

Supporting Information

Substituent effects in halogen bonding complexes between aromatic donors and acceptors: a comprehensive ab initio study.

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Cartesian Coordinates

1.

C	-1.1520788	0.0000000	0.9188985
C	-1.2052966	0.0000000	-0.4867532
C	0.0000000	0.0000000	-1.2084579
C	1.2052966	0.0000000	-0.4867532
C	1.1520788	0.0000000	0.9188985
N	0.0000000	0.0000000	1.6276968
H	0.0000000	0.0000000	-2.3023752
H	-2.0753020	0.0000000	1.5076185
H	-2.1718725	0.0000000	-0.9981956
H	2.1718725	0.0000000	-0.9981956
H	2.0753020	0.0000000	1.5076185

2.

C	1.1513240	0.0000000	-0.9417664
C	1.2147666	0.0000000	0.4633810
C	0.0000000	0.0000000	1.1509359
C	-1.2147666	0.0000000	0.4633810
C	-1.1513240	0.0000000	-0.9417664
N	0.0000000	0.0000000	-1.6502148
H	2.0762010	0.0000000	-1.5268488
H	2.1667517	0.0000000	0.9984150
H	-2.1667517	0.0000000	0.9984150
H	-2.0762010	0.0000000	-1.5268488
F	0.0000000	0.0000000	2.5129173

3.

C	0.0100215	1.6338634	-1.1527888
C	-0.0145074	0.2297103	-1.2108547
C	-0.0291879	-0.4804363	0.0000000
C	-0.0145074	0.2297103	1.2108547
C	0.0100215	1.6338634	1.1527888
N	0.0224918	2.3407313	0.0000000
H	0.0177036	2.2223233	-2.0754678
H	-0.0296825	-0.2892789	-2.1718399
H	-0.0296825	-0.2892789	2.1718399
H	0.0177036	2.2223233	2.0754678
C	-0.0033434	-1.9853345	0.0000000
F	-0.6158724	-2.5056970	1.0944824

F	1.2747138	-2.4568028	0.0000000
F	-0.6158724	-2.5056970	-1.0944824

4.

C	1.1532315	0.0000000	-1.2676707
C	1.2139780	0.0000000	0.1356066
C	0.0000000	0.0000000	0.8531515
C	-1.2139780	0.0000000	0.1356066
C	-1.1532315	0.0000000	-1.2676707
N	0.0000000	0.0000000	-1.9750425
H	2.0760083	0.0000000	-1.8561462
H	2.1739777	0.0000000	0.6576820
H	-2.1739777	0.0000000	0.6576820
H	-2.0760083	0.0000000	-1.8561462
C	0.0000000	0.0000000	2.2967297
N	0.0000000	0.0000000	3.4862178

5.

C	0.0683911	1.8540305	-1.1510011
C	0.3230547	0.4722015	-1.2081666
C	0.4524309	-0.2301892	0.0000000
C	0.3230547	0.4722015	1.2081666
C	0.0683911	1.8540305	1.1510011
N	-0.0619538	2.5522322	0.0000000
H	-0.0322991	2.4314719	-2.0757345
H	0.4331656	-0.0446699	-2.1653954
H	0.4331656	-0.0446699	2.1653954
H	-0.0322991	2.4314719	2.0757345
O	0.7413794	-1.5848111	0.0000000
C	-0.4596449	-2.3827023	0.0000000
H	-0.1329853	-3.4302688	0.0000000
H	-1.0619254	-2.1751644	0.9004885
H	-1.0619254	-2.1751644	-0.9004885

6.

C	-0.0542724	1.4140120	-1.1456776
C	-0.0389217	0.0124537	-1.2018840
C	-0.0287952	-0.7247420	0.0000000
C	-0.0389217	0.0124537	1.2018840
C	-0.0542724	1.4140120	1.1456776
N	-0.0617044	2.1331625	0.0000000
H	-0.0598772	1.9925743	-2.0754466
H	-0.0386746	-0.4966334	-2.1711301
H	-0.0386746	-0.4966334	2.1711301
H	-0.0598772	1.9925743	2.0754466
N	-0.0814379	-2.1231699	0.0000000
H	0.2777147	-2.5650319	-0.8406768
H	0.2777147	-2.5650319	0.8406768

7.

C	0.0024581	2.3923660	-1.1415835
C	0.0938692	0.9939882	-1.2013325
C	0.1573379	0.2422141	0.0000000

C	0.0938692	0.9939882	1.2013325
C	0.0024581	2.3923660	1.1415835
N	-0.0427571	3.1158039	0.0000000
H	-0.0424882	2.9650372	-2.0741267
H	0.1152763	0.5155390	-2.1814739
H	0.1152763	0.5155390	2.1814739
H	-0.0424882	2.9650372	2.0741267
N	0.2978918	-1.1430331	0.0000000
C	-0.0370127	-1.8463812	1.2356725
H	-1.0875612	-1.6791197	1.5473479
H	0.1215212	-2.9218600	1.0795218
H	0.6277009	-1.5270619	2.0511003
C	-0.0370127	-1.8463812	-1.2356725
H	0.6277009	-1.5270619	-2.0511003
H	0.1215212	-2.9218600	-1.0795218
H	-1.0875612	-1.6791197	-1.5473479

8.

C	-1.2275465	0.0000000	-0.3637992
C	0.0000000	0.0000000	-1.0637677
C	1.2275465	0.0000000	-0.3637992
C	1.2193317	0.0000000	1.0407591
C	0.0000000	0.0000000	1.7446669
C	-1.2193317	0.0000000	1.0407591
H	-2.1684709	0.0000000	-0.9204028
H	2.1684709	0.0000000	-0.9204028
H	2.1670080	0.0000000	1.5865139
H	0.0000000	0.0000000	2.8383066
H	-2.1670080	0.0000000	1.5865139
C	0.0000000	0.0000000	-2.5079961
N	0.0000000	0.0000000	-3.6973519

9.

C	-1.2265782	0.0000000	-0.3830790
C	0.0000000	0.0000000	-1.0844126
C	1.2265782	0.0000000	-0.3830790
C	1.2285481	0.0000000	1.0205493
C	0.0000000	0.0000000	1.6906063
C	-1.2285481	0.0000000	1.0205493
H	-2.1691455	0.0000000	-0.9361593
H	2.1691455	0.0000000	-0.9361593
H	2.1601249	0.0000000	1.5909436
H	-2.1601249	0.0000000	1.5909436
C	0.0000000	0.0000000	-2.5277016
N	0.0000000	0.0000000	-3.7169488
F	0.0000000	0.0000000	3.0539476

10.

C	-0.0023389	1.0901502	-1.2270913
C	-0.0209567	-0.3122370	-1.2240700
C	-0.0350471	-1.0067044	0.0000000
C	-0.0209567	-0.3122370	1.2240700
C	-0.0023389	1.0901502	1.2270913

C	0.0082795	1.7909455	0.0000000
H	0.0030125	1.6447044	-2.1687722
H	-0.0339805	-0.8635694	-2.1669823
H	-0.0339805	-0.8635694	2.1669823
H	0.0030125	1.6447044	2.1687722
C	0.0250168	3.2345523	0.0000000
N	0.0384149	4.4240460	0.0000000
C	0.0018447	-2.5115982	0.0000000
F	-0.6066537	-3.0372278	1.0944580
F	1.2833256	-2.9748819	0.0000000
F	-0.6066537	-3.0372278	-1.0944580

11.

C	-0.7005840	1.2273926	0.0000000
C	-1.4024666	0.0000000	0.0000000
C	-0.7005840	-1.2273926	0.0000000
C	0.7005840	-1.2273926	0.0000000
C	1.4024666	0.0000000	0.0000000
C	0.7005840	1.2273926	0.0000000
H	-1.2553992	2.1690372	0.0000000
H	-1.2553992	-2.1690372	0.0000000
H	1.2553992	-2.1690372	0.0000000
H	1.2553992	2.1690372	0.0000000
C	-2.8454685	0.0000000	0.0000000
N	-4.0352553	0.0000000	0.0000000
C	2.8454685	0.0000000	0.0000000
N	4.0352553	0.0000000	0.0000000

12.

C	-0.1508168	-2.0053188	0.0000000
C	-0.2248702	-1.3074328	1.2264234
C	-0.3658667	0.0890943	1.2220912
C	-0.4364294	0.7831585	0.0000000
C	-0.3658667	0.0890943	-1.2220912
C	-0.2248702	-1.3074328	-1.2264234
H	-0.1761209	-1.8595057	2.1686832
H	-0.4385863	0.6482671	2.1590857
H	-0.4385863	0.6482671	-2.1590857
H	-0.1761209	-1.8595057	-2.1686832
O	-0.6155727	2.1573141	0.0000000
C	0.6454859	2.8575777	0.0000000
H	0.4030196	3.9278143	0.0000000
H	1.2293634	2.6025320	0.9004584
H	1.2293634	2.6025320	-0.9004584
C	-0.0070539	-3.4416507	0.0000000
N	0.1135288	-4.6248049	0.0000000

13.

C	-0.0347751	-0.8647076	-1.2208998
C	-0.0351210	-1.5747092	0.0000000
C	-0.0347751	-0.8647076	1.2208998
C	-0.0334786	0.5361311	1.2159468
C	-0.0304891	1.2565750	0.0000000
C	-0.0334786	0.5361311	-1.2159468

H	-0.0344657	-1.4117759	-2.1673892
H	-0.0344657	-1.4117759	2.1673892
H	-0.0391061	1.0800202	2.1661463
H	-0.0391061	1.0800202	-2.1661463
C	-0.0344563	-3.0164505	0.0000000
N	-0.0331739	-4.2059276	0.0000000
N	-0.1007433	2.6570055	0.0000000
H	0.2588174	3.1020857	0.8391315
H	0.2588174	3.1020857	-0.8391315

14.

C	-0.0910186	1.9027027	-1.2168144
C	-0.1220350	0.5024373	-1.2159157
C	-0.1549110	-0.2353810	0.0000000
C	-0.1220350	0.5024373	1.2159157
C	-0.0910186	1.9027027	1.2168144
C	-0.0779321	2.6176489	0.0000000
H	-0.0696955	2.4458532	-2.1654722
H	-0.1248334	-0.0114716	-2.1778281
H	-0.1248334	-0.0114716	2.1778281
H	-0.0696955	2.4458532	2.1654722
C	-0.0414385	4.0580971	0.0000000
N	-0.0116399	5.2474870	0.0000000
N	-0.2417411	-1.6265631	0.0000000
C	0.1075996	-2.3210769	1.2368702
H	0.0101875	-3.4018634	1.0695493
H	1.1418782	-2.1008504	1.5693519
H	-0.5882515	-2.0463752	2.0429773
C	0.1075996	-2.3210769	-1.2368702
H	0.0101875	-3.4018634	-1.0695493
H	-0.5882515	-2.0463752	-2.0429773
H	1.1418782	-2.1008504	-1.5693519

15.

C	-1.2058728	0.0000000	-0.6194676
C	0.0000000	0.0000000	-1.3412966
C	1.2058728	0.0000000	-0.6194676
C	1.1980744	0.0000000	0.7811772
C	0.0000000	0.0000000	1.5003245
C	-1.1980744	0.0000000	0.7811772
H	0.0000000	0.0000000	2.5915050
F	-2.3801759	0.0000000	1.4420584
F	-2.3925500	0.0000000	-1.2646287
F	2.3801759	0.0000000	1.4420584
F	2.3925500	0.0000000	-1.2646287
I	0.0000000	0.0000000	-3.4288115

16.

C	-1.2034789	0.0000000	-0.6404626
C	0.0000000	0.0000000	-1.3650772
C	1.2034789	0.0000000	-0.6404626
C	1.2114481	0.0000000	0.7598809
C	0.0000000	0.0000000	1.4625343

C	-1.2114481	0.0000000	0.7598809
F	-2.3768004	0.0000000	1.4348122
F	-2.3917104	0.0000000	-1.2806328
F	2.3768004	0.0000000	1.4348122
F	2.3917104	0.0000000	-1.2806328
I	0.0000000	0.0000000	-3.4520231
F	0.0000000	0.0000000	2.8073705

17.

C	0.0063678	-0.0525057	-1.2029968
C	0.0324060	-0.7814628	0.0000000
C	0.0063678	-0.0525057	1.2029968
C	0.0038484	1.3476306	1.2000957
C	0.0050014	2.0753186	0.0000000
C	0.0038484	1.3476306	-1.2000957
F	-0.0087058	1.9871739	2.3866843
F	-0.0272513	-0.6764019	2.3969410
F	-0.0272513	-0.6764019	-2.3969410
F	-0.0087058	1.9871739	-2.3866843
I	0.0006073	4.1592366	0.0000000
C	0.0138159	-2.2946109	0.0000000
F	0.6321788	-2.8072037	1.0864377
F	-1.2647064	-2.7558679	0.0000000
F	0.6321788	-2.8072037	-1.0864377

18.

C	-1.2061986	0.0000000	-0.9628510
C	0.0000000	0.0000000	-1.6857700
C	1.2061986	0.0000000	-0.9628510
C	1.2085137	0.0000000	0.4354052
C	0.0000000	0.0000000	1.1569798
C	-1.2085137	0.0000000	0.4354052
F	-2.3808425	0.0000000	1.0968974
F	-2.3893257	0.0000000	-1.6066922
F	2.3808425	0.0000000	1.0968974
F	2.3893257	0.0000000	-1.6066922
I	0.0000000	0.0000000	-3.7698070
C	0.0000000	0.0000000	2.5918306
N	0.0000000	0.0000000	3.7812478

19.

C	-0.3883090	-0.5625483	0.0000000
C	-0.3557481	0.1641189	1.2041546
C	-0.3031845	1.5629372	1.2032181
C	-0.2775133	2.2876622	0.0000000
C	-0.3031845	1.5629372	-1.2032181
C	-0.3557481	0.1641189	-1.2041546
F	-0.2758570	2.2059827	2.3924236
F	-0.3718438	-0.5004694	2.3793819
F	-0.2758570	2.2059827	-2.3924236
F	-0.3718438	-0.5004694	-2.3793819
I	-0.1984104	4.3736324	0.0000000
O	-0.5072947	-1.9216691	0.0000000

C	0.7659042	-2.6270200	0.0000000
H	0.8086666	-3.2516657	0.9025576
H	0.8086666	-3.2516657	-0.9025576
H	1.6015567	-1.9118645	0.0000000

20.

C	0.0557951	-1.1224509	-1.1988994
C	0.0749708	-1.8544068	0.0000000
C	0.0557951	-1.1224509	1.1988994
C	0.0270511	0.2740205	1.1945543
C	0.0147767	1.0146021	0.0000000
C	0.0270511	0.2740205	-1.1945543
F	0.0010034	0.9550055	-2.3711724
F	0.0632147	-1.7579044	-2.3940385
F	0.0010034	0.9550055	2.3711724
F	0.0632147	-1.7579044	2.3940385
I	0.1190282	-3.9406197	0.0000000
N	0.0695208	2.4062352	0.0000000
H	-0.2862126	2.8384239	-0.8474763
H	-0.2862126	2.8384239	0.8474763

21.

C	-0.1831312	0.7646712	-1.1870170
C	-0.2025822	-0.0241595	0.0000000
C	-0.1831312	0.7646712	1.1870170
C	-0.1024313	2.1612543	1.1831616
C	-0.0512360	2.9066357	0.0000000
C	-0.1024313	2.1612543	-1.1831616
F	-0.0811347	2.7867073	2.3846821
F	-0.2801118	0.1958166	2.4197154
F	-0.0811347	2.7867073	-2.3846821
F	-0.2801118	0.1958166	-2.4197154
I	0.0742602	4.9863285	0.0000000
N	-0.3034315	-1.4227356	0.0000000
C	0.1402715	-2.1309304	1.2186550
H	0.0904044	-3.2058788	1.0058414
H	1.1796827	-1.8724112	1.4960169
H	-0.5220549	-1.9222635	2.0626916
C	0.1402715	-2.1309304	-1.2186550
H	1.1796827	-1.8724112	-1.4960169
H	0.0904044	-3.2058788	-1.0058414
H	-0.5220549	-1.9222635	-2.0626916

22.

C	-4.5309893	-1.2083008	0.0000000
C	-3.1304965	-1.2030378	0.0000000
C	-2.4061455	0.0002207	0.0000000
C	-3.1431293	1.1957853	0.0000000
C	-4.5436049	1.1862713	0.0000000
C	-5.2582919	-0.0148143	0.0000000
H	-6.3494120	-0.0205678	0.0000000
F	-2.5072470	2.3922094	0.0000000
F	-5.2127178	2.3671406	0.0000000

F	-5.1876101	-2.3961661	0.0000000
F	-2.4820403	-2.3927244	0.0000000
I	-0.2933836	0.0112970	0.0000000
N	2.4812128	0.0166367	0.0000000
C	3.1709677	-1.1459777	0.0000000
C	3.1840207	1.1713683	0.0000000
C	4.5748779	-1.2027692	0.0000000
H	2.5684398	-2.0600671	0.0000000
C	4.5885055	1.2122733	0.0000000
H	2.5920169	2.0922788	0.0000000
C	5.3005598	0.0006981	0.0000000
H	5.0829210	-2.1707039	0.0000000
H	5.1074414	2.1744139	0.0000000
H	6.3941046	-0.0054642	0.0000000

23.

C	1.2106294	0.0000000	-4.5193595
C	1.1974619	0.0000000	-3.1189357
C	0.0000000	0.0000000	-2.3866401
C	-1.1974619	0.0000000	-3.1189357
C	-1.2106294	0.0000000	-4.5193595
C	0.0000000	0.0000000	-5.2232064
F	-2.3919434	0.0000000	-2.4816193
F	-2.3780792	0.0000000	-5.1965037
F	2.3780792	0.0000000	-5.1965037
F	2.3919434	0.0000000	-2.4816193
I	0.0000000	0.0000000	-0.2716425
N	0.0000000	0.0000000	2.4853671
C	1.1590030	0.0000000	3.1811383
C	-1.1590030	0.0000000	3.1811383
C	1.2075871	0.0000000	4.5852703
H	2.0763566	0.0000000	2.5836889
C	-1.2075871	0.0000000	4.5852703
H	-2.0763566	0.0000000	2.5836889
C	0.0000000	0.0000000	5.3040650
H	2.1725981	0.0000000	5.0988077
H	-2.1725981	0.0000000	5.0988077
H	0.0000000	0.0000000	6.3975932
F	0.0000000	0.0000000	-6.5705102

24.

C	3.6724250	-0.0077558	-1.2020180
C	2.2725086	-0.0056627	-1.1937760
C	1.5364880	-0.0073103	0.0000000
C	2.2725086	-0.0056627	1.1937760
C	3.6724250	-0.0077558	1.2020180
C	4.4035824	-0.0326394	0.0000000
F	1.6359887	0.0062669	2.3866109
F	4.2984397	0.0265332	2.3981528
F	4.2984397	0.0265332	-2.3981528
F	1.6359887	0.0062669	-2.3866109
I	-0.5764917	-0.0041993	0.0000000
N	-3.3216551	-0.0013105	0.0000000

C	-4.0170594	-0.0002608	-1.1593209
C	-4.0170594	-0.0002608	1.1593209
C	-5.4211074	0.0019166	-1.2076428
H	-3.4195587	-0.0011170	-2.0766105
C	-5.4211074	0.0019166	1.2076428
H	-3.4195587	-0.0011170	2.0766105
C	-6.1397689	0.0030282	0.0000000
H	-5.9346331	0.0027271	-2.1726275
H	-5.9346331	0.0027271	2.1726275
H	-7.2332727	0.0047591	0.0000000
C	5.9146887	-0.0127472	0.0000000
F	6.4313320	-0.6304478	-1.0864084
F	6.3797585	1.2660200	0.0000000
F	6.4313320	-0.6304478	1.0864084

25.

C	1.2074489	0.0000000	4.1754008
C	1.1995497	0.0000000	2.7772773
C	0.0000000	0.0000000	2.0457420
C	-1.1995497	0.0000000	2.7772773
C	-1.2074489	0.0000000	4.1754008
C	0.0000000	0.0000000	4.8990039
F	-2.3891174	0.0000000	2.1365582
F	-2.3821015	0.0000000	4.8388982
F	2.3821015	0.0000000	4.8388982
F	2.3891174	0.0000000	2.1365582
I	0.0000000	0.0000000	-0.0684379
N	0.0000000	0.0000000	-2.8046779
C	1.1595184	0.0000000	-3.4998072
C	-1.1595184	0.0000000	-3.4998072
C	1.2076710	0.0000000	-4.9038190
H	2.0768272	0.0000000	-2.9023613
C	-1.2076710	0.0000000	-4.9038190
H	-2.0768272	0.0000000	-2.9023613
C	0.0000000	0.0000000	-5.6224357
H	2.1726283	0.0000000	-5.4173538
H	-2.1726283	0.0000000	-5.4173538
H	0.0000000	0.0000000	-6.7159238
C	0.0000000	0.0000000	6.3338550
N	0.0000000	0.0000000	7.5232880

26.

C	3.4199941	-0.3503978	-1.2032260
C	2.0212929	-0.2957662	-1.1973446
C	1.2885586	-0.2692490	0.0000000
C	2.0212929	-0.2957662	1.1973446
C	3.4199941	-0.3503978	1.2032260
C	4.1476935	-0.3833560	0.0000000
F	1.3811305	-0.2677653	2.3925155
F	4.0866347	-0.3669821	2.3805118
F	4.0866347	-0.3669821	-2.3805118

F	1.3811305	-0.2677653	-2.3925155
I	-0.8224847	-0.1859142	0.0000000
N	-3.5979109	-0.0733669	0.0000000
C	-4.2937480	-0.0460415	-1.1586212
C	-4.2937480	-0.0460415	1.1586212
C	-5.6969060	0.0090630	-1.2075402
H	-3.6968561	-0.0696284	-2.0760886
C	-5.6969060	0.0090630	1.2075402
H	-3.6968561	-0.0696284	2.0760886
C	-6.4152485	0.0372409	0.0000000
H	-6.2100584	0.0290668	-2.1725836
H	-6.2100584	0.0290668	2.1725836
H	-7.5079759	0.0800498	0.0000000
O	5.5093375	-0.5018529	0.0000000
C	6.2104202	0.7716928	0.0000000
H	6.8356238	0.8178862	0.9024288
H	6.8356238	0.8178862	-0.9024288
H	5.4933949	1.6058862	0.0000000

27.

C	3.9609318	-0.0075662	-1.1935021
C	2.5638670	-0.0096359	-1.1933805
C	1.8242972	-0.0146410	0.0000000
C	2.5638670	-0.0096359	1.1933805
C	3.9609318	-0.0075662	1.1935021
C	4.7024004	-0.0097443	0.0000000
F	1.9311713	-0.0047537	2.3943181
F	4.6442625	0.0061123	2.3721608
F	4.6442625	0.0061123	-2.3721608
F	1.9311713	-0.0047537	-2.3943181
I	-0.2868062	-0.0193021	0.0000000
N	-3.0760604	-0.0270438	0.0000000
C	-3.7727399	-0.0300614	-1.1583634
C	-3.7727399	-0.0300614	1.1583634
C	-5.1770429	-0.0360550	-1.2074858
H	-3.1754251	-0.0277217	-2.0758868
C	-5.1770429	-0.0360550	1.2074858
H	-3.1754251	-0.0277217	2.0758868
C	-5.8960021	-0.0390870	0.0000000
H	-5.6905649	-0.0383806	-2.1725666
H	-5.6905649	-0.0383806	2.1725666
H	-6.9895853	-0.0437568	0.0000000
N	6.0965787	-0.0919341	0.0000000
H	6.5281291	0.2708167	-0.8452607
H	6.5281291	0.2708167	0.8452607

28.

C	2.5915946	0.1938139	-1.1862377
C	1.1925217	0.1759015	-1.1778970
C	0.4386084	0.1564888	0.0000000
C	1.1925217	0.1759015	1.1778970
C	2.5915946	0.1938139	1.1862377
C	3.3805189	0.1781719	0.0000000

F	0.5691900	0.1836162	2.3846440
F	3.1655804	0.2692341	2.4204775
F	3.1655804	0.2692341	-2.4204775
F	0.5691900	0.1836162	-2.3846440
I	-1.6680495	0.1266455	0.0000000
N	-4.4647411	0.0842411	0.0000000
C	-5.1615469	0.0741885	-1.1582411
C	-5.1615469	0.0741885	1.1582411
C	-6.5657564	0.0538854	-1.2074694
H	-4.5643850	0.0828938	-2.0758386
C	-6.5657564	0.0538854	1.2074694
H	-4.5643850	0.0828938	2.0758386
C	-7.2847082	0.0435180	0.0000000
H	-7.0792002	0.0465644	-2.1725742
H	-7.0792002	0.0465644	2.1725742
H	-8.3782001	0.0277623	0.0000000
N	4.7870825	0.2167421	0.0000000
C	5.4653060	-0.2810255	-1.2145452
H	6.5428796	-0.2825723	-1.0076531
H	5.1529438	-1.3106109	-1.4748417
H	5.2856169	0.3773260	-2.0681022
C	5.4653060	-0.2810255	1.2145452
H	5.1529438	-1.3106109	1.4748417
H	6.5428796	-0.2825723	1.0076531
H	5.2856169	0.3773260	2.0681022

29.

C	1.1974326	0.0000000	4.5575187
C	1.1999066	0.0000000	3.1570260
C	0.0000000	0.0000000	2.4270369
C	-1.1999066	0.0000000	3.1570260
C	-1.1974326	0.0000000	4.5575187
C	0.0000000	0.0000000	5.2782999
F	-2.3923956	0.0000000	2.5142880
F	-2.3815492	0.0000000	5.2201280
F	2.3815492	0.0000000	5.2201280
F	2.3923956	0.0000000	2.5142880
I	0.0000000	0.0000000	0.3169431
N	0.0000000	0.0000000	-2.4798963
C	1.1574897	0.0000000	-3.1771718
C	-1.1574897	0.0000000	-3.1771718
C	1.2168619	0.0000000	-4.5804735
H	2.0770985	0.0000000	-2.5839999
C	-1.2168619	0.0000000	-4.5804735
H	-2.0770985	0.0000000	-2.5839999
C	0.0000000	0.0000000	-5.2664280
H	2.1675548	0.0000000	-5.1174621
H	-2.1675548	0.0000000	-5.1174621
F	0.0000000	0.0000000	-6.6251083
H	0.0000000	0.0000000	6.3694459

30.

C	1.2107386	0.0000000	-4.5396421
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C	1.1979385	0.0000000	-3.1392425
C	0.0000000	0.0000000	-2.4076026
C	-1.1979385	0.0000000	-3.1392425
C	-1.2107386	0.0000000	-4.5396421
C	0.0000000	0.0000000	-5.2433925
F	-2.3918390	0.0000000	-2.5014164
F	-2.3779542	0.0000000	-5.2165036
F	2.3779542	0.0000000	-5.2165036
F	2.3918390	0.0000000	-2.5014164
I	0.0000000	0.0000000	-0.2955608
N	0.0000000	0.0000000	2.4841393
C	1.1577803	0.0000000	3.1809723
C	-1.1577803	0.0000000	3.1809723
C	1.2169417	0.0000000	4.5841584
H	2.0772354	0.0000000	2.5876250
C	-1.2169417	0.0000000	4.5841584
H	-2.0772354	0.0000000	2.5876250
C	0.0000000	0.0000000	5.2700819
H	2.1675992	0.0000000	5.1211888
H	-2.1675992	0.0000000	5.1211888
F	0.0000000	0.0000000	-6.5903748
F	0.0000000	0.0000000	6.6284297

31.

C	-1.2075727	0.0000000	-4.1947874
C	-1.2000574	0.0000000	-2.7966780
C	0.0000000	0.0000000	-2.0658183
C	1.2000574	0.0000000	-2.7966780
C	1.2075727	0.0000000	-4.1947874
C	0.0000000	0.0000000	-4.9181976
F	2.3890558	0.0000000	-2.1554380
F	2.3819938	0.0000000	-4.8579876
F	-2.3819938	0.0000000	-4.8579876
F	-2.3890558	0.0000000	-2.1554380
I	0.0000000	0.0000000	0.0452071
N	0.0000000	0.0000000	2.8041716
C	-1.1582532	0.0000000	3.5004958
C	1.1582532	0.0000000	3.5004958
C	-1.2170209	0.0000000	4.9034944
H	-2.0777158	0.0000000	2.9072169
C	1.2170209	0.0000000	4.9034944
H	2.0777158	0.0000000	2.9072169
C	0.0000000	0.0000000	5.5894745
H	-2.1676922	0.0000000	5.4404753
H	2.1676922	0.0000000	5.4404753
F	0.0000000	0.0000000	6.9471369
C	0.0000000	0.0000000	-6.3530571
N	0.0000000	0.0000000	-7.5424995

32.

C	-3.9796479	0.0116187	1.1936380
C	-2.5826226	0.0122533	1.1938212
C	-1.8436796	0.0165785	0.0000000

C	-2.5826226	0.0122533	-1.1938212
C	-3.9796479	0.0116187	-1.1936380
C	-4.7210598	0.0146056	0.0000000
F	-1.9494025	0.0067329	-2.3941943
F	-4.6626965	-0.0012925	-2.3720931
F	-4.6626965	-0.0012925	2.3720931
F	-1.9494025	0.0067329	2.3941943
I	0.2648638	0.0188899	0.0000000
N	3.0766779	0.0237158	0.0000000
C	3.7742638	0.0259170	1.1571697
C	3.7742638	0.0259170	-1.1571697
C	5.1777178	0.0302359	1.2168199
H	3.1810839	0.0242343	2.0768016
C	5.1777178	0.0302359	-1.2168199
H	3.1810839	0.0242343	-2.0768016
C	5.8636043	0.0323287	0.0000000
H	5.7146018	0.0319518	2.1675761
H	5.7146018	0.0319518	-2.1675761
F	7.2227708	0.0365460	0.0000000
N	-6.1146320	0.0981400	0.0000000
H	-6.5475704	-0.2620537	-0.8455758
H	-6.5475704	-0.2620537	0.8455758

33.

C	1.1976729	0.0000000	4.9028143
C	1.2005346	0.0000000	3.5023001
C	0.0000000	0.0000000	2.7732632
C	-1.2005346	0.0000000	3.5023001
C	-1.1976729	0.0000000	4.9028143
C	0.0000000	0.0000000	5.6232312
F	-2.3922258	0.0000000	2.8587694
F	-2.3814078	0.0000000	5.5649549
F	2.3814078	0.0000000	5.5649549
F	2.3922258	0.0000000	2.8587694
I	0.0000000	0.0000000	0.6660306
N	0.0000000	0.0000000	-2.1566982
C	1.1590560	0.0000000	-2.8532624
C	-1.1590560	0.0000000	-2.8532624
C	1.2159344	0.0000000	-4.2552403
H	2.0769358	0.0000000	-2.2571972
C	-1.2159344	0.0000000	-4.2552403
H	-2.0769358	0.0000000	-2.2571972
C	0.0000000	0.0000000	-4.9707284
H	2.1746398	0.0000000	-4.7791363
H	-2.1746398	0.0000000	-4.7791363
C	0.0000000	0.0000000	-6.4139990
N	0.0000000	0.0000000	-7.6035175
H	0.0000000	0.0000000	6.7144132

34.

C	1.2109578	0.0000000	4.8849235
C	1.1985876	0.0000000	3.4845478
C	0.0000000	0.0000000	2.7538435

C	-1.1985876	0.0000000	3.4845478
C	-1.2109578	0.0000000	4.8849235
C	0.0000000	0.0000000	5.5884784
F	-2.3916777	0.0000000	2.8459235
F	-2.3778222	0.0000000	5.5613640
F	2.3778222	0.0000000	5.5613640
F	2.3916777	0.0000000	2.8459235
I	0.0000000	0.0000000	0.6449680
N	0.0000000	0.0000000	-2.1605684
C	1.1593091	0.0000000	-2.8567472
C	-1.1593091	0.0000000	-2.8567472
C	1.2159682	0.0000000	-4.2586475
H	2.0770861	0.0000000	-2.2605746
C	-1.2159682	0.0000000	-4.2586475
H	-2.0770861	0.0000000	-2.2605746
C	0.0000000	0.0000000	-4.9740840
H	2.1746755	0.0000000	-4.7825180
H	-2.1746755	0.0000000	-4.7825180
C	0.0000000	0.0000000	-6.4173266
N	0.0000000	0.0000000	-7.6068469
F	0.0000000	0.0000000	6.9349931

35.

C	1.2077680	0.0000000	4.5399427
C	1.2007323	0.0000000	3.1418117
C	0.0000000	0.0000000	2.4119133
C	-1.2007323	0.0000000	3.1418117
C	-1.2077680	0.0000000	4.5399427
C	0.0000000	0.0000000	5.2630830
F	-2.3889284	0.0000000	2.4997965
F	-2.3818550	0.0000000	5.2027150
F	2.3818550	0.0000000	5.2027150
F	2.3889284	0.0000000	2.4997965
I	0.0000000	0.0000000	0.3041454
N	0.0000000	0.0000000	-2.4824288
C	1.1597114	0.0000000	-3.1782157
C	-1.1597114	0.0000000	-3.1782157
C	1.2159770	0.0000000	-4.5799992
H	2.0775642	0.0000000	-2.5822154
C	-1.2159770	0.0000000	-4.5799992
H	-2.0775642	0.0000000	-2.5822154
C	0.0000000	0.0000000	-5.2954186
H	2.1747079	0.0000000	-5.1037901
H	-2.1747079	0.0000000	-5.1037901
C	0.0000000	0.0000000	6.6979523
N	0.0000000	0.0000000	7.8874041
C	0.0000000	0.0000000	-6.7386060
N	0.0000000	0.0000000	-7.9281357

36.

C	-4.3212749	0.0075804	1.1938594
C	-2.9243208	0.0079254	1.1943906
C	-2.1861720	0.0118804	0.0000000

C	-2.9243208	0.0079254	-1.1943906
C	-4.3212749	0.0075804	-1.1938594
C	-5.0625798	0.0107155	0.0000000
F	-2.2903247	0.0025426	-2.3940229
F	-5.0039057	-0.0050468	-2.3719741
F	-5.0039057	-0.0050468	2.3719741
F	-2.2903247	0.0025426	2.3940229
I	-0.0805710	0.0156883	0.0000000
N	2.7571591	0.0233574	0.0000000
C	3.4540363	0.0259542	1.1587568
C	3.4540363	0.0259542	-1.1587568
C	4.8561092	0.0311627	1.2159289
H	2.8579173	0.0237560	2.0766252
C	4.8561092	0.0311627	-1.2159289
H	2.8579173	0.0237560	-2.0766252
C	5.5716062	0.0338321	0.0000000
H	5.3799700	0.0329400	2.1746629
H	5.3799700	0.0329400	-2.1746629
C	7.0148934	0.0386785	0.0000000
N	8.2044005	0.0425395	0.0000000
N	-6.4553758	0.0945703	0.0000000
H	-6.8898871	-0.2624456	-0.8460361
H	-6.8898871	-0.2624456	0.8460361

37.

C	5.1147092	0.0558942	-1.1971101
C	3.7142440	0.0456823	-1.1986619
C	2.9824536	0.0404369	0.0000000
C	3.7142440	0.0456823	1.1986619
C	5.1147092	0.0558942	1.1971101
C	5.8360310	0.0611194	0.0000000
F	3.0728778	0.0409628	2.3926768
F	5.7779755	0.0606382	2.3818444
F	5.7779755	0.0606382	-2.3818444
F	3.0728778	0.0409628	-2.3926768
I	0.8659093	0.0252530	0.0000000
N	-1.8783574	0.0049678	0.0000000
C	-2.5852405	-0.0001540	-1.1525162
C	-2.5852405	-0.0001540	1.1525162
C	-3.9842768	-0.0116224	-1.2045866
H	-1.9980966	0.0037466	-2.0765953
C	-3.9842768	-0.0116224	1.2045866
H	-1.9980966	0.0037466	2.0765953
C	-4.7204882	-0.0189554	0.0000000
H	-4.4945824	-0.0106645	-2.1725895
H	-4.4945824	-0.0106645	2.1725895
N	-6.1122536	0.0363021	0.0000000
H	-6.5678209	-0.2935981	-0.8444629
H	-6.5678209	-0.2935981	0.8444629
H	6.9271266	0.0691061	0.0000000

38.

C	5.0968395	0.0540652	-1.2104727
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C	3.6964030	0.0459027	-1.1967298
C	2.9631045	0.0417073	0.0000000
C	3.6964030	0.0459027	1.1967298
C	5.0968395	0.0540652	1.2104727
C	5.8008154	0.0581088	0.0000000
F	3.0598013	0.0421282	2.3920982
F	5.7744302	0.0579121	2.3782162
F	5.7744302	0.0579121	-2.3782162
F	3.0598013	0.0421282	-2.3920982
I	0.8439565	0.0295450	0.0000000
N	-1.8821505	0.0119541	0.0000000
C	-2.5885080	0.0043012	-1.1528433
C	-2.5885080	0.0043012	1.1528433
C	-3.9873381	-0.0115478	-1.2047072
H	-2.0011698	0.0099584	-2.0767429
C	-3.9873381	-0.0115478	1.2047072
H	-2.0011698	0.0099584	2.0767429
C	-4.7235861	-0.0210911	0.0000000
H	-4.4975720	-0.0123103	-2.1727093
H	-4.4975720	-0.0123103	2.1727093
N	-6.1148630	0.0298080	0.0000000
H	-6.5708035	-0.2983463	-0.8448522
H	-6.5708035	-0.2983463	0.8448522
F	7.1485580	0.0658410	0.0000000

39.

C	4.7544786	0.0479857	-1.2072465
C	3.3563753	0.0418418	-1.1987031
C	2.6236405	0.0386416	0.0000000
C	3.3563753	0.0418418	1.1987031
C	4.7544786	0.0479857	1.2072465
C	5.4784160	0.0511409	0.0000000
F	2.7165083	0.0389612	2.3892934
F	5.4183918	0.0507740	2.3822352
F	5.4183918	0.0507740	-2.3822352
F	2.7165083	0.0389612	-2.3892934
I	0.5051890	0.0293695	0.0000000
N	-2.1984393	0.0146002	0.0000000
C	-2.9042268	0.0056084	-1.1533673
C	-2.9042268	0.0056084	1.1533673
C	-4.3027471	-0.0125075	-1.2048550
H	-2.3169327	0.0121726	-2.0772379
C	-4.3027471	-0.0125075	1.2048550
H	-2.3169327	0.0121726	2.0772379
C	-5.0391706	-0.0230804	0.0000000
H	-4.8128098	-0.0142871	-2.1728802
H	-4.8128098	-0.0142871	2.1728802
N	-6.4293339	0.0252309	0.0000000
H	-6.8871170	-0.2981330	-0.8455488
H	-6.8871170	-0.2981330	0.8455488
C	6.9132142	0.0571949	0.0000000
N	8.1026428	0.0620702	0.0000000

39. (T-shape)

C	0.0170191	-2.9061736	-1.1532443
C	0.0105456	-4.3047967	-1.2047685
C	0.0058720	-5.0413248	0.0000000
C	0.0105456	-4.3047967	1.2047685
C	0.0170191	-2.9061736	1.1532443
N	0.0199358	-2.2002268	0.0000000
H	0.0188521	-2.3189858	-2.0772532
H	0.0130142	-4.8147483	-2.1728326
H	0.0130142	-4.8147483	2.1728326
H	0.0188521	-2.3189858	2.0772532
N	0.0653720	-6.4310884	0.0000000
H	-0.2546832	-6.8913608	0.8454713
H	-0.2546832	-6.8913608	-0.8454713
C	-1.1840611	4.7569512	0.0000000
C	-1.1758561	3.3587445	0.0000000
C	0.0229081	2.6256310	0.0000000
C	1.2218365	3.3584923	0.0000000
C	1.2302518	4.7567300	0.0000000
C	0.0231610	5.4806707	0.0000000
I	0.0226528	0.5064968	0.0000000
F	2.4122594	2.7191689	0.0000000
F	2.4051598	5.4206861	0.0000000
F	-2.3664936	2.7196074	0.0000000
F	-2.3589034	5.4211158	0.0000000
C	0.0232343	6.9155225	0.0000000
N	0.0231751	8.1049530	0.0000000

40.

C	4.5401424	0.0341039	-1.1932991
C	3.1429941	0.0344586	-1.1927584
C	2.4025336	0.0385233	0.0000000
C	3.1429941	0.0344586	1.1927584
C	4.5401424	0.0341039	1.1932991
C	5.2816907	0.0372501	0.0000000
F	2.5109752	0.0286399	2.3944452
F	5.2238382	0.0210987	2.3722938
F	5.2238382	0.0210987	-2.3722938
F	2.5109752	0.0286399	-2.3944452
I	0.2876498	0.0408573	0.0000000
N	-2.4722230	0.0426284	0.0000000
C	-3.1794298	0.0407580	-1.1521981
C	-3.1794298	0.0407580	1.1521981
C	-4.5787057	0.0360551	-1.2044968
H	-2.5922454	0.0418525	-2.0762948
C	-4.5787057	0.0360551	1.2044968
H	-2.5922454	0.0418525	2.0762948
C	-5.3148021	0.0322583	0.0000000
H	-5.0891626	0.0396257	-2.1724570
H	-5.0891626	0.0396257	2.1724570
N	6.6764296	0.1210873	0.0000000
H	7.1071533	-0.2434210	0.8449785
H	7.1071533	-0.2434210	-0.8449785

N	-6.7071155	0.0946728	0.0000000
H	-7.1626412	-0.2368100	-0.8439856
H	-7.1626412	-0.2368100	0.8439856

41.

C	5.4124356	0.0085257	1.1975993
C	4.0119436	0.0028936	1.2003242
C	3.2825686	0.0000877	0.0000000
C	4.0119436	0.0028936	-1.2003242
C	5.4124356	0.0085257	-1.1975993
C	6.1329614	0.0114061	0.0000000
F	3.3686945	0.0002378	-2.3922721
F	6.0748274	0.0111517	-2.3814189
F	6.0748274	0.0111517	2.3814189
F	3.3686945	0.0002378	2.3922721
I	1.1745283	-0.0086252	0.0000000
N	-1.6402525	-0.0183394	0.0000000
C	-2.3360818	-0.0198889	1.1587675
C	-2.3360818	-0.0198889	-1.1587675
C	-3.7391865	-0.0227001	1.2128776
H	-1.7397155	-0.0211885	2.0763351
C	-3.7391865	-0.0227001	-1.2128776
H	-1.7397155	-0.0211885	-2.0763351
C	-4.4469565	-0.0262319	0.0000000
H	-4.2604423	-0.0293285	2.1724582
H	-4.2604423	-0.0293285	-2.1724582
H	7.2241442	0.0158336	0.0000000
C	-5.9528499	0.0226516	0.0000000
F	-6.4794015	-0.5820518	1.0945551
F	-6.4002903	1.3079153	0.0000000
F	-6.4794015	-0.5820518	-1.0945551

42.

C	5.6423021	0.0410791	1.1972924
C	4.2426440	0.0894986	1.1993468
C	3.5122441	0.1145340	0.0000000
C	4.2426440	0.0894986	-1.1993468
C	5.6423021	0.0410791	-1.1972924
C	6.3629111	0.0163124	0.0000000
F	3.6008695	0.1115635	-2.3924671
F	6.3048001	0.0181546	-2.3817158
F	6.3048001	0.0181546	2.3817158
F	3.6008695	0.1115635	2.3924671
I	1.4006251	0.1888486	0.0000000
N	-1.3705920	0.2826286	0.0000000
C	-2.0682998	0.3023705	1.1575847
C	-2.0682998	0.3023705	-1.1575847
C	-3.4711309	0.3377217	1.2103449
H	-1.4736127	0.2931266	2.0766085
C	-3.4711309	0.3377217	-1.2103449
H	-1.4736127	0.2931266	-2.0766085
C	-4.1836070	0.3549753	0.0000000
H	-4.0010442	0.3658860	2.1659876

H	-4.0010442	0.3658860	-2.1659876
H	7.4534079	-0.0213490	0.0000000
O	-5.5633347	0.4298612	0.0000000
C	-6.1687374	-0.8811126	0.0000000
H	-5.8712967	-1.4432953	0.9009344
H	-7.2533801	-0.7169088	0.0000000
H	-5.8712967	-1.4432953	-0.9009344

43.

C	6.4589899	-0.4714890	1.2225074
C	5.0613633	-0.3817590	1.2189130
C	4.3325488	-0.3683360	0.0185280
C	5.0654584	-0.4484410	-1.1767531
C	6.4630803	-0.5380927	-1.1705772
C	7.1810909	-0.5509638	0.0284807
F	4.4277968	-0.4405351	-2.3729739
F	7.1272135	-0.6134857	-2.3527555
F	7.1190734	-0.4809560	2.4093110
F	4.4196214	-0.3073855	2.4106567
I	2.2181427	-0.2323899	0.0111313
N	-0.5035900	-0.0562924	0.0012976
C	-1.2161490	0.0261950	1.1470181
C	-1.2112579	-0.0366799	-1.1502404
C	-2.6114399	0.1224307	1.1971195
H	-0.6351716	0.0199630	2.0751524
C	-2.6063133	0.0565099	-1.2114707
H	-0.6263341	-0.0935855	-2.0741635
C	-3.3612877	0.1249320	-0.0097499
H	-3.0931078	0.1929445	2.1729050
H	-3.0837887	0.0735037	-2.1917064
H	8.2699670	-0.6208620	0.0322876
N	-4.7441883	0.1722940	-0.0139951
C	-5.4123515	0.5075569	-1.2688390
H	-6.4971909	0.4945128	-1.1014785
H	-5.1196147	1.5058827	-1.6488096
H	-5.1840435	-0.2445811	-2.0381718
C	-5.4176471	0.5756445	1.2177692
H	-6.5017648	0.5534532	1.0467420
H	-5.1927503	-0.1332657	2.0280615
H	-5.1263554	1.5932776	1.5438035

44.

C	1.1971391	0.0000000	-6.0448466
C	1.2014668	0.0000000	-4.6444053
C	0.0000000	0.0000000	-3.9150589
C	-1.2014668	0.0000000	-4.6444053
C	-1.1971391	0.0000000	-6.0448466
C	0.0000000	0.0000000	-6.7656602
H	0.0000000	0.0000000	-7.8567357
F	-2.3925803	0.0000000	-4.0026918
F	-2.3811524	0.0000000	-6.7069970
F	2.3811524	0.0000000	-6.7069970
F	2.3925803	0.0000000	-4.0026918

I	0.0000000	0.0000000	-1.8202594
C	1.2290683	0.0000000	4.4935275
C	-1.2290683	0.0000000	4.4935275
C	1.2198605	0.0000000	5.8978756
H	2.1696634	0.0000000	3.9365111
C	-1.2198605	0.0000000	5.8978756
H	-2.1696634	0.0000000	3.9365111
C	0.0000000	0.0000000	6.6009675
H	2.1671308	0.0000000	6.4441328
H	-2.1671308	0.0000000	6.4441328
H	0.0000000	0.0000000	7.6945403
C	0.0000000	0.0000000	3.7962079
C	0.0000000	0.0000000	2.3537951
N	0.0000000	0.0000000	1.1659910

45.

C	1.2104227	0.0000000	-6.0256764
C	1.1994365	0.0000000	-4.6253288
C	0.0000000	0.0000000	-3.8940923
C	-1.1994365	0.0000000	-4.6253288
C	-1.2104227	0.0000000	-6.0256764
C	0.0000000	0.0000000	-6.7295225
F	-2.3919549	0.0000000	-3.9885521
F	-2.3776172	0.0000000	-6.7018872
F	2.3776172	0.0000000	-6.7018872
F	2.3919549	0.0000000	-3.9885521
I	0.0000000	0.0000000	-1.7986198
C	1.2291790	0.0000000	4.4954486
C	-1.2291790	0.0000000	4.4954486
C	1.2198756	0.0000000	5.8997811
H	2.1697870	0.0000000	3.9384717
C	-1.2198756	0.0000000	5.8997811
H	-2.1697870	0.0000000	3.9384717
C	0.0000000	0.0000000	6.6028409
H	2.1671251	0.0000000	6.4460651
H	-2.1671251	0.0000000	6.4460651
H	0.0000000	0.0000000	7.6964006
C	0.0000000	0.0000000	3.7983501
C	0.0000000	0.0000000	2.3560195
N	0.0000000	0.0000000	1.1683332
F	0.0000000	0.0000000	-8.0763538

46.

C	1.2018979	-0.0069959	5.0762330
C	1.1958300	-0.0057705	3.6763585
C	-0.0000014	-0.0075667	2.9415154
C	-1.1958373	-0.0056335	3.6763500
C	-1.2019202	-0.0068679	5.0762253
C	-0.0000148	-0.0318952	5.8071402
F	-2.3866812	0.0061228	3.0402270
F	-2.3976275	0.0275838	5.7014998
F	2.3975992	0.0273433	5.7015264
F	2.3866807	0.0058220	3.0402456

I	0.0000055	-0.0064606	0.8491465
C	1.2292932	0.0000154	-5.4319449
C	-1.2292869	-0.0001952	-5.4319376
C	1.2199133	0.0021392	-6.8362639
H	2.1699182	-0.0007653	-4.8750007
C	-1.2199158	0.0019179	-6.8362566
H	-2.1699085	-0.0011236	-4.8749880
C	-0.0000034	0.0031040	-7.5392288
H	2.1671250	0.0030837	-7.3825918
H	-2.1671308	0.0026757	-7.3825789
H	-0.0000068	0.0047965	-8.6327719
C	0.0000053	-0.0011597	-4.7350753
C	0.0000096	-0.0033867	-3.2928074
N	0.0000130	-0.0053888	-2.1052369
C	0.0000025	-0.0113308	7.3185101
F	1.0863407	-0.6290391	7.8347101
F	0.0002347	1.2676330	7.7822523
F	-1.0865343	-0.6286578	7.8347427

47.

C	1.2073476	0.0000000	-5.6474732
C	1.2017555	0.0000000	-4.2494253
C	0.0000000	0.0000000	-3.5190741
C	-1.2017555	0.0000000	-4.2494253
C	-1.2073476	0.0000000	-5.6474732
C	0.0000000	0.0000000	-6.3708137
F	-2.3892341	0.0000000	-3.6090977
F	-2.3815861	0.0000000	-6.3102051
F	2.3815861	0.0000000	-6.3102051
F	2.3892341	0.0000000	-3.6090977
I	0.0000000	0.0000000	-1.4264708
C	1.2293622	0.0000000	4.8467258
C	-1.2293622	0.0000000	4.8467258
C	1.2199465	0.0000000	6.2510400
H	2.1700252	0.0000000	4.2898421
C	-1.2199465	0.0000000	6.2510400
H	-2.1700252	0.0000000	4.2898421
C	0.0000000	0.0000000	6.9539616
H	2.1671394	0.0000000	6.7973734
H	-2.1671394	0.0000000	6.7973734
H	0.0000000	0.0000000	8.0475056
C	0.0000000	0.0000000	4.1499619
C	0.0000000	0.0000000	2.7077566
N	0.0000000	0.0000000	1.5202273
C	0.0000000	0.0000000	-7.8056134
N	0.0000000	0.0000000	-8.9950010

48.

C	-4.8042701	-0.2785835	1.2030970
C	-3.4047114	-0.2577035	1.1991537
C	-2.6726571	-0.2489255	0.0000000
C	-3.4047114	-0.2577035	-1.1991537
C	-4.8042701	-0.2785835	-1.2030970

C	-5.5325374	-0.2940451	0.0000000
F	-2.7647186	-0.2446664	-2.3925841
F	-5.4702160	-0.2788379	-2.3801219
F	-5.4702160	-0.2788379	2.3801219
F	-2.7647186	-0.2446664	2.3925841
I	-0.5780204	-0.2132958	0.0000000
C	5.7385831	-0.1081499	1.2290448
C	5.7385831	-0.1081499	-1.2290448
C	7.1427492	-0.0857155	1.2198517
H	5.1815118	-0.1171658	2.1695629
C	7.1427492	-0.0857155	-1.2198517
H	5.1815118	-0.1171658	-2.1695629
C	7.8457639	-0.0744295	0.0000000
H	7.6889134	-0.0770735	2.1671432
H	7.6889134	-0.0770735	-2.1671432
H	8.9391973	-0.0570199	0.0000000
C	5.0413158	-0.1193446	0.0000000
C	3.5990923	-0.1424709	0.0000000
N	2.4114240	-0.1618364	0.0000000
O	-6.8962265	-0.3789536	0.0000000
C	-7.5657396	0.9118613	0.0000000
H	-8.1895618	0.9731700	-0.9024211
H	-8.1895618	0.9731700	0.9024211
H	-6.8281716	1.7279122	0.0000000

49.

C	5.4013915	0.0037123	-1.1934113
C	4.0044278	0.0050786	-1.1951168
C	3.2659181	0.0093315	0.0000000
C	4.0044278	0.0050786	1.1951168
C	5.4013915	0.0037123	1.1934113
C	6.1428110	0.0065714	0.0000000
F	3.3722834	-0.0002883	2.3942648
F	6.0839199	-0.0093207	2.3717831
F	6.0839199	-0.0093207	-2.3717831
F	3.3722834	-0.0002883	-2.3942648
I	1.1715752	0.0123633	0.0000000
C	-5.1569095	0.0311206	-1.2289354
C	-5.1569095	0.0311206	1.2289354
C	-6.5612566	0.0372186	-1.2198106
H	-4.5999089	0.0287862	-2.1695379
C	-6.5612566	0.0372186	1.2198106
H	-4.5999089	0.0287862	2.1695379
C	-7.2644485	0.0402614	0.0000000
H	-7.1075162	0.0396701	-2.1670991
H	-7.1075162	0.0396701	2.1670991
H	-8.3580196	0.0450461	0.0000000
C	-4.4593719	0.0281039	0.0000000
C	-3.0169119	0.0219208	0.0000000
N	-1.8290183	0.0167502	0.0000000
N	7.5363487	0.0895660	0.0000000
H	7.9691270	-0.2709347	0.8455481
H	7.9691270	-0.2709347	-0.8455481

50.

C	5.4013915	0.0037123	-1.1934113
C	4.0044278	0.0050786	-1.1951168
C	3.2659181	0.0093315	0.0000000
C	4.0044278	0.0050786	1.1951168
C	5.4013915	0.0037123	1.1934113
C	6.1428110	0.0065714	0.0000000
F	3.3722834	-0.0002883	2.3942648
F	6.0839199	-0.0093207	2.3717831
F	6.0839199	-0.0093207	-2.3717831
F	3.3722834	-0.0002883	-2.3942648
I	1.1715752	0.0123633	0.0000000
C	-5.1569095	0.0311206	-1.2289354
C	-5.1569095	0.0311206	1.2289354
C	-6.5612566	0.0372186	-1.2198106
H	-4.5999089	0.0287862	-2.1695379
C	-6.5612566	0.0372186	1.2198106
H	-4.5999089	0.0287862	2.1695379
C	-7.2644485	0.0402614	0.0000000
H	-7.1075162	0.0396701	-2.1670991
H	-7.1075162	0.0396701	2.1670991
H	-8.3580196	0.0450461	0.0000000
C	-4.4593719	0.0281039	0.0000000
C	-3.0169119	0.0219208	0.0000000
N	-1.8290183	0.0167502	0.0000000
N	7.5363487	0.0895660	0.0000000
H	7.9691270	-0.2709347	0.8455481
H	7.9691270	-0.2709347	-0.8455481

51.

C	1.1971907	0.0000000	-6.0581291
C	1.2015867	0.0000000	-4.6576877
C	0.0000000	0.0000000	-3.9285950
C	-1.2015867	0.0000000	-4.6576877
C	-1.1971907	0.0000000	-6.0581291
C	0.0000000	0.0000000	-6.7788780
F	-2.3925641	0.0000000	-4.0157714
F	-2.3811172	0.0000000	-6.7201622
F	2.3811172	0.0000000	-6.7201622
F	2.3925641	0.0000000	-4.0157714
I	0.0000000	0.0000000	-1.8341373
C	1.2280576	0.0000000	4.4866957
C	-1.2280576	0.0000000	4.4866957
C	1.2290619	0.0000000	5.8899101
H	2.1702520	0.0000000	3.9330723
C	-1.2290619	0.0000000	5.8899101
H	-2.1702520	0.0000000	3.9330723
C	0.0000000	0.0000000	6.5596275
H	2.1603325	0.0000000	6.4607293
H	-2.1603325	0.0000000	6.4607293
C	0.0000000	0.0000000	3.7878397
C	0.0000000	0.0000000	2.3464763

N	0.0000000	0.0000000	1.1587477
F	0.0000000	0.0000000	7.9215584
H	0.0000000	0.0000000	-7.8699533

52.

C	1.2104775	0.0000000	-6.0388861
C	1.1995565	0.0000000	-4.6385499
C	0.0000000	0.0000000	-3.9075584
C	-1.1995565	0.0000000	-4.6385499
C	-1.2104775	0.0000000	-6.0388861
C	0.0000000	0.0000000	-6.7426963
F	-2.3919352	0.0000000	-4.0015568
F	-2.3775761	0.0000000	-6.7150036
F	2.3775761	0.0000000	-6.7150036
F	2.3919352	0.0000000	-4.0015568
I	0.0000000	0.0000000	-1.8125040
C	1.2281501	0.0000000	4.4885843
C	-1.2281501	0.0000000	4.4885843
C	1.2291023	0.0000000	5.8917593
H	2.1703361	0.0000000	3.9349594
C	-1.2291023	0.0000000	5.8917593
H	-2.1703361	0.0000000	3.9349594
C	0.0000000	0.0000000	6.5614534
H	2.1603418	0.0000000	6.4626326
H	-2.1603418	0.0000000	6.4626326
C	0.0000000	0.0000000	3.7899146
C	0.0000000	0.0000000	2.3486557
N	0.0000000	0.0000000	1.1610442
F	0.0000000	0.0000000	7.9231984
F	0.0000000	0.0000000	-8.0893862

53.

C	1.2104775	0.0000000	-6.0388861
C	1.1995565	0.0000000	-4.6385499
C	0.0000000	0.0000000	-3.9075584
C	-1.1995565	0.0000000	-4.6385499
C	-1.2104775	0.0000000	-6.0388861
C	0.0000000	0.0000000	-6.7426963
F	-2.3919352	0.0000000	-4.0015568
F	-2.3775761	0.0000000	-6.7150036
F	2.3775761	0.0000000	-6.7150036
F	2.3919352	0.0000000	-4.0015568
I	0.0000000	0.0000000	-1.8125040
C	1.2281501	0.0000000	4.4885843
C	-1.2281501	0.0000000	4.4885843
C	1.2291023	0.0000000	5.8917593
H	2.1703361	0.0000000	3.9349594
C	-1.2291023	0.0000000	5.8917593
H	-2.1703361	0.0000000	3.9349594
C	0.0000000	0.0000000	6.5614534
H	2.1603418	0.0000000	6.4626326
H	-2.1603418	0.0000000	6.4626326
C	0.0000000	0.0000000	3.7899146

C	0.0000000	0.0000000	2.3486557
N	0.0000000	0.0000000	1.1610442
F	0.0000000	0.0000000	7.9231984
F	0.0000000	0.0000000	-8.0893862

54.

C	5.4133882	0.0006906	-1.1934729
C	4.0164455	0.0025811	-1.1952325
C	3.2781899	0.0070954	0.0000000
C	4.0164455	0.0025811	1.1952325
C	5.4133882	0.0006906	1.1934729
C	6.1547935	0.0032472	0.0000000
F	3.3840763	-0.0024827	2.3942294
F	6.0958197	-0.0125456	2.3717663
F	6.0958197	-0.0125456	-2.3717663
F	3.3840763	-0.0024827	-2.3942294
I	1.1841426	0.0111649	0.0000000
C	-5.1507162	0.0339370	-1.2279241
C	-5.1507162	0.0339370	1.2279241
C	-6.5539582	0.0405152	-1.2290110
H	-4.5972082	0.0314139	-2.1701818
C	-6.5539582	0.0405152	1.2290110
H	-4.5972082	0.0314139	2.1701818
C	-7.2236937	0.0436293	0.0000000
H	-7.1247269	0.0432332	-2.1603170
H	-7.1247269	0.0432332	2.1603170
C	-4.4516602	0.0306242	0.0000000
C	-3.0102613	0.0237689	0.0000000
N	-1.8224468	0.0179976	0.0000000
F	-8.5858562	0.0499958	0.0000000
N	7.5481416	0.0857173	0.0000000
H	7.9812051	-0.2739629	0.8457171
H	7.9812051	-0.2739629	-0.8457171

55.

C	6.6751150	0.0413578	-1.1970068
C	5.2747077	0.0377013	-1.2010669
C	4.5446433	0.0358636	0.0000000
C	5.2747077	0.0377013	1.2010669
C	6.6751150	0.0413578	1.1970068
C	7.3961315	0.0432681	0.0000000
F	4.6334674	0.0359795	2.3926499
F	7.3374528	0.0429892	2.3812400
F	7.3374528	0.0429892	-2.3812400
F	4.6334674	0.0359795	-2.3926499
I	2.4490170	0.0303447	0.0000000
C	-3.8494242	0.0063223	-1.2224198
C	-3.8494242	0.0063223	1.2224198
C	-5.2495444	-0.0020461	-1.2167127
H	-3.3019107	0.0086759	-2.1685651
C	-5.2495444	-0.0020461	1.2167127
H	-3.3019107	0.0086759	2.1685651
C	-5.9699122	-0.0084698	0.0000000

H	-5.7935496	0.0006339	-2.1667180
H	-5.7935496	0.0006339	2.1667180
C	-3.1416962	0.0100192	0.0000000
C	-1.7025372	0.0164053	0.0000000
N	-0.5145646	0.0212511	0.0000000
N	-7.3678329	0.0539815	0.0000000
H	-7.8165352	-0.2960480	-0.8408435
H	-7.8165352	-0.2960480	0.8408435
H	8.4871934	0.0462047	0.0000000

56.

C	6.6558658	0.0413473	-1.2102963
C	5.2555234	0.0375525	-1.1990594
C	4.5236544	0.0356027	0.0000000
C	5.2555234	0.0375525	1.1990594
C	6.6558658	0.0413473	1.2102963
C	7.3598239	0.0432595	0.0000000
F	4.6192206	0.0357698	2.3920363
F	7.3322602	0.0431005	2.3776955
F	7.3322602	0.0431005	-2.3776955
F	4.6192206	0.0357698	-2.3920363
I	2.4271953	0.0298989	0.0000000
C	-3.8510001	0.0059474	-1.2225125
C	-3.8510001	0.0059474	1.2225125
C	-5.2510615	-0.0021509	-1.2167667
H	-3.3035490	0.0082086	-2.1686853
C	-5.2510615	-0.0021509	1.2167667
H	-3.3035490	0.0082086	2.1686853
C	-5.9714649	-0.0084316	0.0000000
H	-5.7950704	0.0005792	-2.1667578
H	-5.7950704	0.0005792	2.1667578
C	-3.1434367	0.0096015	0.0000000
C	-1.7044349	0.0158027	0.0000000
N	-0.5165754	0.0205775	0.0000000
N	-7.3690185	0.0542573	0.0000000
H	-7.8185142	-0.2940978	-0.8410631
H	-7.8185142	-0.2940978	0.8410631
F	8.7069071	0.0469185	0.0000000

57.

C	1.2075384	0.0000000	-6.0295182
C	1.2022620	0.0000000	-4.6314442
C	0.0000000	0.0000000	-3.9020098
C	-1.2022620	0.0000000	-4.6314442
C	-1.2075384	0.0000000	-6.0295182
C	0.0000000	0.0000000	-6.7526273
F	-2.3891609	0.0000000	-3.9903766
F	-2.3814936	0.0000000	-6.6918929
F	2.3814936	0.0000000	-6.6918929
F	2.3891609	0.0000000	-3.9903766
I	0.0000000	0.0000000	-1.8106079
C	1.2290001	0.0000000	4.4926366
C	-1.2290001	0.0000000	4.4926366

C	1.2278617	0.0000000	5.8935980
H	2.1705475	0.0000000	3.9377246
C	-1.2278617	0.0000000	5.8935980
H	-2.1705475	0.0000000	3.9377246
C	0.0000000	0.0000000	6.5949539
H	2.1692020	0.0000000	6.4487841
H	-2.1692020	0.0000000	6.4487841
C	0.0000000	0.0000000	3.7935597
C	0.0000000	0.0000000	2.3522330
N	0.0000000	0.0000000	1.1642365
C	0.0000000	0.0000000	8.0378664
N	0.0000000	0.0000000	9.2276590
C	0.0000000	0.0000000	-8.1874410
N	0.0000000	0.0000000	-9.3768453

58.

C	5.7795847	-0.0002803	-1.1936233
C	4.3826631	0.0012514	-1.1955235
C	3.6449256	0.0056638	0.0000000
C	4.3826631	0.0012514	1.1955235
C	5.7795847	-0.0002803	1.1936233
C	6.5209526	0.0024157	0.0000000
F	3.7498042	-0.0038715	2.3941452
F	6.4617742	-0.0133297	2.3717235
F	6.4617742	-0.0133297	-2.3717235
F	3.7498042	-0.0038715	-2.3941452
I	1.5517080	0.0094220	0.0000000
C	-4.8041762	0.0307849	-1.2285933
C	-4.8041762	0.0307849	1.2285933
C	-6.2051679	0.0371217	-1.2277808
H	-4.2491162	0.0283698	-2.1700607
C	-6.2051679	0.0371217	1.2277808
H	-4.2491162	0.0283698	2.1700607
C	-6.9066102	0.0402518	0.0000000
H	-6.7603723	0.0396856	-2.1691224
H	-6.7603723	0.0396856	2.1691224
C	-4.1043837	0.0275946	0.0000000
C	-2.6629404	0.0209949	0.0000000
N	-1.4745780	0.0153937	0.0000000
C	-8.3495402	0.0466341	0.0000000
N	-9.5393090	0.0517468	0.0000000
N	7.9137537	0.0850161	0.0000000
H	8.3480173	-0.2722985	0.8460274
H	8.3480173	-0.2722985	-0.8460274

59.

C	6.6751150	0.0413578	-1.1970068
C	5.2747077	0.0377013	-1.2010669
C	4.5446433	0.0358636	0.0000000
C	5.2747077	0.0377013	1.2010669
C	6.6751150	0.0413578	1.1970068
C	7.3961315	0.0432681	0.0000000
F	4.6334674	0.0359795	2.3926499

F	7.3374528	0.0429892	2.3812400
F	7.3374528	0.0429892	-2.3812400
F	4.6334674	0.0359795	-2.3926499
I	2.4490170	0.0303447	0.0000000
C	-3.8494242	0.0063223	-1.2224198
C	-3.8494242	0.0063223	1.2224198
C	-5.2495444	-0.0020461	-1.2167127
H	-3.3019107	0.0086759	-2.1685651
C	-5.2495444	-0.0020461	1.2167127
H	-3.3019107	0.0086759	2.1685651
C	-5.9699122	-0.0084698	0.0000000
H	-5.7935496	0.0006339	-2.1667180
H	-5.7935496	0.0006339	2.1667180
C	-3.1416962	0.0100192	0.0000000
C	-1.7025372	0.0164053	0.0000000
N	-0.5145646	0.0212511	0.0000000
N	-7.3678329	0.0539815	0.0000000
H	-7.8165352	-0.2960480	-0.8408435
H	-7.8165352	-0.2960480	0.8408435
H	8.4871934	0.0462047	0.0000000

60.

C	6.6558658	0.0413473	-1.2102963
C	5.2555234	0.0375525	-1.1990594
C	4.5236544	0.0356027	0.0000000
C	5.2555234	0.0375525	1.1990594
C	6.6558658	0.0413473	1.2102963
C	7.3598239	0.0432595	0.0000000
F	4.6192206	0.0357698	2.3920363
F	7.3322602	0.0431005	2.3776955
F	7.3322602	0.0431005	-2.3776955
F	4.6192206	0.0357698	-2.3920363
I	2.4271953	0.0298989	0.0000000
C	-3.8510001	0.0059474	-1.2225125
C	-3.8510001	0.0059474	1.2225125
C	-5.2510615	-0.0021509	-1.2167667
H	-3.3035490	0.0082086	-2.1686853
C	-5.2510615	-0.0021509	1.2167667
H	-3.3035490	0.0082086	2.1686853
C	-5.9714649	-0.0084316	0.0000000
H	-5.7950704	0.0005792	-2.1667578
H	-5.7950704	0.0005792	2.1667578
C	-3.1434367	0.0096015	0.0000000
C	-1.7044349	0.0158027	0.0000000
N	-0.5165754	0.0205775	0.0000000
N	-7.3690185	0.0542573	0.0000000
H	-7.8185142	-0.2940978	-0.8410631
H	-7.8185142	-0.2940978	0.8410631
F	8.7069071	0.0469185	0.0000000

61.

C	6.2801012	0.0376184	-1.2072176
C	4.8820793	0.0343004	-1.2013654

C	4.1510627	0.0325704	0.0000000
C	4.8820793	0.0343004	1.2013654
C	6.2801012	0.0376184	1.2072176
C	7.0036234	0.0392954	0.0000000
F	4.2422396	0.0327276	2.3892947
F	6.9430162	0.0391962	2.3816568
F	6.9430162	0.0391962	-2.3816568
F	4.2422396	0.0327276	-2.3892947
I	2.0574076	0.0273931	0.0000000
C	-4.1995217	0.0050385	-1.2226762
C	-4.1995217	0.0050385	1.2226762
C	-5.5994790	-0.0026856	-1.2168801
H	-3.6523109	0.0070886	-2.1689897
C	-5.5994790	-0.0026856	1.2168801
H	-3.6523109	0.0070886	2.1689897
C	-6.3199550	-0.0086646	0.0000000
H	-6.1435228	0.0000946	-2.1668212
H	-6.1435228	0.0000946	2.1668212
C	-3.4921802	0.0085497	0.0000000
C	-2.0534141	0.0143620	0.0000000
N	-0.8656840	0.0189669	0.0000000
N	-7.7167929	0.0542883	0.0000000
H	-8.1677394	-0.2908062	-0.8415302
H	-8.1677394	-0.2908062	0.8415302
C	8.4384111	0.0426784	0.0000000
N	9.6277967	0.0454153	0.0000000

61. (T-shape)

C	0.0282656	-4.2003916	-1.2226439
C	0.0253131	-5.6003757	-1.2168593
C	0.0217179	-6.3208600	0.0000000
C	0.0253131	-5.6003757	1.2168593
C	0.0282656	-4.2003916	1.2226439
H	0.0284880	-3.6532146	-2.1689825
H	0.0298966	-6.1443837	-2.1668085
H	0.0298966	-6.1443837	2.1668085
H	0.0284880	-3.6532146	2.1689825
N	0.0892990	-7.7174836	0.0000000
H	-0.2543872	-8.1695825	0.8414916
H	-0.2543872	-8.1695825	-0.8414916
C	-1.2025331	6.2764860	0.0000000
C	-1.1912057	4.8784827	0.0000000
C	0.0130379	4.1521169	0.0000000
C	1.2115590	4.8878942	0.0000000
C	1.2118904	6.2859605	0.0000000
C	0.0018384	7.0047320	0.0000000
I	0.0212789	2.0583027	0.0000000
F	2.4019571	4.2528182	0.0000000
F	2.3836606	6.9535265	0.0000000
F	-2.3766445	4.2340736	0.0000000
F	-2.3795424	6.9348303	0.0000000
C	-0.0038209	8.4395054	0.0000000
N	-0.0085781	9.6288859	0.0000000

C	0.0294278	-3.4929550	0.0000000
C	0.0304854	-2.0540991	0.0000000
N	0.0310201	-0.8663213	0.0000000

62.

C	6.0340560	-0.0252037	-1.1932855
C	4.6370705	-0.0259719	-1.1947983
C	3.8980490	-0.0299029	0.0000000
C	4.6370705	-0.0259719	1.1947983
C	6.0340560	-0.0252037	1.1932855
C	6.7755266	-0.0283597	0.0000000
F	4.0053887	-0.0202643	2.3943488
F	6.7167925	-0.0123486	2.3718341
F	6.7167925	-0.0123486	-2.3718341
F	4.0053887	-0.0202643	-2.3943488
I	1.8026448	-0.0322255	0.0000000
C	-4.5103691	-0.0412823	-1.2222929
C	-4.5103691	-0.0412823	1.2222929
C	-5.9105807	-0.0416881	-1.2166340
H	-3.9629125	-0.0402051	-2.1684717
C	-5.9105807	-0.0416881	1.2166340
H	-3.9629125	-0.0402051	2.1684717
C	-6.6309337	-0.0397295	0.0000000
H	-6.4546719	-0.0478505	-2.1665953
H	-6.4546719	-0.0478505	2.1665953
C	-3.8024948	-0.0406102	0.0000000
C	-2.3632088	-0.0378203	0.0000000
N	-1.1751540	-0.0350417	0.0000000
N	-8.0289130	-0.1109480	0.0000000
H	-8.4787970	0.2383043	0.8406009
H	-8.4787970	0.2383043	-0.8406009
N	8.1694131	-0.1118678	0.0000000
H	8.6015590	0.2497630	-0.8454142
H	8.6015590	0.2497630	0.8454142

63.

C	1.1972946	0.0062975	6.9917183
C	1.2018340	0.0036685	5.5912562
C	0.0000097	0.0023648	4.8626244
C	-1.2018284	0.0037174	5.5912334
C	-1.1973155	0.0062747	6.9916957
C	-0.0000173	0.0076223	7.7122873
F	-2.3925052	0.0025907	4.9489703
F	-2.3810628	0.0074019	7.6535645
F	2.3810292	0.0075707	7.6536093
F	2.3925229	0.0023714	4.9490159
I	0.0000292	-0.0017430	2.7686726
C	1.2285106	-0.0165563	-3.5669906
C	-1.2284834	-0.0165053	-3.5669630
C	1.2244851	-0.0214274	-4.9692962
H	2.1697049	-0.0167077	-3.0116571
C	-1.2244901	-0.0214650	-4.9692685
H	-2.1696648	-0.0164826	-3.0116079
C	-0.0000105	-0.0286752	-5.6632040

H	2.1670146	-0.0287669	-5.5212890
H	-2.1670317	-0.0289655	-5.5212386
C	0.0000214	-0.0128905	-2.8685773
C	0.0000335	-0.0103985	-1.4264368
N	0.0000448	-0.0082478	-0.2384694
H	-0.0000275	0.0096721	8.8033778
C	-0.0000227	0.0225506	-7.1684587
F	1.0943637	-0.5809725	-7.6986213
F	0.0000229	1.3085926	-7.6173423
F	-1.0944612	-0.5808909	-7.6986049

64.

C	-7.2509372	-0.0446063	1.1971385
C	-5.8508703	-0.0766269	1.2013930
C	-5.1216051	-0.0932585	0.0000000
C	-5.8508703	-0.0766269	-1.2013930
C	-7.2509372	-0.0446063	-1.1971385
C	-7.9715670	-0.0281096	0.0000000
F	-5.2093649	-0.0912908	-2.3925739
F	-7.9129497	-0.0294325	-2.3811699
F	-7.9129497	-0.0294325	2.3811699
F	-5.2093649	-0.0912908	2.3925739
I	-3.0272142	-0.1417999	0.0000000
C	3.2804833	-0.2839339	1.2279294
C	3.2804833	-0.2839339	-1.2279294
C	4.6834424	-0.3129857	1.2226253
H	2.7257858	-0.2792310	2.1698218
C	4.6834424	-0.3129857	-1.2226253
H	2.7257858	-0.2792310	-2.1698218
C	5.3806151	-0.3279184	0.0000000
H	5.2470947	-0.3409124	2.1592522
H	5.2470947	-0.3409124	-2.1592522
C	2.5815223	-0.2660095	0.0000000
C	1.1403555	-0.2367137	0.0000000
N	-0.0470991	-0.2112081	0.0000000
H	-9.0623637	-0.0032121	0.0000000
O	6.7632766	-0.3977621	0.0000000
C	7.3632155	0.9148944	0.0000000
H	7.0633116	1.4765451	0.9006529
H	8.4488729	0.7560459	0.0000000
H	7.0633116	1.4765451	-0.9006529

65.

C	-8.1881079	0.1154974	1.1969604
C	-6.7877131	0.1104762	1.2009036
C	-6.0573691	0.1077594	0.0000000
C	-6.7877131	0.1104762	-1.2009036
C	-8.1881079	0.1154974	-1.1969604
C	-8.9091946	0.1181078	0.0000000
F	-6.1466883	0.1081908	-2.3926729
F	-8.8505439	0.1178915	-2.3812761
F	-8.8505439	0.1178915	2.3812761
F	-6.1466883	0.1081908	2.3926729

I	-3.9612703	0.1008000	0.0000000
C	2.3315832	0.0719550	1.2184605
C	2.3315832	0.0719550	-1.2184605
C	3.7313293	0.0620253	1.2170064
H	1.7875336	0.0665017	2.1667662
C	3.7313293	0.0620253	-1.2170064
H	1.7875336	0.0665017	-2.1667662
C	4.4696199	0.0735243	0.0000000
H	4.2458664	0.0490331	2.1784132
H	4.2458664	0.0490331	-2.1784132
C	1.6188355	0.0801256	0.0000000
C	0.1807868	0.0860257	0.0000000
N	-1.0074536	0.0913664	0.0000000
H	-10.0002562	0.1220471	0.0000000
N	5.8590326	0.1170623	0.0000000
C	6.5494021	-0.2277341	-1.2403274
H	7.6314600	-0.1611325	-1.0675698
H	6.3042903	-1.2499470	-1.5908928
H	6.2952228	0.4888334	-2.0352050
C	6.5494021	-0.2277341	1.2403274
H	7.6314600	-0.1611325	1.0675698
H	6.2952228	0.4888334	2.0352050
H	6.3042903	-1.2499470	1.5908928

66.

C	-1.3680551	-0.5513272	0.0000000
C	-0.1460312	-1.2364933	0.0000000
C	1.0709289	-0.5525143	0.0000000
C	1.0015155	0.8511667	0.0000000
C	-0.2590710	1.4751359	0.0000000
N	-1.4297497	0.7976825	0.0000000
H	2.0177382	-1.0977386	0.0000000
H	-2.3107626	-1.1061158	0.0000000
H	1.9140424	1.4532809	0.0000000
H	-0.3376628	2.5663023	0.0000000
F	-0.1528925	-2.5993791	0.0000000

67.

C	-1.3511113	-0.2159605	0.0000000
C	-0.1319877	-0.9304519	0.0000000
C	1.0835386	-0.2173074	0.0000000
C	1.0166921	1.1827517	0.0000000
C	-0.2444198	1.8065462	0.0000000
N	-1.4152891	1.1300570	0.0000000
H	2.0392101	-0.7477957	0.0000000
H	-2.3027077	-0.7565618	0.0000000
H	1.9275577	1.7870273	0.0000000
H	-0.3231077	2.8980409	0.0000000
C	-0.1433271	-2.3738391	0.0000000
N	-0.1550480	-3.5625067	0.0000000

68.

C	-1.1086522	-0.7335921	0.0340177
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C	0.3058431	-0.7459982	0.0195030
C	0.9679535	0.4985325	0.0436859
C	0.1978615	1.6707785	0.0784234
C	-1.2045017	1.5709870	0.0923377
N	-1.8581485	0.3865663	0.0701038
H	2.0622921	0.5435388	0.0405575
H	-1.6580823	-1.6832731	0.0184322
H	0.6798594	2.6523474	0.0958507
H	-1.8304093	2.4679144	0.1209288
N	1.0156005	-1.9586306	0.0560816
H	0.4932842	-2.7547025	-0.2997520
H	1.9370998	-1.9144683	-0.3701703

69.

C	-1.0383042	-0.2748744	0.0000000
C	-0.0378800	-1.2724965	0.0000000
C	1.2951538	-0.8547415	0.0000000
C	1.6710817	0.4937321	0.0000000
C	0.6564146	1.4687563	0.0000000
C	-0.6980846	1.0964993	0.0000000
H	-0.2890325	-2.3353060	0.0000000
H	2.7300090	0.7619731	0.0000000
H	0.9281115	2.5276407	0.0000000
H	-1.4883283	1.8508263	0.0000000
F	2.2713974	-1.8050473	0.0000000
C	-2.4275564	-0.6682383	0.0000000
N	-3.5729820	-0.9887238	0.0000000

70.

C	-1.2142864	0.0000000	-0.3884051
C	0.0000000	0.0000000	-1.1053925
C	1.2142864	0.0000000	-0.3884051
C	1.2205046	0.0000000	1.0243133
C	0.0000000	0.0000000	1.7199529
C	-1.2205046	0.0000000	1.0243133
H	0.0000000	0.0000000	-2.1981960
H	2.1722940	0.0000000	1.5614915
H	0.0000000	0.0000000	2.8132195
H	-2.1722940	0.0000000	1.5614915
C	-2.4653512	0.0000000	-1.1107546
C	2.4653512	0.0000000	-1.1107546
N	-3.4973920	0.0000000	-1.7014371
N	3.4973920	0.0000000	-1.7014371

71.

C	-0.6078599	-0.8477453	0.0205988
C	0.8021314	-0.8095488	0.0052433
C	1.4519040	0.4466619	0.0298723
C	0.7076527	1.6372824	0.0661147
C	-0.6966083	1.6094989	0.0805467
H	2.5462406	0.4862941	0.0263092
H	-1.1360535	-1.8063638	0.0094119
H	1.2314379	2.5971912	0.0829585

H	-1.2838849	2.5301120	0.1086361
N	1.5459981	-1.9987470	0.0404121
H	1.0636518	-2.8115765	-0.3317102
H	2.4841170	-1.9209736	-0.3411048
C	-1.3452114	0.3548133	0.0574975
C	-2.7873876	0.2926821	0.0687109
N	-3.9761280	0.2404188	0.0765030

72.

C	3.4442289	-1.3303442	0.0000000
C	4.8444840	-1.4486213	0.0000000
C	5.6311732	-0.2841420	0.0000000
C	4.9513263	0.9364665	0.0000000
C	3.5522290	0.9908187	0.0000000
N	2.8097721	-0.1366707	0.0000000
H	6.7232504	-0.3114484	0.0000000
H	2.8016097	-2.2155471	0.0000000
H	5.3122733	-2.4363724	0.0000000
H	3.0269181	1.9502705	0.0000000
F	5.6548013	2.0982267	0.0000000
C	-4.2424774	-1.0179897	0.0000000
C	-2.8455309	-1.0746385	0.0000000
C	-2.0606533	0.0908420	0.0000000
C	-2.7355160	1.3233339	0.0000000
C	-4.1318466	1.3947037	0.0000000
C	-4.9097603	0.2214805	0.0000000
F	-2.0403907	2.4813791	0.0000000
F	-4.7405873	2.5981225	0.0000000
F	-4.9587586	-2.1607778	0.0000000
F	-2.2593382	-2.2916606	0.0000000
I	0.0471951	-0.0060967	0.0000000
C	-6.3431084	0.2871460	0.0000000
N	-7.5312938	0.3415195	0.0000000

73.

C	3.1796008	-1.4348330	0.0000000
C	4.5773674	-1.5822447	0.0000000
C	5.3834474	-0.4349340	0.0000000
C	4.7444830	0.8217498	0.0000000
C	3.3342048	0.8779798	0.0000000
N	2.5676532	-0.2297971	0.0000000
H	6.4742920	-0.5010951	0.0000000
H	2.5195368	-2.3077222	0.0000000
H	5.0232319	-2.5799553	0.0000000
H	2.8140983	1.8409770	0.0000000
C	-4.5003008	-1.1580953	0.0000000
C	-3.1028393	-1.1997103	0.0000000
C	-2.3319206	-0.0248680	0.0000000
C	-3.0193137	1.2007744	0.0000000
C	-4.4164262	1.2560874	0.0000000
C	-5.1809833	0.0740858	0.0000000
F	-2.3363449	2.3654167	0.0000000
F	-5.0381023	2.4522544	0.0000000

F	-5.2034378	-2.3085193	0.0000000
F	-2.5024123	-2.4095293	0.0000000
I	-0.2267390	-0.0985912	0.0000000
C	-6.6150022	0.1237305	0.0000000
N	-7.8037555	0.1644306	0.0000000
C	5.5131072	2.0433244	0.0000000
N	6.1465552	3.0490840	0.0000000

74.

C	3.0315103	-0.7144566	0.0227128
C	4.4438602	-0.7744046	0.0069797
C	5.1461979	0.4509178	-0.0007187
C	4.4222959	1.6520583	0.0059164
C	3.0182839	1.6095147	0.0234683
H	6.2410075	0.4575391	-0.0071757
H	2.4365722	-1.6359011	0.0314232
H	4.9420036	2.6138154	-0.0014684
H	2.4162360	2.5225788	0.0302967
N	5.1095455	-2.0019947	0.0726128
H	4.5693405	-2.8011604	-0.2454072
H	6.0466310	-2.0043529	-0.3185557
C	-4.5126875	-1.2218474	-0.0100548
C	-3.1191970	-1.1088778	-0.0074282
C	-2.4785920	0.1409078	0.0299378
C	-3.2984183	1.2813262	0.0647605
C	-4.6932884	1.1849780	0.0624796
C	-5.3247891	-0.0725683	0.0249040
I	-0.3668976	0.2987283	0.0333981
F	-2.3917020	-2.2476711	-0.0423760
F	-5.0866255	-2.4426311	-0.0467019
F	-2.7489423	2.5152912	0.1015385
F	-5.4430943	2.3062747	0.0965142
C	-6.7555777	-0.1799850	0.0220865
N	-7.9416577	-0.2693516	0.0195669
N	2.3379850	0.4412725	0.0312905

75.

C	-0.1536828	4.1482058	0.0000000
C	1.0453112	4.8954319	0.0000000
C	0.9376548	6.2883095	0.0000000
C	-0.2927105	6.9568483	0.0000000
C	-1.4716156	6.1886957	0.0000000
C	-1.4148373	4.7851884	0.0000000
H	2.0242340	4.4113419	0.0000000
H	-0.3158096	8.0489912	0.0000000
H	-2.4418631	6.6921501	0.0000000
H	-2.3274520	4.1847575	0.0000000
F	2.0813160	7.0252461	0.0000000
C	-0.0841438	2.7078943	0.0000000
N	-0.0326005	1.5214017	0.0000000
C	0.2249416	-6.3781981	0.0000000
C	1.4088526	-5.6170527	0.0000000
C	1.3591176	-4.2198616	0.0000000

C	0.1345771	-3.5284048	0.0000000
C	-1.0436589	-4.2960838	0.0000000
C	-1.0048087	-5.6935907	0.0000000
F	-2.2506162	-3.6933785	0.0000000
F	-2.1573555	-6.3930607	0.0000000
F	2.6033391	-6.2421032	0.0000000
F	2.5253466	-3.5418978	0.0000000
I	0.0682168	-1.4374832	0.0000000
C	0.2703625	-7.8122756	0.0000000
N	0.3078846	-9.0010715	0.0000000

76.

C	-1.4727055	5.8821689	0.0000000
C	-1.3906486	4.4864526	0.0000000
C	-0.1500053	3.8243419	0.0000000
C	1.0103349	4.6187529	0.0000000
C	0.9387546	6.0149680	0.0000000
C	-0.3067275	6.6705420	0.0000000
F	2.2307726	4.0438906	0.0000000
F	2.0745673	6.7409433	0.0000000
F	-2.6812022	6.4790837	0.0000000
F	-2.5402985	3.7810992	0.0000000
I	-0.0348363	1.7362428	0.0000000
C	-0.7798679	-4.6561207	0.0000000
C	1.6682132	-4.4390547	0.0000000
C	-0.6366414	-6.0587816	0.0000000
H	-1.7721163	-4.1982317	0.0000000
C	1.7877068	-5.8386890	0.0000000
H	2.5544150	-3.7994969	0.0000000
C	0.6442256	-6.6548986	0.0000000
H	2.7801851	-6.2969925	0.0000000
H	0.7336510	-7.7441247	0.0000000
C	0.3813971	-3.8563830	0.0000000
C	0.2498800	-2.4192789	0.0000000
N	0.1484330	-1.2363070	0.0000000
C	-0.3854797	8.1032094	0.0000000
N	-0.4504313	9.2908355	0.0000000
C	-1.8163198	-6.8924636	0.0000000
N	-2.7852560	-7.5817080	0.0000000

77.

C	4.3485573	-0.8478700	0.0339840
C	5.7589550	-0.8128485	0.0310207
C	6.4100800	0.4435668	0.0046471
C	5.6696002	1.6365063	-0.0209526
C	4.2652730	1.6137918	-0.0191887
H	7.5043819	0.4811810	0.0096169
H	3.8172388	-1.8043293	0.0613418
H	6.1962861	2.5945915	-0.0427105
H	3.6795397	2.5355059	-0.0388121
N	6.4992365	-1.9974525	0.1277035
H	6.0226842	-2.8308840	-0.2032097
H	7.4463992	-1.9404026	-0.2338134

C	-6.1124122	-1.2222187	0.0264618
C	-4.7156713	-1.1625233	0.0240739
C	-4.0317670	0.0662668	0.0175029
C	-4.8083483	1.2387109	0.0134915
C	-6.2055682	1.1904975	0.0158232
C	-6.8819359	-0.0437697	0.0223563
I	-1.9401356	0.1469142	0.0140158
F	-4.0302367	-2.3247551	0.0281123
F	-6.7293924	-2.4212980	0.0326904
F	-4.2145868	2.4501816	0.0070985
F	-6.9131915	2.3383583	0.0117331
C	-8.3156348	-0.0991779	0.0246419
N	-9.5041376	-0.1452619	0.0264402
C	3.6173181	0.3587958	0.0085150
C	2.1773592	0.3014701	0.0088967
N	0.9901090	0.2564530	0.0085197

78.

C	-0.0978514	-1.3594398	-2.3006320
C	-0.1215180	-1.4665831	0.0000000
C	-0.0759098	-0.0630893	0.0000000
C	-0.0378150	0.7385603	-1.1518293
C	-0.0523221	0.0719264	-2.3750712
H	-0.1053739	-1.9104612	-3.2481453
C	-0.0378150	0.7385603	1.1518293
H	-0.0289121	0.5694201	-3.3470626
C	-0.0523221	0.0719264	2.3750712
C	-0.0978514	-1.3594398	2.3006320
H	-0.0289121	0.5694201	3.3470626
H	-0.1053739	-1.9104612	3.2481453
N	-0.0873818	2.0887532	-0.7356135
H	0.6447562	2.6970601	-1.1044384
N	-0.0873818	2.0887532	0.7356135
H	0.6447562	2.6970601	1.1044384
N	-0.1363858	-2.1309830	-1.1992343
N	-0.1363858	-2.1309830	1.1992343

79.

C	-0.0688188	-1.2775037	-2.3074353
C	-0.0648209	-1.2236746	0.0000000
C	-0.0487625	0.2177541	0.0000000
C	-0.0384513	0.8974775	-1.2486959
C	-0.0495896	0.1494419	-2.4251866
H	-0.0824610	-1.8823443	-3.2240833
C	-0.0384513	0.8974775	1.2486959
H	-0.0290129	1.9936165	-1.2764952
C	-0.0495896	0.1494419	2.4251866
C	-0.0688188	-1.2775037	2.3074353
H	-0.0290129	1.9936165	1.2764952
H	-0.0824610	-1.8823443	3.2240833
N	-0.0725005	-1.9519889	-1.1593853

N	-0.0725005	-1.9519889	1.1593853
N	-0.1163041	0.7340955	3.6992536
H	0.2679223	0.1579686	4.4430652
H	0.2460076	1.6821970	3.7483736
N	-0.1163041	0.7340955	-3.6992536
H	0.2460076	1.6821970	-3.7483736
H	0.2679223	0.1579686	-4.4430652

80.

C	-0.0465844	-0.5704825	-2.4551684
C	-0.0663133	-0.7956996	0.0000000
C	-0.0496388	0.6197387	0.0000000
C	-0.0301429	1.4409653	-1.1487614
C	-0.0357794	0.8489700	-2.4125698
H	-0.0437325	-1.0657579	-3.4306568
C	-0.0301429	1.4409653	1.1487614
H	-0.0294488	1.4296604	-3.3379237
C	-0.0357794	0.8489700	2.4125698
C	-0.0465844	-0.5704825	2.4551684
H	-0.0294488	1.4296604	3.3379237
H	-0.0437325	-1.0657579	3.4306568
N	-0.1052072	2.7867608	-0.7299338
H	0.6096208	3.4120958	-1.1043200
N	-0.1052072	2.7867608	0.7299338
H	0.6096208	3.4120958	1.1043200
C	-0.0673047	-1.3901445	-1.3073338
C	-0.0673047	-1.3901445	1.3073338
C	-0.0889742	-2.8175921	-1.5023960
C	-0.0889742	-2.8175921	1.5023960
N	-0.1044706	-3.9864949	-1.7278670
N	-0.1044706	-3.9864949	1.7278670

81.

C	3.4994151	0.0000000	-0.5395186
C	2.8428400	0.0000000	0.6874539
C	1.4223628	0.0000000	0.7085376
C	0.7286550	0.0000000	-0.5473226
C	2.7179248	0.0000000	-1.7244213
C	0.6887494	0.0000000	1.9473902
C	-0.7286550	0.0000000	-0.5473226
C	-1.4223628	0.0000000	0.7085376
C	-0.6887494	0.0000000	1.9473902
C	-2.8428400	0.0000000	0.6874539
H	-3.3987079	0.0000000	1.6311252
C	-3.4994151	0.0000000	-0.5395186
C	-2.7179248	0.0000000	-1.7244213
H	1.2465473	0.0000000	2.8898984
H	4.5911555	0.0000000	-0.6017973
H	3.3987079	0.0000000	1.6311252
H	3.2105774	0.0000000	-2.7032325
H	-1.2465473	0.0000000	2.8898984
H	-4.5911555	0.0000000	-0.6017973
H	-3.2105774	0.0000000	-2.7032325

N	1.3790248	0.0000000	-1.7481131
N	-1.3790248	0.0000000	-1.7481131

82.

C	0.0251995	0.9113009	-3.4896882
C	0.0150554	-0.3352179	-2.8582621
C	0.0561521	-0.3544768	-1.4277300
C	0.0530966	0.8998228	-0.7289405
C	0.0535295	2.0839973	-2.7015051
C	0.1200283	-1.5845914	-0.6905124
C	0.0530966	0.8998228	0.7289405
C	0.0561521	-0.3544768	1.4277300
C	0.1200283	-1.5845914	0.6905124
C	0.0150554	-0.3352179	2.8582621
C	0.0251995	0.9113009	3.4896882
C	0.0535295	2.0839973	2.7015051
H	0.2156699	-2.5371204	-1.2197028
H	0.0021180	0.9853847	-4.5818698
H	0.0611629	3.0615688	-3.1970787
H	0.2156699	-2.5371204	1.2197028
H	0.0021180	0.9853847	4.5818698
H	0.0611629	3.0615688	3.1970787
N	0.0382240	-1.5314251	-3.5879200
H	-0.4887870	-2.2947447	-3.1733914
H	-0.2070512	-1.4137871	-4.5671959
N	0.0382240	-1.5314251	3.5879200
H	-0.2070512	-1.4137871	4.5671959
H	-0.4887870	-2.2947447	3.1733914
N	0.0556018	2.1092888	-1.3631452
N	0.0556018	2.1092888	1.3631452

83.

C	-2.4379759	0.0000000	-0.3779763
C	-1.2358453	0.0000000	-1.0712144
C	0.0000000	0.0000000	-0.3408850
C	0.0000000	0.0000000	1.1310461
C	-1.2882530	0.0000000	1.7956748
C	-2.4545037	0.0000000	1.0230191
C	1.2358453	0.0000000	-1.0712144
C	1.2882530	0.0000000	1.7956748
C	2.4545037	0.0000000	1.0230191
C	2.4379759	0.0000000	-0.3779763
I	-1.7732411	0.0000000	3.8538091
I	1.7732411	0.0000000	3.8538091
F	3.6767949	0.0000000	1.5873351
F	3.6098376	0.0000000	-1.0334273
F	-3.6767949	0.0000000	1.5873351
F	-3.6098376	0.0000000	-1.0334273
C	-1.3597232	0.0000000	-2.5041424
C	1.3597232	0.0000000	-2.5041424
N	-1.6140481	0.0000000	-3.6681581
N	1.6140481	0.0000000	-3.6681581

84.

C	-0.0812129	1.3000650	-1.1548687
C	-0.0710007	-0.1115495	-1.2139007
C	-0.0701165	-0.8230925	0.0000000
C	-0.0710007	-0.1115495	1.2139007
C	-0.0812129	1.3000650	1.1548687
N	-0.0874208	1.9957861	0.0000000
H	-0.0851610	-1.9194836	0.0000000
H	-0.0869140	1.8881139	-2.0801014
H	-0.0869140	1.8881139	2.0801014
N	-0.1398787	-0.7833077	-2.4501613
H	0.1893311	-0.2255188	-3.2338325
H	0.3110244	-1.6944078	-2.4504326
N	-0.1398787	-0.7833077	2.4501613
H	0.3110244	-1.6944078	2.4504326
H	0.1893311	-0.2255188	3.2338325

85.

C	-0.0333689	2.3787293	-2.3006203
C	-0.0564736	2.2828780	0.0000000
C	-0.0366097	3.6831425	0.0000000
C	-0.0119908	4.4821627	-1.1533592
C	-0.0134769	3.8092382	-2.3759824
H	-0.0300518	1.8235429	-3.2452263
C	-0.0119908	4.4821627	1.1533592
H	0.0030454	4.3039889	-3.3492146
C	-0.0134769	3.8092382	2.3759824
C	-0.0333689	2.3787293	2.3006203
H	0.0030454	4.3039889	3.3492146
H	-0.0300518	1.8235429	3.2452263
N	-0.0876471	5.8253654	-0.7330577
H	0.6052605	6.4709460	-1.1127656
N	-0.0876471	5.8253654	0.7330577
H	0.6052605	6.4709460	1.1127656
N	-0.0586868	1.6132600	-1.1933875
N	-0.0586868	1.6132600	1.1933875
C	-0.0492628	-5.6188065	-1.2069981
C	-0.0471556	-6.3428533	0.0000000
C	-0.0492628	-5.6188065	1.2069981
C	-0.0531343	-4.2208281	1.2011578
C	-0.0551919	-3.4887664	0.0000000
C	-0.0531343	-4.2208281	-1.2011578
I	-0.0606682	-1.3943067	0.0000000
F	-0.0546988	-3.5829857	2.3902586
F	-0.0471873	-6.2823831	2.3818572
F	-0.0546988	-3.5829857	-2.3902586
F	-0.0471873	-6.2823831	-2.3818572
C	-0.0427101	-7.7775543	0.0000000
N	-0.0387917	-8.9669998	0.0000000

86.

C	-0.0659174	2.1427790	-2.3077021
C	-0.0603643	2.2158311	0.0000000

C	-0.0111724	3.6535872	0.0000000
C	0.0146532	4.3243212	-1.2528655
C	-0.0140317	3.5691576	-2.4274774
H	-0.0936635	1.5308008	-3.2186243
C	0.0146532	4.3243212	1.2528655
H	0.0495888	5.4193614	-1.2890590
C	-0.0140317	3.5691576	2.4274774
C	-0.0659174	2.1427790	2.3077021
H	0.0495888	5.4193614	1.2890590
H	-0.0936635	1.5308008	3.2186243
N	-0.0849971	1.4812394	-1.1521689
N	-0.0849971	1.4812394	1.1521689
N	-0.0683074	4.1492441	3.6997588
H	0.2876945	3.5646277	4.4503511
H	0.2980491	5.0947881	3.7580023
N	-0.0683074	4.1492441	-3.6997588
H	0.2980491	5.0947881	-3.7580023
H	0.2876945	3.5646277	-4.4503511
C	-0.0404004	-5.6990999	-1.2068800
C	-0.0336713	-6.4234004	0.0000000
C	-0.0404004	-5.6990999	1.2068800
C	-0.0533024	-4.3012175	1.2005696
C	-0.0599697	-3.5684678	0.0000000
C	-0.0533024	-4.3012175	-1.2005696
F	-0.0588135	-3.6637110	2.3904682
F	-0.0340098	-6.3627310	2.3819310
F	-0.0588135	-3.6637110	-2.3904682
F	-0.0340098	-6.3627310	-2.3819310
I	-0.0799286	-1.4712753	0.0000000
C	-0.0198656	-7.8579853	0.0000000
N	-0.0081130	-9.0474093	0.0000000

87.

C	-0.0438044	3.4127574	-2.4562662
C	-0.0682442	3.1907908	0.0000000
C	-0.0254107	4.6042929	0.0000000
C	0.0099318	5.4243051	-1.1494601
C	-0.0058885	4.8313070	-2.4138542
H	-0.0497920	2.9172776	-3.4316296
C	0.0099318	5.4243051	1.1494601
H	0.0123775	5.4112641	-3.3394045
C	-0.0058885	4.8313070	2.4138542
C	-0.0438044	3.4127574	2.4562662
H	0.0123775	5.4112641	3.3394045
H	-0.0497920	2.9172776	3.4316296
N	-0.0414021	6.7678718	-0.7282768
H	0.6691278	7.3937539	-1.1091396
N	-0.0414021	6.7678718	0.7282768
H	0.6691278	7.3937539	1.1091396
C	-0.0084502	-7.1742158	-1.2072174
C	0.0104583	-7.8975343	0.0000000
C	-0.0084502	-7.1742158	1.2072174
C	-0.0448856	-5.7767029	1.2027998

C	-0.0637331	-5.0469952	0.0000000
C	-0.0448856	-5.7767029	-1.2027998
I	-0.1179610	-2.9624314	0.0000000
F	-0.0614227	-5.1384426	2.3899754
F	0.0089785	-7.8375670	2.3816667
F	-0.0614227	-5.1384426	-2.3899754
F	0.0089785	-7.8375670	-2.3816667
C	0.0483279	-9.3317578	0.0000000
N	0.0799891	-10.5207283	0.0000000
C	-0.0802038	2.5958198	-1.3071832
C	-0.0802038	2.5958198	1.3071832
C	-0.1287998	1.1677055	-1.4792658
C	-0.1287998	1.1677055	1.4792658
N	-0.1674797	-0.0129522	-1.6274155
N	-0.1674797	-0.0129522	1.6274155

88.

C	0.0000000	0.0000000	-6.3617231
C	1.2070416	0.0000000	-5.6375096
C	1.1999049	0.0000000	-4.2395872
C	0.0000000	0.0000000	-3.5063661
C	-1.1999049	0.0000000	-4.2395872
C	-1.2070416	0.0000000	-5.6375096
C	0.0000000	0.0000000	-7.7964173
N	0.0000000	0.0000000	-8.9858756
F	-2.3904437	0.0000000	-3.6012605
F	2.3904437	0.0000000	-3.6012605
F	2.3821260	0.0000000	-6.3011276
F	-2.3821260	0.0000000	-6.3011276
I	0.0000000	0.0000000	-1.4049407
C	3.4880368	0.0000000	2.5185683
C	2.8470099	0.0000000	3.7559722
C	1.4268212	0.0000000	3.7976235
C	0.7255248	0.0000000	2.5497851
C	2.6974543	0.0000000	1.3401506
C	0.6897434	0.0000000	5.0354508
C	-0.7255248	0.0000000	2.5497851
C	-1.4268212	0.0000000	3.7976235
C	-0.6897434	0.0000000	5.0354508
C	-2.8470099	0.0000000	3.7559722
H	-3.4181763	0.0000000	4.6901593
C	-3.4880368	0.0000000	2.5185683
C	-2.6974543	0.0000000	1.3401506
H	1.2446932	0.0000000	5.9794072
H	4.5788855	0.0000000	2.4455368
H	3.4181763	0.0000000	4.6901593
H	3.1712904	0.0000000	0.3515985
H	-1.2446932	0.0000000	5.9794072
H	-4.5788855	0.0000000	2.4455368
H	-3.1712904	0.0000000	0.3515985
N	1.3588327	0.0000000	1.3428941
N	-1.3588327	0.0000000	1.3428941

89.

C	0.0094850	-1.9415192	-3.4782344
C	0.0014776	-3.1996379	-2.8631273
C	0.0345168	-3.2398494	-1.4320551
C	0.0269982	-1.9942514	-0.7257763
C	0.0279775	-0.7768401	-2.6806801
C	0.0934578	-4.4690143	-0.6915451
C	0.0269982	-1.9942514	0.7257763
C	0.0345168	-3.2398494	1.4320551
C	0.0934578	-4.4690143	0.6915451
C	0.0014776	-3.1996379	2.8631273
C	0.0094850	-1.9415192	3.4782344
C	0.0279775	-0.7768401	2.6806801
H	0.1814887	-5.4239408	-1.2177206
H	-0.0071775	-1.8558685	-4.5692945
H	0.0318230	0.2110600	-3.1564362
H	0.1814887	-5.4239408	1.2177206
H	-0.0071775	-1.8558685	4.5692945
H	0.0318230	0.2110600	3.1564362
N	0.0346348	-4.3796478	3.6086132
H	-0.2044537	-4.2609453	4.5887594
H	-0.4548453	-5.1698670	3.2002557
N	0.0346348	-4.3796478	-3.6086132
H	-0.4548453	-5.1698670	-3.2002557
H	-0.2044537	-4.2609453	-4.5887594
N	0.0264397	-0.7788333	-1.3422559
N	0.0264397	-0.7788333	1.3422559
C	0.0301164	4.0392742	0.0000000
C	0.0303243	4.7738136	1.1991638
C	0.0308657	6.1717349	1.2068161
C	0.0310788	6.8963198	0.0000000
C	0.0308657	6.1717349	-1.2068161
C	0.0303243	4.7738136	-1.1991638
F	0.0298711	4.1366347	-2.3906976
F	0.0309325	6.8358307	-2.3823006
F	0.0298711	4.1366347	2.3906976
F	0.0309325	6.8358307	2.3823006
I	0.0287783	1.9352744	0.0000000
C	0.0312430	8.3309702	0.0000000
N	0.0311512	9.5204439	0.0000000

89. (T-shape)

C	0.0042112	-1.9368023	-3.4784893
C	-0.0136629	-3.1945836	-2.8630124
C	0.0192643	-3.2340202	-1.4318645
C	0.0218958	-1.9884298	-0.7256930
C	0.0322259	-0.7723782	-2.6810690
C	0.0686271	-4.4636681	-0.6914741
C	0.0218958	-1.9884298	0.7256930
C	0.0192643	-3.2340202	1.4318645
C	0.0686271	-4.4636681	0.6914741
C	-0.0136629	-3.1945836	2.8630124

C	0.0042112	-1.9368023	3.4784893
C	0.0322259	-0.7723782	2.6810690
H	0.1492388	-5.4192013	-1.2176864
H	-0.0119594	-1.8512561	-4.5695473
H	0.0438394	0.2147346	-3.1582671
H	0.1492388	-5.4192013	1.2176864
H	-0.0119594	-1.8512561	4.5695473
H	0.0438394	0.2147346	3.1582671
N	0.0098726	-4.3748660	3.6079082
H	-0.2279240	-4.2549999	4.5882045
H	-0.4846194	-5.1617174	3.1991704
N	0.0098726	-4.3748660	-3.6079082
H	-0.4846194	-5.1617174	-3.1991704
H	-0.2279240	-4.2549999	-4.5882045
N	0.0310267	-0.7732108	-1.3427617
N	0.0310267	-0.7732108	1.3427617
C	-1.1468914	4.7667938	0.0000000
C	0.0502920	4.0286964	0.0000000
C	1.2517483	4.7598538	0.0000000
C	1.2629189	6.1576166	0.0000000
C	0.0584864	6.8860783	0.0000000
C	-1.1500979	6.1645497	0.0000000
F	2.4404297	6.8184346	0.0000000
F	2.4402886	4.1180839	0.0000000
F	-2.3393306	4.1318806	0.0000000
F	-2.3239181	6.8320969	0.0000000
C	0.0624976	8.3205577	0.0000000
N	0.0655998	9.5100463	0.0000000
I	0.0439044	1.9261100	0.0000000

90.

C	-2.4388990	0.0000000	-3.4077972
C	-1.2371861	0.0000000	-4.1026367
C	0.0000000	0.0000000	-3.3740623
C	0.0000000	0.0000000	-1.9031404
C	-1.2880528	0.0000000	-1.2354182
C	-2.4540636	0.0000000	-2.0067491
C	1.2371861	0.0000000	-4.1026367
C	1.2880528	0.0000000	-1.2354182
C	2.4540636	0.0000000	-2.0067491
C	2.4388990	0.0000000	-3.4077972
I	-1.7387130	0.0000000	0.8271521
I	1.7387130	0.0000000	0.8271521
F	3.6755690	0.0000000	-1.4395966
F	3.6117978	0.0000000	-4.0635856
F	-3.6755690	0.0000000	-1.4395966
F	-3.6117978	0.0000000	-4.0635856
C	-1.3623043	0.0000000	-5.5355742
C	1.3623043	0.0000000	-5.5355742
N	-1.6153475	0.0000000	-6.6998340
N	1.6153475	0.0000000	-6.6998340
C	1.1515932	0.0000000	4.5903911
C	1.2057962	0.0000000	5.9953741

C	0.0000000	0.0000000	6.7164951
C	-1.2057962	0.0000000	5.9953741
C	-1.1515932	0.0000000	4.5903911
N	0.0000000	0.0000000	3.8800333
H	0.0000000	0.0000000	7.8101225
H	2.0796621	0.0000000	4.0073337
H	2.1723032	0.0000000	6.5062164
H	-2.1723032	0.0000000	6.5062164
H	-2.0796621	0.0000000	4.0073337

91.

C	3.9327992	-0.0318793	-2.4388459
C	4.6279735	-0.0339682	-1.2373414
C	3.8996402	-0.0318288	0.0000000
C	2.4287884	-0.0274326	0.0000000
C	1.7602693	-0.0254073	-1.2879781
C	2.5317487	-0.0276520	-2.4538309
C	4.6279735	-0.0339682	1.2373414
C	1.7602693	-0.0254073	1.2879781
C	2.5317487	-0.0276520	2.4538309
C	3.9327992	-0.0318793	2.4388459
I	-0.3029168	-0.0196210	-1.7356281
I	-0.3029168	-0.0196210	1.7356281
F	1.9646574	-0.0258495	3.6755325
F	4.5886889	-0.0337557	3.6120004
F	1.9646574	-0.0258495	-3.6755325
F	4.5886889	-0.0337557	-3.6120004
C	6.0609018	-0.0381036	-1.3627310
C	6.0609018	-0.0381036	1.3627310
N	7.2252137	-0.0413718	-1.6155277
N	7.2252137	-0.0413718	1.6155277
C	-4.0551246	-0.0005217	1.1451135
C	-5.4554620	0.0122017	1.2026023
C	-6.1938010	0.0199829	0.0000000
C	-5.4554620	0.0122017	-1.2026023
C	-4.0551246	-0.0005217	-1.1451135
N	-3.3337018	-0.0067822	0.0000000
H	-3.4826273	-0.0048361	2.0799846
H	-5.9632065	0.0115522	2.1720570
H	-5.9632065	0.0115522	-2.1720570
H	-3.4826273	-0.0048361	-2.0799846
N	-7.5867294	-0.0354049	0.0000000
H	-8.0400135	0.2999449	0.8437245
H	-8.0400135	0.2999449	-0.8437245

92.

C	4.1792066	-0.0645501	-2.4388154
C	4.8744928	-0.0774984	-1.2374250
C	4.1465257	-0.0642443	0.0000000
C	2.6758234	-0.0371627	0.0000000
C	2.0071145	-0.0250129	-1.2878502
C	2.7784277	-0.0384038	-2.4536623
C	4.8744928	-0.0774984	1.2374250

C	2.0071145	-0.0250129	1.2878502
C	2.7784277	-0.0384038	2.4536623
C	4.1792066	-0.0645501	2.4388154
I	-0.0557656	0.0136523	-1.7341214
I	-0.0557656	0.0136523	1.7341214
F	2.2112723	-0.0272235	3.6753394
F	4.8348303	-0.0762501	3.6121096
F	2.2112723	-0.0272235	-3.6753394
F	4.8348303	-0.0762501	-3.6121096
C	6.3071725	-0.1036795	-1.3629549
C	6.3071725	-0.1036795	1.3629549
N	7.4713026	-0.1247014	-1.6156961
N	7.4713026	-0.1247014	1.6156961
C	-3.7643379	0.0750441	1.1546838
C	-5.1741750	0.0027586	1.2152990
C	-5.8830446	-0.0366488	0.0000000
C	-5.1741750	0.0027586	-1.2152990
C	-3.7643379	0.0750441	-1.1546838
N	-3.0688027	0.1102014	0.0000000
H	-6.9766760	-0.1117538	0.0000000
H	-3.1831912	0.1043506	2.0851932
H	-3.1831912	0.1043506	-2.0851932
N	-5.8370149	-0.1055611	2.4486118
H	-5.3099742	0.2598444	3.2370292
H	-6.7862737	0.2570350	2.4494711
N	-5.8370149	-0.1055611	-2.4486118
H	-6.7862737	0.2570350	-2.4494711
H	-5.3099742	0.2598444	-3.2370292

93.

C	-2.4382345	0.0000000	-4.5360983
C	-1.2368337	0.0000000	-5.2308479
C	0.0000000	0.0000000	-4.5018115
C	0.0000000	0.0000000	-3.0311101
C	-1.2879228	0.0000000	-2.3623717
C	-2.4531803	0.0000000	-3.1350582
C	1.2368337	0.0000000	-5.2308479
C	1.2879228	0.0000000	-2.3623717
C	2.4531803	0.0000000	-3.1350582
C	2.4382345	0.0000000	-4.5360983
I	-1.7428500	0.0000000	-0.3004770
I	1.7428500	0.0000000	-0.3004770
F	3.6755787	0.0000000	-2.5691676
F	3.6114805	0.0000000	-5.1921372
F	-3.6755787	0.0000000	-2.5691676
F	-3.6114805	0.0000000	-5.1921372
C	-1.3620601	0.0000000	-6.6637948
C	1.3620601	0.0000000	-6.6637948
N	-1.6152650	0.0000000	-7.8279702
N	1.6152650	0.0000000	-7.8279702
C	0.0000000	0.0000000	5.3349971
C	1.2287425	0.0000000	6.0332437
C	1.2197902	0.0000000	7.4376974

C	0.0000000	0.0000000	8.1408484
C	-1.2197902	0.0000000	7.4376974
C	-1.2287425	0.0000000	6.0332437
H	2.1699109	0.0000000	5.4771233
H	2.1671057	0.0000000	7.9838629
H	0.0000000	0.0000000	9.2343956
H	-2.1671057	0.0000000	7.9838629
H	-2.1699109	0.0000000	5.4771233
C	0.0000000	0.0000000	3.8922036
N	0.0000000	0.0000000	2.7024684

94.

C	5.1189184	0.0263551	-2.4381782
C	5.8138429	0.0276678	-1.2369052
C	5.0848887	0.0262618	0.0000000
C	3.6142095	0.0233201	0.0000000
C	2.9450953	0.0219950	-1.2879250
C	3.7179092	0.0235616	-2.4530533
C	5.8138429	0.0276678	1.2369052
C	2.9450953	0.0219950	1.2879250
C	3.7179092	0.0235616	2.4530533
C	5.1189184	0.0263551	2.4381782
I	0.8830514	0.0178166	-1.7415074
I	0.8830514	0.0178166	1.7415074
F	3.1521404	0.0224120	3.6755944
F	5.7750714	0.0276996	3.6115824
F	3.1521404	0.0224120	-3.6755944
F	5.7750714	0.0276996	-3.6115824
C	7.2467789	0.0303182	-1.3623604
C	7.2467789	0.0303182	1.3623604
N	8.4109376	0.0323985	-1.6155937
N	8.4109376	0.0323985	1.6155937
C	-4.7478178	0.0034879	0.0000000
C	-5.4566285	0.0012603	1.2220058
C	-6.8568747	-0.0041158	1.2166607
C	-7.5775020	-0.0086919	0.0000000
C	-6.8568747	-0.0041158	-1.2166607
C	-5.4566285	0.0012603	-1.2220058
H	-4.9102483	0.0022280	2.1688539
H	-7.4008255	-0.0004507	2.1666961
H	-7.4008255	-0.0004507	-2.1666961
H	-4.9102483	0.0022280	-2.1688539
C	-3.3082146	0.0076649	0.0000000
N	-2.1182363	0.0109880	0.0000000
N	-8.9746472	0.0569903	0.0000000
H	-9.4255086	-0.2891568	-0.8412267
H	-9.4255086	-0.2891568	0.8412267

95.

C	-0.0526146	-0.6125529	-2.4668731
C	-0.0569042	-1.3470799	-1.2742871
C	-0.0483740	-0.6884447	0.0000000
C	-0.0325978	0.7588630	0.0000000

C	-0.0199265	1.4723238	-1.2319967
C	-0.0308454	0.8082461	-2.4603494
H	-0.0720151	-1.1550595	-3.4176109
C	-0.0569042	-1.3470799	1.2742871
C	-0.0199265	1.4723238	1.2319967
H	-0.0090977	2.5680549	-1.2039670
C	-0.0308454	0.8082461	2.4603494
C	-0.0526146	-0.6125529	2.4668731
H	-0.0090977	2.5680549	1.2039670
H	-0.0720151	-1.1550595	3.4176109
N	-0.0976681	1.5006848	3.6771441
H	0.2923051	1.0020508	4.4716526
H	0.2371676	2.4591059	3.6406531
N	-0.0976681	1.5006848	-3.6771441
H	0.2371676	2.4591059	-3.6406531
H	0.2923051	1.0020508	-4.4716526
C	-0.0706073	-2.7820724	-1.4222367
C	-0.0706073	-2.7820724	1.4222367
N	-0.0793080	-3.9489108	-1.6632920
N	-0.0793080	-3.9489108	1.6632920

96.

C	-0.0682094	-1.6241059	-3.4595480
C	-0.0153912	-1.4792446	-1.1634706
C	-0.0307618	-0.0329297	-1.2144663
C	-0.0339576	0.6146464	-2.5049306
C	-0.0646876	-0.2039558	-3.6216901
C	-0.0549224	0.6779178	0.0000000
C	-0.0307618	-0.0329297	1.2144663
C	-0.0153912	-1.4792446	1.1634706
C	-0.0682094	-1.6241059	3.4595480
C	-0.0646876	-0.2039558	3.6216901
C	-0.0339576	0.6146464	2.5049306
H	-0.0856576	-2.2537603	-4.3567459
H	-0.0715199	0.2241051	-4.6292641
H	-0.1597824	1.7671315	0.0000000
H	-0.0856576	-2.2537603	4.3567459
H	-0.0715199	0.2241051	4.6292641
N	-0.0327798	-2.2650815	-2.3002016
N	-0.0084661	-2.1642893	0.0000000
N	-0.0327798	-2.2650815	2.3002016
N	-0.0813489	2.0132691	-2.5819277
H	0.4915490	2.4929190	-1.8926472
H	0.1043501	2.3737584	-3.5143155
N	-0.0813489	2.0132691	2.5819277
H	0.1043501	2.3737584	3.5143155
H	0.4915490	2.4929190	1.8926472

97.

C	-3.6581468	0.0000000	-0.4540938
C	-2.4689390	0.0000000	-1.1667527
C	-1.2235445	0.0000000	-0.4511924
C	-1.2287648	0.0000000	0.9997425

C	-2.4849892	0.0000000	1.6965522
C	-3.6640231	0.0000000	0.9651705
C	0.0000000	0.0000000	-1.1452543
C	0.0000000	0.0000000	1.6863405
C	1.2287648	0.0000000	0.9997425
C	1.2235445	0.0000000	-0.4511924
C	2.4689390	0.0000000	-1.1667527
C	3.6581468	0.0000000	-0.4540938
C	3.6640231	0.0000000	0.9651705
C	2.4849892	0.0000000	1.6965522
H	0.0000000	0.0000000	-2.2411915
H	0.0000000	0.0000000	2.7778965
F	4.8694345	0.0000000	1.5655523
F	4.8448385	0.0000000	-1.0890578
F	-4.8694345	0.0000000	1.5655523
F	-4.8448385	0.0000000	-1.0890578
C	-2.4894109	0.0000000	-2.6013408
C	2.4894109	0.0000000	-2.6013408
N	-2.4612541	0.0000000	-3.7917199
N	2.4612541	0.0000000	-3.7917199
I	-2.6132541	0.0000000	3.7882443
I	2.6132541	0.0000000	3.7882443

98.

C	0.0358400	3.2476787	-2.4520820
C	0.0338402	2.4748320	-1.2891277
C	0.0351934	3.1470479	0.0000000
C	0.0381331	4.6179927	0.0000000
C	0.0396359	5.3452568	-1.2383643
C	0.0385536	4.6488845	-2.4392616
C	0.0338402	2.4748320	1.2891277
C	0.0396359	5.3452568	1.2383643
C	0.0385536	4.6488845	2.4392616
C	0.0358400	3.2476787	2.4520820
F	0.0399535	5.3061229	3.6138568
F	0.0347709	2.6779360	3.6748447
F	0.0399535	5.3061229	-3.6138568
F	0.0347709	2.6779360	-3.6748447
I	0.0291389	0.3975596	-1.7132552
I	0.0291389	0.3975596	1.7132552
C	0.0421041	6.7782945	-1.3651917
C	0.0421041	6.7782945	1.3651917
N	0.0438951	7.9427749	-1.6168565
N	0.0438951	7.9427749	1.6168565
C	0.0062637	-4.8133150	-2.3792823
C	0.0161096	-5.4760037	-1.1515393
C	0.0287321	-4.6709224	0.0000000
C	0.0271233	-3.2670969	0.0000000
C	0.0048130	-3.3858095	-2.3082570
H	-0.0033577	-5.3140272	-3.3493078
C	0.0161096	-5.4760037	1.1515393
H	-0.0071575	-2.8356904	-3.2562901
C	0.0048130	-3.3858095	2.3082570

C	0.0062637	-4.8133150	2.3792823
H	-0.0071575	-2.8356904	3.2562901
H	-0.0033577	-5.3140272	3.3493078
N	0.0192117	-2.6107252	-1.2053556
N	0.0192117	-2.6107252	1.2053556
N	0.1119423	-6.8130978	-0.7297680
H	-0.5501483	-7.4841817	-1.1189840
N	0.1119423	-6.8130978	0.7297680
H	-0.5501483	-7.4841817	1.1189840

99.

C	-0.0344193	3.1502734	-2.3141366
C	-0.0298588	3.1957087	0.0000000
C	-0.0095515	4.6379446	0.0000000
C	0.0027501	5.3192968	-1.2469910
C	-0.0110873	4.5763513	-2.4284660
H	-0.0492551	2.5463491	-3.2315152
C	0.0027501	5.3192968	1.2469910
H	0.0159076	6.4150518	-1.2707940
C	-0.0110873	4.5763513	2.4284660
C	-0.0344193	3.1502734	2.3141366
H	0.0159076	6.4150518	1.2707940
H	-0.0492551	2.5463491	3.2315152
N	-0.0399026	2.4741160	-1.1646703
N	-0.0399026	2.4741160	1.1646703
N	-0.0775998	5.1619598	3.6953441
H	0.2813924	4.5894718	4.4536049
H	0.2630686	6.1170298	3.7508667
N	-0.0775998	5.1619598	-3.6953441
H	0.2630686	6.1170298	-3.7508667
H	0.2813924	4.5894718	-4.4536049
C	-0.0321838	-4.8053895	-2.4395734
C	-0.0299443	-5.5013938	-1.2383187
C	-0.0322807	-4.7738760	0.0000000
C	-0.0368414	-3.3026391	0.0000000
C	-0.0389715	-2.6317145	-1.2896002
C	-0.0364653	-3.4042935	-2.4529116
C	-0.0299443	-5.5013938	1.2383187
C	-0.0389715	-2.6317145	1.2896002
C	-0.0364653	-3.4042935	2.4529116
C	-0.0321838	-4.8053895	2.4395734
I	-0.0450230	-0.5551607	-1.7104770
I	-0.0450230	-0.5551607	1.7104770
F	-0.0379950	-2.8343687	3.6753984
F	-0.0299235	-5.4627877	3.6138277
F	-0.0379950	-2.8343687	-3.6753984
F	-0.0299235	-5.4627877	-3.6138277
C	-0.0251404	-6.9344176	-1.3648573
C	-0.0251404	-6.9344176	1.3648573
N	-0.0209415	-8.0989429	-1.6163968
N	-0.0209415	-8.0989429	1.6163968

100.

C	6.0747511	-0.0539640	-2.4374900
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C	6.7701122	-0.0563196	-1.2369211
C	6.0406581	-0.0537819	0.0000000
C	4.5693477	-0.0486215	0.0000000
C	3.8971910	-0.0462967	-1.2882642
C	4.6736153	-0.0490478	-2.4505124
C	6.7701122	-0.0563196	1.2369211
C	3.8971910	-0.0462967	1.2882642
C	4.6736153	-0.0490478	2.4505124
C	6.0747511	-0.0539640	2.4374900
I	1.8295213	-0.0388515	-1.7467412
I	1.8295213	-0.0388515	1.7467412
F	4.1090030	-0.0470128	3.6754063
F	6.7317367	-0.0562301	3.6122311
F	4.1090030	-0.0470128	-3.6754063
F	6.7317367	-0.0562301	-3.6122311
C	8.2032644	-0.0611369	-1.3631310
C	8.2032644	-0.0611369	1.3631310
N	9.3674409	-0.0649132	-1.6158434
N	9.3674409	-0.0649132	1.6158434
C	-4.6072659	0.0097630	-2.4576129
C	-3.7866334	-0.0060785	-1.3091940
C	-4.3768332	-0.0101372	0.0000000
C	-5.7923986	-0.0047052	0.0000000
C	-6.6151059	0.0094071	-1.1488456
C	-6.0247110	0.0105251	-2.4148826
H	-4.1126269	0.0175771	-3.4333759
C	-3.7866334	-0.0060785	1.3091940
C	-6.6151059	0.0094071	1.1488456
H	-6.6059182	0.0145651	-3.3396909
C	-6.0247110	0.0105251	2.4148826
C	-4.6072659	0.0097630	2.4576129
H	-6.6059182	0.0145651	3.3396909
H	-4.1126269	0.0175771	3.4333759
C	-2.3625143	-0.0176124	-1.5144751
C	-2.3625143	-0.0176124	1.5144751
N	-1.1978982	-0.0258185	-1.7564294
N	-1.1978982	-0.0258185	1.7564294
N	-7.9531162	-0.0779591	-0.7259799
H	-8.6112331	0.5980268	-1.1144029
N	-7.9531162	-0.0779591	0.7259799
H	-8.6112331	0.5980268	1.1144029

101.

C	6.2946360	-0.0310095	-2.4376460
C	6.9899863	-0.0294435	-1.2369169
C	6.2605954	-0.0309927	0.0000000
C	4.7895461	-0.0340629	0.0000000
C	4.1175726	-0.0354738	-1.2883198
C	4.8936702	-0.0339245	-2.4508102
C	6.9899863	-0.0294435	1.2369169
C	4.1175726	-0.0354738	1.2883198
C	4.8936702	-0.0339245	2.4508102
C	6.2946360	-0.0310095	2.4376460

I	2.0502780	-0.0394407	-1.7444998
I	2.0502780	-0.0394407	1.7444998
F	4.3286387	-0.0350428	3.6755030
F	6.9516611	-0.0295825	3.6122137
F	4.3286387	-0.0350428	-3.6755030
F	6.9516611	-0.0295825	-3.6122137
C	8.4230502	-0.0261683	-1.3630745
C	8.4230502	-0.0261683	1.3630745
N	9.5872509	-0.0233255	-1.6158725
N	9.5872509	-0.0233255	1.6158725
C	-4.3164973	-0.0214220	-2.4691964
C	-4.2382901	-0.0171937	0.0000000
C	-5.6863003	-0.0058596	0.0000000
C	-6.3999221	0.0042846	-1.2315231
C	-5.7375307	-0.0044118	-2.4620781
H	-3.7740629	-0.0385171	-3.4200019
C	-6.3999221	0.0042846	1.2315231
H	-7.4954618	0.0115286	-1.2023961
C	-5.7375307	-0.0044118	2.4620781
C	-4.3164973	-0.0214220	2.4691964
H	-7.4954618	0.0115286	1.2023961
H	-3.7740629	-0.0385171	3.4200019
N	-6.4292443	-0.0735183	3.6748842
H	-5.9334514	0.3005584	4.4782215
H	-7.3928779	0.2452840	3.6433124
N	-6.4292443	-0.0735183	-3.6748842
H	-7.3928779	0.2452840	-3.6433124
H	-5.9334514	0.3005584	-4.4782215
C	-3.5828558	-0.0235139	-1.2753718
C	-3.5828558	-0.0235139	1.2753718
C	-2.1502401	-0.0332973	-1.4309448
C	-2.1502401	-0.0332973	1.4309448
N	-0.9873754	-0.0395097	-1.6856301
N	-0.9873754	-0.0395097	1.6856301

102.

C	-0.0613300	2.9712401	-3.4658804
C	-0.0037331	3.1176919	-1.1622847
C	0.0017763	4.5647938	-1.2159274
C	0.0055950	5.2085872	-2.5096825
C	-0.0401373	4.3881079	-3.6265155
C	-0.0124408	5.2739488	0.0000000
C	0.0017763	4.5647938	1.2159274
C	-0.0037331	3.1176919	1.1622847
C	-0.0613300	2.9712401	3.4658804
C	-0.0401373	4.3881079	3.6265155
C	0.0055950	5.2085872	2.5096825
H	-0.0874969	2.3366030	-4.3592856
H	-0.0442383	4.8142704	-4.6342378
H	-0.0994654	6.3645465	0.0000000
H	-0.0874969	2.3366030	4.3592856
H	-0.0442383	4.8142704	4.6342378
N	-0.0211085	6.6012312	2.5921114

H	0.1568379	6.9673476	3.5232795
H	0.5301392	7.0896517	1.8926771
N	-0.0211085	6.6012312	-2.5921114
H	0.5301392	7.0896517	-1.8926771
H	0.1568379	6.9673476	-3.5232795
N	-0.0326354	2.3351268	-2.3023446
N	-0.0068695	2.4314140	0.0000000
N	-0.0326354	2.3351268	2.3023446
C	-0.0259284	-4.8550718	-3.6624581
C	-0.0256612	-5.5907641	-2.4858574
C	-0.0266569	-4.8963125	-1.2274432
C	-0.0277961	-3.4445589	-1.2303015
C	-0.0280764	-2.7123053	-2.4709512
C	-0.0270712	-3.4332173	-3.6537610
C	-0.0261357	-5.5909149	0.0000000
C	-0.0296875	-2.7666499	0.0000000
C	-0.0277961	-3.4445589	1.2303015
C	-0.0266569	-4.8963125	1.2274432
C	-0.0256612	-5.5907641	2.4858574
C	-0.0259284	-4.8550718	3.6624581
C	-0.0270712	-3.4332173	3.6537610
C	-0.0280764	-2.7123053	2.4709512
H	-0.0253005	-6.6872613	0.0000000
H	-0.0306292	-1.6763942	0.0000000
F	-0.0268863	-2.8215041	-4.8573199
F	-0.0247613	-5.4781813	-4.8604640
F	-0.0268863	-2.8215041	4.8573199
F	-0.0247613	-5.4781813	4.8604640
C	-0.0239679	-7.0252585	-2.5326934
C	-0.0239679	-7.0252585	2.5326934
I	-0.0292615	-0.5960380	-2.4756142
I	-0.0292615	-0.5960380	2.4756142
N	-0.0223375	-8.2157843	-2.5220947
N	-0.0223375	-8.2157843	2.5220947

103.

C	1.1446590	0.0000000	-1.0081078
C	1.1801751	0.0000000	0.4007884
C	0.0000000	0.0000000	1.1982416
C	-1.1801751	0.0000000	0.4007884
C	-1.1446590	0.0000000	-1.0081078
N	0.0000000	0.0000000	-1.7299324
H	2.0750199	0.0000000	-1.5900638
H	2.1752343	0.0000000	0.8681454
H	-2.1752343	0.0000000	0.8681454
H	-2.0750199	0.0000000	-1.5900638
Li	0.0000000	0.0000000	3.1901664

104.

C	1.14425020	0.00000000	-1.03586350
C	1.17950760	0.00000000	0.37396380
C	0.00000000	0.00000000	1.16838490
C	-1.17950760	0.00000000	0.37396380

C	-1.14425020	0.00000000	-1.03586350
N	0.00000000	0.00000000	-1.75814000
H	2.07517740	0.00000000	-1.61766270
H	2.17556320	0.00000000	0.83981310
H	-2.17556320	0.00000000	0.83981310
H	-2.07517740	0.00000000	-1.61766270
Na	0.00000000	0.00000000	3.46925390

105.

C	1.2035790	0.00000000	-0.6973602
C	1.1670915	0.00000000	0.7032132
C	0.00000000	0.00000000	1.4651979
C	-1.1670915	0.00000000	0.7032132
C	-1.2035790	0.00000000	-0.6973602
C	0.00000000	0.00000000	-1.4226152
F	-2.3873324	0.00000000	1.3520357
F	2.3873324	0.00000000	1.3520357
F	2.3959695	0.00000000	-1.3502291
F	-2.3959695	0.00000000	-1.3502291
I	0.00000000	0.00000000	-3.5126283
Li	0.00000000	0.00000000	3.4547263

106.

C	1.2038781	0.00000000	-0.7199627
C	1.1653731	0.00000000	0.6808590
C	0.00000000	0.00000000	1.4349920
C	-1.1653731	0.00000000	0.6808590
C	-1.2038781	0.00000000	-0.7199627
C	0.00000000	0.00000000	-1.4458809
F	-2.3965364	0.00000000	-1.3767914
F	-2.3903554	0.00000000	1.3293337
F	2.3965364	0.00000000	-1.3767914
F	2.3903554	0.00000000	1.3293337
I	0.00000000	0.00000000	-3.5365126
Na	0.00000000	0.00000000	3.7205242

107.

C	1.1010796	0.0174534	3.1160017
C	1.1088599	0.0279490	4.5232981
C	-0.0855713	0.0397253	5.2999829
C	-1.2557598	0.0394036	4.4871664
C	-1.2050944	0.0285812	3.0807535
N	-0.0412597	0.0177660	2.3930769
H	2.0324809	0.0085320	2.5371041
H	2.0946814	0.0266720	5.0077215
H	-2.2558866	0.0477571	4.9412423
H	-2.1184222	0.0285085	2.4736820
Li	-0.1157044	0.0549759	7.2978553
C	-1.1214913	-0.0295086	-4.5677243
C	0.0872406	-0.0391933	-5.2694000
C	1.2715143	-0.0382511	-4.5271245
C	1.2482784	-0.0279702	-3.1268565
C	0.0388448	-0.0181249	-2.4134301

C	-1.1457442	-0.0192466	-3.1674583
H	0.1056938	-0.0471711	-6.3602955
F	2.4681342	-0.0475071	-5.1714035
F	2.4331486	-0.0275661	-2.4669173
F	-2.2955830	-0.0301015	-5.2522759
F	-2.3523133	-0.0102014	-2.5481881
I	0.0028738	-0.0024821	-0.2868108

108.

C	-1.15316800	0.00000000	-3.07880400
C	-1.18163490	0.00000000	-4.48661280
C	0.00000000	0.00000000	-5.27927550
C	1.18163490	0.00000000	-4.48661280
C	1.15316800	0.00000000	-3.07880400
N	0.00000000	0.00000000	-2.37356660
H	-2.07583750	0.00000000	-2.48536750
H	-2.17596270	0.00000000	-4.95404470
H	2.17596270	0.00000000	-4.95404470
H	2.07583750	0.00000000	-2.48536750
Na	0.00000000	0.00000000	-7.58866560
C	1.19653530	0.00000000	4.55546270
C	0.00000000	0.00000000	5.27778390
C	-1.19653530	0.00000000	4.55546270
C	-1.19685960	0.00000000	3.15496850
C	0.00000000	0.00000000	2.42080280
C	1.19685960	0.00000000	3.15496850
H	0.00000000	0.00000000	6.36884650
F	-2.38233850	0.00000000	5.22025150
F	-2.39322360	0.00000000	2.51569930
F	2.38233850	0.00000000	5.22025150
F	2.39322360	0.00000000	2.51569930
I	0.00000000	0.00000000	0.29096870

109.

C	-4.5611188	-1.1372077	0.0013021
C	-3.1621965	-1.2072895	0.0013268
C	-2.3964526	-0.0296185	-0.0002052
C	-3.0980202	1.1874133	-0.0016593
C	-4.4988546	1.1944459	-0.0016066
C	-5.2937628	0.0489733	-0.0001740
F	-5.1148531	2.4341379	-0.0030941
F	-2.4162095	2.3677709	-0.0031632
F	-2.5454480	-2.4226930	0.0028464
F	-5.2454888	-2.3417347	0.0029028
I	-0.2899729	-0.0857306	-0.0002035
Li	-7.2781073	0.0733171	0.0002951
C	3.3174726	-1.2116857	-0.0010908
C	4.7228245	-1.1872096	-0.0009166
C	5.3773524	0.0564336	0.0003239
C	4.5951759	1.2240427	0.0013375
C	3.1952340	1.0998389	0.0010689
N	2.5592905	-0.0928652	-0.0001178
H	6.4695101	0.1141994	0.0004799

H	2.7704576	-2.1600760	-0.0020503
H	5.2865403	-2.1239751	-0.0017376
H	5.0567914	2.2150896	0.0023076
H	2.5498356	1.9844230	0.0018282

110.

C	1.1986276	0.0000000	3.1250873
C	1.1643836	0.0000000	4.5258235
C	0.0000000	0.0000000	5.2818037
C	-1.1643836	0.0000000	4.5258235
C	-1.1986276	0.0000000	3.1250873
C	0.0000000	0.0000000	2.3910536
F	-2.3969853	0.0000000	2.4717049
F	-2.3917627	0.0000000	5.1758156
F	2.3969853	0.0000000	2.4717049
F	2.3917627	0.0000000	5.1758156
I	0.0000000	0.0000000	0.2842454
Na	0.0000000	0.0000000	7.5626780
C	1.1571970	0.0000000	-3.2747105
C	1.2073445	0.0000000	-4.6793967
C	0.0000000	0.0000000	-5.3987549
C	-1.2073445	0.0000000	-4.6793967
C	-1.1571970	0.0000000	-3.2747105
N	0.0000000	0.0000000	-2.5765937
H	0.0000000	0.0000000	-6.4924613
H	2.0749065	0.0000000	-2.6774376
H	2.1725779	0.0000000	-5.1928720
H	-2.1725779	0.0000000	-5.1928720
H	-2.0749065	0.0000000	-2.6774376

111.

C	0.0094452	1.6214054	-1.1486936
C	-0.0102764	0.2166408	-1.1977916
C	-0.0173655	-0.5233107	0.0000000
C	-0.0102764	0.2166408	1.1977916
C	0.0094452	1.6214054	1.1486936
N	0.0204300	2.3351864	0.0000000
H	0.0137481	2.2052690	-2.0751774
H	-0.0235200	-0.2923773	-2.1671351
H	-0.0235200	-0.2923773	2.1671351
H	0.0137481	2.2052690	2.0751774
C	-0.0033589	-2.0342915	0.0000000
H	-0.5060294	-2.4348703	-0.8936245
H	1.0335593	-2.4097193	0.0000000
H	-0.5060294	-2.4348703	0.8936245

112.

C	0.0029620	-0.0684791	-1.1908856
C	0.0069054	-0.8094023	0.0000000
C	0.0029620	-0.0684791	1.1908856
C	0.0004571	1.3311637	1.2009624
C	-0.0018540	2.0589420	0.0000000
C	0.0004571	1.3311637	-1.2009624

F	-0.0006694	1.9720507	2.3920341
F	0.0029054	-0.7223580	2.3803284
F	0.0029054	-0.7223580	-2.3803284
F	-0.0006694	1.9720507	-2.3920341
I	-0.0080636	4.1456660	0.0000000
C	0.0030522	-2.3177947	0.0000000
H	0.5093574	-2.7006178	0.8963630
H	-1.0300649	-2.7009298	0.0000000
H	0.5093574	-2.7006178	-0.8963630

113.

C	-0.0049995	-2.3248524	-1.1554166
C	-0.0120096	-3.7281080	-1.2000958
C	-0.0127084	-4.4657269	0.0000000
C	-0.0120096	-3.7281080	1.2000958
C	-0.0049995	-2.3248524	1.1554166
N	-0.0005736	-1.6237669	0.0000000
H	-0.0058186	-1.7323940	-2.0761552
H	-0.0202497	-4.2387534	-2.1680737
H	-0.0202497	-4.2387534	2.1680737
H	-0.0058186	-1.7323940	2.0761552
C	0.0144765	-5.9759004	0.0000000
H	-0.4838603	-6.3806870	0.8938185
H	1.0554372	-6.3398213	0.0000000
H	-0.4838603	-6.3806870	-0.8938185
C	0.0007018	3.9843824	1.1991220
C	-0.0010054	5.3848711	1.1972279
C	-0.0020371	6.1059824	0.0000000
C	-0.0010054	5.3848711	-1.1972279
C	0.0007018	3.9843824	-1.1991220
C	0.0018532	3.2531804	0.0000000
H	-0.0035559	7.1971167	0.0000000
I	0.0026531	1.1391894	0.0000000
F	-0.0017451	6.0479278	2.3817323
F	0.0012140	3.3424868	2.3925324
F	-0.0017451	6.0479278	-2.3817323
F	0.0012140	3.3424868	-2.3925324

114.

C	-0.0222906	-3.6981633	-1.1900211
C	-0.0243470	-4.4405845	0.0000000
C	-0.0222906	-3.6981633	1.1900211
C	-0.0136437	-2.2986074	1.1949506
C	-0.0098146	-1.5623932	0.0000000
C	-0.0136437	-2.2986074	-1.1949506
F	-0.0094185	-1.6606272	2.3920376
F	-0.0279498	-4.3541946	2.3815800
F	-0.0279498	-4.3541946	-2.3815800
F	-0.0094185	-1.6606272	-2.3920376
I	0.0015763	0.5489313	0.0000000
C	-0.0421686	-5.9490846	0.0000000
H	0.4607980	-6.3368889	0.8962348
H	-1.0783585	-6.3242630	0.0000000

H	0.4607980	-6.3368889	-0.8962348
C	0.0253689	4.0301595	1.1585060
C	0.0391534	5.4343662	1.2075168
C	0.0462123	6.1532825	0.0000000
C	0.0391534	5.4343662	-1.2075168
C	0.0253689	4.0301595	-1.1585060
N	0.0183501	3.3336159	0.0000000
H	0.0569287	7.2468111	0.0000000
H	0.0195635	3.4329293	2.0760627
H	0.0442295	5.9478688	2.1725737
H	0.0442295	5.9478688	-2.1725737
H	0.0195635	3.4329293	-2.0760627

115.

C	-1.3997889	-1.2051536	0.0005052
C	0.0065081	-1.2192541	0.0001845
C	0.6503036	0.0236868	-0.0000864
C	-0.0822177	1.2164927	-0.0000160
C	-1.4837617	1.1001134	0.0003160
N	-2.1481284	-0.0782499	0.0005908
H	-1.9542249	-2.1484784	0.0006885
H	0.5770949	-2.1490530	0.0001446
H	0.4192061	2.1853417	-0.0003173
H	-2.1053584	2.0006011	0.0003154
N	2.1276804	0.0775074	-0.0006406
O	2.6562815	1.1979443	-0.0007574
O	2.7364054	-1.0014983	-0.0009271

116.

C	-1.1434008	-0.7166558	0.0001419
C	0.2600135	-0.6868537	0.0001242
C	0.9611611	0.5235067	-0.0000991
C	0.1902324	1.6954969	-0.0002877
C	-1.2128739	1.5918132	-0.0002353
N	-1.8788369	0.4154634	-0.0000266
H	2.0524323	0.5333435	-0.0002077
H	-1.6770396	-1.6690423	0.0003017
H	0.6688773	2.6781064	-0.0005334
H	-1.8350210	2.4920118	-0.0003827
N	1.0115533	-1.9591353	0.0003404
O	2.2476531	-1.8895390	0.0002185
O	0.3552491	-3.0085158	0.0006458

117.

C	-0.5130743	-1.2315571	0.0005567
C	0.8890006	-1.2279183	0.0009757
C	1.5905610	-0.0000891	0.0003991
C	0.8891395	1.2278170	-0.0005717
C	-0.5129358	1.2316141	-0.0010148
C	-1.1862862	0.0000668	-0.0004044
H	-1.0827700	-2.1620286	0.0009614
H	1.4439166	-2.1694310	0.0018162
H	1.4441623	2.1692673	-0.0008501

H	-1.0825313	2.1621467	-0.0018237
C	3.0333159	-0.0001700	0.0009889
N	4.2232230	-0.0002258	0.0015131
N	-2.6649201	0.0001482	-0.0007590
O	-3.2353394	1.0998803	-0.0015182
O	-3.2354617	-1.0995204	-0.0002691

118.

C	-0.7403705	-0.7736960	0.0002965
C	0.6588125	-0.8151664	0.0008036
C	1.3502738	0.4144271	0.0002213
C	0.6511140	1.6418785	-0.0008229
C	-0.7536320	1.6358908	-0.0013278
C	-1.4679488	0.4246672	-0.0007521
H	1.1870911	-1.7698485	0.0015956
H	1.2078652	2.5822500	-0.0011324
H	-1.2994132	2.5830016	-0.0022159
H	-2.5586275	0.3977738	-0.0011836
C	2.7951635	0.4137601	0.0007592
N	3.9841037	0.4210190	0.0012155
N	-1.4816278	-2.0570457	0.0007463
O	-2.7181692	-1.9991689	0.0002789
O	-0.8146350	-3.0997425	0.0015179

119.

C	2.6567927	-1.1541938	0.0090014
C	4.0616036	-1.1466878	0.0039124
C	4.6876340	0.1059238	-0.0013195
C	3.9422379	1.2914151	-0.0014156
C	2.5435017	1.1614938	0.0039626
N	1.9045619	-0.0304309	0.0092280
H	2.1066275	-2.0999826	0.0132077
H	4.6460921	-2.0676997	0.0039810
H	4.4339839	2.2650991	-0.0055201
H	1.9027817	2.0485914	0.0040881
N	6.1648820	0.1781973	-0.0067875
O	6.6773911	1.3056907	-0.0117300
O	6.7850411	-0.8938841	-0.0060781
C	-5.1580609	-1.2788601	-0.0037790
C	-3.7574949	-1.2803311	-0.0009931
C	-3.0298763	-0.0788831	0.0014169
C	-3.7600937	1.1209796	0.0010029
C	-5.1606440	1.1165313	-0.0017550
C	-5.8797009	-0.0819343	-0.0041533
H	-6.9708820	-0.0830989	-0.0062479
F	-3.1178465	2.3133387	0.0032078
F	-5.8238531	2.2995453	-0.0020723
F	-5.8187339	-2.4632711	-0.0061663
F	-3.1125684	-2.4711267	-0.0007256
I	-0.9233767	-0.0764218	0.0057344

120.

C	2.8371738	-0.9709922	-0.0186711
C	4.2338363	-0.8446363	-0.0255671
C	4.8507436	0.4108948	-0.0253271
C	4.0059786	1.5315604	-0.0179460
C	2.6138012	1.3382855	-0.0112334
N	2.0378445	0.1159644	-0.0115382
H	5.9389646	0.4925666	-0.0307067
H	2.3615733	-1.9539776	-0.0188669
H	4.4199996	2.5428221	-0.0173757
H	1.9259483	2.1895224	-0.0053505
N	5.0690711	-2.0645454	-0.0331925
O	6.2969729	-1.9106627	-0.0377237
O	4.4816017	-3.1533693	-0.0344973
C	-5.0764182	-0.9829127	0.0263656
C	-3.6766361	-1.0302271	0.0183421
C	-2.9107502	0.1472781	0.0162940
C	-3.6013529	1.3703655	0.0225831
C	-5.0011628	1.4113459	0.0305978
C	-5.7587262	0.2368645	0.0326060
H	-6.8493528	0.2710367	0.0388555
F	-2.9206943	2.5413892	0.0210049
F	-5.6256751	2.6153693	0.0364788
F	-5.7754187	-2.1449372	0.0280679
F	-3.0707206	-2.2406672	0.0125553
I	-0.8066016	0.0816624	0.0042453

121.

C	-5.2675472	-1.1971461	0.0035752
C	-3.8656840	-1.2076192	0.0013562
C	-3.1551750	0.0151016	-0.0026857
C	-3.8426597	1.2509264	-0.0044933
C	-5.2444736	1.2667204	-0.0022912
C	-5.9287197	0.0410883	0.0016857
H	-5.8465655	-2.1218556	0.0066830
H	-3.3191610	-2.1539677	0.0026928
H	-3.2784999	2.1868646	-0.0076169
H	-5.8060728	2.2021160	-0.0036005
C	-1.7140256	0.0016655	-0.0050829
N	-0.5256215	-0.0092243	-0.0070894
N	-7.4077382	0.0549433	0.0039928
O	-7.9669582	1.1602209	0.0021953
O	-7.9875620	-1.0396619	0.0075560
C	5.3063249	-1.2370669	-0.0025913
C	6.7068039	-1.2379830	-0.0006977
C	7.4320610	-0.0434954	0.0022747
C	6.7163364	1.1567311	0.0033335
C	5.3158949	1.1669666	0.0014545
C	4.5828153	-0.0321478	-0.0015385
H	8.5231434	-0.0478385	0.0037409
F	4.6780975	2.3599732	0.0025954
F	7.3828494	2.3377185	0.0062169
F	4.6590543	-2.4249489	-0.0054543

F	7.3638907	-2.4242412	-0.0017952
I	2.4891923	-0.0238401	-0.0044161
122.			
C	-5.4337277	-0.8694101	-0.0178187
C	-4.0402122	-0.9996078	-0.0205194
C	-3.2750274	0.1849122	0.0094814
C	-3.8929269	1.4547643	0.0410218
C	-5.2952201	1.5365003	0.0424906
C	-6.0835610	0.3723883	0.0130332
H	-3.5731560	-1.9854382	-0.0450248
H	-3.2776076	2.3575669	0.0639022
H	-5.7805199	2.5156123	0.0667940
H	-7.1738160	0.4139809	0.0135800
C	-1.8342541	0.0953028	0.0079808
N	-0.6483175	0.0349331	0.0071529
N	-6.2547566	-2.1032688	-0.0490857
O	-7.4848374	-1.9666681	-0.0460506
O	-5.6539100	-3.1849128	-0.0760082
C	5.2255513	-1.0403650	0.0459859
C	6.6253532	-0.9943692	0.0437511
C	7.3101527	0.2228576	-0.0030902
C	6.5547305	1.3976101	-0.0478772
C	5.1547502	1.3609017	-0.0459850
C	4.4620803	0.1388710	0.0011667
H	8.4007672	0.2549785	-0.0045761
F	4.4773942	2.5312096	-0.0906032
F	7.1813336	2.5994595	-0.0942119
F	7.3218183	-2.1570105	0.0879638
F	4.6184530	-2.2481164	0.0923683
I	2.3694655	0.0773177	0.0041784