.710302	6.157844	1.000000
47	6	0	-0.710302	6.157844	1.000000
48	6	0	-4.977698	3.694062	1.000000
49	6	0	-5.688001	2.463782	1.000000
50	6	0	-5.688001	-2.463782	1.000000
51	6	0	-4.977698	-3.694062	1.000000

52	6	0	-0.710302	-6.157844	1.000000
53	6	0	0.710302	-6.157844	1.000000
54	6	0	4.977698	-3.694062	1.000000
55	6	0	7.123200	0.000000	1.000000
56	6	0	3.561600	6.168872	1.000000
57	6	0	-3.561600	6.168872	1.000000
58	6	0	-7.123200	0.000000	1.000000
59	6	0	-3.561600	-6.168872	1.000000
60	6	0	3.561600	-6.168872	1.000000
61	6	0	7.126173	-2.454947	1.000000
62	6	0	7.126173	2.454947	1.000000
63	6	0	5.689133	4.943974	1.000000
64	6	0	1.437041	7.398921	1.000000
65	6	0	-1.437041	7.398921	1.000000
66	6	0	-5.689133	4.943974	1.000000
67	6	0	-7.126173	2.454947	1.000000
68	6	0	-7.126173	-2.454947	1.000000
69	6	0	-5.689133	-4.943974	1.000000
70	6	0	-1.437041	-7.398921	1.000000
71	6	0	1.437041	-7.398921	1.000000
72	6	0	5.689133	-4.943974	1.000000
73	6	0	7.804018	-1.241703	1.000000
74	6	0	7.804018	1.241703	1.000000
75	6	0	4.977355	6.137627	1.000000
76	6	0	2.826663	7.379329	1.000000
77	6	0	-2.826663	7.379329	1.000000
78	6	0	-4.977355	6.137627	1.000000
79	6	0	-7.804018	1.241703	1.000000
80	6	0	-7.804018	-1.241703	1.000000
81	6	0	-4.977355	-6.137627	1.000000
82	6	0	-2.826663	-7.379329	1.000000
83	6	0	2.826663	-7.379329	1.000000
84	6	0	4.977355	-6.137627	1.000000
85	6	0	7.811121	-3.725024	1.000000
86	6	0	7.811121	3.725024	1.000000
87	6	0	7.131526	4.902117	1.000000
88	6	0	0.679595	8.627141	1.000000
89	6	0	-0.679595	8.627141	1.000000

90	6	0	-7.131526	4.902117	1.000000
91	6	0	-7.811121	3.725024	1.000000
92	6	0	-7.811121	-3.725024	1.000000
93	6	0	-7.131526	-4.902117	1.000000
94	6	0	-0.679595	-8.627141	1.000000
95	6	0	0.679595	-8.627141	1.000000
96	6	0	7.131526	-4.902117	1.000000
97	1	0	8.892018	-1.240852	1.000000
98	1	0	8.892018	1.240852	1.000000
99	1	0	5.520618	7.080287	1.000000
100	1	0	3.371400	8.321139	1.000000
101	1	0	-3.371400	8.321139	1.000000
102	1	0	-5.520618	7.080287	1.000000
103	1	0	-8.892018	1.240852	1.000000
104	1	0	-8.892018	-1.240852	1.000000
105	1	0	-5.520618	-7.080287	1.000000
106	1	0	-3.371400	-8.321139	1.000000
107	1	0	3.371400	-8.321139	1.000000
108	1	0	5.520618	-7.080287	1.000000
109	1	0	8.898409	-3.719972	1.000000
110	1	0	8.898409	3.719972	1.000000
111	1	0	7.670795	5.846262	1.000000
112	1	0	1.227614	9.566234	1.000000
113	1	0	-1.227614	9.566234	1.000000
114	1	0	-7.670795	5.846262	1.000000
115	1	0	-8.898409	3.719972	1.000000
116	1	0	-8.898409	-3.719972	1.000000
117	1	0	-7.670795	-5.846262	1.000000
118	1	0	-1.227614	-9.566234	1.000000
119	1	0	1.227614	-9.566234	1.000000
120	1	0	7.670795	-5.846262	1.000000
121	6	0	0.645200	0.000000	-3.090000
122	6	0	1.476888	-1.304061	-3.090000
123	6	0	1.476888	1.304061	-3.090000
124	9	0	-0.135946	0.000000	-4.194359
125	9	0	-0.135946	0.000000	-1.985641
126	9	0	0.648783	-2.354625	-3.090000
127	9	0	2.252758	-1.359072	-4.180655

128	9	0	2.252758	-1.359072	-1.999345
129	9	0	0.648783	2.354625	-3.090000
130	9	0	2.254378	1.326634	-4.180655
131	9	0	2.254378	1.326634	-1.999345

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### ***n*-fluoropentane**

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.423200	0.000000	1.000000
2	6	0	0.711600	1.232527	1.000000
3	6	0	-0.711600	1.232527	1.000000
4	6	0	-1.423200	0.000000	1.000000
5	6	0	-0.711600	-1.232527	1.000000
6	6	0	0.711600	-1.232527	1.000000
7	6	0	2.842500	0.000000	1.000000
8	6	0	1.421250	2.461677	1.000000
9	6	0	-1.421250	2.461677	1.000000
10	6	0	-2.842500	0.000000	1.000000
11	6	0	-1.421250	-2.461677	1.000000
12	6	0	1.421250	-2.461677	1.000000
13	6	0	3.553392	-1.233398	1.000000
14	6	0	3.553392	1.233398	1.000000
15	6	0	2.844850	2.460629	1.000000
16	6	0	0.708542	3.694026	1.000000
17	6	0	-0.708542	3.694026	1.000000
18	6	0	-2.844850	2.460629	1.000000
19	6	0	-3.553392	1.233398	1.000000
20	6	0	-3.553392	-1.233398	1.000000
21	6	0	-2.844850	-2.460629	1.000000
22	6	0	-0.708542	-3.694026	1.000000
23	6	0	0.708542	-3.694026	1.000000
24	6	0	2.844850	-2.460629	1.000000
25	6	0	4.980792	-1.232765	1.000000
26	6	0	4.980792	1.232765	1.000000

27	6	0	3.558002	3.697110	1.000000
28	6	0	1.422790	4.929875	1.000000
29	6	0	-1.422790	4.929875	1.000000
30	6	0	-3.558002	3.697110	1.000000
31	6	0	-4.980792	1.232765	1.000000
32	6	0	-4.980792	-1.232765	1.000000
33	6	0	-3.558002	-3.697110	1.000000
34	6	0	-1.422790	-4.929875	1.000000
35	6	0	1.422790	-4.929875	1.000000
36	6	0	3.558002	-3.697110	1.000000
37	6	0	5.690400	0.000000	1.000000
38	6	0	2.845200	4.928031	1.000000
39	6	0	-2.845200	4.928031	1.000000
40	6	0	-5.690400	0.000000	1.000000
41	6	0	-2.845200	-4.928031	1.000000
42	6	0	2.845200	-4.928031	1.000000
43	6	0	5.688001	-2.463782	1.000000
44	6	0	5.688001	2.463782	1.000000
45	6	0	4.977698	3.694062	1.000000
46	6	0	0.710302	6.157844	1.000000
47	6	0	-0.710302	6.157844	1.000000
48	6	0	-4.977698	3.694062	1.000000
49	6	0	-5.688001	2.463782	1.000000
50	6	0	-5.688001	-2.463782	1.000000
51	6	0	-4.977698	-3.694062	1.000000
52	6	0	-0.710302	-6.157844	1.000000
53	6	0	0.710302	-6.157844	1.000000
54	6	0	4.977698	-3.694062	1.000000
55	6	0	7.123200	0.000000	1.000000
56	6	0	3.561600	6.168872	1.000000
57	6	0	-3.561600	6.168872	1.000000
58	6	0	-7.123200	0.000000	1.000000
59	6	0	-3.561600	-6.168872	1.000000
60	6	0	3.561600	-6.168872	1.000000
61	6	0	7.126173	-2.454947	1.000000
62	6	0	7.126173	2.454947	1.000000
63	6	0	5.689133	4.943974	1.000000
64	6	0	1.437041	7.398921	1.000000



65	6	0	-1.437041	7.398921	1.000000
66	6	0	-5.689133	4.943974	1.000000
67	6	0	-7.126173	2.454947	1.000000
68	6	0	-7.126173	-2.454947	1.000000
69	6	0	-5.689133	-4.943974	1.000000
70	6	0	-1.437041	-7.398921	1.000000
71	6	0	1.437041	-7.398921	1.000000
72	6	0	5.689133	-4.943974	1.000000
73	6	0	7.804018	-1.241703	1.000000
74	6	0	7.804018	1.241703	1.000000
75	6	0	4.977355	6.137627	1.000000
76	6	0	2.826663	7.379329	1.000000
77	6	0	-2.826663	7.379329	1.000000
78	6	0	-4.977355	6.137627	1.000000
79	6	0	-7.804018	1.241703	1.000000
80	6	0	-7.804018	-1.241703	1.000000
81	6	0	-4.977355	-6.137627	1.000000
82	6	0	-2.826663	-7.379329	1.000000
83	6	0	2.826663	-7.379329	1.000000
84	6	0	4.977355	-6.137627	1.000000
85	6	0	7.811121	-3.725024	1.000000
86	6	0	7.811121	3.725024	1.000000
87	6	0	7.131526	4.902117	1.000000
88	6	0	0.679595	8.627141	1.000000
89	6	0	-0.679595	8.627141	1.000000
90	6	0	-7.131526	4.902117	1.000000
91	6	0	-7.811121	3.725024	1.000000
92	6	0	-7.811121	-3.725024	1.000000
93	6	0	-7.131526	-4.902117	1.000000
94	6	0	-0.679595	-8.627141	1.000000
95	6	0	0.679595	-8.627141	1.000000
96	6	0	7.131526	-4.902117	1.000000
97	1	0	8.892018	-1.240852	1.000000
98	1	0	8.892018	1.240852	1.000000
99	1	0	5.520618	7.080287	1.000000
100	1	0	3.371400	8.321139	1.000000
101	1	0	-3.371400	8.321139	1.000000
102	1	0	-5.520618	7.080287	1.000000

103	1	0	-8.892018	1.240852	1.000000
104	1	0	-8.892018	-1.240852	1.000000
105	1	0	-5.520618	-7.080287	1.000000
106	1	0	-3.371400	-8.321139	1.000000
107	1	0	3.371400	-8.321139	1.000000
108	1	0	5.520618	-7.080287	1.000000
109	1	0	8.898409	-3.719972	1.000000
110	1	0	8.898409	3.719972	1.000000
111	1	0	7.670795	5.846262	1.000000
112	1	0	1.227614	9.566234	1.000000
113	1	0	-1.227614	9.566234	1.000000
114	1	0	-7.670795	5.846262	1.000000
115	1	0	-8.898409	3.719972	1.000000
116	1	0	-8.898409	-3.719972	1.000000
117	1	0	-7.670795	-5.846262	1.000000
118	1	0	-1.227614	-9.566234	1.000000
119	1	0	1.227614	-9.566234	1.000000
120	1	0	7.670795	-5.846262	1.000000
121	6	0	0.645200	0.000000	-3.120000
122	6	0	1.486425	-1.305431	-3.120000
123	6	0	1.486425	1.305431	-3.120000
124	6	0	0.643574	-2.609932	-3.120000
125	6	0	0.643574	2.609932	-3.120000
126	9	0	-0.139795	0.000000	-4.224204
127	9	0	-0.139795	0.000000	-2.015796
128	9	0	2.267443	-1.324745	-4.224035
129	9	0	2.267443	-1.324745	-2.015965
130	9	0	2.267443	1.324745	-2.015965
131	9	0	2.267443	1.324745	-4.224035
132	9	0	-0.129837	-2.670325	-4.210766
133	9	0	-0.129837	-2.670325	-2.029234
134	9	0	1.477757	-3.656699	-3.120000
135	9	0	-0.129837	2.670325	-2.029234
136	9	0	-0.129837	2.670325	-4.210766
137	9	0	1.477757	3.656699	-3.120000

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## *n*-fluoroheptane

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

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34	6	0	-1.422790	-4.929875	1.000000
35	6	0	1.422790	-4.929875	1.000000
36	6	0	3.558002	-3.697110	1.000000
37	6	0	5.690400	0.000000	1.000000
38	6	0	2.845200	4.928031	1.000000
39	6	0	-2.845200	4.928031	1.000000
40	6	0	-5.690400	0.000000	1.000000
41	6	0	-2.845200	-4.928031	1.000000
42	6	0	2.845200	-4.928031	1.000000
43	6	0	5.688001	-2.463782	1.000000
44	6	0	5.688001	2.463782	1.000000
45	6	0	4.977698	3.694062	1.000000
46	6	0	0.710302	6.157844	1.000000
47	6	0	-0.710302	6.157844	1.000000
48	6	0	-4.977698	3.694062	1.000000
49	6	0	-5.688001	2.463782	1.000000
50	6	0	-5.688001	-2.463782	1.000000
51	6	0	-4.977698	-3.694062	1.000000
52	6	0	-0.710302	-6.157844	1.000000
53	6	0	0.710302	-6.157844	1.000000
54	6	0	4.977698	-3.694062	1.000000
55	6	0	7.123200	0.000000	1.000000
56	6	0	3.561600	6.168872	1.000000
57	6	0	-3.561600	6.168872	1.000000
58	6	0	-7.123200	0.000000	1.000000
59	6	0	-3.561600	-6.168872	1.000000
60	6	0	3.561600	-6.168872	1.000000
61	6	0	7.126173	-2.454947	1.000000
62	6	0	7.126173	2.454947	1.000000
63	6	0	5.689133	4.943974	1.000000
64	6	0	1.437041	7.398921	1.000000
65	6	0	-1.437041	7.398921	1.000000
66	6	0	-5.689133	4.943974	1.000000
67	6	0	-7.126173	2.454947	1.000000
68	6	0	-7.126173	-2.454947	1.000000
69	6	0	-5.689133	-4.943974	1.000000
70	6	0	-1.437041	-7.398921	1.000000
71	6	0	1.437041	-7.398921	1.000000

72	6	0	5.689133	-4.943974	1.000000
73	6	0	7.804018	-1.241703	1.000000
74	6	0	7.804018	1.241703	1.000000
75	6	0	4.977355	6.137627	1.000000
76	6	0	2.826663	7.379329	1.000000
77	6	0	-2.826663	7.379329	1.000000
78	6	0	-4.977355	6.137627	1.000000
79	6	0	-7.804018	1.241703	1.000000
80	6	0	-7.804018	-1.241703	1.000000
81	6	0	-4.977355	-6.137627	1.000000
82	6	0	-2.826663	-7.379329	1.000000
83	6	0	2.826663	-7.379329	1.000000
84	6	0	4.977355	-6.137627	1.000000
85	6	0	7.811121	-3.725024	1.000000
86	6	0	7.811121	3.725024	1.000000
87	6	0	7.131526	4.902117	1.000000
88	6	0	0.679595	8.627141	1.000000
89	6	0	-0.679595	8.627141	1.000000
90	6	0	-7.131526	4.902117	1.000000
91	6	0	-7.811121	3.725024	1.000000
92	6	0	-7.811121	-3.725024	1.000000
93	6	0	-7.131526	-4.902117	1.000000
94	6	0	-0.679595	-8.627141	1.000000
95	6	0	0.679595	-8.627141	1.000000
96	6	0	7.131526	-4.902117	1.000000
97	1	0	8.892018	-1.240852	1.000000
98	1	0	8.892018	1.240852	1.000000
99	1	0	5.520618	7.080287	1.000000
100	1	0	3.371400	8.321139	1.000000
101	1	0	-3.371400	8.321139	1.000000
102	1	0	-5.520618	7.080287	1.000000
103	1	0	-8.892018	1.240852	1.000000
104	1	0	-8.892018	-1.240852	1.000000
105	1	0	-5.520618	-7.080287	1.000000
106	1	0	-3.371400	-8.321139	1.000000
107	1	0	3.371400	-8.321139	1.000000
108	1	0	5.520618	-7.080287	1.000000
109	1	0	8.898409	-3.719972	1.000000

110	1	0	8.898409	3.719972	1.000000
111	1	0	7.670795	5.846262	1.000000
112	1	0	1.227614	9.566234	1.000000
113	1	0	-1.227614	9.566234	1.000000
114	1	0	-7.670795	5.846262	1.000000
115	1	0	-8.898409	3.719972	1.000000
116	1	0	-8.898409	-3.719972	1.000000
117	1	0	-7.670795	-5.846262	1.000000
118	1	0	-1.227614	-9.566234	1.000000
119	1	0	1.227614	-9.566234	1.000000
120	1	0	7.670795	-5.846262	1.000000
121	6	0	0.645200	0.000000	-3.130000
122	6	0	1.495986	-1.307341	-3.130000
123	6	0	1.495986	1.307341	-3.130000
124	6	0	0.651492	-2.613399	-3.130000
125	6	0	0.651492	2.613399	-3.130000
126	6	0	1.494467	-3.918177	-3.130000
127	6	0	1.494467	3.918177	-3.130000
128	9	0	-0.136217	0.000000	-4.234412
129	9	0	-0.136217	0.000000	-2.025588
130	9	0	2.278837	-1.313592	-4.234114
131	9	0	2.278837	-1.313592	-2.025886
132	9	0	2.278837	1.313592	-2.025886
133	9	0	2.278837	1.313592	-4.234114
134	9	0	-0.129255	-2.634923	-4.234064
135	9	0	-0.129255	-2.634923	-2.025936
136	9	0	-0.129255	2.634923	-2.025936
137	9	0	-0.129255	2.634923	-4.234064
138	9	0	0.659147	-4.964421	-3.130000
139	9	0	2.267735	-3.979744	-2.039198
140	9	0	2.267735	-3.979744	-4.220802
141	9	0	0.659147	4.964421	-3.130000
142	9	0	2.267735	3.979744	-4.220802
143	9	0	2.267735	3.979744	-2.039198

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## XYZ coordinates of each optimized geometry on C<sub>54</sub>H<sub>18</sub>

### propane

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.329143	-0.019410	-0.282007
2	6	0	-2.757188	-0.040143	-0.319518
3	6	0	-3.483578	1.179865	-0.338153
4	6	0	-3.447912	-1.280681	-0.338033
5	6	0	-4.913267	1.153718	-0.375685
6	6	0	-4.877758	-1.295987	-0.375563
7	6	0	-5.575278	-0.080990	-0.393467
8	6	0	-5.616653	2.406764	-0.393729
9	6	0	-5.544529	-2.568896	-0.393483
10	1	0	-6.662857	-0.096755	-0.422014
11	1	0	-6.703408	2.386452	-0.422257
12	1	0	-6.631416	-2.580096	-0.422012
13	6	0	-0.601930	-1.238152	-0.263291
14	6	0	-1.298072	-2.485705	-0.282039
15	6	0	-2.717442	-2.504988	-0.319263
16	6	0	-0.569447	-3.704381	-0.263298
17	6	0	-3.409639	-3.756636	-0.337849
18	6	0	-1.271108	-4.950743	-0.282122
19	6	0	-2.671721	-4.947514	-0.318878
20	6	0	-4.846124	-3.739463	-0.375542
21	6	0	-0.502499	-6.164848	-0.262352
22	1	0	-3.201854	-5.897592	-0.333106
23	1	0	-5.371910	-4.691099	-0.389656
24	1	0	-1.036237	-7.112042	-0.276672
25	6	0	0.816683	-1.217586	-0.226060
26	6	0	1.548686	-2.444442	-0.207306
27	6	0	0.855697	-3.683721	-0.225891
28	6	0	2.968025	-2.422569	-0.170034
29	6	0	1.593188	-4.909220	-0.206938
30	6	0	3.696211	-3.653624	-0.151331
31	6	0	2.993119	-4.865393	-0.170184

32	6	0	0.860092	-6.145094	-0.226586
33	6	0	5.131594	-3.594820	-0.113641
34	1	0	3.550566	-5.799706	-0.155864
35	1	0	1.421060	-7.076419	-0.212173
36	1	0	5.684740	-4.530814	-0.099435
37	6	0	1.508219	0.021709	-0.207553
38	6	0	2.936313	0.042401	-0.170070
39	6	0	3.662701	-1.177601	-0.151395
40	6	0	3.627035	1.282945	-0.151512
41	6	0	5.092391	-1.151454	-0.113862
42	6	0	5.056881	1.298250	-0.113982
43	6	0	5.754401	0.083253	-0.096079
44	6	0	5.795777	-2.404500	-0.095816
45	6	0	5.723653	2.571160	-0.096062
46	1	0	6.841981	0.099019	-0.067532
47	1	0	6.882531	-2.384188	-0.067290
48	1	0	6.810540	2.582359	-0.067534
49	6	0	0.781063	1.240454	-0.226152
50	6	0	1.477185	2.487975	-0.207543
51	6	0	2.896566	2.507251	-0.170278
52	6	0	0.748573	3.706644	-0.226255
53	6	0	3.588763	3.758899	-0.151697
54	6	0	1.450232	4.953007	-0.207425
55	6	0	2.850845	4.949777	-0.170669
56	6	0	5.025247	3.741727	-0.114003
57	6	0	0.681622	6.167111	-0.227194
58	1	0	3.380978	5.899855	-0.156441
59	1	0	5.551033	4.693362	-0.099890
60	1	0	1.215362	7.114306	-0.212873
61	6	0	-0.637510	1.219776	-0.263437
62	6	0	-1.369561	2.446705	-0.282292
63	6	0	-0.676574	3.685984	-0.263660
64	6	0	-2.788901	2.424832	-0.319512
65	6	0	-1.414065	4.911485	-0.282608
66	6	0	-3.517086	3.655888	-0.338216
67	6	0	-2.813995	4.867657	-0.319363
68	6	0	-0.680968	6.147357	-0.262959
69	6	0	-4.952470	3.597084	-0.375905



70	1	0	-3.371442	5.801969	-0.333683
71	1	0	-1.241936	7.078683	-0.277374
72	1	0	-5.505617	4.533078	-0.390112
73	6	0	-0.588606	-0.004645	3.211574
74	1	0	0.052959	0.006699	2.323113
75	1	0	0.088086	0.007014	4.077143
76	6	0	-1.416785	-1.293130	3.223882
77	1	0	-2.026720	-1.361346	4.133669
78	1	0	-2.097023	-1.328437	2.365862
79	6	0	-1.461065	1.254281	3.224118
80	1	0	-2.141719	1.266317	2.365782
81	1	0	-2.073420	1.300845	4.133646
82	1	0	-0.854585	2.166200	3.178317
83	1	0	-0.779011	-2.183407	3.177381

## fluoropropane

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.079420	0.178362	-0.974740
2	6	0	2.477127	0.431885	-1.127100
3	6	0	3.390343	-0.653155	-1.200100
4	6	0	2.951154	1.768035	-1.204972
5	6	0	4.788899	-0.394352	-1.352548
6	6	0	4.351543	2.016303	-1.357470
7	6	0	5.235570	0.931567	-1.427573
8	6	0	5.684920	-1.515615	-1.423163
9	6	0	4.796628	3.380631	-1.433054
10	1	0	6.300105	1.124464	-1.543535
11	1	0	6.747897	-1.318369	-1.539084
12	1	0	5.861230	3.568911	-1.548958
13	6	0	0.165583	1.262053	-0.901354
14	6	0	0.643754	2.606111	-0.980121
15	6	0	2.033216	2.856597	-1.131457
16	6	0	-0.271445	3.689422	-0.906733

17	6	0	2.506742	4.204099	-1.209668
18	6	0	0.212236	5.033254	-0.985916
19	6	0	1.587034	5.258458	-1.135213
20	6	0	3.919028	4.421398	-1.362739
21	6	0	-0.741400	6.105518	-0.908270
22	1	0	1.951093	6.282064	-1.195082
23	1	0	4.278566	5.445832	-1.422151
24	1	0	-0.373329	7.126868	-0.968514
25	6	0	-1.222839	1.010395	-0.750089
26	6	0	-2.142740	2.101208	-0.676494
27	6	0	-1.666387	3.436653	-0.754721
28	6	0	-3.531768	1.848205	-0.525077
29	6	0	-2.591362	4.525232	-0.680430
30	6	0	-4.448527	2.943781	-0.451808
31	6	0	-3.957760	4.253723	-0.531041
32	6	0	-2.075115	5.863844	-0.762947
33	6	0	-5.847248	2.651717	-0.298586
34	1	0	-4.658233	5.084431	-0.474917
35	1	0	-2.778552	6.691032	-0.706438
36	1	0	-6.543781	3.484786	-0.242927
37	6	0	-1.697816	-0.324799	-0.672107
38	6	0	-3.095647	-0.578079	-0.519766
39	6	0	-4.008824	0.506887	-0.446636
40	6	0	-3.569549	-1.914387	-0.441741
41	6	0	-5.407327	0.247966	-0.294132
42	6	0	-4.969986	-2.162641	-0.289263
43	6	0	-5.854016	-1.077904	-0.219200
44	6	0	-6.303364	1.369278	-0.223578
45	6	0	-5.415071	-3.526969	-0.213687
46	1	0	-6.918549	-1.270799	-0.103206
47	1	0	-7.366341	1.172032	-0.107658
48	1	0	-6.479673	-3.715248	-0.097783
49	6	0	-0.784084	-1.408398	-0.745221
50	6	0	-1.262143	-2.752470	-0.666672
51	6	0	-2.651659	-3.002934	-0.515285
52	6	0	-0.347002	-3.835759	-0.740031
53	6	0	-3.125184	-4.350436	-0.437072
54	6	0	-0.830680	-5.179591	-0.660826

55	6	0	-2.205478	-5.404794	-0.511529
56	6	0	-4.537471	-4.567736	-0.284002
57	6	0	0.122957	-6.251853	-0.738472
58	1	0	-2.569538	-6.428399	-0.451659
59	1	0	-4.897008	-5.592169	-0.224591
60	1	0	-0.245115	-7.273203	-0.678228
61	6	0	0.604408	-1.156683	-0.896526
62	6	0	1.524260	-2.247522	-0.970369
63	6	0	1.047944	-3.582990	-0.892018
64	6	0	2.913341	-1.994644	-1.121598
65	6	0	1.972919	-4.671570	-0.966311
66	6	0	3.830100	-3.090103	-1.194925
67	6	0	3.339315	-4.400060	-1.115719
68	6	0	1.456671	-6.010179	-0.883795
69	6	0	5.228807	-2.798053	-1.348151
70	1	0	4.039790	-5.230769	-1.171825
71	1	0	2.160109	-6.837368	-0.940305
72	1	0	5.925337	-3.631123	-1.403815
73	6	0	0.596188	0.113181	3.172866
74	6	0	1.033674	1.581711	2.947661
75	6	0	1.763358	-0.897825	3.266162
76	9	0	2.391457	-0.998259	2.090394
77	9	0	-0.201837	-0.260692	2.151048
78	9	0	1.914075	1.659374	1.942270
79	9	0	2.641733	-0.499198	4.199717
80	9	0	-0.103791	0.058843	4.330395
81	9	0	1.603416	2.064466	4.060629
82	9	0	1.281644	-2.099248	3.606751
83	9	0	-0.038420	2.323736	2.649090

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XYZ coordinates of molecules at an initial position for horizontal displacement on  $C_{54}H_{18}$

**propane**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.419200	0.000000	1.000000
2	6	0	2.848000	0.000000	1.000000
3	6	0	3.556875	-1.230405	1.000000
4	6	0	3.556875	1.230405	1.000000
5	6	0	4.987265	-1.224985	1.000000
6	6	0	4.987265	1.224985	1.000000
7	6	0	5.667400	0.000000	1.000000
8	6	0	5.672661	-2.488111	1.000000
9	6	0	5.672661	2.488111	1.000000
10	1	0	6.755500	0.000000	1.000000
11	1	0	6.759952	-2.483557	1.000000
12	1	0	6.759952	2.483557	1.000000
13	6	0	0.709600	1.229063	1.000000
14	6	0	1.424000	2.466440	1.000000
15	6	0	2.843999	2.465142	1.000000
16	6	0	0.712876	3.695547	1.000000
17	6	0	3.554500	3.706606	1.000000
18	6	0	1.432764	4.931590	1.000000
19	6	0	2.833700	4.908112	1.000000
20	6	0	4.991098	3.668613	1.000000
21	6	0	0.681563	6.156724	1.000000
22	1	0	3.377750	5.850435	1.000000
23	1	0	5.530799	4.612511	1.000000
24	1	0	1.229152	7.096068	1.000000
25	6	0	-0.709600	1.229063	1.000000
26	6	0	-1.424000	2.466440	1.000000
27	6	0	-0.712876	3.695547	1.000000
28	6	0	-2.843999	2.465142	1.000000
29	6	0	-1.432764	4.931590	1.000000
30	6	0	-3.554500	3.706606	1.000000

31	6	0	-2.833700	4.908112	1.000000
32	6	0	-0.681563	6.156724	1.000000
33	6	0	-4.991098	3.668613	1.000000
34	1	0	-3.377750	5.850435	1.000000
35	1	0	-1.229152	7.096068	1.000000
36	1	0	-5.530799	4.612511	1.000000
37	6	0	-1.419200	0.000000	1.000000
38	6	0	-2.848000	0.000000	1.000000
39	6	0	-3.556875	1.230405	1.000000
40	6	0	-3.556875	-1.230405	1.000000
41	6	0	-4.987265	1.224985	1.000000
42	6	0	-4.987265	-1.224985	1.000000
43	6	0	-5.667400	0.000000	1.000000
44	6	0	-5.672661	2.488111	1.000000
45	6	0	-5.672661	-2.488111	1.000000
46	1	0	-6.755500	0.000000	1.000000
47	1	0	-6.759952	2.483557	1.000000
48	1	0	-6.759952	-2.483557	1.000000
49	6	0	-0.709600	-1.229063	1.000000
50	6	0	-1.424000	-2.466440	1.000000
51	6	0	-2.843999	-2.465142	1.000000
52	6	0	-0.712876	-3.695547	1.000000
53	6	0	-3.554500	-3.706606	1.000000
54	6	0	-1.432764	-4.931590	1.000000
55	6	0	-2.833700	-4.908112	1.000000
56	6	0	-4.991098	-3.668613	1.000000
57	6	0	-0.681563	-6.156724	1.000000
58	1	0	-3.377750	-5.850435	1.000000
59	1	0	-5.530799	-4.612511	1.000000
60	1	0	-1.229152	-7.096068	1.000000
61	6	0	0.709600	-1.229063	1.000000
62	6	0	1.424000	-2.466440	1.000000
63	6	0	0.712876	-3.695547	1.000000
64	6	0	2.843999	-2.465142	1.000000
65	6	0	1.432764	-4.931590	1.000000
66	6	0	3.554500	-3.706606	1.000000
67	6	0	2.833700	-4.908112	1.000000
68	6	0	0.681563	-6.156724	1.000000

69	6	0	4.991098	-3.668613	1.000000
70	1	0	3.377750	-5.850435	1.000000
71	1	0	1.229152	-7.096068	1.000000
72	1	0	5.530799	-4.612511	1.000000
73	6	0	0.641200	0.000000	-2.500000
74	6	0	1.491030	-1.275162	-2.500000
75	6	0	1.491030	1.275162	-2.500000
76	1	0	-0.018533	0.000000	-3.378325
77	1	0	-0.018533	0.000000	-1.621675
78	1	0	0.866970	-2.176386	-2.500000
79	1	0	2.138732	-1.316125	-3.384800
80	1	0	2.138732	-1.316125	-1.615200
81	1	0	0.866970	2.176386	-2.500000
82	1	0	2.139359	1.245732	-3.384800
83	1	0	2.139359	1.245732	-1.615200

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### fluoropropane

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.419200	0.000000	1.000000
2	6	0	2.848000	0.000000	1.000000
3	6	0	3.556875	-1.230405	1.000000
4	6	0	3.556875	1.230405	1.000000
5	6	0	4.987265	-1.224985	1.000000
6	6	0	4.987265	1.224985	1.000000
7	6	0	5.667400	0.000000	1.000000
8	6	0	5.672661	-2.488111	1.000000
9	6	0	5.672661	2.488111	1.000000
10	1	0	6.755500	0.000000	1.000000
11	1	0	6.759952	-2.483557	1.000000
12	1	0	6.759952	2.483557	1.000000
13	6	0	0.709600	1.229063	1.000000
14	6	0	1.424000	2.466440	1.000000
15	6	0	2.843999	2.465142	1.000000
16	6	0	0.712876	3.695547	1.000000

17	6	0	3.554500	3.706606	1.000000
18	6	0	1.432764	4.931590	1.000000
19	6	0	2.833700	4.908112	1.000000
20	6	0	4.991098	3.668613	1.000000
21	6	0	0.681563	6.156724	1.000000
22	1	0	3.377750	5.850435	1.000000
23	1	0	5.530799	4.612511	1.000000
24	1	0	1.229152	7.096068	1.000000
25	6	0	-0.709600	1.229063	1.000000
26	6	0	-1.424000	2.466440	1.000000
27	6	0	-0.712876	3.695547	1.000000
28	6	0	-2.843999	2.465142	1.000000
29	6	0	-1.432764	4.931590	1.000000
30	6	0	-3.554500	3.706606	1.000000
31	6	0	-2.833700	4.908112	1.000000
32	6	0	-0.681563	6.156724	1.000000
33	6	0	-4.991098	3.668613	1.000000
34	1	0	-3.377750	5.850435	1.000000
35	1	0	-1.229152	7.096068	1.000000
36	1	0	-5.530799	4.612511	1.000000
37	6	0	-1.419200	0.000000	1.000000
38	6	0	-2.848000	0.000000	1.000000
39	6	0	-3.556875	1.230405	1.000000
40	6	0	-3.556875	-1.230405	1.000000
41	6	0	-4.987265	1.224985	1.000000
42	6	0	-4.987265	-1.224985	1.000000
43	6	0	-5.667400	0.000000	1.000000
44	6	0	-5.672661	2.488111	1.000000
45	6	0	-5.672661	-2.488111	1.000000
46	1	0	-6.755500	0.000000	1.000000
47	1	0	-6.759952	2.483557	1.000000
48	1	0	-6.759952	-2.483557	1.000000
49	6	0	-0.709600	-1.229063	1.000000
50	6	0	-1.424000	-2.466440	1.000000
51	6	0	-2.843999	-2.465142	1.000000
52	6	0	-0.712876	-3.695547	1.000000
53	6	0	-3.554500	-3.706606	1.000000
54	6	0	-1.432764	-4.931590	1.000000

55	6	0	-2.833700	-4.908112	1.000000
56	6	0	-4.991098	-3.668613	1.000000
57	6	0	-0.681563	-6.156724	1.000000
58	1	0	-3.377750	-5.850435	1.000000
59	1	0	-5.530799	-4.612511	1.000000
60	1	0	-1.229152	-7.096068	1.000000
61	6	0	0.709600	-1.229063	1.000000
62	6	0	1.424000	-2.466440	1.000000
63	6	0	0.712876	-3.695547	1.000000
64	6	0	2.843999	-2.465142	1.000000
65	6	0	1.432764	-4.931590	1.000000
66	6	0	3.554500	-3.706606	1.000000
67	6	0	2.833700	-4.908112	1.000000
68	6	0	0.681563	-6.156724	1.000000
69	6	0	4.991098	-3.668613	1.000000
70	1	0	3.377750	-5.850435	1.000000
71	1	0	1.229152	-7.096068	1.000000
72	1	0	5.530799	-4.612511	1.000000
73	6	0	0.641200	0.000000	-3.090000
74	6	0	1.472888	-1.304061	-3.090000
75	6	0	1.472888	1.304061	-3.090000
76	9	0	-0.139946	0.000000	-4.194359
77	9	0	-0.139946	0.000000	-1.985641
78	9	0	0.644783	-2.354625	-3.090000
79	9	0	2.248758	-1.359072	-4.180655
80	9	0	2.248758	-1.359072	-1.999345
81	9	0	0.644783	2.354625	-3.090000
82	9	0	2.250378	1.326634	-4.180655
83	9	0	2.250378	1.326634	-1.999345

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