Supporting Information

Theoretical Study of Hydrogen Bonding Interaction in Substituted Nitroxide Radicals

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Benchmark study

The performance of the functional UM06L/6-311++G(d,p) for the calculation of E_{int} is compared with high level *ab initio* methods *viz*. UMP2/6-311++G(d,p), UMP4(SDQ)/6-311++G(d,p) and UCCSD(T)/6-311++G(d,p)//UMP4(SDQ)/6-311++G(d,p). We have selected ten representative complexes of unsubstituted nitroxide radicals with HF, namely **3, 4, 11, 12, 13, 16**, **17, 21, 24,** and **25** for this study. All calculated E_{int} values are presented in Table S1. When compared to UCCSD(T)/6-311++G(d,p)//UMP4(SDQ)/6-311++G(d,p) method, UM06L/6-311++G(d,p) method slightly overestimate the E_{int} of nitroxide radicals, whereas E_{int} values of iminoxyl radicals are more or less comparable. The E_{int} values calculated at UCCSD(T)/6-311++G(d,p)//UMP4(SDQ)/6-311++G(d,p) level of theory deviates from UM06L/6-311++G(d,p) by 0.38 – -1.67 kcal/mol. A reasonably good correlation exist between the E_{int} values calculated at the UM06L method and the values calculated using wavefunction methods. The correlation coefficients are respectively 0.983, 0.964 and 0.945 for single point calculations at UCCSD(T), UMP4(SDQ) and UMP2 methods. The decent correlation of the E_{int} values calculated using the *ab initio* methods with UM06L method clearly justify the use of UM06L method for the calculations in this manuscript.

Table S1. E_{int} of ten unsubstituted NO···HF complexes namely, **3**, **4**, **11**, **12**, **13**, **16**, **17**, **21**, **24**, and **25** computed with UM06L, UMP2, UMP4(SDQ), and UCCSD(T)//UMP4(SDQ) level of theories.

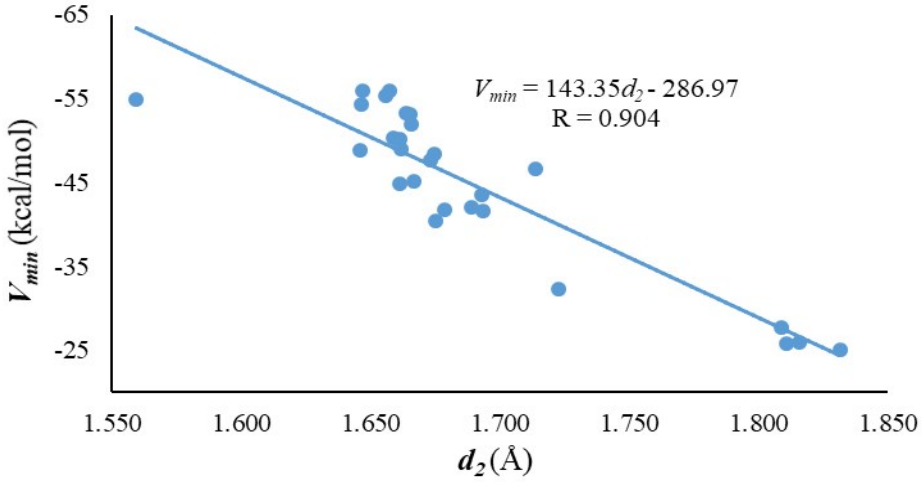
Structure	E_{int} (in kcal/mol)			
	UM06L /6-311++G(d,p)	UMP2 /6-311++G(d,p)	UMP4(SDQ) /6-311++G(d,p)	UCCSD(T)/ 6-311 ++G(d,p)// UMP4(SDQ)/ 6-311++G(d,p)
3	-12.35	-12.85	-11.63	-11.70
4	-12.51	-13.24	-11.76	-11.70
11	-12.22	-12.67	-11.46	-11.50
12	-11.69	-12.29	-10.99	-10.98
13	-14.99	-15.77	-13.34	-13.32
16	-10.65	-10.10	-9.25	-9.63
17	-9.05	-7.20	-6.89	-7.52
21	-11.95	-11.07	-11.25	-11.62
24	-5.42	-6.40	-5.88	-5.68
25	-6.11	-7.59	-6.77	-6.49

Table S2. N–O distance (d_1) of nitroxide radicals with and without substituents (X = H, CH_3, and F).

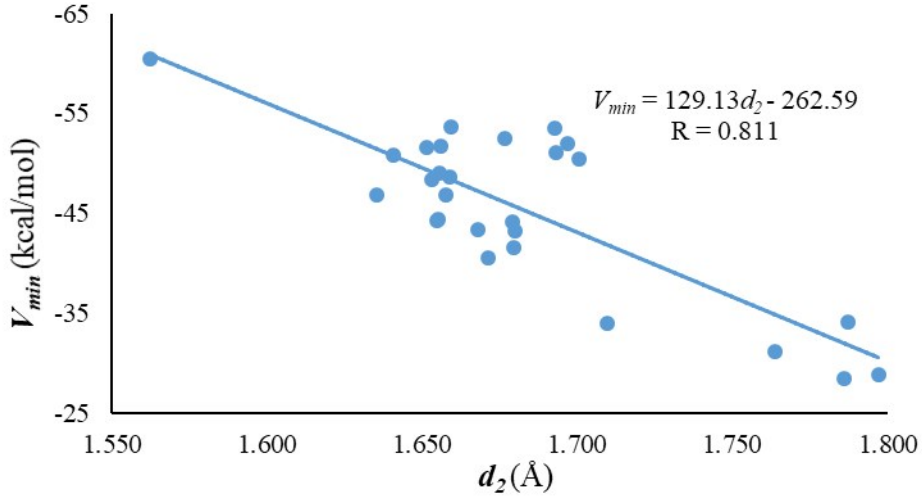
Structure	d_1 (Å)		
	X =H	X =CH_3	X =F
1	1.270	1.275	1.147
2	1.264	1.266	1.258
3	1.263	1.265	1.258
4	1.274	1.275	1.267
5	1.276	1.277	1.266
6	1.261	1.262	1.259
7	1.262	1.264	1.257
8	1.271	1.271	1.266
9	1.269	1.271	1.265
10	1.272	1.272	1.271
11	1.262	1.264	1.255
12	1.262	1.264	1.256
13	1.268	1.283	1.274
14	1.262	1.265	1.258
15	1.258	1.262	1.253
16	1.269	1.271	1.264
17	1.260	1.263	1.260
18	1.277	1.277	1.268
19	1.268	1.269	1.266
20	1.263	1.266	1.260
21	1.260	1.268	1.259
22	1.273	1.275	1.265
23	1.262	1.266	1.264
24	1.216	1.230	1.243
25	1.224	1.227	1.234
26	1.223	1.226	1.233
27	1.224	1.224	1.216

Table S3. Spin densities on N and O atoms of NO unit in nitroxide and iminoxyl radicals with and without substituents (X = H, CH_3, and F).

Structure	Spin density (in au)					
	X = H		X = CH_3		X = F	
	N	O	N	O	N	O
1	0.4351	0.5984	0.4191	0.5296	0.3650	0.2187
2	0.4327	0.5121	0.4532	0.5038	0.3223	0.6195
3	0.4273	0.5224	0.4687	0.5072	0.3315	0.6169
4	0.4501	0.5365	0.4407	0.5206	0.3268	0.6291
5	0.4038	0.5243	0.4491	0.5225	0.3597	0.5896
6	0.3231	0.4538	0.3424	0.4453	0.3016	0.5051
7	0.4206	0.5194	0.4793	0.5002	0.3197	0.6105
8	0.3403	0.4673	0.3565	0.4752	0.3159	0.5292
9	0.3110	0.4443	0.3386	0.4400	0.2774	0.5191
10	0.2948	0.4443	0.2957	0.4420	0.2825	0.4696
11	0.4344	0.5131	0.4789	0.4954	0.3096	0.6218
12	0.4347	0.5170	0.4701	0.5000	0.3254	0.6169
13	0.3254	0.5322	0.3406	0.5273	0.1828	0.6298
14	0.4235	0.5234	0.4721	0.5047	0.3237	0.6216
15	0.3150	0.4753	0.3482	0.4750	0.2688	0.5884
16	0.3208	0.5048	0.3290	0.4970	0.2805	0.5764
17	0.2426	0.4501	0.2706	0.4525	0.2132	0.5638
18	0.4005	0.5224	0.4588	0.5221	0.3817	0.5774
19	0.3343	0.4576	0.3444	0.4499	0.3195	0.5057
20	0.4144	0.5320	0.4486	0.5193	0.2989	0.6326
21	0.2487	0.3309	0.2780	0.3150	0.2079	0.3739
22	0.2447	0.3409	0.2545	0.3316	0.2201	0.3752
23	0.1687	0.3455	0.1797	0.3367	0.1654	0.3491
24	0.4731	0.5591	0.4401	0.5872	0.3448	0.6723
25	0.4458	0.5750	0.4523	0.5790	0.4130	0.6170
26	0.4449	0.5743	0.4633	0.5797	0.4156	0.6190
27	0.4619	0.5878	0.4532	0.5770	0.4663	0.5807



(a)



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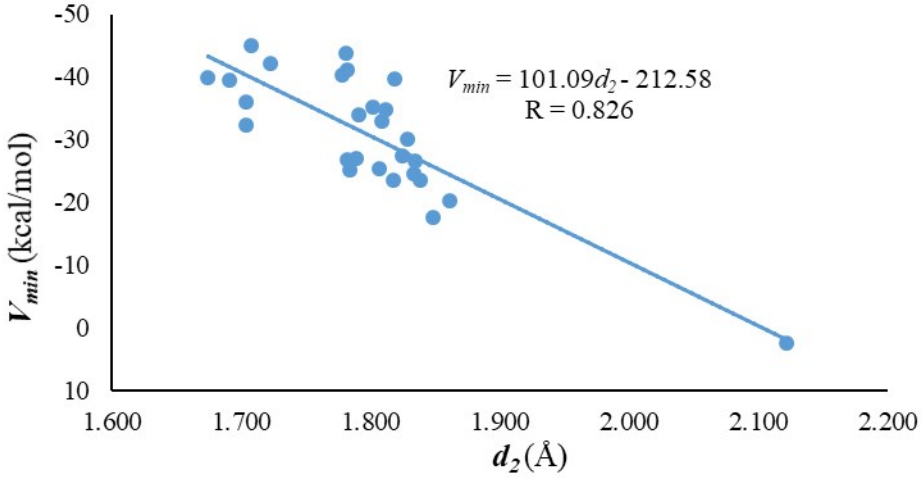

(c)

Fig. S1 Correlation between the NO···H distance (d_2) and V_{min} of nitroxide radicals with different substituents (a) for X = H (b) for X = CH_3, and (c) for X = F.

Table S4. Spin densities on atoms nitrogen, oxygen, hydrogen, and fluorine calculated for NO···HF complexes of unsubstituted nitroxide radicals.

Structure	Spin density (in au)			
	N	O	H	F
1	0.4833	0.5596	-0.0076	-0.0004
2	0.4659	0.4839	-0.0142	0.0049
3	0.4599	0.4943	-0.0141	0.0050
4	0.4826	0.5023	-0.0127	0.0039
5	0.4542	0.4767	-0.0114	0.0076
6	0.3464	0.4203	-0.0128	0.0047
7	0.4464	0.4991	-0.0155	0.0060
8	0.3669	0.4303	-0.0137	0.0047
9	0.3368	0.4042	-0.0121	0.0057
10	0.3412	0.3698	-0.0025	0.0068
11	0.4684	0.4835	-0.0135	0.0046
12	0.4732	0.4826	-0.0122	0.0040
13	0.3864	0.4792	-0.0102	0.0016
14	0.4578	0.4949	-0.0127	0.0043
15	0.3442	0.4451	-0.0114	0.0043
16	0.3509	0.4761	-0.0125	0.0042
17	0.2782	0.4154	0.0005	0.0007
18	0.4401	0.4851	-0.0095	0.0032
19	0.3603	0.4164	-0.0114	0.0037
20	0.4460	0.4988	-0.0122	0.0044
21	0.2563	0.2907	-0.0076	0.0028
22	0.2520	0.2914	-0.0069	0.0026
23	0.1616	0.2897	-0.0069	0.0017
24	0.4953	0.5346	-0.0052	0.0023
25	0.4702	0.5469	-0.0064	0.0026
26	0.4686	0.5450	-0.0067	0.0027
27	0.4840	0.5573	-0.0090	0.0038

Table S5. AIM parameters at the bcp of NO···H bond for all complexes with and without substituents. All ρ, $\nabla^2\rho$, and H values are in atomic units.

Structure	X= H			X = CH_3			X = F		
	ρ	$\nabla^2\rho$	H	ρ	$\nabla^2\rho$	H	ρ	$\nabla^2\rho$	H
1	0.0434	0.1385	-0.0029	0.0478	0.1501	-0.0042	0.0125	0.0560	0.0029
2	0.0483	0.1501	-0.0044	0.0406	0.1425	-0.0010	0.0305	0.1175	0.0020
3	0.0474	0.1489	-0.0041	0.0401	0.1415	-0.0008	0.0308	0.1184	0.0020
4	0.0482	0.1504	-0.0043	0.0401	0.1433	-0.0008	0.0297	0.1156	0.0022
5	0.0489	0.1526	-0.0046	0.0431	0.1459	-0.0021	0.0323	0.1236	0.0013
6	0.0471	0.1493	-0.0043	0.0459	0.1498	-0.0029	0.0399	0.1414	-0.0007
7	0.0451	0.1480	-0.0036	0.0361	0.1404	-0.0006	0.0306	0.1187	0.0017
8	0.0469	0.1507	-0.0040	0.0453	0.1506	-0.0028	0.0325	0.1261	0.0016
9	0.0471	0.1502	-0.0037	0.0423	0.1438	-0.0017	0.0321	0.1194	0.0014
10	0.0424	0.1474	-0.0016	0.0418	0.1445	-0.0013	0.0387	0.1421	-0.0002
11	0.0473	0.1488	-0.0040	0.0467	0.1527	-0.0034	0.0290	0.1128	0.0023
12	0.0461	0.1472	-0.0035	0.0466	0.1518	-0.0034	0.0296	0.1149	0.0021
13	0.0653	0.1642	-0.0138	0.0631	0.1637	-0.0122	0.0488	0.1498	-0.0054
14	0.0464	0.1472	-0.0037	0.0475	0.1526	-0.0038	0.0295	0.1120	0.0019
15	0.0439	0.1428	-0.0027	0.0436	0.1478	-0.0021	0.0279	0.1097	0.0025
16	0.0427	0.1417	-0.0021	0.0432	0.1492	-0.0018	0.0342	0.1223	0.0005
17	0.0405	0.1376	-0.0013	0.0397	0.1426	-0.0005	0.0329	0.1180	0.0007
18	0.0490	0.1530	-0.0046	0.0459	0.1561	-0.0028	0.0320	0.1222	0.0013
19	0.0451	0.1503	-0.0032	0.0461	0.1535	-0.0031	0.0371	0.1387	0.0003
20	0.0475	0.1485	-0.0042	0.0463	0.1537	-0.0032	0.0285	0.1117	0.0024
21	0.0490	0.1499	-0.0049	0.0491	0.1577	-0.0044	0.0335	0.1260	0.0012
22	0.0503	0.1526	-0.0054	0.0480	0.1563	-0.0039	0.0430	0.1407	-0.0025
23	0.0467	0.1456	-0.0040	0.0438	0.1380	-0.0026	0.0406	0.1375	-0.0018
24	0.0279	0.1118	0.0026	0.0333	0.1221	0.0009	0.0285	0.1075	0.0017
25	0.0298	0.1031	0.0025	0.0318	0.1196	0.0016	0.0303	0.1157	0.0018
26	0.0297	0.1150	0.0021	0.0338	0.1236	0.0013	0.0330	0.1185	0.0011
27	0.0301	0.1152	0.0018	0.0306	0.1110	0.0015	0.0283	0.1108	0.0022

Table S6. E_{int} values of unsubstituted NO···H_2O complexes. All values are in kcal/mol.

Structure	E_{int}
1	-8.29
2	-8.15
3	-8.04
4	-7.84
5	-8.84
6	-7.88
7	-8.04
8	-7.81
9	-7.89
10	-6.23
11	-7.96
12	-7.88
13	-12.04
14	-8.13
15	-7.11
16	-7.20
17	-6.51
18	-8.73
19	-7.53
20	-7.69
21	-8.41
22	-7.91
23	-7.94
24	-4.60
25	-3.74
26	-3.89
27	-4.16

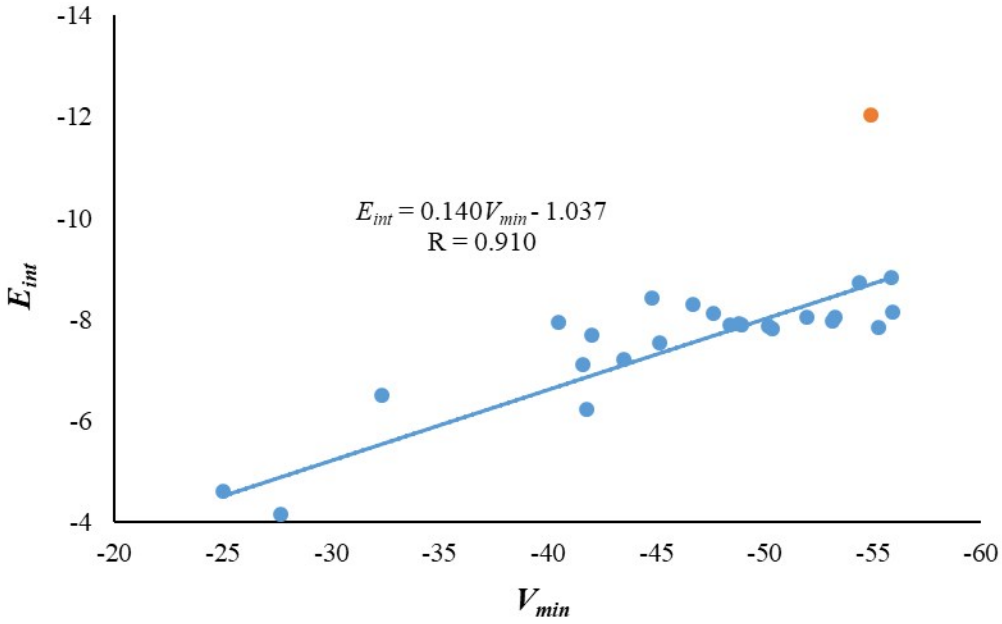

Fig. S2 Correlation between values of V_{min} and E_{int} for unsubstituted NO···H_2O complexes. All values are in kcal/mol. The values of V_{min} and E_{int} for radical **13** (indicated as red circle) is excluded in the correlation curve. This is due to the interaction between phosphorus atom and water molecule in NO···H_2O complex of **13**.

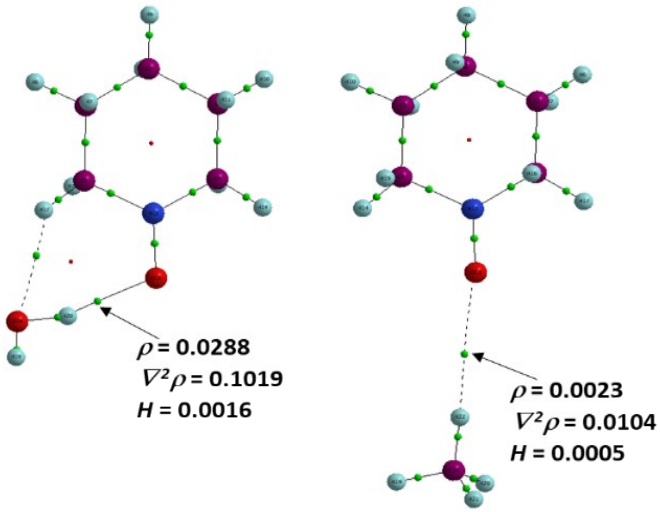

Fig. S3 QTAIM topological plot and QTAIM parameters (in au) of hydrogen bonded complex of unsubstituted nitroxide radical **4** with water and methane molecule.

Table S7. Values of QTAIM parameters for H_2O and CH_4 -interacted radicals of **3**, **4**, **11**, **12**, **13**, **16**, **17**, **21**, **24**, and **25**. The values of ρ, $\nabla^2\rho$ and H at the bcp of NO···H bond are given in atomic units.

Structure	Complexes with H_2O			Complexes with CH_4		
	ρ	$\nabla^2\rho$	H	ρ	$\nabla^2\rho$	H
3	0.0286	0.1013	0.0017	0.0023	0.0104	0.0005
4	0.0288	0.1019	0.0016	0.0023	0.0104	0.0005
11	0.0287	0.1021	0.0017	0.0074	0.0239	0.0006
12	0.0280	0.1004	0.0018	0.0067	0.0213	0.0005
13	0.0369	0.1242	-0.0002	0.0106	0.0303	0.0007
16	0.0264	0.0956	0.0020	0.0023	0.0104	0.0005
17	0.0248	0.0911	0.0021	0.0023	0.0103	0.0005
21	0.0277	0.0984	0.0017	0.0023	0.0105	0.0005
24	0.0153	0.0582	0.0020	0.0022	0.0102	0.0005
25	0.0160	0.0671	0.0026	0.0013	0.0063	0.0004

Table S8. The SAPT partitioning of interaction energy for unsubstituted complexes of **3**, **4**, **11**, **12**, **13**, **16**, **17**, **21**, **24**, and **25** nitroxide radical with HF. All energy values are in kcal/mol.

Structure	E_{elst}	E_{exch}	E_{ind}	E_{disp}	E_{int}^{SAPT}
3	-17.62	16.78	-8.44	-4.32	-13.60
4	-18.31	18.08	-8.82	-4.47	-13.52
11	-17.73	16.96	-8.45	-4.35	-13.57
12	-16.96	16.48	-8.07	-4.29	-12.83
13	-27.53	31.60	-14.94	-7.28	-18.14
16	-15.21	15.82	-7.63	-4.20	-11.22
17	-13.04	13.94	-6.88	-3.94	-9.91
21	-19.06	17.96	-9.11	-4.70	-14.92
24	-7.59	7.22	-3.81	-2.23	-6.41
25	-7.58	8.34	-4.17	-2.84	-6.25

Table S9. The SAPT partitioning of interaction energy for unsubstituted complexes of **3**, **4**, **11**, **12**, **13**, **16**, **17**, **21**, **24**, and **25** nitroxide radical with H_2O. All energy values are in kcal/mol.

Structure	E_{elst}	E_{exch}	E_{ind}	E_{disp}	E_{int}^{SAPT}
3	-11.33	11.04	-3.77	-4.22	-8.27
4	-11.89	12.18	-4.00	-4.21	-7.91
11	-11.74	11.70	-3.93	-4.26	-8.23
12	-11.60	11.60	-3.78	-4.28	-8.06
13	-21.51	22.57	-7.67	-6.92	-13.52
16	-10.34	10.79	-3.38	-4.05	-6.98
17	-9.52	10.37	-3.17	-4.10	-6.43
21	-14.10	13.66	-4.61	-4.70	-9.74
24	-5.98	6.38	-1.86	-3.14	-4.60
25	-5.33	5.79	-1.58	-3.03	-4.15

Table S10. The SAPT partitioning of interaction energy for unsubstituted complexes of **3**, **4**, **11**, **12**, **13**, **16**, **17**, **21**, **24**, and **25** nitroxide radical with CH_4. All energy values are in kcal/mol.

Structure	E_{elst}	E_{exch}	E_{ind}	E_{disp}	E_{int}^{SAPT}
3	-0.26	0.21	-0.13	-0.48	-0.66
4	-0.27	0.22	-0.13	-0.49	-0.67
11	-1.24	2.74	-0.44	-2.99	-1.93
12	-1.43	3.19	-0.44	-3.39	-2.06
13	-2.21	4.22	-1.03	-3.05	-2.07
16	-0.22	0.21	-0.08	-0.49	-0.58
17	-0.21	0.21	-0.06	-0.48	-0.54
21	-0.26	0.21	-0.12	-0.51	-0.68
24	-0.17	0.20	-0.05	-0.43	-0.44
25	-0.09	0.08	-0.03	-0.32	-0.36

Coordinates of optimized structures of 27 Nitroxide radicals (X = H, CH_3, and F)

1 (X = H)

N	0.537495000000	0.000000000000	-0.036151000000
O	-0.731688000000	0.000000000000	0.009042000000
H	1.045519000000	-0.874577000000	0.090361000000
H	1.045518000000	0.874577000000	0.090361000000

1 (X = CH_3)

N	0.000002000	0.122099000	-0.148152000
O	-0.000032000	1.382584000	0.042137000
C	-1.247001000	-0.602122000	0.024185000
H	-2.056618000	0.017633000	-0.357814000
H	-1.211174000	-1.547024000	-0.522509000
H	-1.435657000	-0.815764000	1.084994000
C	1.247026000	-0.602080000	0.024227000
H	1.211408000	-1.546800000	-0.522799000
H	2.056664000	0.017883000	-0.357382000
H	1.435462000	-0.816079000	1.085004000

1 (X = F)

N	-0.725236000	-0.093385000	0.277312000
O	0.184874000	-0.633741000	-0.204987000
F	-0.917127000	1.337786000	-0.071799000
F	-2.050222000	-0.667855000	0.003138000
H	2.252139000	-0.156355000	-0.218889000
F	3.116851000	-0.016599000	0.059505000

2 (X = H)

C	0.021501000	1.214460000	-0.127598000
C	-1.374766000	0.731180000	0.228229000
C	0.021379000	-1.214429000	0.126689000
C	-1.375248000	-0.730975000	-0.227079000
H	-1.523499000	0.786306000	1.311562000
H	-2.161827000	-1.323284000	0.243425000
H	-1.525585000	-0.786074000	-1.310210000
H	-2.161925000	1.323597000	-0.241180000
N	0.832543000	-0.000267000	-0.002098000
O	2.096177000	-0.000044000	0.001338000
H	0.086489000	1.592786000	-1.157943000
H	0.422755000	1.987063000	0.533505000
H	0.420769000	-1.988306000	-0.534099000
H	0.088409000	-1.591273000	1.157479000

2 (X = CH_3)

C	1.253800000	0.130191000	0.013611000
C	0.702674000	1.529313000	0.300026000
C	-1.253856000	0.130328000	-0.013693000
C	-0.702673000	1.529461000	-0.299743000
H	0.654556000	1.691199000	1.382670000
H	-1.340212000	2.313805000	0.116060000
H	-0.654501000	1.691599000	-1.382358000
H	1.340273000	2.313698000	-0.115616000
N	-0.000033000	-0.671677000	-0.000733000
O	-0.000092000	-1.937682000	-0.000541000
C	-2.180135000	-0.399690000	-1.094178000
H	-3.100909000	0.188594000	-1.130860000
H	-1.701315000	-0.354343000	-2.076034000
H	-2.440280000	-1.441011000	-0.893181000
C	-1.908614000	0.026419000	1.362915000
H	-1.264407000	0.439067000	2.144624000
H	-2.859048000	0.567440000	1.381624000
H	-2.103360000	-1.021138000	1.604426000
C	1.909584000	0.026919000	-1.362554000
H	1.265920000	0.439966000	-2.144503000
H	2.860043000	0.567928000	-1.380331000
H	2.104475000	-1.020524000	-1.604436000
C	2.179284000	-0.400312000	1.094572000
H	2.439968000	-1.441423000	0.893172000
H	3.099809000	0.188284000	1.132445000

2 (X = F)

C	-1.207933000	-0.106039000	0.020582000
C	-0.705662000	-1.504375000	0.291723000
C	1.208004000	-0.105987000	-0.020661000
C	0.705929000	-1.504228000	-0.292565000
H	-0.685280000	-1.654751000	1.373336000
H	1.365132000	-2.249139000	0.150724000
H	0.685715000	-1.654237000	-1.374224000
H	-1.364853000	-2.249185000	-0.151717000
N	-0.000060000	0.710838000	-0.000152000
O	-0.000088000	1.968607000	-0.000090000
F	2.069443000	0.365053000	-0.939025000
F	1.841213000	-0.009108000	1.183688000
F	-2.068953000	0.364463000	0.939732000
F	-1.841883000	-0.008590000	-1.183375000

H	1.699572000	-0.355718000	2.076025000

3 (X = H)

C	-0.047561000	1.218258000	-0.000009000
C	-1.431046000	0.666379000	0.000013000
C	-0.047489000	-1.218221000	-0.000092000
C	-1.430988000	-0.666445000	0.000234000
N	0.767845000	0.000024000	-0.000522000
O	2.030723000	0.000016000	0.000272000
H	0.186250000	1.830396000	0.882347000
H	0.186001000	1.830882000	-0.882005000
H	0.186100000	-1.830352000	0.882378000
H	0.186363000	-1.830886000	-0.881967000
H	-2.311395000	-1.296605000	-0.000213000
H	-2.311514000	1.296451000	0.000064000

3 (X = CH_3)

C	-1.249042000	0.174776000	0.000021000
C	-0.665307000	1.556449000	0.000446000
C	1.249042000	0.174773000	0.000020000
C	0.665312000	1.556447000	0.000443000
N	-0.000002000	-0.632231000	-0.000495000
O	-0.000006000	-1.897471000	-0.000563000
C	2.056902000	-0.140420000	1.256885000
H	2.981196000	0.442834000	1.278950000
H	1.483095000	0.085909000	2.158637000
H	2.316396000	-1.201641000	1.270271000
C	2.057278000	-0.139523000	-1.256832000
H	1.483658000	0.087287000	-2.158581000
H	2.981502000	0.443862000	-1.278315000
H	2.316919000	-1.200702000	-1.270818000
C	-2.056902000	-0.140418000	1.256882000
H	-1.483088000	0.085887000	2.158636000
H	-2.981183000	0.442855000	1.278960000
H	-2.316420000	-1.201634000	1.270260000
C	-2.057275000	-0.139519000	-1.256834000
H	-2.316906000	-1.200700000	-1.270827000
H	-2.981505000	0.443858000	-1.278309000
H	-1.483658000	0.087305000	-2.158582000
H	-1.297889000	2.437448000	0.000753000
H	1.297896000	2.437444000	0.000739000

3 (X = F)

C	-1.200970000	0.143179000	-0.000094000
C	-0.663720000	1.535501000	-0.000112000
C	1.200973000	0.143186000	0.000021000
C	0.663716000	1.535507000	0.000152000
N	0.000000000	-0.679275000	-0.000133000
O	0.000011000	-1.936971000	-0.000129000
F	-1.967094000	-0.129930000	-1.081171000
F	-1.966778000	-0.129673000	1.081445000
F	1.966901000	-0.130018000	1.081310000
F	1.966963000	-0.129577000	-1.081307000
H	-1.326771000	2.389619000	-0.000337000
H	1.326756000	2.389633000	-0.000003000

4 (X = H)

C	-1.054702000	1.249396000	-0.259533000
C	-1.798364000	-0.000075000	0.194071000
C	-1.054570000	-1.249416000	-0.259685000
C	0.377530000	-1.247959000	0.250383000
C	0.377437000	1.248092000	0.250297000
H	-1.558839000	2.156515000	0.087249000
H	-1.045693000	1.292781000	-1.355433000
H	-2.821118000	-0.000061000	-0.193984000
H	-1.881772000	-0.000154000	1.289630000
H	-1.558628000	-2.156651000	0.086900000
H	-1.045493000	-1.292571000	-1.355598000
N	1.060313000	-0.000070000	-0.094703000
O	2.332786000	0.000043000	-0.162385000
H	0.977738000	-2.055042000	-0.172023000
H	0.393598000	-1.362314000	1.347430000
H	0.394063000	1.362548000	1.347242000
H	0.977682000	2.054868000	-0.172607000

4 (X = CH_3)

C	1.236373000	1.384472000	-0.502946000
C	-0.000068000	2.108691000	-0.002947000
C	-1.236455000	1.384401000	-0.503067000
C	-1.322694000	-0.068464000	-0.028983000
C	1.322790000	-0.068368000	-0.028931000
H	2.153948000	1.896738000	-0.192136000
H	1.233218000	1.395509000	-1.600950000
H	-0.000032000	3.144611000	-0.355292000
H	-0.000163000	2.164903000	1.092526000

4 (X = F)

C	1.242903000	1.352121000	-0.466173000
C	0.000102000	2.067529000	0.037907000
C	-1.242800000	1.352143000	-0.466028000
C	-1.264453000	-0.088944000	-0.027053000
C	1.264658000	-0.088850000	-0.026858000
H	2.164256000	1.813903000	-0.104778000
H	1.277197000	1.359780000	-1.560388000
H	0.000131000	3.103184000	-0.307607000
H	0.000249000	2.101486000	1.132019000

H	-2.154094000	1.896547000	-0.192278000
H	-1.233170000	1.395378000	-1.601040000
N	-0.000004000	-0.750488000	-0.234974000
O	0.000030000	-2.017277000	-0.087160000
C	-2.350550000	-0.824905000	-0.861658000
H	-2.060731000	-0.843140000	-1.915109000
H	-2.451367000	-1.854794000	-0.519133000
H	-3.322017000	-0.329655000	-0.780710000
C	2.350532000	-0.824770000	-0.861760000
H	3.322064000	-0.329597000	-0.781050000
H	2.451444000	-1.854639000	-0.519185000
H	2.060575000	-0.843162000	-1.915173000
C	-1.703082000	-0.156885000	1.451779000
H	-2.743400000	0.152212000	1.588887000
H	-1.602361000	-1.187906000	1.798753000
H	-1.081543000	0.480766000	2.083386000
C	1.703145000	-0.156955000	1.451775000
H	1.603135000	-1.188218000	1.798325000
H	2.743226000	0.152813000	1.589061000
H	1.081103000	0.479964000	2.083647000

H	-2.164135000	1.813785000	-0.104318000
H	-1.277384000	1.360212000	-1.560189000
N	-0.000031000	-0.792282000	-0.295096000
O	0.000131000	-2.057700000	-0.224311000
F	1.519575000	-0.173364000	1.315654000
F	2.238758000	-0.777246000	-0.646022000
F	-1.519560000	-0.173223000	1.315815000
F	-2.239174000	-0.777142000	-0.646042000

5 (X = H)

C	0.572062000	1.596878000	0.376340000
C	1.408213000	0.786733000	-0.618437000
C	1.796296000	-0.603390000	-0.112440000
C	-0.931043000	1.350349000	0.278034000
C	0.652663000	-1.603058000	0.009368000
C	-0.536696000	-1.097805000	0.820828000
H	0.923258000	1.387224000	1.395078000
H	0.870732000	0.702531000	-1.572401000
H	2.282728000	-0.489382000	0.866798000
H	0.271946000	-1.872475000	-0.982837000
H	0.733091000	2.669891000	0.228408000
H	2.327371000	1.338856000	-0.838572000
H	2.559908000	-1.026523000	-0.773882000
H	1.021808000	-2.529808000	0.462198000
N	-1.269434000	-0.061360000	0.098184000
O	-1.950961000	-0.415632000	-0.920945000
H	-1.356924000	1.849502000	-0.594429000
H	-1.443763000	1.742683000	1.166985000
H	-1.244934000	-1.908251000	1.012952000
H	-0.220465000	-0.687911000	1.787824000

5 (X = CH_3)

C	1.675393000	0.949524000	-0.589562000
C	0.985253000	2.211162000	-0.100484000
C	-0.519817000	2.237010000	-0.315674000
C	1.315922000	-0.396330000	0.065896000
C	-1.274696000	1.248657000	0.563983000
C	-1.374644000	-0.207663000	0.091808000
H	1.510313000	0.838934000	-1.669268000
H	1.199183000	2.367568000	0.965725000
H	-0.747044000	2.056455000	-1.374268000
H	-0.872291000	1.295094000	1.582211000
H	2.757457000	1.076428000	-0.463559000
H	1.439176000	3.064034000	-0.617105000
H	-0.889781000	3.245286000	-0.101797000
H	-2.315597000	1.577296000	0.662991000
N	-0.070149000	-0.829258000	-0.345992000
O	-0.196562000	-2.007910000	-0.821787000
C	1.441881000	-0.367783000	1.590740000
H	0.775612000	0.347824000	2.071487000
H	1.233716000	-1.358130000	2.003866000
H	2.465229000	-0.097445000	1.869657000
C	2.289624000	-1.439072000	-0.474611000
H	2.089190000	-2.427763000	-0.064077000
H	2.229566000	-1.514988000	-1.561197000
H	3.305049000	-1.141563000	-0.200349000
C	-2.306019000	-0.286087000	-1.119355000
H	-1.934982000	0.320254000	-1.949435000
H	-2.390303000	-1.315022000	-1.466567000
H	-3.299663000	0.078284000	-0.846212000
C	-1.939024000	-1.066271000	1.225436000
H	-2.011137000	-2.107225000	0.905652000
H	-1.305927000	-1.018664000	2.115491000
H	-2.937456000	-0.717457000	1.503936000

5 (X = F)

C	-1.175775000	1.242190000	0.581692000
C	-0.296725000	2.069024000	-0.358414000

6 (X = H)

C	-2.567604000	0.268336000	0.000015000
C	-1.597629000	1.277082000	0.000005000

C	1.200387000	1.968425000	-0.062617000
C	-1.355705000	-0.195799000	0.142266000
C	1.867929000	0.643168000	-0.416318000
C	1.180924000	-0.563222000	0.169440000
H	-0.770493000	1.244976000	1.595972000
H	-0.503238000	1.794860000	-1.400701000
H	1.365268000	2.182643000	0.999939000
H	1.879852000	0.480424000	-1.498780000
H	-2.185851000	1.655758000	0.642924000
H	-0.591216000	3.117402000	-0.264107000
H	1.725134000	2.755413000	-0.611507000
H	2.905902000	0.629528000	-0.073476000
N	-0.135535000	-0.819272000	-0.444644000
O	-0.118998000	-1.120767000	-1.674265000
F	-1.764603000	-0.967879000	1.183156000
F	-2.298798000	-0.281116000	-0.811618000
F	0.979482000	-0.427522000	1.509870000
F	1.922715000	-1.672671000	-0.016956000

C	-2.196084000	-1.078512000	0.000019000
H	-1.893513000	2.322070000	-0.000007000
H	-2.965229000	-1.844397000	0.000036000
C	-0.261626000	0.922926000	0.000018000
C	-0.858968000	-1.454704000	0.000006000
H	-0.540512000	-2.490510000	0.000021000
C	0.087125000	-0.430841000	0.000009000
H	-3.619004000	0.534670000	0.000018000
C	2.130233000	0.756061000	0.000179000
C	0.981461000	1.771784000	-0.000126000
H	1.018981000	2.425655000	-0.876446000
H	1.018953000	2.426172000	0.875794000
N	1.466594000	-0.567405000	-0.000052000
O	2.108122000	-1.653044000	-0.000077000
H	2.774162000	0.814910000	-0.881540000
H	2.773585000	0.814823000	0.882350000

6 (X = CH_3)

C	3.083488000	-0.594348000	0.019851000
C	1.968418000	-1.437992000	-0.029775000
C	2.926369000	0.793987000	0.030785000
H	2.096798000	-2.516592000	-0.041861000
H	3.804864000	1.430032000	0.068843000
C	0.704470000	-0.879882000	-0.065431000
C	1.665284000	1.374994000	-0.001884000
H	1.514250000	2.448258000	0.010567000
C	0.569710000	0.512570000	-0.046444000
H	4.080289000	-1.021619000	0.049995000
C	-1.656712000	-0.361224000	0.009246000
C	-0.650909000	-1.520388000	-0.156716000
H	-0.781426000	-2.014002000	-1.126950000
H	-0.799426000	-2.291114000	0.606119000
N	-0.769400000	0.856765000	-0.072351000
O	-1.235428000	2.029380000	-0.048647000
C	-2.311563000	-0.350616000	1.384483000
H	-1.560759000	-0.409015000	2.177356000
H	-2.886020000	0.568166000	1.521934000
H	-2.987966000	-1.202937000	1.489497000
C	-2.690259000	-0.278843000	-1.098831000
H	-3.280489000	0.634262000	-0.997329000
H	-2.214613000	-0.270831000	-2.082881000
H	-3.366057000	-1.136554000	-1.051367000

6 (X = F)

C	3.054890000	-0.581160000	0.000310000
C	1.945464000	-1.431390000	-0.000101000
C	2.893462000	0.806312000	0.000238000
H	2.078598000	-2.508863000	0.000010000
H	3.769535000	1.446007000	0.000454000
C	0.679897000	-0.876596000	-0.000531000
C	1.629374000	1.382082000	-0.000116000
H	1.473255000	2.454527000	-0.000101000
C	0.542379000	0.514156000	-0.000422000
H	4.053872000	-1.003807000	0.000730000
C	-1.644804000	-0.351624000	0.000123000
C	-0.674058000	-1.524618000	-0.001346000
H	-0.847219000	-2.144004000	-0.884353000
H	-0.847801000	-2.146281000	0.879888000
N	-0.805890000	0.859219000	-0.000584000
O	-1.295199000	2.018736000	-0.000193000
F	-2.459054000	-0.326555000	-1.081198000
F	-2.456175000	-0.327331000	1.083428000

7 (X = H)

C	1.195083000	-1.226708000	0.000069000
C	1.195099000	1.226708000	0.000133000
N	1.999214000	0.000006000	0.000095000
O	3.260988000	-0.000007000	-0.000224000
C	-1.396552000	-1.403558000	0.000012000
C	-2.595527000	-0.696675000	-0.000034000
C	-0.200484000	-0.698232000	0.000031000
H	-3.537912000	-1.234777000	-0.000050000
C	-2.595522000	0.696683000	-0.000077000
C	-0.200482000	0.698223000	0.000021000
H	-3.537904000	1.234790000	-0.000130000
C	-1.396540000	1.403559000	-0.000030000
H	-1.399004000	2.489567000	-0.000047000

7 (X = CH_3)

C	0.709423000	1.258945000	-0.000503000
C	0.709633000	-1.258825000	-0.000416000
N	1.504168000	0.000067000	-0.004854000
O	2.768326000	0.000197000	-0.002900000
C	1.038017000	-2.064032000	-1.255197000
H	0.474303000	-3.000450000	-1.269285000
H	0.792623000	-1.501126000	-2.158842000
H	2.104565000	-2.299688000	-1.272433000
C	1.039854000	-2.056691000	1.258745000
H	0.796308000	-1.488224000	2.159415000
H	0.475603000	-2.992662000	1.279426000
H	2.106318000	-2.292709000	1.275554000

H	-1.399029000	-2.489567000	0.000030000
H	1.440141000	1.832302000	0.883124000
H	1.440342000	1.832449000	-0.882685000
H	1.440218000	-1.832392000	0.882966000
H	1.440299000	-1.832351000	-0.882833000

C	1.037906000	2.064110000	-1.255150000
H	0.792844000	1.501120000	-2.158827000
H	0.474062000	3.000458000	-1.269449000
H	2.104415000	2.300001000	-1.272198000
C	1.039247000	2.056778000	1.258857000
H	2.105581000	2.293419000	1.275792000
H	0.474587000	2.992496000	1.279795000
H	0.795937000	1.488052000	2.159417000
C	-1.882411000	1.401197000	-0.000366000
C	-3.083029000	0.696710000	0.000090000
C	-0.684670000	0.696807000	-0.000658000
H	-4.025044000	1.235312000	0.000319000
C	-3.082940000	-0.697050000	0.000176000
C	-0.684560000	-0.696891000	-0.000590000
H	-4.024891000	-1.235764000	0.000538000
C	-1.882238000	-1.401403000	-0.000211000
H	-1.884042000	-2.488263000	-0.000190000
H	-1.884347000	2.488059000	-0.000513000

7 (X = F)

C	0.724718000	-1.214903000	-0.000137000
C	0.724738000	1.214735000	-0.000227000
N	1.534841000	0.000092000	0.000451000
O	2.791440000	0.000140000	0.001068000
C	-1.855008000	-1.413807000	-0.000297000
C	-3.047824000	-0.698247000	0.000084000
C	-0.670698000	-0.694013000	-0.001008000
H	-3.992529000	-1.231427000	0.000503000
C	-3.047830000	0.698175000	0.000024000
C	-0.670725000	0.693897000	-0.001085000
H	-3.992526000	1.231369000	0.000557000
C	-1.855011000	1.413717000	-0.000444000
H	-1.846782000	2.498310000	-0.000193000
H	-1.846796000	-2.498401000	0.000042000
F	1.023097000	-1.977646000	-1.079949000
F	1.020956000	-1.977694000	1.080107000
F	1.022998000	1.977864000	-1.079827000
F	1.020622000	1.977594000	1.080328000

8 (X = H)

C	2.757039000	-0.471876000	0.024247000
C	1.688005000	-1.358044000	-0.061516000
C	2.510794000	0.899891000	0.086535000
H	1.873783000	-2.428361000	-0.102783000
H	3.338299000	1.598765000	0.154468000
C	0.370685000	-0.912588000	-0.093174000
C	1.214189000	1.378672000	0.065442000
H	0.989237000	2.436924000	0.112501000
C	0.141535000	0.478838000	-0.024820000
H	3.774318000	-0.847893000	0.047150000
C	-2.321254000	0.089596000	-0.159018000
C	-2.031504000	-1.270027000	0.441649000
C	-0.785476000	-1.864512000	-0.195689000
H	-2.899238000	-1.919925000	0.300641000
N	-1.162573000	0.986402000	-0.048652000
O	-1.385125000	2.237274000	-0.040477000
H	-1.882934000	-1.166334000	1.522453000
H	-0.989878000	-2.086086000	-1.252983000
H	-0.523073000	-2.820972000	0.265991000
H	-3.142821000	0.607520000	0.337823000
H	-2.582758000	0.003641000	-1.222814000

8 (X = CH_3)

C	3.271827000	-0.377094000	0.195578000
C	2.346302000	0.656901000	0.138269000
C	2.834874000	-1.695925000	0.072125000
H	2.694863000	1.682879000	0.218211000
H	3.547038000	-2.513862000	0.108078000
C	0.980897000	0.426153000	-0.033026000
C	1.490031000	-1.967273000	-0.084650000
H	1.114765000	-2.979309000	-0.167725000
C	0.557319000	-0.916791000	-0.125275000
H	4.325571000	-0.156461000	0.328204000
C	-1.845998000	-0.225049000	0.071246000
C	-1.379668000	1.096230000	-0.537297000
C	0.019446000	1.599539000	-0.151350000
H	-2.122764000	1.869838000	-0.308868000
N	-0.801348000	-1.250012000	-0.242353000

8 (X = F)

C	3.302039000	-0.117040000	0.022362000
C	2.311809000	0.854432000	-0.025943000
C	2.945361000	-1.466193000	0.039016000
H	2.567074000	1.908200000	-0.042569000
H	3.715640000	-2.229216000	0.079504000
C	0.969711000	0.494877000	-0.062132000
C	1.616172000	-1.846998000	0.004043000
H	1.314111000	-2.886453000	0.017005000
C	0.619642000	-0.865440000	-0.049832000
H	4.346040000	0.173820000	0.046565000
C	-1.813462000	-0.286782000	-0.063958000
C	-1.404392000	1.042593000	-0.643556000
C	-0.099749000	1.539483000	-0.071939000
H	-2.198625000	1.768111000	-0.463099000
N	-0.725302000	-1.277671000	-0.093011000

C	-3.150140000	-0.648080000	-0.586467000
H	-3.915840000	0.103818000	-0.379121000
H	-3.036959000	-0.735062000	-1.669289000
H	-3.490559000	-1.609869000	-0.205080000
C	-2.010834000	-0.203045000	1.591665000
H	-1.056073000	-0.074530000	2.104354000
H	-2.677893000	0.608207000	1.896489000
H	-2.442381000	-1.148658000	1.927925000
O	-1.158373000	-2.464306000	-0.356796000
C	0.485885000	2.539279000	-1.274380000
H	0.596984000	2.002731000	-2.220318000
H	-0.244872000	3.340859000	-1.423415000
H	1.444135000	3.008823000	-1.039787000
C	-0.004951000	2.414034000	1.151196000
H	-0.693165000	3.260160000	1.054430000
H	-0.314455000	1.827742000	2.016273000
H	0.986327000	2.819870000	1.370797000
H	-1.408246000	0.964083000	-1.626133000
O	-1.049262000	-2.498576000	-0.014548000
H	-1.283471000	0.916775000	-1.721847000
F	0.304492000	2.634005000	-0.793090000
F	-0.303700000	2.004817000	1.207783000
F	-2.849141000	-0.791863000	-0.755529000
F	-2.226356000	-0.159462000	1.225673000

9 (X = H)			
C	-2.737713000	0.416169000	0.000722000
C	-1.702702000	1.343355000	-0.000074000
C	-2.443030000	-0.949161000	0.000988000
H	-1.920626000	2.407785000	-0.000676000
H	-3.248519000	-1.676460000	0.001661000
C	-0.367656000	0.938379000	-0.000374000
C	-1.130261000	-1.388065000	0.000530000
H	-0.872847000	-2.439752000	0.000527000
C	-0.089907000	-0.451144000	0.000194000
H	-3.768554000	0.752892000	0.001029000
C	2.375210000	0.025587000	0.005008000
C	2.004015000	1.463922000	-0.000649000
C	0.731979000	1.878456000	-0.002318000
H	2.826758000	2.171787000	-0.002660000
H	0.497004000	2.938592000	-0.005922000
N	1.228638000	-0.896366000	-0.001110000
O	1.508302000	-2.134362000	-0.003799000
H	2.984096000	-0.233178000	0.883170000
H	2.996192000	-0.237200000	-0.863136000

9 (X = CH_3)			
C	-3.336328000	0.295085000	0.000047000
C	-2.352136000	1.275504000	-0.000024000
C	-2.968040000	-1.052272000	0.000057000
H	-2.625770000	2.326831000	-0.000064000
H	-3.732661000	-1.822636000	0.000147000
C	-0.997297000	0.941024000	-0.000094000
C	-1.633440000	-1.420264000	0.000003000
H	-1.322722000	-2.457243000	-0.000012000
C	-0.641963000	-0.428959000	-0.000058000
H	-4.383865000	0.575551000	0.000088000
C	1.837911000	0.180126000	0.000019000
C	1.341291000	1.592137000	0.000010000
C	0.049512000	1.936762000	-0.000046000
H	2.120247000	2.350627000	0.000126000
H	-0.241749000	2.983277000	-0.000025000
N	0.698497000	-0.801833000	-0.000043000
C	2.669617000	-0.090351000	1.256860000
H	3.539799000	0.570201000	1.276740000
H	2.081982000	0.088830000	2.160148000
H	3.012275000	-1.126336000	1.259938000
C	2.669725000	-0.090343000	-1.256733000
H	2.082200000	0.088857000	-2.160082000
H	3.539938000	0.570171000	-1.276513000
H	3.012365000	-1.126336000	-1.259750000
O	1.024422000	-2.029957000	-0.000084000

9 (X = F)			
C	3.299036000	0.307620000	-0.000005000
C	2.313127000	1.282793000	-0.000003000
C	2.940625000	-1.043002000	0.000028000
H	2.580804000	2.335207000	-0.000026000
H	3.710587000	-1.807372000	0.000047000
C	0.958867000	0.937546000	-0.000016000
C	1.608954000	-1.420114000	0.000028000
H	1.304851000	-2.459212000	0.000024000
C	0.619398000	-0.432716000	0.000003000
H	4.344871000	0.593541000	-0.000024000
C	-1.820293000	0.167015000	-0.000021000

10 (X = H)			
C	-3.632612000	0.581964000	-0.014220000
C	-2.412390000	1.231615000	-0.004963000
C	-3.685335000	-0.811598000	-0.014610000
H	-2.333446000	2.311039000	-0.005328000
H	-4.641752000	-1.323722000	-0.022855000
C	-1.229426000	0.483434000	0.004672000
C	-2.505522000	-1.543608000	-0.004541000
H	-2.541482000	-2.630060000	-0.004029000
C	-1.260042000	-0.918422000	0.006182000
H	-4.548904000	1.162708000	-0.021820000
C	0.000003000	-1.728991000	0.024656000

C	-1.386592000	1.577619000	-0.000040000
C	-0.092841000	1.922944000	-0.000021000
H	-2.193636000	2.300615000	0.000039000
H	0.189461000	2.971466000	0.000043000
N	-0.726285000	-0.813166000	-0.000025000
O	-1.072386000	-2.029577000	-0.000028000
F	-2.606422000	-0.100239000	-1.082889000
F	-2.606417000	-0.100172000	1.082952000

N	-0.000003000	1.178651000	0.011691000
O	-0.000009000	2.451069000	0.015460000
C	2.505523000	-1.543606000	-0.004560000
C	3.685337000	-0.811595000	-0.014636000
C	1.260046000	-0.918417000	0.006217000
H	4.641754000	-1.323717000	-0.022888000
C	3.632615000	0.581966000	-0.014213000
C	1.229425000	0.483437000	0.004715000
H	4.548908000	1.162708000	-0.021822000
C	2.412392000	1.231617000	-0.004931000
H	2.333448000	2.311041000	-0.005288000
H	2.541484000	-2.630058000	-0.004098000
H	-0.000058000	-2.380933000	0.909731000
H	0.000064000	-2.424897000	-0.825733000

10 (X = CH_3)

C	3.631301000	0.969710000	-0.000522000
C	2.406245000	1.608367000	-0.000271000
C	3.689748000	-0.423164000	-0.000417000
H	2.318182000	2.686950000	-0.000297000
H	4.647262000	-0.932796000	-0.000583000
C	1.226286000	0.852550000	0.000033000
C	2.513013000	-1.159575000	-0.000114000
H	2.569292000	-2.244130000	0.000120000
C	1.257341000	-0.549743000	0.000088000
H	4.543793000	1.556337000	-0.000828000
C	0.000050000	-1.402924000	0.000226000
C	0.000016000	-2.295579000	1.255974000
H	0.000038000	-1.692809000	2.167319000
H	-0.882053000	-2.940223000	1.276771000
H	0.882273000	-2.940031000	1.277020000
C	0.000191000	-2.296561000	-1.254893000
H	0.000401000	-1.694007000	-2.166392000
H	0.882432000	-2.940963000	-1.275345000
H	-0.882036000	-2.940994000	-1.275657000
N	-0.000094000	1.549231000	0.000287000
O	-0.000089000	2.821064000	0.000714000
C	-2.512904000	-1.159629000	-0.000348000
C	-3.689722000	-0.423349000	-0.000484000
C	-1.257264000	-0.549764000	-0.000126000
H	-4.647155000	-0.933129000	-0.000671000
C	-3.631415000	0.969517000	-0.000404000
C	-1.226426000	0.852528000	0.000011000
H	-4.543943000	1.556088000	-0.000538000
C	-2.406391000	1.608271000	-0.000134000
H	-2.318420000	2.686859000	-0.000030000
H	-2.569106000	-2.244206000	-0.000322000

10 (X = F)

C	-3.625728000	0.914882000	-0.000072000
C	-2.415163000	1.580072000	0.000005000
C	-3.669984000	-0.481308000	-0.000134000
H	-2.349272000	2.660263000	0.000046000
H	-4.623893000	-0.997292000	-0.000212000
C	-1.225290000	0.842877000	0.000023000
C	-2.489714000	-1.207185000	-0.000098000
H	-2.506942000	-2.291848000	-0.000137000
C	-1.256824000	-0.557349000	-0.000015000
H	-4.547672000	1.486678000	-0.000084000
C	0.000007000	-1.356862000	0.000078000
N	-0.000009000	1.539279000	0.000068000
O	-0.000036000	2.809924000	0.000133000
C	2.489724000	-1.207169000	-0.000024000
C	3.669990000	-0.481288000	-0.000080000
C	1.256831000	-0.557338000	0.000015000
H	4.623901000	-0.997271000	-0.000097000
C	3.625726000	0.914901000	-0.000117000
C	1.225285000	0.842890000	0.000004000
H	4.547668000	1.486697000	-0.000186000
C	2.415158000	1.580088000	-0.000075000
H	2.349266000	2.660277000	-0.000095000
H	2.506955000	-2.291832000	-0.000012000
F	0.000027000	-2.218600000	-1.087842000
F	-0.000001000	-2.218431000	1.088084000

11 (X = H)

C	0.015603000	-1.209555000	-0.136461000
C	1.383919000	-0.660703000	0.212397000
C	-0.009959000	1.197451000	0.076968000
H	1.537609000	-0.703615000	1.303692000
H	2.199996000	-1.203382000	-0.268564000
N	-0.818837000	-0.018254000	0.013268000
O	-2.080705000	-0.021063000	0.026499000
N	1.301773000	0.708517000	-0.308069000
H	-0.038063000	-1.576004000	-1.169880000

11 (X = CH_3)

C	-1.350912000	-0.373718000	0.002171000
C	-0.310446000	-1.452912000	0.287251000
C	0.976083000	0.490117000	-0.023467000
H	-0.198069000	-1.599811000	1.379604000
H	-0.577031000	-2.421525000	-0.148521000
N	-0.467481000	0.818865000	-0.007487000
O	-0.897007000	2.007515000	0.024304000
C	1.671830000	1.261793000	-1.128374000

H	-0.340220000	-1.996919000	0.531730000
H	-0.400147000	1.941811000	-0.625048000
H	-0.071082000	1.616630000	1.099121000
H	2.039623000	1.294984000	0.063142000

H	2.737774000	1.021781000	-1.155237000
H	1.231848000	1.015765000	-2.096204000
H	1.565595000	2.334364000	-0.954138000
C	1.564552000	0.828573000	1.348035000
H	1.114881000	0.220127000	2.137830000
H	2.646720000	0.675021000	1.365346000
H	1.363825000	1.877796000	1.574538000
C	-1.988156000	-0.525322000	-1.376228000
H	-1.221970000	-0.691370000	-2.137091000
H	-2.683640000	-1.369348000	-1.390340000
H	-2.542884000	0.380331000	-1.632279000
C	-2.399687000	-0.225796000	1.089067000
H	-3.028277000	0.644091000	0.889215000
H	-3.038025000	-1.112364000	1.127189000
H	-1.935744000	-0.090228000	2.069387000
N	0.902526000	-0.944378000	-0.336014000
C	2.083483000	-1.714344000	-0.024219000
H	2.286883000	-1.798388000	1.058012000
H	1.967748000	-2.726742000	-0.420016000
H	2.960616000	-1.271375000	-0.502635000

11 (X = F)

C	-1.298298000	-0.364003000	0.009855000
C	-0.271740000	-1.480079000	0.102378000
C	0.946788000	0.492176000	-0.014814000
H	-0.086808000	-1.725626000	1.153635000
H	-0.574669000	-2.366893000	-0.451377000
N	-0.470642000	0.832553000	0.002904000
O	-0.906900000	2.008666000	-0.022400000
N	0.897387000	-0.855171000	-0.524474000
F	1.476842000	0.587179000	1.226709000
F	1.636653000	1.306916000	-0.798621000
F	-2.044727000	-0.419963000	-1.112580000
F	-2.156373000	-0.347579000	1.044650000
F	2.050823000	-1.538447000	-0.077556000

12 (X = H)

C	-0.007580000	-1.183513000	0.054966000
C	-0.049882000	1.206836000	-0.158098000
C	-1.380482000	0.598673000	0.243435000
H	-2.249411000	1.059293000	-0.225811000
H	-1.512070000	0.617519000	1.334978000
N	0.815254000	0.022795000	-0.110932000
O	2.059561000	0.047272000	0.099029000
O	-1.306516000	-0.751843000	-0.219839000
H	0.111215000	-1.560288000	1.086335000
H	0.281793000	-1.961348000	-0.656498000
H	0.328874000	1.962665000	0.532738000
H	-0.063876000	1.627195000	-1.170560000

12 (X = CH_3)

C	-1.226272000	-0.128383000	0.005994000
C	1.238597000	-0.137268000	-0.010279000
C	0.596754000	-1.466130000	-0.405587000
H	1.112842000	-2.336319000	0.005069000
H	0.552713000	-1.570797000	-1.500567000
N	0.009919000	0.692772000	0.053820000
O	0.005108000	1.956031000	0.090092000
C	2.186009000	0.426011000	-1.051744000
H	3.083056000	-0.193634000	-1.131049000
H	1.708573000	0.473373000	-2.033985000
H	2.488901000	1.438072000	-0.775762000
C	1.877871000	-0.186016000	1.374290000
H	1.205214000	-0.655716000	2.096343000
H	2.811366000	-0.755626000	1.350760000
H	2.102270000	0.826185000	1.719239000
C	-1.913584000	0.069901000	-1.336301000
H	-1.255874000	-0.216817000	-2.160222000
H	-2.823626000	-0.530994000	-1.389093000
H	-2.175258000	1.122803000	-1.463089000
C	-2.124898000	0.191554000	1.176999000

12 (X = F)

C	1.185939000	-0.122144000	-0.025445000
C	-1.200411000	-0.110458000	0.000172000
C	-0.619238000	-1.496623000	0.196773000
H	-1.108215000	-2.245849000	-0.422383000
H	-0.670589000	-1.777831000	1.252259000
N	-0.008372000	0.714696000	-0.008260000
O	0.001598000	1.970349000	0.034158000
O	0.743709000	-1.389910000	-0.231734000
F	2.026559000	0.235393000	-0.990416000
F	1.857446000	0.004318000	1.142641000
F	-2.037166000	0.259924000	0.984637000
F	-1.882704000	0.028438000	-1.161355000

H	-2.411027000	1.244264000	1.139180000
H	-3.026676000	-0.422428000	1.142000000
H	-1.604710000	0.002185000	2.117321000
O	-0.710614000	-1.442526000	0.158268000

13 (X = H)

C	1.434317000	0.992718000	-0.318254000
C	1.599153000	-0.455083000	0.191418000
H	1.474002000	0.987845000	-1.414747000
H	2.350963000	-1.068832000	-0.313965000
H	1.811517000	-0.471634000	1.265285000
H	2.297522000	1.570181000	0.023492000
N	-0.960896000	0.322276000	0.003234000
O	-2.225698000	0.286809000	-0.071654000
B	0.030796000	1.578776000	0.243492000
P	-0.050778000	-1.132499000	-0.020754000
H	-0.432132000	-2.070765000	0.959169000
H	-0.197055000	-1.879803000	-1.208804000
H	-0.432612000	2.509116000	-0.351978000
H	0.066521000	1.741288000	1.447000000

13 (X = CH_3)

C	-0.971757000	1.538734000	-0.529621000
C	0.417822000	1.766419000	0.105759000
H	-0.866687000	1.562970000	-1.623210000
H	1.040996000	2.533985000	-0.365433000
H	0.330192000	2.018145000	1.167887000
H	-1.611122000	2.386845000	-0.263961000
N	-0.226733000	-0.797468000	-0.089822000
O	-0.089570000	-2.073517000	-0.075122000
C	2.171563000	-0.367630000	1.420581000
H	3.147624000	0.119760000	1.442612000
H	1.625580000	-0.146488000	2.338485000
H	2.306644000	-1.450142000	1.349169000
C	2.199619000	-0.090756000	-1.464771000
H	1.670543000	0.304760000	-2.332845000
H	3.170924000	0.399182000	-1.372925000
H	2.347044000	-1.164247000	-1.604655000
C	-2.027661000	0.135051000	1.540069000
H	-1.269504000	0.555360000	2.218591000
H	-2.933798000	0.736743000	1.682000000
H	-2.252950000	-0.871040000	1.912203000
C	-2.679547000	-0.545701000	-0.999511000
H	-2.949965000	-1.562301000	-0.693781000
H	-3.607313000	0.039166000	-1.001885000
H	-2.340568000	-0.606205000	-2.041365000
B	-1.590478000	0.106030000	-0.021958000
P	1.185880000	0.144471000	0.006240000

13 (X = F)

C	-0.967709000	1.521829000	-0.516686000
C	0.423736000	1.686981000	0.132285000
H	-0.869704000	1.537239000	-1.606364000
H	1.085686000	2.429546000	-0.321482000
H	0.340252000	1.911890000	1.201254000
H	-1.582487000	2.380547000	-0.236623000
N	-0.204640000	-0.890618000	-0.084056000
O	-0.171879000	-2.163437000	-0.114629000
B	-1.612419000	0.135902000	-0.005140000
P	1.129813000	0.068509000	0.007651000
F	2.124044000	-0.279483000	1.171119000
F	2.140407000	-0.034036000	-1.196382000
F	-1.919750000	0.139408000	1.343290000
F	-2.543312000	-0.456712000	-0.797362000

14 (X = H)

N	-1.441165000	-0.710462000	-0.001531000
C	-0.082370000	-1.186810000	0.001254000
C	-1.425680000	0.564214000	-0.000994000
C	-0.079983000	1.209330000	0.001266000
N	0.761780000	0.017763000	0.002358000
H	-2.355022000	1.131764000	-0.003982000
O	2.023533000	0.016427000	-0.002363000
H	0.107850000	1.835090000	-0.882003000
H	0.103784000	1.834237000	0.886049000
H	0.117409000	-1.801800000	0.887748000
H	0.121606000	-1.802221000	-0.883852000

14 (X = CH_3)

N	-0.715234000	-1.538461000	-0.007684000
C	-1.227519000	-0.173794000	-0.000568000
C	0.557171000	-1.514437000	-0.007529000
C	1.228676000	-0.169942000	-0.000538000
N	0.007533000	0.660806000	0.005349000
H	1.132687000	-2.442182000	-0.012474000

14 (X = F)

N	-0.719347000	-1.513749000	0.001177000
C	-1.185064000	-0.149301000	-0.000405000
C	0.550745000	-1.501381000	0.001404000
C	1.186529000	-0.134441000	-0.000295000
N	0.008888000	0.699308000	-0.002609000
H	1.146507000	-2.410965000	0.002502000

O	0.012807000	1.925295000	0.009121000
C	-2.033945000	0.091883000	1.260668000
H	-2.310527000	1.147602000	1.298049000
H	-2.940350000	-0.515875000	1.267726000
H	-1.448761000	-0.145906000	2.151580000
C	-2.031597000	0.105654000	-1.260345000
H	-1.444738000	-0.122168000	-2.152777000
H	-2.937701000	-0.502398000	-1.275783000
H	-2.308553000	1.161575000	-1.286642000
C	2.049241000	0.100072000	-1.258903000
H	2.948922000	-0.520068000	-1.278940000
H	1.468642000	-0.100294000	-2.162309000
H	2.351797000	1.149831000	-1.272893000
C	2.051604000	0.086148000	1.259167000
H	1.472488000	-0.123578000	2.161382000
H	2.951149000	-0.534417000	1.271008000
H	2.354611000	1.135602000	1.283741000

O	0.006102000	1.956819000	-0.000672000
F	-1.933425000	0.091827000	1.081680000
F	-1.935392000	0.089360000	-1.081152000
F	1.961237000	0.083930000	-1.082977000
F	1.959205000	0.086911000	1.083414000

15 (X = H)

N	0.788300000	0.005712000	0.000024000
C	-1.479610000	-0.513466000	0.000036000
C	-0.100610000	-1.176710000	-0.000056000
C	-0.006936000	1.142224000	0.000017000
N	-1.274409000	0.942640000	-0.000067000
O	2.045118000	-0.042281000	0.000006000
H	0.483619000	2.108966000	0.000026000
H	0.117479000	-1.779161000	-0.885124000
H	0.117423000	-1.779287000	0.884953000
H	-2.077104000	-0.781585000	-0.875875000
H	-2.076666000	-0.781443000	0.876297000

15 (X = CH_3)

N	-0.963591000	0.598538000	-0.172126000
C	0.939071000	-0.724197000	-0.034687000
C	0.505086000	0.771048000	0.074464000
C	-1.304464000	-0.731503000	0.079020000
N	-0.291227000	-1.508866000	0.245395000
C	2.033240000	-1.123526000	0.942090000
H	2.284617000	-2.176594000	0.799164000
H	2.940138000	-0.532674000	0.776433000
H	1.724503000	-0.995399000	1.980478000
C	1.362801000	-1.102607000	-1.454871000
H	0.599027000	-0.829710000	-2.187938000
H	2.300605000	-0.614608000	-1.735061000
H	1.507384000	-2.183231000	-1.512491000
C	-2.734633000	-1.102072000	0.134127000
H	-3.251913000	-0.525234000	0.904860000
H	-3.225522000	-0.860781000	-0.812078000
H	-2.835741000	-2.166057000	0.337625000
C	1.094647000	1.732952000	-0.936792000
H	2.172541000	1.829523000	-0.779951000
H	0.923235000	1.412943000	-1.965135000
H	0.643319000	2.720018000	-0.814508000
C	0.634601000	1.343539000	1.484557000
H	1.682785000	1.507781000	1.745108000
H	0.113820000	2.302849000	1.532829000
H	0.195145000	0.678297000	2.231767000
O	-1.771539000	1.552921000	-0.342679000

15 (X = F)

N	1.031065000	0.566816000	-0.000028000
C	-0.948843000	-0.681673000	-0.000023000
C	-0.425327000	0.796685000	-0.000034000
C	1.212996000	-0.815144000	-0.000041000
N	0.182245000	-1.561435000	-0.000011000
O	1.907687000	1.462629000	0.000060000
F	2.436918000	-1.233585000	-0.000018000
F	-0.779820000	1.485451000	-1.083042000
F	-0.779831000	1.485496000	1.082964000
F	-1.704538000	-0.898530000	1.087845000
F	-1.704686000	-0.898599000	-1.087707000

16 (X = H)

N	0.947865000	-1.365293000	-0.003359000
C	1.755638000	-0.172994000	0.192709000
C	1.111236000	1.095160000	-0.343443000
C	-0.288574000	1.239776000	0.217870000
C	-0.320232000	-1.214844000	-0.089422000
H	1.706997000	1.978502000	-0.098887000
H	1.058725000	1.038590000	-1.436285000
N	-1.023707000	-0.017222000	0.015746000
O	-2.291810000	-0.001375000	-0.023770000
H	-0.985072000	-2.062745000	-0.246294000
H	-0.872922000	2.021983000	-0.269601000

H	-0.276651000	1.454162000	1.293723000
H	1.957015000	-0.077507000	1.269470000
H	2.728867000	-0.346969000	-0.274968000

16 (X = CH_3)

N	-1.215567000	1.368621000	-0.127497000
C	-1.538487000	-0.061571000	-0.053084000
C	-0.392874000	-0.928212000	-0.595993000
C	1.019190000	-0.606743000	-0.093678000
C	0.013584000	1.712830000	-0.071148000
H	-0.598041000	-1.989327000	-0.411400000
H	-0.391781000	-0.805125000	-1.685921000
N	1.128399000	0.881397000	0.019153000
O	2.278513000	1.395537000	0.185101000
C	2.048997000	-1.062669000	-1.123250000
H	1.879757000	-0.581544000	-2.089541000
H	3.060367000	-0.824158000	-0.792533000
H	1.970275000	-2.144013000	-1.261346000
C	1.362894000	-1.216899000	1.263132000
H	1.333862000	-2.307424000	1.192002000
H	2.371886000	-0.919704000	1.556696000
H	0.675505000	-0.912081000	2.051441000
C	-1.898738000	-0.357531000	1.406393000
H	-2.099390000	-1.423853000	1.548558000
H	-1.107400000	-0.059116000	2.095366000
H	-2.795448000	0.200269000	1.685150000
C	-2.774677000	-0.291141000	-0.919723000
H	-3.599583000	0.335396000	-0.574504000
H	-2.573114000	-0.036437000	-1.963018000
H	-3.091406000	-1.337661000	-0.877687000
H	0.307249000	2.761978000	-0.071550000

16 (X = F)

N	-1.160190000	1.376676000	-0.064073000
C	-1.486492000	-0.012256000	-0.057442000
C	-0.436422000	-0.939836000	-0.634588000
C	0.933094000	-0.645908000	-0.081337000
C	0.076695000	1.689241000	-0.035212000
H	-0.693666000	-1.982043000	-0.442119000
H	-0.402873000	-0.782761000	-1.714717000
N	1.166081000	0.814263000	-0.029654000
O	2.350039000	1.243868000	0.073914000
H	0.399550000	2.727986000	-0.008274000
F	1.102322000	-1.132053000	1.169178000
F	1.890195000	-1.187825000	-0.850900000
F	-2.633608000	-0.177629000	-0.763386000
F	-1.766221000	-0.368954000	1.231925000

17 (X = H)

N	0.952245000	0.041306000	0.000066000
C	0.210155000	-1.250713000	0.000221000
N	-1.210805000	-1.133163000	-0.000147000
C	-1.717867000	0.043369000	-0.000019000
C	0.237527000	1.207025000	0.000154000
N	-1.060284000	1.268385000	0.000068000
H	0.858059000	2.100741000	0.000111000
O	2.211932000	0.021094000	-0.000273000
H	-2.803250000	0.121031000	-0.000978000
H	0.551619000	-1.812443000	-0.878827000
H	0.551133000	-1.811867000	0.879834000

17 (X = CH_3)

N	0.059653000	0.955990000	-0.000021000
C	0.647705000	-0.447478000	0.000000000
N	-0.375437000	-1.464374000	-0.000062000
C	-1.608900000	-1.123445000	-0.000036000
C	-1.295453000	1.124555000	-0.000005000
N	-2.158045000	0.153524000	-0.000004000
C	1.490601000	-0.579546000	-1.262020000
H	1.964474000	-1.561500000	-1.273780000
H	0.868189000	-0.487151000	-2.154286000
H	2.257768000	0.196053000	-1.281003000
C	1.490421000	-0.579510000	1.262148000
H	2.257526000	0.196147000	1.281188000
H	0.867870000	-0.487129000	2.154316000
H	1.964384000	-1.561421000	1.273994000
H	-1.605194000	2.168049000	0.000002000
O	0.843052000	1.946997000	-0.000037000
H	-2.348878000	-1.922461000	-0.000047000

17 (X = F)

N	-0.188559000	0.923778000	-0.000309000
C	-0.604901000	-0.510010000	0.000408000
N	0.448804000	-1.430341000	0.000271000
C	1.653438000	-0.983903000	-0.001498000

18 (X = H)

C	0.648071000	-1.574883000	-0.015095000
N	1.756763000	-0.651810000	-0.159111000
C	1.420474000	0.686692000	-0.630030000
C	-0.544990000	-1.089106000	0.819079000

C	1.155657000	1.222659000	0.001023000
N	2.089015000	0.330738000	0.000488000
H	1.363511000	2.290370000	0.002909000
O	-1.070717000	1.823487000	-0.001664000
H	2.453203000	-1.721215000	-0.002117000
F	-1.384568000	-0.683732000	-1.084528000
F	-1.384427000	-0.682797000	1.085615000

C	0.628875000	1.571339000	0.346470000
C	-0.885201000	1.367778000	0.307568000
H	0.260849000	-1.820758000	-1.011356000
H	0.867842000	0.580463000	-1.572069000
H	1.012576000	1.397744000	1.360208000
H	1.033061000	-2.504985000	0.414844000
H	2.360848000	1.188629000	-0.879342000
H	0.825979000	2.628620000	0.136035000
N	-1.269950000	-0.033332000	0.122277000
O	-1.935359000	-0.361874000	-0.917055000
H	-1.250734000	-1.908709000	0.985831000
H	-0.220854000	-0.707346000	1.794820000
H	-1.351849000	1.759348000	1.221012000
H	-1.332509000	1.889243000	-0.540173000
H	2.266592000	-0.582188000	0.716512000

18 (X = CH_3)

C	-1.523767000	0.544301000	-0.841002000
N	-1.924000000	-0.813711000	-0.576003000
C	-0.869175000	-1.798506000	-0.695282000
C	-0.442106000	1.262081000	0.011241000
C	0.225194000	-1.718579000	0.369583000
C	1.365136000	-0.718447000	0.135902000
H	-1.169424000	0.592008000	-1.880694000
H	-0.429870000	-1.706441000	-1.697342000
H	-0.239537000	-1.558155000	1.348396000
H	-2.426416000	1.165392000	-0.789009000
H	-1.338109000	-2.788550000	-0.655508000
H	0.715354000	-2.696107000	0.451726000
N	0.911138000	0.664832000	-0.261142000
O	1.867012000	1.469144000	-0.528291000
C	-0.733596000	1.265539000	1.512600000
H	-0.721702000	0.273591000	1.961995000
H	0.007698000	1.879421000	2.032376000
H	-1.720469000	1.700277000	1.701413000
C	-0.409496000	2.706899000	-0.476840000
H	0.338101000	3.292239000	0.056414000
H	-0.175124000	2.765000000	-1.541277000
H	-1.392099000	3.156385000	-0.310283000
C	2.254266000	-1.215227000	-1.005441000
H	1.688297000	-1.331704000	-1.933190000
H	3.060565000	-0.506311000	-1.190413000
H	2.687321000	-2.184189000	-0.743393000
C	2.199641000	-0.589611000	1.411563000
H	3.012264000	0.122443000	1.257448000
H	1.593448000	-0.247408000	2.254684000
H	2.631808000	-1.558103000	1.679523000
C	-2.838312000	-1.035040000	0.520455000
H	-2.392570000	-1.024847000	1.529681000
H	-3.617355000	-0.268075000	0.502983000
H	-3.324947000	-2.008321000	0.394131000

18 (X = F)

C	-1.662081000	0.479975000	-0.673630000
N	-1.740619000	-0.965309000	-0.677570000
C	-0.492721000	-1.720607000	-0.791040000
C	-0.579059000	1.146151000	0.166021000
C	0.506572000	-1.583405000	0.359683000
C	1.441936000	-0.404428000	0.217764000
H	-1.476909000	0.782978000	-1.709515000
H	-0.055974000	-1.416824000	-1.750084000
H	-0.032825000	-1.504832000	1.303614000
H	-2.636694000	0.869420000	-0.375045000
H	-0.785931000	-2.766861000	-0.893296000
H	1.135673000	-2.474475000	0.419302000
N	0.771148000	0.817141000	-0.323991000
O	1.021005000	1.181643000	-1.511982000
F	-2.280296000	-1.331311000	0.617544000
F	-0.721911000	2.482925000	0.085927000
F	-0.641769000	0.791669000	1.467793000
F	2.436741000	-0.683413000	-0.639571000
F	2.005351000	-0.083370000	1.405975000

19 (X = H)

C	-2.736636000	-0.367319000	-0.005178000
C	-1.709295000	-1.303433000	0.072534000
C	-2.442915000	0.994805000	-0.086274000
H	-1.931839000	-2.364911000	0.131571000
H	-3.247632000	1.718792000	-0.152353000
C	-0.386070000	-0.883816000	0.083113000

19 (X = CH_3)

C	-3.285984000	-0.338366000	-0.008487000
C	-2.268720000	-1.287461000	-0.014693000
C	-2.976276000	1.023079000	-0.015358000
H	-2.501698000	-2.348354000	-0.009740000
H	-3.772615000	1.759526000	-0.014342000

C	-1.128726000	1.430066000	-0.084461000
H	-0.865903000	2.479593000	-0.140347000
C	-0.091989000	0.495885000	0.007096000
H	-3.767093000	-0.705013000	-0.012559000
C	2.280124000	-0.142524000	0.116140000
N	0.690724000	-1.770144000	0.278050000
N	1.237619000	0.897316000	0.046950000
O	1.596394000	2.113191000	0.079737000
O	1.830245000	-1.310677000	-0.494519000
H	0.504572000	-2.689954000	-0.111273000
H	3.135867000	0.215112000	-0.457142000
H	2.553563000	-0.305919000	1.167533000

C	-0.939384000	-0.883392000	-0.018449000
C	-1.657071000	1.441442000	-0.024049000
H	-1.382703000	2.489163000	-0.022091000
C	-0.626985000	0.493088000	-0.023052000
H	-4.320606000	-0.663342000	-0.007213000
C	1.795220000	-0.149202000	-0.021237000
N	0.129285000	-1.785645000	0.099834000
N	0.705836000	0.889622000	0.007000000
C	2.898547000	0.326110000	-0.936711000
H	3.699213000	-0.414227000	-0.955281000
H	2.519003000	0.467722000	-1.949422000
H	3.290023000	1.275168000	-0.573993000
C	2.257700000	-0.407941000	1.399030000
H	1.447292000	-0.811058000	2.007035000
H	3.083816000	-1.121825000	1.396265000
H	2.599257000	0.529260000	1.842132000
O	1.041430000	2.106590000	0.141010000
O	1.255911000	-1.295363000	-0.660064000
H	-0.067832000	-2.683831000	-0.330723000

19 (X = F)

C	-3.256389000	-0.353136000	-0.023799000
C	-2.237048000	-1.299272000	0.024966000
C	-2.955205000	1.008539000	-0.066370000
H	-2.464730000	-2.360163000	0.061443000
H	-3.755963000	1.738192000	-0.110825000
C	-0.914108000	-0.880417000	0.042142000
C	-1.637989000	1.438073000	-0.056364000
H	-1.370227000	2.487247000	-0.081575000
C	-0.614486000	0.492397000	-0.000938000
H	-4.289133000	-0.682982000	-0.037763000
C	1.777862000	-0.137907000	-0.058939000
N	0.172238000	-1.752125000	0.237251000
N	0.726724000	0.883965000	0.056871000
O	1.089910000	2.088265000	0.199620000
O	1.287619000	-1.304568000	-0.582584000
H	0.003191000	-2.685683000	-0.124917000
F	2.355987000	-0.310852000	1.144443000
F	2.709355000	0.277660000	-0.907299000

20 (X = H)

C	-0.741141000	1.221762000	0.154114000
C	0.741234000	1.221783000	-0.154049000
C	0.000058000	-1.078817000	-0.000287000
H	0.951749000	1.465335000	-1.203564000
H	1.331918000	1.886923000	0.477559000
N	-1.132044000	-0.168934000	-0.111141000
O	-2.326904000	-0.568204000	-0.020784000
N	1.131917000	-0.168947000	0.110233000
O	2.326894000	-0.568265000	0.021685000
H	-1.331786000	1.887361000	-0.477052000
H	-0.951755000	1.464353000	1.203799000
H	0.086885000	-1.717922000	-0.888684000
H	-0.086943000	-1.717500000	0.888424000

20 (X = CH_3)

C	-1.341079000	0.294129000	-0.020086000
C	-0.454475000	1.494137000	-0.334205000
C	1.051569000	-0.400243000	-0.028715000
H	-0.439824000	1.721518000	-1.410367000
H	-0.731567000	2.402106000	0.205705000
N	-0.357237000	-0.818857000	-0.176620000
O	-0.699406000	-2.029864000	-0.042549000
C	1.681422000	-0.979108000	1.223106000
H	2.680057000	-0.557973000	1.352696000
H	1.083850000	-0.746433000	2.106382000
H	1.754855000	-2.063442000	1.128890000
C	1.841597000	-0.739712000	-1.282987000
H	1.378183000	-0.296754000	-2.167767000
H	2.859133000	-0.355404000	-1.191062000
H	1.873726000	-1.823226000	-1.411859000

20 (X = F)

C	1.297680000	0.328048000	-0.012567000
C	0.393393000	1.531722000	-0.192179000
C	-1.000173000	-0.443334000	-0.011337000
H	0.630063000	2.330417000	0.511406000
H	0.457238000	1.912052000	-1.216785000
N	0.401209000	-0.817098000	-0.119791000
O	0.791827000	-2.012020000	-0.040954000
N	-0.943091000	0.999389000	0.074937000
O	-1.989080000	1.701925000	0.056690000
F	-1.693750000	-0.862675000	-1.078733000
F	-1.577226000	-0.981688000	1.065343000
F	2.266503000	0.247818000	-0.938344000
F	1.908749000	0.314727000	1.195064000

C	-1.843114000	0.309583000	1.421779000
H	-1.032287000	0.527031000	2.122299000
H	-2.617065000	1.070780000	1.550141000
H	-2.268888000	-0.663465000	1.676249000
C	-2.477496000	0.096015000	-1.004767000
H	-2.989119000	-0.846350000	-0.800003000
H	-3.203877000	0.908005000	-0.919213000
H	-2.108253000	0.067257000	-2.032713000
N	0.875017000	1.063400000	0.098840000
O	1.872665000	1.841832000	0.103840000

21 (X = H)

N	-1.113912000	0.233637000	-0.000158000
C	0.760118000	-1.213256000	0.000184000
C	-0.760296000	-1.213175000	-0.000192000
C	0.000097000	0.982580000	-0.000035000
N	1.113974000	0.233843000	-0.000077000
O	2.311837000	0.624733000	0.000017000
O	-2.311753000	0.624919000	0.000189000
H	1.209162000	-1.666140000	0.886000000
H	1.209822000	-1.666442000	-0.885128000
H	-1.209740000	-1.666453000	0.885260000
H	-1.209432000	-1.666446000	-0.885787000
H	-0.000431000	2.059011000	-0.000084000

21 (X = CH_3)

N	-0.666236000	-1.079872000	0.127415000
C	0.828472000	0.748096000	0.122676000
C	0.793837000	-0.785192000	-0.121479000
C	-1.411650000	0.033077000	-0.001672000
N	-0.617550000	1.112961000	-0.129926000
O	-0.991147000	2.317664000	-0.255982000
C	1.722028000	1.536117000	-0.812932000
H	1.617449000	2.601916000	-0.605077000
H	2.766991000	1.254893000	-0.655844000
H	1.472857000	1.374522000	-1.861894000
C	1.104246000	1.134924000	1.572216000
H	0.465742000	0.584819000	2.267728000
H	2.147003000	0.946060000	1.837317000
H	0.905173000	2.201265000	1.697029000
C	-2.879190000	0.057508000	0.000649000
H	-3.278810000	-0.477868000	-0.865027000
H	-3.264300000	-0.447254000	0.889861000
H	-3.220808000	1.091673000	-0.020220000
C	1.648245000	-1.612739000	0.816796000
H	2.705411000	-1.379788000	0.662698000
H	1.403689000	-1.439923000	1.865041000
H	1.495970000	-2.672694000	0.608648000
C	1.058103000	-1.182767000	-1.570348000
H	2.108065000	-1.033523000	-1.832668000
H	0.818220000	-2.240561000	-1.695988000
H	0.443132000	-0.608352000	-2.267467000
O	-1.106831000	-2.262785000	0.250733000

21 (X = F)

N	0.656447000	-1.134167000	0.028825000
C	-0.781667000	0.780289000	0.032296000
C	-0.781752000	-0.780200000	-0.032306000
C	1.377979000	-0.000068000	0.000003000
N	0.656643000	1.134112000	-0.028846000
O	1.072532000	2.322337000	-0.057435000
O	1.072250000	-2.322432000	0.057441000
F	2.662470000	-0.000220000	-0.000005000
F	-1.303782000	1.225313000	1.173298000
F	-1.429336000	1.327719000	-0.986992000
F	-1.303978000	-1.225170000	-1.173289000
F	-1.429513000	-1.327529000	0.987003000

22 (X = H)

N	1.188067000	-0.436155000	0.021302000
C	1.244753000	1.026659000	0.209387000
C	0.000082000	1.678268000	-0.354157000
C	-1.244908000	1.026725000	0.208772000
C	0.000018000	-1.061068000	-0.074843000
H	0.000034000	2.744781000	-0.120073000
H	0.000374000	1.589432000	-1.445154000
N	-1.188040000	-0.436163000	0.021270000
O	-2.285559000	-1.078668000	-0.027232000
H	0.000014000	-2.131584000	-0.213897000
O	2.285620000	-1.078574000	-0.027596000
H	2.158455000	1.350844000	-0.288839000
H	1.360938000	1.218049000	1.282285000
H	-2.158312000	1.350650000	-0.290175000
H	-1.361852000	1.218485000	1.281516000

22 (X = CH_3)

N	-1.227076000	0.946429000	-0.092661000
C	-1.307518000	-0.553548000	-0.019296000
C	-0.012994000	-1.107059000	-0.617400000
C	1.316384000	-0.529957000	-0.126067000
C	-0.037942000	1.566891000	-0.001439000
H	0.003982000	-2.192269000	-0.471102000
H	-0.068890000	-0.948486000	-1.700647000
N	1.157513000	0.954923000	0.061204000
O	2.218374000	1.633712000	0.260932000
C	2.380492000	-0.727597000	-1.201604000
H	2.089687000	-0.245418000	-2.137993000
H	3.332552000	-0.306328000	-0.879481000
H	2.511066000	-1.796138000	-1.391126000
C	1.818448000	-1.114819000	1.190338000
H	2.026350000	-2.180261000	1.062511000
H	2.744322000	-0.613258000	1.477447000
H	1.105518000	-1.004000000	2.006482000
C	-1.550137000	-0.912530000	1.445595000
H	-1.515527000	-1.996700000	1.582017000
H	-0.816759000	-0.457558000	2.112345000
H	-2.536782000	-0.557482000	1.750271000
C	-2.486302000	-1.004852000	-0.867353000
H	-3.415466000	-0.573061000	-0.498085000
H	-2.363063000	-0.704405000	-1.910220000
H	-2.561603000	-2.094408000	-0.827842000
H	-0.043450000	2.645025000	0.066201000
O	-2.309322000	1.618301000	-0.115584000

22 (X = F)

N	-1.197244000	0.937653000	-0.038085000
C	-1.258316000	-0.549418000	-0.068984000
C	0.000047000	-1.139055000	-0.651499000
C	1.258407000	-0.549232000	-0.069061000
C	-0.000201000	1.557072000	-0.007314000
H	0.000209000	-2.218225000	-0.494420000
H	-0.000052000	-0.942916000	-1.725880000
N	1.197028000	0.937754000	-0.037736000
O	2.289904000	1.570582000	0.028378000
H	-0.000165000	2.634649000	0.063017000
O	-2.290296000	1.570188000	0.027617000
F	2.317925000	-0.896201000	-0.805233000
F	1.479432000	-0.972807000	1.194602000
F	-2.318045000	-0.896583000	-0.804496000
F	-1.478753000	-0.972599000	1.195263000

23 (X = H)

N	-1.201881000	-1.113020000	-0.000180000
C	-1.982953000	0.000012000	-0.000160000
N	-1.201877000	1.113029000	-0.000028000
O	-1.587022000	2.314699000	0.000025000
O	-1.587054000	-2.314685000	-0.000287000
C	2.503992000	0.700868000	0.000255000
C	1.319532000	1.432222000	0.000210000
C	2.503988000	-0.700879000	0.000158000
H	1.296608000	2.515253000	0.000280000
H	3.451527000	-1.228593000	0.000200000
C	0.149643000	0.695711000	0.000061000
C	1.319527000	-1.432233000	0.000014000
H	1.296615000	-2.515265000	-0.000062000
C	0.149632000	-0.695725000	-0.000035000
H	3.451537000	1.228575000	0.000369000
H	-3.057538000	0.000000000	-0.000252000

23 (X = CH_3)

N	0.857476000	-1.105909000	0.000459000
C	1.650033000	0.003276000	-0.000027000
N	0.852739000	1.111273000	0.000588000
O	1.240492000	2.316297000	0.000723000
C	3.113696000	0.002210000	-0.001570000
H	3.508770000	-0.456180000	0.909524000
H	3.500937000	-0.574879000	-0.845217000
H	3.466421000	1.031223000	-0.068087000
O	1.261054000	-2.306198000	0.000463000
C	-2.853131000	0.694414000	-0.000446000
C	-1.668044000	1.427659000	-0.000246000
C	-2.850500000	-0.705841000	-0.000188000
H	-1.646875000	2.510761000	-0.000494000
H	-3.796753000	-1.235908000	-0.000196000
C	-0.497415000	0.694292000	0.000171000
C	-1.662791000	-1.434818000	0.000080000
H	-1.638001000	-2.517858000	0.000211000
C	-0.494694000	-0.697281000	0.000256000
H	-3.801294000	1.221046000	-0.000731000

23 (X = F)

N	-0.890620000	-1.123241000	-0.000124000
C	-1.647750000	0.000127000	-0.000154000
N	-0.890553000	1.123374000	0.000038000
O	-1.300910000	2.318338000	0.000082000
O	-1.301395000	-2.318151000	-0.000246000

24 (X = H)

N	-0.070523000	-0.341081000	-0.000010000
O	-1.187278000	0.140049000	-0.000003000
C	1.124660000	0.114438000	0.000009000
H	1.314042000	1.186634000	0.000050000
H	1.929883000	-0.606087000	-0.000009000

C	2.816712000	0.699294000	0.000265000
C	1.629839000	1.431208000	0.000218000
C	2.816663000	-0.699467000	0.000174000
H	1.605958000	2.514184000	0.000293000
H	3.763332000	-1.228398000	0.000221000
C	0.461770000	0.696525000	0.000082000
C	1.629787000	-1.431360000	0.000029000
H	1.605978000	-2.514338000	-0.000041000
C	0.461679000	-0.696695000	-0.000012000
H	3.763419000	1.228155000	0.000383000
F	-2.940471000	0.000020000	-0.000282000

24 (X = CH_3)

N	-0.795060000	-0.619293000	-0.000032000
O	-1.961462000	-0.229624000	0.000017000
C	0.341924000	-0.017427000	0.000010000
C	0.426401000	1.475820000	-0.000017000
C	1.584600000	-0.838475000	0.000004000
H	1.354760000	-1.903621000	0.000207000
H	2.200314000	-0.617560000	-0.878537000
H	2.200406000	-0.617237000	0.878407000
H	0.974954000	1.830624000	-0.878850000
H	0.973633000	1.830758000	0.879614000
H	-0.564495000	1.929574000	-0.000734000

24 (X = F)

N	0.793868000	-0.534133000	0.000022000
O	1.918840000	-0.005320000	0.000010000
C	-0.362098000	-0.041181000	0.000000000
F	-0.650513000	1.241967000	-0.000046000
F	-1.431177000	-0.794347000	0.000020000

25 (X = H)

C	-1.468628000	-0.994573000	-0.000113000
N	-2.569456000	-0.320463000	-0.000143000
O	-2.829144000	0.875392000	-0.000117000
C	-0.128528000	-0.429471000	-0.000025000
C	0.962440000	-1.312401000	0.000063000
C	0.116070000	0.950818000	-0.000027000
C	2.261808000	-0.828103000	0.000155000
C	1.419791000	1.427666000	0.000063000
C	2.495709000	0.544381000	0.000155000
H	0.779209000	-2.383111000	0.000062000
H	-0.716641000	1.645622000	-0.000100000
H	3.094910000	-1.523362000	0.000226000
H	1.596938000	2.498136000	0.000060000
H	3.512039000	0.923876000	0.000228000
H	-1.599075000	-2.070953000	-0.000163000

25 (X = CH_3)

C	1.422521000	0.417476000	-0.000333000
N	2.297478000	-0.539511000	-0.000070000
O	2.232462000	-1.764531000	0.000441000
C	-0.021742000	0.162065000	-0.000260000
C	-0.909431000	1.251441000	0.000054000
C	-0.561094000	-1.133806000	-0.000280000
C	-2.282465000	1.050265000	0.000201000
C	-1.935370000	-1.327221000	-0.000119000
C	-2.803123000	-0.239446000	0.000148000
H	-0.522801000	2.264433000	0.000025000
H	0.099977000	-1.992295000	-0.000565000
H	-2.948524000	1.907053000	0.000268000
H	-2.330852000	-2.337655000	-0.000084000
H	-3.876678000	-0.396109000	0.000279000
C	1.972161000	1.807787000	0.000048000
H	3.060907000	1.781231000	-0.000218000
H	1.643434000	2.367612000	-0.880746000
H	1.643755000	2.367190000	0.881253000

25 (X = F)

C	1.389834000	0.479387000	-0.000051000
N	2.371371000	-0.344160000	-0.000189000
O	2.411935000	-1.577761000	-0.000280000
C	-0.029216000	0.184733000	0.000024000
C	-0.953816000	1.240014000	0.000074000
C	-0.491398000	-1.138426000	0.000045000
C	-2.313778000	0.968427000	0.000141000
C	-1.854555000	-1.395735000	0.000117000
C	-2.769291000	-0.346630000	0.000164000

26 (X = H)

C	-1.832981000	-1.222027000	0.000227000
N	-3.123992000	-1.151560000	-0.000206000
O	-3.926402000	-0.227967000	-0.000545000
H	0.463009000	-2.482986000	0.000108000
C	1.086619000	-1.597020000	0.000161000
C	2.451822000	-1.758245000	0.000180000
C	3.304755000	-0.638963000	-0.000112000
C	2.768096000	0.623412000	-0.000381000
C	1.367223000	0.824541000	-0.000227000

H	-0.596732000	2.262747000	0.000061000
H	0.217397000	-1.959164000	0.000007000
H	-3.022443000	1.789886000	0.000177000
H	-2.203884000	-2.422608000	0.000136000
H	-3.834150000	-0.553856000	0.000216000
F	1.742005000	1.773730000	-0.000013000

C	0.495445000	-0.311221000	-0.000025000
C	-0.924629000	-0.085943000	0.000242000
C	-1.407161000	1.214434000	0.000464000
C	-0.538952000	2.316464000	0.000321000
C	0.820378000	2.128262000	-0.000094000
H	2.874160000	-2.757703000	0.000514000
H	4.380686000	-0.777712000	-0.000202000
H	3.412740000	1.497741000	-0.000679000
H	1.498257000	2.976760000	-0.000451000
H	-0.953774000	3.318703000	0.000706000
H	-2.477479000	1.385111000	0.000666000
H	-1.462126000	-2.237426000	0.000605000

26 (X = CH_3)

C	1.893398000	-0.746078000	0.198529000
N	3.040606000	-0.473241000	-0.337017000
O	3.482002000	0.450270000	-1.011818000
C	1.826618000	-2.019961000	0.991989000
H	1.636066000	-2.899628000	0.369927000
H	2.773420000	-2.190665000	1.506978000
H	1.032935000	-1.966052000	1.738385000
H	-0.224674000	-2.281511000	-0.379324000
C	-0.979611000	-1.516601000	-0.250859000
C	-2.304348000	-1.859207000	-0.373323000
C	-3.310757000	-0.881544000	-0.253898000
C	-2.963821000	0.428939000	-0.046843000
C	-1.607993000	0.819418000	0.068820000
C	-0.582839000	-0.179850000	-0.000908000
C	0.783483000	0.229919000	0.128241000
C	1.078266000	1.577841000	0.232555000
C	0.067383000	2.551071000	0.280088000
C	-1.251673000	2.178813000	0.219488000
H	-2.576655000	-2.890110000	-0.575718000
H	-4.354360000	-1.164600000	-0.345085000
H	-3.727840000	1.198630000	0.019285000
H	-2.042159000	2.922246000	0.269342000
H	0.339418000	3.596682000	0.380079000
H	2.114953000	1.888980000	0.306518000

26 (X = F)

C	1.862108000	-0.803175000	0.138758000
N	3.093792000	-0.613156000	-0.162353000
O	3.712046000	0.364117000	-0.589830000
H	-0.372872000	-2.345896000	-0.172084000
C	-1.075500000	-1.527024000	-0.125968000
C	-2.419742000	-1.799517000	-0.216277000
C	-3.372915000	-0.765973000	-0.166880000
C	-2.954014000	0.533807000	-0.048485000
C	-1.578098000	0.855315000	0.033637000
C	-0.604480000	-0.197769000	0.015480000
C	0.781405000	0.173256000	0.100207000
C	1.136092000	1.513390000	0.145943000
C	0.169177000	2.527416000	0.153251000
C	-1.163076000	2.203817000	0.110194000
H	-2.747257000	-2.827715000	-0.329875000
H	-4.430529000	-0.998378000	-0.232392000
H	-3.672725000	1.347843000	-0.024668000
H	-1.922655000	2.979963000	0.121401000
H	0.484905000	3.563602000	0.201917000
H	2.184505000	1.784760000	0.197700000
F	1.604219000	-2.045142000	0.583773000

27 (X = H)

C	0.019305000	0.845845000	0.017940000
N	0.028878000	2.147304000	0.028256000
O	-0.842092000	3.007351000	0.012170000
C	-1.251617000	0.097561000	-0.022845000
C	-1.303011000	-1.162917000	-0.636396000
C	-2.430504000	0.632086000	0.512139000
C	-2.496900000	-1.867977000	-0.702802000
C	-3.619048000	-0.082896000	0.453115000
C	-3.658493000	-1.334357000	-0.153795000
H	-0.403562000	-1.580369000	-1.076426000
H	-2.414527000	1.609016000	0.982127000
H	-2.519875000	-2.836584000	-1.191616000
H	-4.520535000	0.342337000	0.881860000
H	-4.590572000	-1.887389000	-0.204567000
C	1.340832000	0.194799000	0.034965000
C	2.443678000	0.812280000	-0.568893000
C	1.532275000	-1.028812000	0.688332000
C	3.699444000	0.224618000	-0.518785000

27 (X = CH_3)

C	0.050519000	0.662492000	-0.085631000
N	0.077449000	1.961172000	-0.154237000
O	-0.772696000	2.824926000	-0.322920000
C	-1.248571000	-0.047704000	-0.203635000
C	-1.375099000	-1.030516000	-1.192428000
C	-2.334063000	0.246192000	0.640901000
C	-2.570356000	-1.709333000	-1.372612000
C	-3.526887000	-0.456325000	0.444655000
C	-3.653804000	-1.416420000	-0.549455000
H	-0.519348000	-1.253996000	-1.822998000
H	-2.655910000	-2.462166000	-2.149045000
H	-4.367937000	-0.244735000	1.099431000
H	-4.594193000	-1.943026000	-0.676446000
C	1.312457000	-0.070014000	0.092147000
C	2.574431000	0.443411000	-0.291854000
C	1.245638000	-1.344955000	0.675753000
C	3.702828000	-0.345958000	-0.065974000

C	2.790392000	-1.616209000	0.733724000
C	3.878238000	-0.994219000	0.129917000
H	2.300250000	1.757078000	-1.083858000
H	0.692801000	-1.510928000	1.179094000
H	4.541517000	0.715400000	-0.995967000
H	2.922207000	-2.561130000	1.250804000
H	4.859350000	-1.456195000	0.163698000
C	2.383757000	-2.105788000	0.893838000
C	3.623923000	-1.603303000	0.520230000
H	0.276087000	-1.734463000	0.969274000
H	4.670954000	0.042522000	-0.370395000
H	2.300214000	-3.084649000	1.353983000
H	4.525284000	-2.186583000	0.677584000
C	2.749514000	1.780871000	-0.942920000
H	3.762229000	1.882296000	-1.338413000
H	2.045339000	1.933067000	-1.765444000
H	2.582859000	2.604526000	-0.242305000
C	-2.231015000	1.253887000	1.742387000
H	-2.981413000	1.068887000	2.512887000
H	-1.244491000	1.239495000	2.213709000
H	-2.379869000	2.271991000	1.368773000

27 (X = F)

C	0.044650000	0.671207000	-0.062932000
N	0.051108000	1.970199000	-0.140653000
O	-0.815610000	2.807056000	-0.306717000
C	-1.232305000	-0.066497000	-0.167724000
C	-1.366663000	-1.139008000	-1.058577000
C	-2.352997000	0.280749000	0.586032000
C	-2.570311000	-1.814140000	-1.194414000
C	-3.564849000	-0.378451000	0.466774000
C	-3.671731000	-1.430311000	-0.433251000
H	-0.504973000	-1.429785000	-1.651726000
F	-2.247685000	1.270717000	1.487574000
H	-2.652193000	-2.635168000	-1.898066000
H	-4.398116000	-0.064666000	1.084332000
H	-4.616649000	-1.953277000	-0.535736000
C	1.315611000	-0.038442000	0.098610000
C	2.551499000	0.491868000	-0.293460000
C	1.341333000	-1.321352000	0.667025000
C	3.743832000	-0.189381000	-0.133387000
C	2.526149000	-2.021619000	0.837124000
C	3.732530000	-1.455987000	0.438051000
F	2.594630000	1.705761000	-0.869125000
H	0.402695000	-1.762372000	0.986536000
H	4.661703000	0.282089000	-0.464882000
H	2.507310000	-3.008697000	1.285928000
H	4.664356000	-1.996074000	0.566652000