

Supporting Information

Better Sensing through Stacking: The Role of Non-Covalent Interactions in Guanine Binding Sensors

Drew P. Harding, Andrea N. Bootsma, and Steven E. Wheeler*

Department of Chemistry, Texas A&M University, College Station, TX 77842

Center for Computational Quantum Chemistry, Department of Chemistry, University of Georgia, Athens, GA 30602

E-mail: : swheele2@uga.edu

Contents

	Page
Table S1. Incremental focal point tables for interaction energies and binding energies (in kcal mol ⁻¹) for complexes of 9-methyl-guanine (G) with 1 and 1-methyl-cytosine (C).	2
Table S2. Gas-phase binding energies (in kcal mol ⁻¹) for complexes of 9-methyl-guanine (G) with 1 and 1-methyl-cytosine (C), as well as the difference between the two, computed at M06-2X/6-31G(d) optimized geometries.	2
Table S3. IEFPCM M06-2X/6-311+G(d)//6-31G(d) solution-phase (dichloromethane) binding energies of 1-methyl-cytosine and sensors 1 , 4-10 with 9-methyl-guanine in kcal mol ⁻¹ .	3
Table S4. Bond distances and angles of N ⁺ H-N hydrogen bonds between 1-methyl-guanine and sensors 4-9 and 10a-10j and their respective correlation to gas phase interaction energies and M4 interaction energies.	3
Table S5. Single point electronic energies for 1-methyl-guanine optimized at IEFPCM M06-2X/6-31G(d).	4
Table S6. IEFPCM-M06-2X/6-311+G(d) solution-phase (dichloromethane) electronic energies of 1-methyl-cytosine and sensors 1,4-10 with and without 9-methyl-guanine (at IEFPCM-M06-2X/6-31G(d) optimized geometries).	4
Table S7. Gas-phase electronic energies at various levels of theory for the 1 ...9-methyl-guanine complex and corresponding monomers at the complex geometry optimized at the IEFPCM M06-2X/6-31G(d) level of theory.	4
Table S8. Gas-phase electronic energies at various levels of theory for the 1-methyl-cytosine...9-methyl-guanine complex and corresponding monomers at the complex geometry optimized at the IEFPCM M06-2X/6-31G(d) level of theory.	5
Table S9. Gas-phase M06-2X/6-311+G(d) electronic energies for sensors 4-10 complexed with 9-methyl-guanine and corresponding monomers at the complex geometry.	5
Table S10. M06-2X/6-311+G(d) electronic energies for truncated models for sensors 4-10 with and without 9-methyl-guanine at the complex geometry.	6
Optimized Cartesian Coordinates	6

Table S1. Incremental focal point tables for interaction energies and binding energies (in kcal mol⁻¹) for complexes of 9-methyl-guanine (G) with **1** and 1-methyl-cytosine (C).^a

Interaction Energies					
C ^{...} G	df-HF	+ δ (SL-MP2)	+ δ (DLPNO-CCSD)	+ δ [DLPNO-CCSD(T)]	=DLPNO-CCSD(T)
cc-pVDZ	-29.67	-5.85	2.59	-0.35	[-33.28]
cc-pVTZ	-26.43	-7.28	2.21	-0.45	[-31.94]
cc-pVQZ	-25.64	-7.48	2.06	-0.43	[-31.48]
CBS limit	[-25.39]	[-7.63]	[+1.96]	[-0.41]	[-31.47]
1^{...}G					
cc-pVDZ	-25.63	-6.60	1.67	-0.37	[-30.92]
cc-pVTZ	-22.34	-7.91	1.26	-0.40	[-29.39]
cc-pVQZ	-21.57	-8.18	1.11	-0.43	[-29.07]
CBS limit	[-21.34]	[-8.37]	[+1.01]	[-0.45]	[-29.16]
Binding Energies					
C ^{...} G	df-HF	+ δ (SL-MP2)	+ δ (DLPNO-CCSD)	+ δ [DLPNO-CCSD(T)]	=DLPNO-CCSD(T)
cc-pVDZ	-24.83	-7.19	3.20	-0.42	[-29.25]
cc-pVTZ	-21.65	-8.63	2.82	-0.55	[-28.01]
cc-pVQZ	-20.92	-8.88	2.67	-0.61	[-27.73]
CBS limit	[-20.71]	[-9.06]	[+2.56]	[-0.65]	[-27.85]
1^{...}G					
cc-pVDZ	-21.51	-8.03	2.15	-0.51	[-27.91]
cc-pVTZ	-18.20	-9.57	1.83	-0.61	[-26.55]
cc-pVQZ	-17.46	-9.86	1.69	-0.68	[-26.31]
CBS limit	[-17.25]	[-10.07]	[+1.58]	[-0.73]	[-26.48]

^a Numbers in brackets are the results of basis set extrapolations.

Table S2. Gas-phase binding energies (in kcal mol⁻¹) for complexes of 9-methyl-guanine (G) with **1** and 1-methyl-cytosine (C), as well as the difference between the two, computed at M06-2X/6-31G(d) optimized geometries.

	1^{...}G	C^{...}G	Diff.
M06-2X/6-311+G(d)	-26.9	-28.4	-1.5
DLPNO-CCSD(T)/CBS ^a	-26.5	-27.9	-1.5

^a DLPNO-CCSD(T) energies extrapolated to the complete basis set limit.

Table S3. IEFPCM M06-2X/6-311+G(d)//6-31G(d) solution-phase (dichloromethane) binding energies of 1-methyl-cytosine and sensors **1**, **4-10** with 9-methyl-guanine in kcal mol⁻¹.

	E _{bind}		E _{bind}
C	-18.2	9b	-25.6
1	-17.6	9c	-28.2
4a	-24.0	9d	-26.0
5a	-25.4	10a	-25.4
5b	-23.9	10b	-27.5
6a	-24.4	10c	-25.5
6b	-26.5	10d	-26.6
6c	-25.0	10e	-27.2
7a	-26.6	10f	-28.0
8a	-26.0	10g	-22.6
8b	-27.4	10h	-26.2
8c	-26.0	10i	-26.9
9a	-27.4	10j	-27.9

Table S4. Bond distances N⁺H-N hydrogen bonds between 1-methyl-guanine and sensors **4-9** and **10a-10j** and their respective correlation to gas phase interaction energies and M4 interaction energies.

Sensor	r1	r2	r3
4a	3.338	2.201	2.118
5a	3.286	2.172	2.144
6b	2.446	2.051	2.154
7a	3.232	2.125	2.204
8b	2.529	2.067	2.195
9c	2.567	2.085	2.208
10f	2.310	1.901	-
Correl. with E _{int} (r ²)	0.97	0.81	0.28
Correl. with E _{M4} (r ²)	0.92	0.82	0.34

Sensor	r1	r2	r3
10a	3.219	2.109	2.314
10b	3.216	2.172	2.300
10c	3.138	2.065	2.208
10d	2.954	2.681	1.895
10e	3.107	2.122	2.140
10f	2.310	1.901	-
10g	2.966	2.648	2.174
10h	3.275	2.152	2.230
10i	3.092	1.930	1.988
10j	2.552	2.069	2.198
Correl. with E _{int} (r ²)	0.49	0.36	0.57
Correl. with E _{M4} (r ²)	0.18	0.61	0.25

Table S5. Single point electronic energies for 1-methyl-guanine optimized at IEFPCM M06-2X/6-31G(d) .

IEFPCM M06-2X/6-31G(d) Solvent DCM	IEFPCM M06-2X/6-311+G(d) Solvent DCM	M06-2X/6-311+G(d)
-581.65828843	-581.81858224	-581.7961856690

Table S6. IEFPCM-M06-2X/6-311+G(d) solution-phase (dichloromethane) electronic energies of 1-methyl-cytosine and sensors 1,4-10 with and without 9-methyl-guanine (at IEFPCM-M06-2X/6-31G(d) optimized geometries).

	complex	sensor
C	-1016.046359	-434.1988354
1	-1207.754623	-625.90798
4a	-1974.533926	-1392.677138
5a	-2128.157492	-1546.298389
5b	-2128.155513	-1546.298915
6a	-2281.772553	-1699.915101
6b	-2281.772040	-1699.911149
6c	-2281.766705	-1699.908312
7a	-2435.404862	-1853.543816
8a	-2358.008086	-1776.148062
8b	-2358.008524	-1776.146337
8c	-2358.007925	-1776.147901
9a	-2281.782524	-1699.920165
9b	-2281.783086	-1699.923725
9c	-2281.782712	-1699.919207
9d	-2281.782235	-1699.922158
10a	-2511.626106	-1929.766995
10b	-2511.625285	-1929.762830
10c	-2511.624741	-1929.765591
10d	-2511.625726	-1929.764744
10e	-2511.621081	-1929.759207
10f	-2511.626086	-1929.762897
10g	-2511.621469	-1929.766871
10h	-2511.626591	-1929.766313
10i	-2511.626431	-1929.764945
10j	-2511.626622	-1929.763519

Table S7. Gas-phase electronic energies at various levels of theory for the 1⁺9-methyl-guanine complex and corresponding monomers at the complex geometry optimized at the IEFPCM M06-2X/6-31G(d) level of theory.

	Complex	1	Guanine
M06-2X/6-31G(d)	-1207.422342	-625.7356946	-581.6345965
M06-2X/6-311+G(d)	-1207.733569	-625.8932008	-581.7929687
wB97X-D/def2-TZVP	-1207.956383	-626.009083	-581.8984112
DLPNO-CCSD/cc-pVQZ	-1205.978624	-624.9610432	-580.9719463
SCS-MP2/cc-pVTZ	-1205.584373	-624.753322	-580.784702
SCS-MP2/cc-pVQZ	-1205.938369	-624.937349	-580.956681
DLPNO-CCSD(T)/cc-pVQZ	-1206.220601	-625.0897962	-581.0844857

Table S8. Gas-phase electronic energies at various levels of theory for the 1-methyl-cytosine ...9-methyl-guanine complex and corresponding monomers at the complex geometry optimized at the IEFPCM M06-2X/6-31G(d) level of theory.

	Complex	1-methyl-cytosine	Guanine
M06-2X/6-31G(d)	-1015.747576	-434.0572223	-581.6341812
M06-2X/6-311+G(d)	-1016.021567	-434.177902	-581.7925802
wB97X-D/def2-TZVP	-1016.217687	-434.2677661	-581.8980515
SCS-MP2/cc-pVTZ	-1014.258924	-433.425559	-580.784161
SCS-MP2/cc-pVQZ	-1014.559445	-433.555599	-580.956160
DLPNO-CCSD/cc-pVQZ	-1014.592985	-433.5721273	-580.9713723
DLPNO-CCSD(T)/cc-pVQZ	-1014.78875	-433.6546863	-581.0838994

Table S9. Gas-phase M06-2X/6-311+G(d) electronic energies for sensors **4-10** complexed with 9-methyl-guanine and corresponding monomers at the complex geometry.

	Complex	Sensor	Guanine
4a	-1974.51031021	-1392.646024	-581.791715
5a	-2128.13346029	-1546.267225	-581.791554
6b	-2281.74792404	-1699.873772	-581.789477
7a	-2435.37983556	-1853.511743	-581.791687
8b	-2357.98409113	-1776.110963	-581.790726
9c	-2281.75847695	-1699.885911	-581.790726
10a	-2511.60001655	-1929.728558	-581.791802
10b	-2511.59990859	-1929.729765	-581.791423
10c	-2511.59920100	-1929.730530	-581.791369
10d	-2511.60081224	-1929.734877	-581.791856
10e	-2511.59539825	-1929.727090	-581.791675
10f	-2511.60092291	-1929.725345	-581.789438
10g	-2511.59559600	-1929.726610	-581.792267
10h	-2511.60165800	-1929.731438	-581.791698
10i	-2511.60065500	-1929.732672	-581.791471
10j	-2511.60160784	-1929.729408	-581.790642

Table S10. M06-2X/6-311+G(*d*) electronic energies for truncated models for sensors **4-10** with and without 9-methyl-guanine at the complex geometry.

Sensor	M1 complex	M1	M2 complex	M2	M3 complex	M3	M4 complex	M4
4a	-790.980471	-209.178227	-999.707767	-417.886392	-811.568692	-229.763992	-813.995846	-232.190051
5a	-790.980134	-209.178220	-999.707649	-417.886257	-811.568799	-229.764049	-967.612362	-385.804134
6b	-790.978606	-209.178461	-999.704854	-417.886394	-811.568833	-229.761371	-1121.223041	-539.410995
7a	-790.980910	-209.178405	-999.707576	-417.886420	-811.568505	-229.762512	-1274.846886	-693.037296
8b	-790.980191	-209.178545	-999.706245	-417.886197	-811.570538	-229.762081	-1197.455761	-615.644121
9c	-790.979061	-209.178373	-999.705826	-417.886376	-811.569807	-229.762461	-1121.232535	-539.421345
10a	-790.981488	-209.178511	-999.707897	-417.886512	-811.568947	-229.762687	-1351.068618	-769.255193
10b	-790.980840	-209.178552	-999.707450	-417.886112	-811.569851	-229.764456	-1351.068347	-769.256099
10c	-790.980793	-209.178476	-999.707479	-417.886287	-811.566998	-229.762209	-1351.067403	-769.256375
10d	-790.981554	-209.178608	-999.707228	-417.886398	-811.565893	-229.762884	-1351.066051	-769.255798
10e	-790.980893	-209.178371	-999.707484	-417.886340	-811.566796	-229.761599	-1351.066631	-769.255390
10f	-790.978651	-209.178508	-999.704807	-417.886352	-811.564979	-229.755975	-1351.069165	-769.256096
10g	-790.982343	-209.178612	-999.707666	-417.886231	-811.568127	-229.761800	-1351.065331	-769.256227
10h	-790.980525	-209.178234	-999.707659	-417.886209	-811.570412	-229.764340	-1351.067451	-769.255686
10i	-790.980819	-209.178446	-999.707490	-417.886359	-811.566866	-229.762368	-1351.067862	-769.256454
10j	-790.979733	-209.178390	-999.706112	-417.886248	-811.570349	-229.762181	-1351.067314	-769.256001

Optimized Cartesian Coordinates (Å) at the IEFPCM M06-2X/6-31G(*d*) level of theory (solvent = dichloromethane)

19

9-methyl-guanine

N	1.9233310	-0.4033040	-0.0001550
C	2.3629550	0.9001780	0.0017120
H	3.4212950	1.1270300	0.0007530
N	1.3934800	1.7766770	0.0037880
C	0.2495810	1.0090970	0.0039430
C	-1.1335710	1.3937790	0.0014340
O	-1.6395730	2.5038470	-0.0015570
N	-1.9579460	0.2408760	-0.0027220
H	-2.9520360	0.4407290	-0.0406860
C	-1.5342160	-1.0643900	-0.0005610
N	-2.5036870	-2.0218730	-0.0680090
H	-3.4150530	-1.8113880	0.3167600
H	-2.1715000	-2.9558380	0.1342720
N	-0.2719560	-1.4146190	0.0064180
C	0.5611420	-0.3441630	0.0008820
C	2.7226230	-1.6153990	-0.0019010
H	2.5046300	-2.2069110	0.8892930
H	2.4995780	-2.2076810	-0.8912660
H	3.7760320	-1.3356240	-0.0049650

35

1-methyl-cytosine complex

N	4.6299920	-0.3533300	-0.0012330
C	4.9593160	0.9822230	0.0708150
H	5.9956430	1.2944710	0.0930890
N	3.9219950	1.7742490	0.1032790
C	2.8437250	0.9138420	0.0516360
C	1.4369280	1.1691670	0.0514010
O	0.8578100	2.2584430	0.1019130
N	0.7033850	-0.0195410	-0.0157540
H	-0.3276740	0.0882260	-0.0084130
C	1.2313970	-1.2866190	-0.0816770
N	0.3444570	-2.2939160	-0.1820520
H	-0.6577550	-2.1490500	-0.0258590
H	0.7170660	-3.2287090	-0.1066320
N	2.5278170	-1.5385710	-0.0789130
C	3.2664600	-0.4100250	-0.0135230
C	5.5282000	-1.4918860	-0.0480780
H	5.4392390	-2.0839510	0.8652990
H	5.2836010	-2.1181390	-0.9077630
H	6.5499110	-1.1241850	-0.1448870
N	-4.3629860	-0.6786730	0.0392880
C	-4.9485420	0.5434300	-0.0540470
H	-6.0327790	0.5489740	-0.0796030
C	-4.2136590	1.6789120	-0.1098860
H	-4.6805430	2.6515910	-0.1839320
C	-2.7884500	1.5273800	-0.0646690
N	-1.9917620	2.5961610	-0.1105210
H	-0.9739730	2.4862650	-0.0434060
H	-2.3843450	3.5240150	-0.1622680
N	-2.2140640	0.3252400	0.0218590
C	-2.9676660	-0.8010440	0.0766520
O	-2.4861680	-1.9366820	0.1594450
C	-5.1465100	-1.9090180	0.0963620

H	-4.8943450	-2.5467670	-0.7522300
H	-4.9220360	-2.4468410	1.0186300
H	-6.2041670	-1.6495020	0.0655110
16			
1-methyl-cytosine			
N	1.1087670	0.4413600	-0.0006890
C	0.2590220	1.4965390	0.0006060
H	0.7181630	2.4797070	-0.0005940
C	-1.0848970	1.3199290	0.0034280
H	-1.7676980	2.1585170	0.0099700
C	-1.5423070	-0.0383940	0.0023750
N	-2.8694770	-0.2872530	0.0316190
H	-3.1760810	-1.2410900	-0.0957480
H	-3.5363780	0.4499750	-0.1377830
N	-0.7263980	-1.0781490	-0.0006160
C	0.6240850	-0.8882660	0.0011960
O	1.4437050	-1.8006470	0.0010560
C	2.5557250	0.6179650	-0.0043660
H	2.9882190	0.1501790	0.8817810
H	2.9842350	0.1449600	-0.8896600
H	2.7798830	1.6845910	-0.0080440
42			
1 complex			
C	-2.5429100	-3.4886570	-0.1358890
C	-3.9508910	-3.5721990	-0.1794430
N	-1.8667010	-2.3588900	-0.0769230
C	-4.6705200	-2.4035960	-0.1505040
H	-4.4335690	-4.5408430	-0.2312360
C	-2.5641340	-1.1930310	-0.0558250
C	-3.9810240	-1.1743390	-0.0860370
H	-5.7568180	-2.4051430	-0.1767230
N	-1.8235270	-0.0568410	-0.0047980
C	-4.6176680	0.0935450	-0.0469090
C	-2.4472780	1.1086670	0.0196310
C	-3.8727640	1.2335610	0.0082030
H	-5.7028160	0.1439230	-0.0636060
N	-1.6055030	2.2079240	0.0466090
H	-4.3181650	2.2160210	0.0394500
C	-1.9352890	3.5441160	0.1386240
H	-0.6044170	1.9831530	-0.0341110
C	-0.7340270	4.4600780	0.1955140
O	-3.0782510	3.9649630	0.2019520
H	0.1583330	4.0103010	-0.2421020
H	-0.5258980	4.6896990	1.2455960
H	-0.9832100	5.3925550	-0.3121490
N	5.1469460	-0.4386030	-0.0329520
C	5.3688200	0.9000220	-0.2694880
H	6.3761620	1.2851820	-0.3623170
N	4.2723720	1.6028360	-0.3621480
C	3.2670020	0.6762070	-0.1762870
C	1.8471980	0.8232460	-0.1620300
O	1.1835160	1.8533300	-0.3184450
N	1.2065720	-0.3992360	0.0639350
H	0.1757880	-0.3608750	0.0699030
C	1.8345270	-1.6075030	0.2608890
N	1.0277580	-2.6580900	0.5125560
H	0.0300670	-2.5940990	0.2871820
H	1.4688150	-3.5662060	0.4915490
N	3.1441670	-1.7585220	0.2492490

C	3.7933300	-0.5948090	0.0296930
C	6.1322310	-1.4922360	0.1269230
H	6.0376980	-1.9454620	1.1155830
H	5.9857830	-2.2591790	-0.6359160
H	7.1257720	-1.0570960	0.0189350
H	-1.9498490	-4.4007580	-0.1491750
23			
1			
C	-3.5848970	-1.2128610	-0.0001620
C	-4.0354880	0.1289120	-0.0001520
N	-2.3219920	-1.5805420	-0.0000470
C	-3.0972220	1.1282870	-0.0000640
H	-5.0980820	0.3427390	-0.0002230
C	-1.3815150	-0.5979780	0.0000780
C	-1.7281750	0.7788950	0.0000320
H	-3.3824500	2.1770660	-0.0000770
N	-0.0894600	-1.0142430	0.0001420
C	-0.6707070	1.7241150	0.0001310
C	0.8612740	-0.1065730	0.0002340
C	0.6272520	1.3022120	0.0002270
H	-0.9053010	2.7851990	0.0001010
N	2.1491010	-0.6467880	0.0002120
H	1.4622420	1.9862630	0.0002940
C	3.3704680	-0.0087420	-0.0000900
H	2.1476500	-1.6607320	0.0004090
C	4.5446950	-0.9618360	-0.0001000
O	3.4996700	1.2025010	-0.0003530
H	4.5166140	-1.6039920	-0.8851120
H	4.5169990	-1.6036840	0.8851370
H	5.4653620	-0.3804840	-0.0004390
H	-4.3180480	-2.0179650	-0.0002210
77			
4a complex			
C	1.1746210	-4.4254330	-0.2183200
N	0.0689220	-2.2777940	-0.3874650
C	-0.0276040	-5.0736710	-0.1399540
H	2.1185680	-4.9561800	-0.1890390
C	2.4522080	-2.3534630	-0.3841490
C	-1.1267570	-2.9113220	-0.2904780
C	-1.2213650	-4.3206840	-0.1665180
H	-0.0784480	-6.1550720	-0.0487170
C	3.6060800	-1.9717680	-0.3541130
N	-2.2258290	-2.1130240	-0.3045010
C	-2.5169060	-4.8872940	-0.0695990
C	4.9849180	-1.6142620	-0.2786540
C	-3.4203490	-2.6717040	-0.1912290
C	-3.6182760	-4.0840460	-0.0795990
H	-2.6201420	-5.9651810	0.0195200
C	5.9389060	-2.6375260	-0.1571460
C	5.3943170	-0.2537000	-0.2810910
N	-4.4742270	-1.7760300	-0.1757880
H	-4.6213490	-4.4738640	-0.0012700
C	7.2873990	-2.3486950	-0.0254740
H	5.5907750	-3.6659730	-0.1597290
C	6.7666040	0.0191740	-0.1235480
N	4.4771980	0.7458450	-0.4592870
C	-5.8292920	-2.0332650	-0.1096370
H	-4.2037590	-0.7819210	-0.1892290
C	7.6880450	-1.0105020	-0.0037350

H	8.0145140	-3.1472330	0.0694730
H	7.1097690	1.0469360	-0.0997860
C	4.7640800	2.1248440	-0.1222030
H	3.4973140	0.4983770	-0.3547400
C	-6.6655800	-0.7741130	-0.1212820
O	-6.3143320	-3.1505640	-0.0615340
H	8.7392300	-0.7631600	0.1122100
H	5.0473530	2.2247780	0.9376870
H	5.6092670	2.4904500	-0.7149720
H	-6.5893240	-0.2912870	-1.1004180
H	-6.3033230	-0.0580650	0.6200690
H	-7.7031540	-1.0391440	0.0769650
N	-1.5676020	4.7974780	-0.8107140
C	-2.8464270	5.1163240	-0.4094420
H	-3.1418970	6.1492480	-0.2762900
N	-3.6101030	4.0730910	-0.2254840
C	-2.7905970	3.0033710	-0.5225770
C	-3.0160260	1.5959270	-0.4405970
O	-4.0481340	1.0073770	-0.1015390
N	-1.8746740	0.8695130	-0.7890310
H	-1.9408260	-0.1502360	-0.6480650
C	-0.6562800	1.4026060	-1.1236080
N	0.3321480	0.5237910	-1.4130970
H	1.2588910	0.9205500	-1.2666130
H	0.2247190	-0.4256400	-1.0405210
N	-0.4363110	2.7032170	-1.2102130
C	-1.5210830	3.4365470	-0.8830650
C	3.5458530	2.9901210	-0.4450210
H	3.4644170	3.1012320	-1.5306430
H	3.7095870	3.9900190	-0.0116340
N	2.3129490	2.3647580	0.0170880
H	1.5090570	2.8502550	-0.3868530
C	2.1630900	2.3361760	1.4743570
H	2.2474640	3.3440410	1.9143410
H	2.9799210	1.7337200	1.8911900
C	0.8375870	1.7154340	1.8494460
C	0.6803950	0.3266450	1.8336790
C	-0.2650670	2.5147910	2.1562980
C	-0.5493600	-0.2509780	2.1389450
H	1.5282400	-0.3037900	1.5679190
C	-1.5000290	1.9415210	2.4575050
H	-0.1566020	3.5979810	2.1526710
C	-1.6423080	0.5555600	2.4545240
H	-0.6573610	-1.3311130	2.1214250
H	-2.3514620	2.5773940	2.6830520
H	-2.6059250	0.1056830	2.6757500
C	-0.4556260	5.6956430	-1.0592630
H	0.3321520	5.5319060	-0.3191860
H	-0.0525340	5.5208380	-2.0583980
H	-0.8138880	6.7224950	-0.9858880
C	1.1750310	-3.0070010	-0.3388250
58			
4a			
C	-0.4572440	3.5350250	0.0186860
N	-0.1664140	1.2479660	-0.7362560
C	0.8984730	3.7331410	0.0369140
H	-1.1573650	4.3123880	0.3011960
C	-2.3422490	1.9481460	-0.3209420
C	1.1741210	1.4373310	-0.7137270

C	1.7580240	2.6708750	-0.3209650
H	1.3220140	4.6881890	0.3361310
C	-3.4767150	1.5217930	-0.2589230
N	1.9199080	0.3592910	-1.0539020
C	3.1736760	2.7468930	-0.2914460
C	-4.6703410	0.7501210	-0.1872340
C	3.2260410	0.4554120	-0.9661890
C	3.9227860	1.6482650	-0.5997320
H	3.6515340	3.6811410	-0.0091090
C	-5.9239170	1.3051040	0.0918540
C	-4.5220770	-0.6569790	-0.3624070
N	3.8932840	-0.7261310	-1.2893100
H	5.0020500	1.6526950	-0.5698480
C	-7.0449200	0.4974880	0.2154090
H	-5.9979630	2.3808420	0.2185440
C	-5.6668290	-1.4586200	-0.2088790
N	-3.2976040	-1.1801580	-0.6918190
C	5.1841610	-1.0928560	-0.9754780
H	3.2508590	-1.4655580	-1.5540040
C	-6.9001440	-0.8842210	0.0693270
H	-8.0146600	0.9323530	0.4302670
H	-5.5878260	-2.5349660	-0.3136250
C	-2.9662540	-2.5756560	-0.4954230
H	-2.5146530	-0.5405520	-0.5952630
C	5.4807130	-2.5458610	-1.2720660
O	6.0063130	-0.3272320	-0.5046610
H	-7.7662740	-1.5310550	0.1754520
H	-3.0934860	-2.8686380	0.5594000
H	-3.6387280	-3.2058920	-1.0884900
H	5.2702960	-2.7768670	-2.3200480
H	4.8510850	-3.1916850	-0.6512940
H	6.5292550	-2.7438040	-1.0550480
C	-1.5305410	-2.8546930	-0.9598980
H	-1.4801210	-2.7310390	-2.0465160
H	-1.3245560	-3.9108630	-0.7414290
N	-0.4694380	-2.0472500	-0.3794710
H	-0.3808780	-1.1248690	-0.8068470
C	-0.5016760	-1.9151920	1.0718010
H	-0.6224790	-2.9232670	1.4922280
H	-1.3517780	-1.3140180	1.4410600
C	0.7913300	-1.3059670	1.5631170
C	0.8241870	-0.0276260	2.1160460
C	1.9907020	-2.0092740	1.4138350
C	2.0358620	0.5555580	2.4872830
H	-0.1045900	0.5279920	2.2295180
C	3.1990340	-1.4419100	1.8024040
H	1.9663470	-3.0049280	0.9763480
C	3.2265120	-0.1484890	2.3265710
H	2.0488900	1.5630760	2.8934440
H	4.1255790	-2.0000860	1.6919000
H	4.1722990	0.3046250	2.6093200
C	-0.9433020	2.2566260	-0.3650530
83			
5a complex			
C	1.1965040	-4.2184300	-0.5352480
N	0.1819520	-2.0481770	-0.8820320
C	-0.0322400	-4.8189890	-0.4895990
H	2.1176170	-4.7777050	-0.4240740
C	2.5585860	-2.2076120	-0.7322730

C	-1.0407940	-2.6301830	-0.8106440
C	-1.1926810	-4.0272620	-0.6185390
H	-0.1291170	-5.8910560	-0.3416650
C	3.7288300	-1.8888310	-0.6525530
N	-2.1046280	-1.7927840	-0.9001210
C	-2.5100730	-4.5412630	-0.5362880
C	5.1214840	-1.6078950	-0.5222400
C	-3.3200550	-2.2984980	-0.7702180
C	-3.5772940	-3.6962690	-0.6049810
H	-2.6572310	-5.6096150	-0.4027770
C	6.0290650	-2.6782000	-0.5512950
C	5.5858760	-0.2831380	-0.3064100
N	-4.3387290	-1.3636130	-0.7937480
H	-4.5968310	-4.0417250	-0.5304710
C	7.3855910	-2.4724510	-0.3587370
H	5.6384150	-3.6774320	-0.7182670
C	6.9637660	-0.0981290	-0.0877660
N	4.7083630	0.7679820	-0.3371340
C	-5.6892990	-1.5538350	-0.5846950
H	-4.0256590	-0.3827540	-0.8229950
C	7.8400050	-1.1732480	-0.1194810
H	8.0770250	-3.3071460	-0.3829450
H	7.3479550	0.8975770	0.1022600
C	5.0111990	2.0442710	0.2778960
H	3.7205060	0.5330670	-0.2971750
C	-6.4687760	-0.2587130	-0.5719590
O	-6.2154800	-2.6433210	-0.4301120
H	8.8976860	-0.9927030	0.0485090
H	5.2354010	1.9251120	1.3500390
H	5.8965630	2.4896990	-0.1872630
H	-7.5173170	-0.4815770	-0.3800810
H	-6.3648090	0.2529810	-1.5330300
H	-6.0756990	0.4153100	0.1938540
N	-1.1104810	5.0915210	-0.7267750
C	-2.4162040	5.4393890	-0.4577300
H	-2.6847880	6.4710190	-0.2692830
N	-3.2372620	4.4238490	-0.4594860
C	-2.4293640	3.3430090	-0.7496020
C	-2.7210590	1.9469370	-0.8290190
O	-3.8121100	1.3912830	-0.6655950
N	-1.5791340	1.1940770	-1.1164280
H	-1.7053510	0.1695480	-1.0869570
C	-0.3063410	1.6925320	-1.2458810
N	0.6739260	0.7996490	-1.5004980
H	0.4825370	-0.1844680	-1.2823990
H	1.5939350	1.1305180	-1.2143340
N	-0.0227270	2.9830470	-1.1703070
C	-1.1090980	3.7404560	-0.9138920
C	3.8324280	2.9968840	0.0692200
H	3.8218190	3.3289680	-0.9733110
H	3.9860330	3.8816060	0.7081020
N	2.5613180	2.3281210	0.3183930
H	1.7955890	2.9042140	-0.0372960
C	2.3161520	2.0043230	1.7263500
H	2.4117370	2.8960340	2.3697420
H	3.0779560	1.2871750	2.0545490
C	0.0562660	5.9526410	-0.7788140
H	0.7838750	5.6407310	-0.0250660
H	0.5177100	5.8987250	-1.7667870

H	-0.2568610	6.9772760	-0.5780150
C	1.2551140	-2.8101440	-0.7308420
C	0.9446130	1.3933060	1.8948060
C	0.7707280	0.0310280	1.9430470
C	-0.1969400	2.2388770	1.9650570
C	-0.5206890	-0.5459060	2.0870440
H	1.6347280	-0.6300220	1.8836950
C	-1.4599060	1.7149160	2.0671760
H	-0.0567060	3.3180010	1.9312270
C	-1.6584190	0.3082210	2.1276810
C	-0.7089660	-1.9478480	2.2175520
H	-2.3281980	2.3688370	2.1057650
C	-2.9516430	-0.2672650	2.2500080
C	-1.9671900	-2.4743770	2.3692950
H	0.1640210	-2.5975090	2.1911310
C	-3.1020560	-1.6256860	2.3755640
H	-3.8179010	0.3895530	2.2492290
H	-2.1006860	-3.5479270	2.4677230
H	-4.0941290	-2.0594110	2.4690270
64			
5a			
C	-0.6847600	-3.2310080	-1.0522580
N	-0.5965430	-0.8196100	-1.2980550
C	0.6788150	-3.3211560	-1.1531000
H	-1.3114640	-4.1033320	-0.9082100
C	-2.6836160	-1.7608880	-0.8963710
C	0.7516000	-0.9047250	-1.3965860
C	1.4403540	-2.1430020	-1.3129320
H	1.1841280	-4.2813290	-1.0899060
C	-3.8277080	-1.4518590	-0.6347010
N	1.4007910	0.2774360	-1.5334700
C	2.8585550	-2.1106550	-1.3486370
C	-5.0438840	-0.8148220	-0.2597910
C	2.7127890	0.2667650	-1.5272810
C	3.5104140	-0.9160890	-1.4453050
H	3.4146080	-3.0416570	-1.2803750
C	-6.2359280	-1.5122460	-0.0369040
C	-4.9783220	0.5948100	-0.0560530
N	3.2833800	1.5366610	-1.6370370
H	4.5874860	-0.8389740	-1.4438120
C	-7.3742930	-0.8491580	0.3977860
H	-6.2471660	-2.5851900	-0.2021120
C	-6.1365480	1.2422240	0.4088380
N	-3.8188230	1.2732410	-0.3330800
C	4.5363340	1.9412740	-1.2289960
H	2.5808730	2.2598090	-1.7513090
C	-7.3077550	0.5277110	0.6238890
H	-8.2960810	-1.3934070	0.5700000
H	-6.1171950	2.3098080	0.5972470
C	-3.5353220	2.5881220	0.2018290
H	-3.0018240	0.6896510	-0.4858790
C	4.7144430	3.4430620	-1.2480070
O	5.4135240	1.1716820	-0.8793770
H	-8.1868400	1.0584580	0.9779810
H	-4.2952770	3.3008540	-0.1386100
H	-3.5660050	2.5831770	1.3034210
H	4.0594370	3.9047080	-0.5014340
H	4.4515170	3.8538310	-2.2267210
H	5.7516150	3.6791700	-1.0148230

C	-2.1703960	3.0850250	-0.2937030
H	-1.9962070	4.0609580	0.1780460
H	-2.2255690	3.2504060	-1.3744970
N	-1.0168660	2.2354950	-0.0401090
H	-0.9304560	1.4633720	-0.7021590
C	-0.8977940	1.7308240	1.3221700
H	-1.6706570	0.9882160	1.5883980
H	-1.0300190	2.5837300	2.0030460
C	-1.2780340	-1.9418570	-1.1113880
C	0.4693290	1.1237480	1.5262570
C	0.6361160	-0.2232870	1.7244110
C	1.6166660	1.9616140	1.4564330
C	1.9313150	-0.7999780	1.8307410
H	-0.2327250	-0.8791060	1.7667920
C	2.8778390	1.4425980	1.5801810
H	1.4721390	3.0270780	1.2941880
C	3.0735600	0.0445150	1.7528750
C	2.1200860	-2.1976000	1.9926620
H	3.7537210	2.0870230	1.5367590
C	4.3683040	-0.5330110	1.8331880
C	3.3831350	-2.7304760	2.0660110
H	1.2431130	-2.8391140	2.0414830
C	4.5200760	-1.8884730	1.9859920
H	5.2344700	0.1183060	1.7534190
H	3.5168200	-3.8016340	2.1855250
H	5.5135700	-2.3228390	2.0433280
78			
83			
5b complex			
C	-0.9706760	4.8122850	-0.1813870
N	0.0515970	2.6236480	-0.3318670
C	0.2565030	5.4192610	-0.1672940
H	-1.8933170	5.3781520	-0.1349090
C	-2.3187370	2.7703380	-0.2330190
C	1.2695590	3.2155950	-0.2825400
C	1.4216720	4.6231620	-0.2096300
H	0.3476290	6.5004910	-0.1129720
C	-3.4720050	2.3959500	-0.1511460
N	2.3333160	2.3742600	-0.2918600
C	2.7424190	5.1386820	-0.1744070
C	-4.8518390	2.0575630	-0.0208350
C	3.5515430	2.8838350	-0.2309320
C	3.8105530	4.2903610	-0.1867970
H	2.8919370	6.2138420	-0.1281560
C	-5.7401410	3.0385250	0.4471590
C	-5.3314810	0.7641110	-0.3579620
N	4.5605860	1.9388220	-0.1878110
H	4.8309920	4.6408230	-0.1554980
C	-7.0919750	2.7716850	0.5942280
H	-5.3388660	4.0167090	0.6944770
C	-6.7070840	0.5111770	-0.1982110
N	-4.4800550	-0.1863320	-0.8543230
C	5.9261340	2.1293030	-0.2263930
H	4.2345700	0.9646510	-0.0995510
C	-7.5635990	1.4989860	0.2664330
H	-7.7674380	3.5374560	0.9585170
H	-7.1043300	-0.4681960	-0.4380110
C	-4.8879950	-1.5636250	-1.0311000
H	-3.4879420	-0.0601670	-0.6809320

C	6.7001080	0.8364260	-0.1078360
O	6.4626390	3.2184770	-0.3375110
H	-8.6189280	1.2680150	0.3782350
H	-5.2564990	-1.9971420	-0.0875580
H	-5.7119440	-1.6181750	-1.7518300
H	6.5703930	0.4195920	0.8956270
H	7.7549840	1.0384650	-0.2879570
H	6.3266270	0.0932030	-0.8165350
N	1.5103880	-4.4510720	-1.2581830
C	2.7385490	-4.8272850	-0.7637110
H	3.0202090	-5.8718700	-0.7223310
N	3.4787080	-3.8211980	-0.3808940
C	2.6912730	-2.7166670	-0.6306070
C	2.9144770	-1.3288320	-0.3808930
O	3.9221380	-0.7920220	0.0941470
N	1.8057700	-0.5569230	-0.7387780
H	1.8877950	0.4514900	-0.5342870
C	0.6292240	-1.0355440	-1.2553250
N	-0.3289950	-0.1172040	-1.5407260
H	-0.2443460	0.7833570	-1.0603390
H	-1.2632660	-0.5209690	-1.5110840
N	0.4206420	-2.3117350	-1.5171720
C	1.4645420	-3.0923860	-1.1657080
C	-3.7178790	-2.3773760	-1.5710270
H	-3.4793670	-2.0336280	-2.5828380
H	-4.0349860	-3.4311640	-1.6335670
N	-2.5279060	-2.1969430	-0.7468410
H	-1.7150660	-2.6062460	-1.2117340
C	-2.6526180	-2.8078420	0.5836910
H	-3.1529990	-3.7883930	0.5239410
H	-3.2864820	-2.1675150	1.2106410
C	0.4474890	-5.3048420	-1.7509710
H	-0.5004320	-4.9797510	-1.3163420
H	0.3842820	-5.2535210	-2.8403360
H	0.6520110	-6.3314850	-1.4446550
C	-1.0253300	3.3926920	-0.2631220
C	-1.2939920	-2.9946090	1.2139870
C	-0.7631670	-4.2573310	1.3264850
C	-0.5250770	-1.8684900	1.6511540
C	0.5389030	-4.4731700	1.8433860
H	-1.3568010	-5.1120940	1.0098500
C	0.7862610	-2.0842850	2.1661480
C	-1.0205060	-0.5374940	1.5991380
C	1.2992080	-3.4086680	2.2461640
H	0.9295920	-5.4844410	1.9080710
C	1.5604580	-0.9709110	2.5890690
C	-0.2566920	0.5171300	2.0340410
H	-2.0144210	-0.3526630	1.2009260
H	2.3075010	-3.5555260	2.6247300
C	1.0545530	0.3027270	2.5213700
H	2.5681010	-1.1489250	2.9558390
H	-0.6573600	1.5244740	1.9892240
H	1.6557890	1.1496350	2.8378600
64			
5b			
C	0.9499570	3.5950370	0.0523230
N	0.5454880	1.3838410	-0.8586320
C	-0.3909180	3.8773000	0.0444320
H	1.6868590	4.3078130	0.4033800

C	2.7481230	1.9246780	-0.3490290
C	-0.7828500	1.6473010	-0.8425960
C	-1.3019150	2.8932570	-0.3985050
H	-0.7642730	4.8371990	0.3908330
C	3.8589320	1.4395520	-0.2833890
N	-1.5825890	0.6332680	-1.2481290
C	-2.7101540	3.0508290	-0.3930130
C	5.0182000	0.6143380	-0.2282470
C	-2.8843760	0.8044940	-1.1888990
C	-3.5166630	2.0174580	-0.7763660
H	-3.1391850	3.9936420	-0.0641460
C	6.2881280	1.1012760	0.0995690
C	4.8172290	-0.7750860	-0.4750830
N	-3.6067790	-0.3257360	-1.5659990
H	-4.5938450	2.0858220	-0.7681110
C	7.3719540	0.2412920	0.2016960
H	6.4050410	2.1652150	0.2813190
C	5.9236590	-1.6316200	-0.3445270
N	3.5773770	-1.2287500	-0.8478590
C	-4.9644010	-0.5449680	-1.5197680
H	-3.0059940	-1.1175800	-1.7672620
C	7.1741700	-1.1243630	-0.0165330
H	8.3542270	0.6234630	0.4561120
H	5.7995530	-2.6964670	-0.5087600
C	3.1704230	-2.6097380	-0.6920560
H	2.8266280	-0.5551570	-0.7305800
C	-5.3795150	-1.9295430	-1.9628430
O	-5.7764760	0.3045160	-1.1954860
H	8.0110640	-1.8110540	0.0713850
H	3.7758470	-3.2574370	-1.3365780
H	3.3215070	-2.9519370	0.3444460
H	-4.6045330	-2.6779170	-1.7861490
H	-5.6027910	-1.9036680	-3.0341920
H	-6.2892050	-2.2065310	-1.4289400
C	1.6983450	-2.7682040	-1.1017270
H	1.4124640	-3.8064660	-0.8865240
H	1.6128580	-2.6235060	-2.1833900
N	0.7401660	-1.8791970	-0.4660830
H	0.7156760	-0.9436010	-0.8738110
C	0.8357950	-1.7922720	0.9851410
H	1.8092610	-1.4097600	1.3385750
H	0.7357720	-2.8098460	1.3905540
C	1.3699070	2.3173920	-0.4055750
C	-0.2504400	-0.8945000	1.5282850
C	0.0812080	0.3136830	2.0926370
C	-1.6290650	-1.2650720	1.4246620
C	-0.9102260	1.2170900	2.5456820
H	1.1300600	0.5946230	2.1629490
C	-2.6267590	-0.3649170	1.8961270
C	-2.0450410	-2.5091500	0.8750360
C	-2.2361690	0.8883670	2.4413460
H	-0.6108170	2.1736790	2.9639130
C	-3.9961470	-0.7352780	1.8127430
C	-3.3751310	-2.8504270	0.8298450
H	-1.2949040	-3.1861280	0.4801870
H	-3.0088410	1.5756900	2.7769450
C	-4.3647140	-1.9550070	1.3041310
H	-4.7472640	-0.0329060	2.1661270
H	-3.6744760	-3.8132130	0.4249620

H	-5.4137940	-2.2332670	1.2545850
89			
6a complex			
C	1.0744340	-2.6740440	-1.0909680
C	0.7496450	-4.0591550	-1.0690550
N	0.1680560	-1.7141490	-1.1992390
C	-0.5668750	-4.4212010	-1.1657210
H	1.5437790	-4.7901900	-0.9765820
C	2.4620290	-2.3270560	-0.9598150
C	-1.1412650	-2.0622200	-1.2618880
C	-1.5544880	-3.4185620	-1.2612450
H	-0.8637660	-5.4665450	-1.1565150
C	3.6627420	-2.2373640	-0.7934470
N	-2.0290260	-1.0364860	-1.2946930
C	-2.9451620	-3.6832830	-1.3236500
C	5.0725010	-2.2325900	-0.5724490
C	-3.3221160	-1.3198750	-1.2999090
C	-3.8365130	-2.6527340	-1.3441910
H	-3.2903690	-4.7135520	-1.3314330
C	5.7687930	-3.4487260	-0.6500120
C	5.7580270	-1.0383220	-0.2247210
H	-4.9040790	-2.8068280	-1.3654850
C	7.1259830	-3.5158520	-0.3787490
H	5.2132400	-4.3418190	-0.9193950
C	7.1306950	-1.1312570	0.0709770
N	5.0913760	0.1580670	-0.2069380
C	7.7954550	-2.3463610	-0.0107220
H	7.6530780	-4.4612450	-0.4414750
H	7.6784810	-0.2416450	0.3601930
C	5.5827430	1.3030690	0.5326590
H	4.0766690	0.1102460	-0.2360030
H	8.8562860	-2.3801530	0.2195580
H	5.7322240	1.0548540	1.5957100
H	6.5531810	1.6230440	0.1391840
N	0.1771280	5.4989450	-0.4332440
C	-1.0560300	6.0597500	-0.1824410
H	-1.1429410	7.1053290	0.0839400
N	-2.0463960	5.2169090	-0.3030100
C	-1.4338530	4.0321070	-0.6579380
C	-1.9683790	2.7248560	-0.8702630
O	-3.1468180	2.3650480	-0.7801550
N	-0.9706190	1.8031700	-1.1994140
H	-1.2822540	0.8207210	-1.2722370
C	0.3769460	2.0642420	-1.2304510
N	1.1897630	1.0284160	-1.5272570
H	0.8134480	0.0820370	-1.3970280
H	2.1408060	1.1606400	-1.1877800
N	0.8865410	3.2678430	-1.0206840
C	-0.0565970	4.1902250	-0.7388730
C	4.5983620	2.4644450	0.3777520
H	4.7012560	2.8903190	-0.6248530
H	4.8672190	3.2439690	1.1088640
N	3.2197440	2.0097760	0.5097650
H	2.5852680	2.7454650	0.1922880
C	2.8494980	1.5905030	1.8642940
H	3.0578830	2.3814040	2.6054710
H	3.4608130	0.7223870	2.1374630
C	1.4819620	6.1299050	-0.3620030
H	2.0847330	5.6569350	0.4175690

H	1.9945040	6.0335230	-1.3209240
H	1.3462670	7.1853050	-0.1254070
C	1.3899910	1.2074660	1.9142240
C	0.9954620	-0.0991510	1.8521360
C	0.3942200	2.2375390	1.9852920
C	-0.3892010	-0.4642960	1.8752480
H	1.7386010	-0.8932770	1.7903970
C	-0.9356340	1.9367670	1.9675510
H	0.7173540	3.2755950	2.0450290
C	-0.8020980	-1.7985320	1.8938820
C	-1.3789060	0.5761230	1.9003790
H	-1.6840900	2.7248160	2.0098870
C	-2.1570380	-2.1415100	1.9274900
H	-0.0526810	-2.5893890	1.8821630
C	-2.7342680	0.2353880	1.8821890
C	-2.5923530	-3.5038980	1.9817570
C	-3.1468070	-1.1004310	1.9025820
H	-3.4814340	1.0271620	1.8638040
C	-3.9211070	-3.8135080	1.9926210
H	-1.8369780	-4.2860880	2.0083790
C	-4.5297220	-1.4689390	1.8906690
C	-4.9048950	-2.7806380	1.9344220
H	-4.2405260	-4.8505130	2.0322440
H	-5.2766830	-0.6790300	1.8507280
H	-5.9574780	-3.0464220	1.9224290
N	-4.1518730	-0.2153900	-1.2409190
C	-5.5279040	-0.1719640	-1.1481330
H	-3.6664980	0.6845050	-1.1151180
C	-6.0549460	1.2297860	-0.9385170
O	-6.2570740	-1.1466220	-1.2201880
H	-5.7038800	1.8970120	-1.7300810
H	-5.6797000	1.6319940	0.0074110
H	-7.1434420	1.1981060	-0.9260140
70			
6a			
C	0.7353770	-0.7197090	-1.2669000
C	0.7893550	0.5950960	-1.8143960
N	-0.3825250	-1.3880340	-1.0405350
C	-0.3896050	1.2228250	-2.1070370
H	1.7540170	1.0755890	-1.9413540
C	1.9760930	-1.3404200	-0.8915520
C	-1.5544120	-0.7636950	-1.3203580
C	-1.6077750	0.5508780	-1.8544070
H	-0.4072300	2.2331220	-2.5078550
C	3.0423660	-1.8049380	-0.5428350
N	-2.6781440	-1.4698210	-1.0363600
C	-2.8856990	1.1176060	-2.0847840
C	4.3390340	-2.2151150	-0.1129960
C	-3.8437380	-0.8985380	-1.2420290
C	-4.0145790	0.4102730	-1.7847210
H	-2.9556120	2.1210950	-2.4967140
C	4.5761830	-3.4986970	0.3931180
C	5.3903870	-1.2574270	-0.1594640
H	-5.0077300	0.8063340	-1.9331640
C	5.8303200	-3.8546700	0.8692380
H	3.7530620	-4.2063340	0.4159660
C	6.6473080	-1.6293240	0.3460490
N	5.1557230	-0.0222040	-0.7054920
C	6.8567850	-2.9079480	0.8467630

H	6.0050170	-4.8501520	1.2620940
H	7.4615060	-0.9120950	0.3338460
C	5.9416880	1.1424910	-0.3557030
H	4.1767260	0.2123470	-0.8574730
H	7.8403440	-3.1693890	1.2263760
H	6.0610760	1.2280660	0.7362300
H	6.9491040	1.0807950	-0.7832080
C	5.2447440	2.3829840	-0.9252920
H	5.3925080	2.4099720	-2.0088420
H	5.7174760	3.2792730	-0.4933390
N	3.8041470	2.3219430	-0.6860080
H	3.3402800	3.0398440	-1.2387510
C	3.4345670	2.4814410	0.7238510
H	3.8336520	3.4195430	1.1471080
H	3.8814240	1.6537070	1.2858990
C	1.9354540	2.4326690	0.8756070
C	1.3025110	1.3121020	1.3347240
C	1.1533080	3.5596400	0.4642400
C	-0.1246680	1.2352040	1.4035320
H	1.8824770	0.4402580	1.6324050
C	-0.2095470	3.5296710	0.5151750
H	1.6643010	4.4542290	0.1136250
C	-0.7808330	0.0804920	1.8372260
C	-0.9006620	2.3681100	0.9855550
H	-0.7948060	4.3914180	0.2040840
C	-2.1757240	0.0063410	1.8755220
H	-0.1920770	-0.7858290	2.1321410
C	-2.2951030	2.2955720	1.0255310
C	-2.8594740	-1.1760900	2.3043800
C	-2.9515490	1.1408450	1.4601290
H	-2.8834960	3.1523310	0.7021880
C	-4.2228460	-1.2216560	2.3382410
H	-2.2656880	-2.0354810	2.6042040
C	-4.3796610	1.0460250	1.4934480
C	-4.9945800	-0.0917030	1.9283930
H	-4.7305960	-2.1210470	2.6754200
H	-4.9641530	1.9023290	1.1664440
H	-6.0795550	-0.1462820	1.9523080
N	-4.9286300	-1.7091180	-0.8994210
C	-6.2512370	-1.3635420	-0.7421800
H	-4.6345670	-2.6108000	-0.5402580
C	-7.0928860	-2.4672920	-0.1410680
O	-6.7075210	-0.2730520	-1.0393380
H	-6.9204080	-3.4212540	-0.6460900
H	-8.1436370	-2.1916480	-0.2196520
H	-6.8326530	-2.5918810	0.9157780
89			
6b complex			
C	-0.7802070	-3.4215330	-0.7057190
C	-0.5041470	-4.7930980	-0.4513890
N	0.1593950	-2.5053590	-0.8868830
C	0.8041650	-5.1888550	-0.3710580
H	-1.3253940	-5.4879190	-0.3228290
C	-2.1492350	-2.9941940	-0.7269850
C	1.4552570	-2.8842890	-0.7865460
C	1.8272100	-4.2292370	-0.5290980
H	1.0658560	-6.2250010	-0.1742370
C	-3.3281420	-2.7097660	-0.6600370
N	2.3701150	-1.8935630	-0.9203860

C	3.2099880	-4.5175590	-0.4167530
C	-4.7052430	-2.3688300	-0.5280800
C	3.6498130	-2.1898960	-0.7723740
C	4.1283630	-3.5154550	-0.5291380
H	3.5270920	-5.5395910	-0.2273520
C	-5.6084860	-3.3144950	-0.0182400
C	-5.1445980	-1.0569790	-0.8517390
H	5.1898990	-3.6869630	-0.4353180
C	-6.9355340	-2.9865250	0.2053600
H	-5.2363950	-4.3083270	0.2113610
C	-6.4908950	-0.7355560	-0.5886530
N	-4.2813510	-0.1630400	-1.4269850
C	-7.3611540	-1.6854860	-0.0755010
H	-7.6253240	-3.7217450	0.6039890
H	-6.8589610	0.2626960	-0.7967560
C	-4.5120160	1.2684600	-1.4194570
H	-3.3213200	-0.4671080	-1.5364410
H	-8.3939560	-1.4040730	0.1081420
H	-3.7708270	1.7182100	-2.0891550
H	-5.4937110	1.4852220	-1.8522640
N	0.2824660	4.7696170	-1.2848760
C	1.5526440	5.2991590	-1.2447080
H	1.7036140	6.3708870	-1.2210560
N	2.4962800	4.3955350	-1.2434250
C	1.8097930	3.2006230	-1.2824100
C	2.2760330	1.8533220	-1.2419140
O	3.4475870	1.4638380	-1.2082660
N	1.2173130	0.9366250	-1.2285130
H	1.4991380	-0.0506830	-1.1246540
C	-0.1167260	1.2623620	-1.2133300
N	-1.0149120	0.2403120	-1.1299550
H	-1.8084660	0.5088120	-0.5349190
H	-0.6144120	-0.6790360	-0.9225340
N	-0.5552310	2.5032160	-1.2887300
C	0.4382150	3.4158960	-1.2952230
C	-4.3909920	1.9026210	-0.0307010
H	-4.9655000	1.3118920	0.6943470
H	-4.8311690	2.9142660	-0.0476850
N	-2.9914210	1.9155570	0.3753780
H	-2.4611240	2.4891960	-0.2856920
C	-2.7680200	2.4676210	1.7160800
H	-3.1038950	1.7319400	2.4580210
H	-3.3605900	3.3819900	1.8823110
C	-0.9801110	5.4832880	-1.2888340
H	-1.3654670	5.5870370	-2.3057910
H	-1.6983090	4.9267310	-0.6835060
H	-0.8304720	6.4714620	-0.8515040
C	-1.3054370	2.8045950	1.8887660
C	-0.3096210	1.7614660	1.9623380
C	-0.9054990	4.1118570	1.8955910
C	-0.6444990	0.4058500	2.0242090
C	1.0811830	2.1297300	1.9885760
C	0.4740730	4.4789000	1.9306820
H	-1.6574810	4.8968800	1.8557660
C	0.3319210	-0.5893750	2.1423020
H	-1.6889570	0.1054130	1.9858370
C	2.0581610	1.1332060	2.0674880
C	1.4379730	3.5170080	1.9554450
H	0.7455060	5.5304460	1.9174930

C	-0.0134450	-1.9719250	2.2782860
C	1.7183890	-0.2194170	2.1604480
H	3.1076950	1.4213090	2.0756540
H	2.4923860	3.7808420	1.9507690
C	0.9533910	-2.9201060	2.4423090
H	-1.0654090	-2.2476360	2.2516030
C	2.7040790	-1.2466350	2.3122410
C	2.3342020	-2.5522300	2.4561800
H	0.6795870	-3.9657580	2.5492760
H	3.7535060	-0.9612770	2.3152790
H	3.0897130	-3.3226360	2.5771870
N	4.4978680	-1.1014220	-0.8639270
C	5.8676190	-1.0537700	-0.7190540
H	4.0189440	-0.2029850	-1.0221900
C	6.4279630	0.3395430	-0.8935600
O	6.5692000	-2.0249420	-0.4893710
H	5.8444690	1.0716500	-0.3305350
H	6.3755390	0.6240110	-1.9492850
H	7.4676750	0.3445660	-0.5689130
70			
6b			
C	2.3126300	2.3763930	-0.3136640
C	2.1031180	3.6906270	0.1826050
N	1.3517310	1.6083250	-0.8072480
C	0.8261720	4.1888850	0.1781130
H	2.9434050	4.2614660	0.5600030
C	3.6035070	1.7548120	-0.2514470
C	0.0851410	2.0873790	-0.7926770
C	-0.2291140	3.3827420	-0.3021090
H	0.6117470	5.1851610	0.5554800
C	4.6114690	1.0818500	-0.1831020
N	-0.8637670	1.2349800	-1.2459330
C	-1.5947800	3.7639840	-0.2902380
C	5.6099120	0.0680880	-0.1335460
C	-2.1216750	1.6110910	-1.1851000
C	-2.5543300	2.8894080	-0.7136790
H	-1.8693030	4.7501900	0.0747860
C	6.9340590	0.3182070	0.2426890
C	5.1818630	-1.2567700	-0.4396020
H	-3.6067120	3.1305070	-0.7024280
C	7.8522250	-0.7177810	0.3344100
H	7.2243300	1.3393770	0.4699320
C	6.1226130	-2.2942820	-0.3196620
N	3.8938290	-1.4777100	-0.8558560
C	7.4311200	-2.0204160	0.0565710
H	8.8775300	-0.5187960	0.6256780
H	5.8245110	-3.3158010	-0.5289550
C	3.2582770	-2.7765630	-0.7847620
H	3.2633200	-0.6923500	-0.7265780
H	8.1365070	-2.8425060	0.1361390
H	3.7729160	-3.4852020	-1.4442370
H	3.3105270	-3.1879680	0.2361570
C	1.7972790	-2.6688040	-1.2468870
H	1.3372430	-3.6550090	-1.0997580
H	1.7793120	-2.4570930	-2.3207220
N	0.9722590	-1.6671460	-0.5914440
H	1.1189310	-0.7213490	-0.9465790
C	1.0330630	-1.6667110	0.8647330
H	2.0402160	-1.4487450	1.2609090

H	0.7728370	-2.6769610	1.2130280
C	0.0734500	-0.6462960	1.4262510
C	-1.3517830	-0.8156400	1.2738700
C	0.5528160	0.4705350	2.0494710
C	-1.9123490	-1.9513520	0.6839310
C	-2.2292990	0.2130200	1.7643410
C	-0.3162360	1.5005770	2.5194540
H	1.6276840	0.5964690	2.1610750
C	-3.2988520	-2.1224620	0.5925290
H	-1.2615780	-2.7226870	0.2823320
C	-3.6115820	0.0603060	1.6384090
C	-1.6647660	1.3817280	2.3699620
H	0.1114600	2.3849070	2.9825400
C	-3.8800430	-3.3074660	0.0374670
C	-4.1713240	-1.0909220	1.0768240
H	-4.2689480	0.8512030	1.9945370
H	-2.3379760	2.1636290	2.7119220
C	-5.2359910	-3.4579370	-0.0281110
H	-3.2156880	-4.0884490	-0.3236970
C	-5.5862620	-1.2765210	0.9694830
C	-6.1023730	-2.4252360	0.4425010
H	-5.6646680	-4.3645070	-0.4439210
H	-6.2396910	-0.4823410	1.3213990
H	-7.1774310	-2.5589620	0.3715170
N	-3.0103270	0.6433450	-1.6450290
C	-4.3893570	0.6489800	-1.6523490
H	-2.5410380	-0.2031490	-1.9491960
C	-4.9861000	-0.5802520	-2.2956450
O	-5.0615010	1.5655150	-1.2131020
H	-6.0625800	-0.5757810	-2.1309500
H	-4.5568830	-1.4938950	-1.8726030
H	-4.7790340	-0.5672580	-3.3706250
89			
6c complex			
C	-1.7548260	3.0546510	-0.4427530
C	-1.8106860	4.4383250	-0.1234930
N	-0.6257670	2.4144710	-0.7025710
C	-0.6348870	5.1407190	-0.0602870
H	-2.7703260	4.9038610	0.0672130
C	-2.9720170	2.2908550	-0.5005900
C	0.5400730	3.0950820	-0.6314860
C	0.5854730	4.4731700	-0.3020890
H	-0.6269530	6.1982610	0.1894170
C	-4.0181190	1.6820550	-0.5978120
N	1.6587340	2.3662950	-0.8697680
C	1.8648650	5.0754120	-0.1990050
C	-5.2611260	1.0104240	-0.8151600
C	2.8363630	2.9510930	-0.7451470
C	2.9916940	4.3319690	-0.4026160
H	1.9385880	6.1294260	0.0542340
C	-6.2719360	1.6791470	-1.5222180
C	-5.4562720	-0.3290280	-0.3845400
H	3.9830340	4.7500730	-0.3183800
C	-7.4621660	1.0461770	-1.8440090
H	-6.0898980	2.7045870	-1.8290400
C	-6.6580450	-0.9639300	-0.7501500
N	-4.5156470	-0.9552490	0.3948030
C	-7.6368570	-0.2847080	-1.4610570
H	-8.2337480	1.5719630	-2.3950520

H	-6.8297230	-1.9964110	-0.4700980
C	-4.4576990	-2.3978920	0.5438400
H	-3.6209750	-0.4860650	0.4876950
H	-8.5532850	-0.8071260	-1.7192630
H	-5.4292080	-2.7710020	0.8816660
H	-4.2268270	-2.8935650	-0.4125740
N	1.2567130	-4.5473530	-1.4471820
C	2.5872930	-4.7469480	-1.7402680
H	2.9899560	-5.7482000	-1.8269540
N	3.2574350	-3.6384300	-1.9060630
C	2.3188440	-2.6490030	-1.7040430
C	2.4467570	-1.2281630	-1.6776760
O	3.4658860	-0.5475580	-1.8423930
N	1.2219930	-0.6072750	-1.4179070
H	1.2697110	0.4150420	-1.2948320
C	0.0339120	-1.2495260	-1.1658370
N	-1.0486290	-0.4649000	-0.9704490
H	-1.7371290	-0.8875970	-0.3516360
H	-0.8781030	0.5338320	-0.8175940
N	-0.0899140	-2.5653170	-1.1483110
C	1.0743760	-3.1964690	-1.4108180
C	-3.4248670	-2.7626850	1.6003960
H	-3.4235600	-3.8530000	1.7494360
H	-3.7293370	-2.3028000	2.5482760
N	-2.1123320	-2.2272580	1.2497910
H	-1.7008440	-2.7743380	0.4881950
C	-1.1758840	-2.2459630	2.3814420
H	-0.8970320	-3.2675020	2.6659200
H	-1.7074180	-1.8371960	3.2477330
C	0.2508460	-5.5455350	-1.1439220
H	0.0061290	-5.5258630	-0.0781400
H	-0.6519010	-5.3445330	-1.7232540
H	0.6411180	-6.5287590	-1.4082430
C	0.0478280	-1.3908540	2.1280010
C	-0.0929690	0.0114820	2.2136860
C	1.3090000	-1.9555780	1.8516800
C	-1.3567740	0.6460480	2.4623830
C	1.0586470	0.8569740	2.0781960
C	2.4473600	-1.0937750	1.6556270
C	1.5345480	-3.3709130	1.7497260
C	-1.4456780	1.9956200	2.6509160
H	-2.2598040	0.0451670	2.4962410
C	0.9251910	2.2661300	2.2903960
C	2.2963450	0.2867760	1.7755810
C	3.7265880	-1.6670890	1.3599190
H	0.7049090	-4.0573960	1.8789330
C	2.7729010	-3.8785030	1.4841470
C	-0.2839350	2.8199000	2.5900720
H	-2.4137940	2.4521900	2.8364980
H	1.8170840	2.8851170	2.2067310
H	3.1647480	0.9323140	1.6518650
C	3.8909370	-3.0165120	1.2820580
H	4.5622710	-0.9909900	1.1965750
H	2.9099650	-4.9537640	1.4113120
H	-0.3745340	3.8889960	2.7571700
H	4.8620930	-3.4426930	1.0522060
N	3.9145480	2.1126020	-0.9820710
C	5.2576610	2.3770180	-0.8234090
H	3.6566160	1.1636270	-1.2891920

C	6.1567680	1.2198790	-1.1960560
O	5.7030540	3.4427970	-0.4298800
H	6.6790070	1.4765380	-2.1226650
H	5.6111530	0.2865470	-1.3419150
H	6.9094080	1.1012380	-0.4139770
70			
6c			
C	1.7282060	2.1788120	-1.0841180
C	1.4007620	3.5449570	-0.8808710
N	0.8324860	1.2234140	-1.2906470
C	0.0763120	3.8903080	-0.8207300
H	2.1923830	4.2718290	-0.7419230
C	3.0772780	1.7103910	-0.9620770
C	-0.4786210	1.5621000	-1.2433050
C	-0.9074510	2.8893430	-0.9791450
H	-0.2281080	4.9166600	-0.6332840
C	4.1291680	1.1453060	-0.7416740
N	-1.3513840	0.5449560	-1.4416050
C	-2.3035870	3.1151840	-0.8718960
C	5.1727570	0.2264590	-0.4420780
C	-2.6377280	0.7942150	-1.3405230
C	-3.1806110	2.0811790	-1.0343830
H	-2.6653830	4.1159330	-0.6515730
C	6.5095600	0.6028410	-0.2763840
C	4.7772960	-1.1350640	-0.2799010
H	-4.2495250	2.2060870	-0.9485630
C	7.4763620	-0.3366000	0.0510240
H	6.7729550	1.6477730	-0.4087230
C	5.7715930	-2.0693080	0.0652380
N	3.4693200	-1.4891530	-0.4428880
C	7.0914140	-1.6687450	0.2230510
H	8.5114110	-0.0395590	0.1770260
H	5.5024320	-3.1084500	0.2189730
C	2.9915290	-2.8530150	-0.4481030
H	2.8321050	-0.7723080	-0.7732780
H	7.8355330	-2.4141370	0.4890640
H	3.6748040	-3.4970820	-1.0182500
H	2.9537640	-3.2510050	0.5763020
C	1.6050190	-2.9368810	-1.1042290
H	1.2615130	-3.9743500	-0.9939950
H	1.7086090	-2.7413620	-2.1767890
N	0.5735920	-2.0484850	-0.5962530
H	0.6474280	-1.0973630	-0.9597630
C	0.4441500	-2.0283910	0.8555910
H	1.3665340	-1.7256640	1.3714710
H	0.2464940	-3.0552200	1.1901700
C	-0.7016580	-1.1335910	1.2733540
C	-2.0232640	-1.6078400	1.1544000
C	-0.4664190	0.1738900	1.7430280
C	-2.3289270	-2.8934060	0.5947660
C	-3.1223920	-0.7924090	1.5878940
C	-1.5754810	0.9932120	2.1551430
C	0.8414950	0.7643030	1.7918790
C	-3.6158810	-3.3452160	0.5228900
H	-1.5228150	-3.5024890	0.2006280
C	-4.4570940	-1.3024650	1.5000590
C	-2.8730390	0.4888350	2.0781490
C	-1.3354850	2.3226560	2.6297140
H	1.6978680	0.2070340	1.4230480

C	1.0285600	2.0415320	2.2347680
C	-4.6996890	-2.5452040	0.9949730
H	-3.8226810	-4.3221870	0.0954220
H	-5.2730840	-0.6693400	1.8392000
H	-3.7075140	1.1100640	2.3976020
C	-0.0732470	2.8334740	2.6755990
H	-2.1909010	2.9156570	2.9434250
H	2.0277650	2.4680650	2.2361720
H	-5.7144200	-2.9267000	0.9327380
H	0.1002620	3.8445720	3.0312790
N	-3.4391440	-0.3191940	-1.5911720
C	-4.8114890	-0.4140330	-1.6344490
H	-2.8959970	-1.1578520	-1.7663900
C	-5.3243060	-1.7459880	-2.1331550
O	-5.5605120	0.5065670	-1.3541110
H	-4.6138380	-2.5598100	-1.9767490
H	-5.5264000	-1.6547390	-3.2053200
H	-6.2617500	-1.9724090	-1.6240790
95			
7a complex			
C	1.0557430	-2.2510190	-1.3488360
C	0.9534400	-3.6653410	-1.4479330
N	0.0065320	-1.4414310	-1.3500370
C	-0.2912240	-4.2227910	-1.5601590
H	1.8551420	-4.2652990	-1.4265220
C	2.3778890	-1.7013700	-1.2313500
C	-1.2308390	-1.9857620	-1.4412800
C	-1.4268410	-3.3852400	-1.5617630
H	-0.4195800	-5.2989430	-1.6409440
C	3.5604940	-1.4477160	-1.1091500
N	-2.2686770	-1.1109090	-1.4013490
C	-2.7593750	-3.8541610	-1.6806290
C	4.9699190	-1.2904760	-0.9406730
C	-3.4998140	-1.5848470	-1.4669590
C	-3.7991110	-2.9737860	-1.6395560
H	-2.9397350	-4.9191460	-1.7997660
C	5.7627690	-2.4484870	-0.8892350
C	5.5726460	-0.0114080	-0.8063390
N	-4.4929020	-0.6234190	-1.3752980
H	-4.8287010	-3.2882500	-1.7135440
C	7.1345150	-2.3737160	-0.7064580
H	5.2702910	-3.4107900	-0.9930670
C	6.9655510	0.0437900	-0.6138290
N	4.8142960	1.1270780	-0.8860710
C	-5.8344920	-0.8167310	-1.1195120
H	-4.1426400	0.3295580	-1.2101680
C	7.7258740	-1.1160800	-0.5690340
H	7.7338600	-3.2764550	-0.6699300
H	7.4516370	1.0063110	-0.5027570
C	5.3083470	2.4011460	-0.4030390
H	3.8122290	1.0132190	-0.7621030
C	-6.5948800	0.4773430	-0.9388620
O	-6.3726890	-1.9102550	-1.0626260
H	8.7988360	-1.0354200	-0.4214280
H	5.7124390	2.3049830	0.6170720
H	6.1293750	2.7565890	-1.0359780
H	-6.7671140	0.9326260	-1.9197470
H	-6.0274170	1.1924050	-0.3384800
H	-7.5564600	0.2586030	-0.4753870

N	-0.9993590	5.6090910	-0.0596450
C	-2.2974450	5.9544280	0.2494570
H	-2.5399540	6.9603260	0.5677200
N	-3.1445320	4.9704460	0.1163180
C	-2.3632290	3.9114910	-0.3015700
C	-2.7017080	2.5608290	-0.6217130
O	-3.8182460	2.0308470	-0.6021050
N	-1.5752380	1.8185280	-0.9847580
H	-1.7445310	0.8128500	-1.1488390
C	-0.2855000	2.2934180	-1.0411060
N	0.6684730	1.4147170	-1.3972250
H	0.4461480	0.4145460	-1.3436790
H	1.6111490	1.6930310	-1.1267540
N	0.0323060	3.5549700	-0.7938990
C	-1.0312420	4.2932460	-0.4180950
C	4.1816290	3.4364110	-0.4459690
H	4.0067380	3.7359270	-1.4836110
H	4.5084450	4.3264020	0.1138540
N	2.9342320	2.8672600	0.0508750
H	2.1462380	3.4782030	-0.1756610
C	2.9193890	2.5769870	1.4900180
H	2.9268970	3.4960380	2.0971230
H	3.8267640	2.0154550	1.7371970
C	0.1852720	6.4455210	-0.0155280
H	0.9272130	6.0052830	0.6553500
H	0.6162500	6.5425960	-1.0140280
H	-0.0979050	7.4306270	0.3555990
C	1.7075060	1.7338150	1.7969510
C	0.4650590	2.3299010	2.0513570
C	1.7785480	0.3541890	1.7076150
H	0.3944900	3.4096120	2.1628320
C	-0.6763330	1.5563170	2.1115980
C	0.6375550	-0.4626180	1.8246550
H	2.7485720	-0.0941210	1.5115730
C	-0.6255530	0.1571270	1.9521400
H	-1.6258790	2.0534010	2.2759620
C	0.7354190	-1.9269500	1.8340120
C	-1.8471600	-0.6521770	1.8927920
C	-0.4394920	-2.7122090	1.8343450
C	1.9855210	-2.5757600	1.8730660
C	-1.7566010	-2.0606850	1.8123530
C	-3.1198900	-0.0493410	1.8596940
C	-0.3130790	-4.1153300	1.8644790
C	2.0857570	-3.9533950	1.8941270
H	2.8981810	-1.9916940	1.8949420
C	-2.9452490	-2.8068080	1.6955560
C	-4.2728650	-0.8048710	1.7689190
H	-3.2164770	1.0297600	1.8717680
C	0.9231910	-4.7314490	1.8896530
H	-1.1985250	-4.7398500	1.8799810
H	3.0635270	-4.4243910	1.9260750
C	-4.1861410	-2.1976830	1.6818020
H	-2.9027240	-3.8847720	1.5921850
H	-5.2413780	-0.3125370	1.7437940
H	0.9872500	-5.8149570	1.9145990
H	-5.0849370	-2.7972750	1.5741750
76			
7a			
C	1.0805410	-1.0273020	-1.2895860

C	0.9936490	0.3159770	-1.7560850
N	0.0387620	-1.8184010	-1.0951290
C	-0.2446650	0.8338710	-2.0118140
H	1.9025340	0.9004220	-1.8532840
C	2.3895690	-1.5208680	-0.9602910
C	-1.1931630	-1.3033860	-1.3390620
C	-1.3851600	0.0256600	-1.8039800
H	-0.3720060	1.8616160	-2.3445320
C	3.5210380	-1.8277410	-0.6443620
N	-2.2384940	-2.1296540	-1.0782630
C	-2.7133100	0.4713430	-2.0108050
C	4.8704740	-2.0469300	-0.2372370
C	-3.4552000	-1.6622930	-1.2435380
C	-3.7614280	-0.3605170	-1.7384060
H	-2.8854540	1.4867010	-2.3614840
C	5.3234600	-3.3112810	0.1579920
C	5.7473960	-0.9252070	-0.1960950
N	-4.4604380	-2.5784610	-0.9159890
H	-4.7906970	-0.0554560	-1.8552070
C	6.6250700	-3.4949970	0.6033770
H	4.6294690	-4.1452150	0.1159650
C	7.0558000	-1.1282100	0.2757300
N	5.3050450	0.2954810	-0.6328980
C	-5.7702970	-2.3175130	-0.5821380
H	-4.0881480	-3.4878310	-0.6645900
C	7.4804030	-2.3927540	0.6627580
H	6.9672280	-4.4775570	0.9085740
H	7.7409190	-0.2890770	0.3319970
C	5.9424870	1.5420360	-0.2678630
H	4.2969780	0.3993980	-0.7288350
C	-6.5125520	-3.5316310	-0.0688840
O	-6.2887690	-1.2188160	-0.6861170
H	8.4983480	-2.5182940	1.0202280
H	6.0306710	1.6434840	0.8261580
H	6.9583040	1.5940420	-0.6756200
H	-6.4540350	-4.3534270	-0.7878930
H	-7.5544610	-3.2627920	0.0989380
H	-6.0694930	-3.8746370	0.8716520
C	5.1227860	2.6924800	-0.8640900
H	5.2688380	2.6976000	-1.9480040
H	5.5020070	3.6464090	-0.4668810
N	3.6973370	2.4860780	-0.6197620
H	3.1474040	3.0076480	-1.2972680
C	3.2491010	2.8287290	0.7339850
H	3.1361220	3.9145920	0.8728910
H	4.0194190	2.4919790	1.4362290
C	1.9569630	2.1096500	1.0343010
C	1.9910470	0.7829300	1.4858050
C	0.7292990	2.6928530	0.7820610
H	2.9491650	0.2985140	1.6620840
C	0.8189170	0.0890100	1.6992760
C	-0.4824790	1.9921790	0.9518420
H	0.7208880	3.7215750	0.4360620
C	-0.4400720	0.6696330	1.4444170
H	0.8892460	-0.9345190	2.0473980
C	-1.7698870	2.5865330	0.5718160
C	-1.6876930	-0.0667550	1.6853980
C	-2.9704320	1.8757260	0.7946330
C	-1.8364990	3.8420420	-0.0672860

C	-2.9311170	0.5388040	1.3973460
C	-1.6790100	-1.3745950	2.2103500
C	-4.1862310	2.4522120	0.3736180
C	-3.0391650	4.3895830	-0.4676400
H	-0.9288940	4.3970280	-0.2719370
C	-4.1145220	-0.1788680	1.6666850
C	-2.8497540	-2.0619270	2.4622870
H	-0.7394400	-1.8678130	2.4267720
C	-4.2284110	3.6863710	-0.2435020
H	-5.1174250	1.9143660	0.5050680
H	-3.0569880	5.3558190	-0.9620400
C	-4.0810380	-1.4539670	2.1951430
H	-5.0820500	0.2600050	1.4573870
H	-2.8086250	-3.0675750	2.8689850
H	-5.1796760	4.0998080	-0.5634560
H	-5.0109700	-1.9768720	2.4009160
91			
8a complex			
C	1.1640510	-4.1541500	-0.9116400
N	0.2729030	-1.9172490	-1.1398130
C	-0.0910350	-4.6950600	-0.9850900
H	2.0503850	-4.7668800	-0.7969010
C	2.6280260	-2.2051440	-0.8738090
C	-0.9756670	-2.4405120	-1.1858140
C	-1.2053590	-3.8393600	-1.1173340
H	-0.2439620	-5.7696490	-0.9328870
C	3.8093280	-1.9509780	-0.7381930
N	-1.9920320	-1.5451160	-1.2819930
C	-2.5481460	-4.2897190	-1.1784790
C	5.2167840	-1.7816690	-0.5650050
C	-3.2347630	-1.9955800	-1.2824890
C	-3.5665640	-3.3880650	-1.2578080
H	-2.7531060	-5.3564650	-1.1514280
C	6.0186030	-2.9328460	-0.4996120
C	5.8081700	-0.4963220	-0.4368730
N	-4.2063060	-1.0121670	-1.3320780
H	-4.6036630	-3.6854740	-1.2863120
C	7.3874760	-2.8464990	-0.3035570
H	5.5354270	-3.8997160	-0.6030660
C	7.1981370	-0.4300280	-0.2245290
N	5.0450620	0.6359750	-0.5423260
C	-5.5533630	-1.1353260	-1.0615320
H	-3.8454980	-0.0487420	-1.3776250
C	7.9666930	-1.5832920	-0.1636790
H	7.9935430	-3.7442400	-0.2567930
H	7.6760570	0.5360680	-0.1102050
C	5.5206070	1.9224970	-0.0751140
H	4.0404560	0.5195850	-0.4489170
C	-6.2761180	0.1922670	-1.0571680
O	-6.1199180	-2.1959940	-0.8565210
H	9.0368290	-1.4930830	-0.0017450
H	5.8589900	1.8627650	0.9714600
H	6.3824140	2.2467400	-0.6686530
H	-5.7242240	0.9358000	-0.4761590
H	-7.2758600	0.0467720	-0.6494300
H	-6.3519160	0.5732680	-2.0806490
N	-0.7054780	5.2709730	-0.6791660
C	-2.0207400	5.6807740	-0.6425090
H	-2.2705180	6.7174910	-0.4563460

N	-2.8734570	4.7135110	-0.8474340
C	-2.0783580	3.6005030	-1.0326220
C	-2.4176260	2.2288090	-1.2417020
O	-3.5430560	1.7322060	-1.3511480
N	-1.2787990	1.4217340	-1.3102610
H	-1.4577880	0.4070080	-1.3622470
C	0.0221080	1.8557680	-1.1990110
N	0.9820210	0.9217600	-1.3080450
H	0.7209980	-0.0654580	-1.2119800
H	1.8899850	1.2035380	-0.9385470
N	0.3479850	3.1277380	-1.0265690
C	-0.7318400	3.9297230	-0.9280120
C	4.4121000	2.9662670	-0.2307490
H	4.3081440	3.2240290	-1.2888810
H	4.7137940	3.8750590	0.3128460
N	3.1267400	2.4349720	0.2070190
H	2.3663670	3.0404380	-0.1119630
C	3.0024080	2.2254540	1.6541960
H	3.0102440	3.1753590	2.2117590
H	3.8632130	1.6387630	1.9933340
C	0.4879120	6.0739030	-0.4905500
H	1.0748820	5.6802770	0.3429830
H	1.0976990	6.0616210	-1.3962130
H	0.1873940	7.0980840	-0.2688050
C	1.2995380	-2.7401510	-0.9895340
C	1.7311780	1.4533270	1.9080450
C	0.5100270	2.1211160	1.9650150
C	1.7565060	0.0583090	1.9389120
C	-0.6995720	1.4185060	1.9918670
H	0.4889020	3.2097740	1.9452460
C	0.5747760	-0.6861930	2.0038210
H	2.7110790	-0.4649730	1.8991810
C	-0.6713940	-0.0023990	1.9963800
C	-1.9755770	2.0883090	1.9742570
C	0.5742090	-2.1268640	2.0718930
C	-1.8931260	-0.7405400	1.9986920
C	-3.1349550	1.3862660	1.9371080
H	-1.9873250	3.1756960	1.9645690
C	-0.5854030	-2.8275380	2.0964040
H	1.5331740	-2.6397200	2.0909900
C	-3.1370270	-0.0548750	1.9525420
C	-1.8640550	-2.1615650	2.0447380
H	-4.0906980	1.9024910	1.8944830
H	-0.5739360	-3.9140260	2.1388190
C	-4.3232650	-0.8001430	1.9354010
C	-3.0723170	-2.8656910	2.0255800
C	-4.2892320	-2.1903850	1.9643040
H	-5.2770520	-0.2782180	1.8979030
H	-3.0523600	-3.9523980	2.0482810
H	-5.2175820	-2.7516180	1.9294490
72			
8a			
C	0.8662860	0.1844000	-1.8470160
N	-0.1392230	-1.8171990	-0.9035060
C	-0.3601850	0.6979470	-2.1640900
H	1.7893630	0.7256790	-2.0264460
C	2.2111400	-1.5687020	-0.7938120
C	-1.3592300	-1.3018320	-1.1990620
C	-1.5198590	-0.0414860	-1.8350030

H	-0.4619200	1.6710320	-2.6380430
C	3.3194910	-1.8906830	-0.4167790
N	-2.4231500	-2.0537160	-0.8188780
C	-2.8392160	0.4157560	-2.0692650
C	4.6548670	-2.1110220	0.0333800
C	-3.6304190	-1.5773130	-1.0269940
C	-3.9079740	-0.3368090	-1.6716450
H	-2.9892790	1.3800710	-2.5483090
C	5.0482230	-3.3174820	0.6242960
C	5.5803370	-1.0359140	-0.0866940
N	-4.6455930	-2.4095510	-0.5453540
H	-4.9293750	-0.0173020	-1.8115590
C	6.3378210	-3.4842580	1.1100600
H	4.3182250	-4.1171500	0.7042140
C	6.8755870	-1.2174470	0.4268960
N	5.1922420	0.1213460	-0.7085330
C	-5.9933930	-2.1613090	-0.4239760
H	-4.2823940	-3.2523710	-0.1146150
C	7.2409610	-2.4237090	1.0106130
H	6.6347810	-4.4214310	1.5677100
H	7.5957640	-0.4089150	0.3579610
C	5.8568290	1.3879470	-0.4890090
H	4.1897420	0.2370950	-0.8423190
C	-6.7382400	-3.2339350	0.3399630
O	-6.5429300	-1.1663760	-0.8642150
H	8.2498470	-2.5368140	1.3966960
H	5.9813150	1.5928030	0.5864300
H	6.8600860	1.3870700	-0.9308590
H	-6.4234940	-4.2371240	0.0419380
H	-7.8062020	-3.1132460	0.1626450
H	-6.5398240	-3.1177210	1.4107010
C	5.0285530	2.4872150	-1.1647760
H	5.1608000	2.4139380	-2.2480650
H	5.4110920	3.4674570	-0.8396280
N	3.6044570	2.3053570	-0.8900290
H	3.0586820	2.8732590	-1.5346410
C	3.2208750	2.6402810	0.4841720
H	3.4203790	3.6987300	0.7201920
H	3.8347950	2.0357980	1.1606410
C	0.9202370	-1.0850780	-1.2006530
C	1.7644690	2.3132110	0.7121460
C	0.7709050	3.1862380	0.2676830
C	1.3990300	1.1085100	1.3107570
C	-0.5858250	2.8758300	0.4103600
H	1.0510300	4.1307990	-0.1969400
C	0.0546170	0.7583740	1.4802730
H	2.1716450	0.4178480	1.6443840
C	-0.9539150	1.6514360	1.0311350
C	-1.6293590	3.7540990	-0.0569010
C	-0.3427480	-0.4887480	2.0828910
C	-2.3320250	1.3130390	1.1875180
C	-2.9382610	3.4342990	0.0953770
H	-1.3404270	4.6859950	-0.5361810
C	-1.6509560	-0.8109630	2.2306630
H	0.4370940	-1.1751120	2.4025130
C	-3.3408080	2.2030710	0.7285870
C	-2.6950500	0.0795210	1.7918140
H	-3.7149060	4.1061610	-0.2609600
H	-1.9397640	-1.7601700	2.6742810

C	-4.6847600	1.8484640	0.8822600
C	-4.0528660	-0.2364660	1.9282140
C	-5.0357770	0.6378810	1.4749290
H	-5.4559060	2.5256260	0.5242220
H	-4.3317550	-1.1819870	2.3876860
H	-6.0832660	0.3711830	1.5742780
91			
8b complex			
C	0.6924610	-4.6652310	-0.7888560
N	0.0165770	-2.3555870	-1.0342710
C	-0.6125770	-5.0801550	-0.8255170
H	1.5152460	-5.3621990	-0.6838720
C	2.3217640	-2.8207960	-0.8161140
C	-1.2764310	-2.7548010	-1.0437020
C	-1.6420100	-4.1213810	-0.9454500
H	-0.8672990	-6.1337370	-0.7501550
C	3.4869870	-2.5034030	-0.6875550
N	-2.1955860	-1.7604090	-1.1133880
C	-3.0253160	-4.4308080	-0.9399030
C	4.8522740	-2.1417260	-0.4933820
C	-3.4747610	-2.0788850	-1.0419730
C	-3.9478900	-3.4266050	-0.9760820
H	-3.3397690	-5.4697820	-0.8910010
C	5.7445630	-3.0827080	0.0442760
C	5.2953420	-0.8273630	-0.8024720
N	-4.3392180	-0.9964110	-1.0570600
H	-5.0102960	-3.6157610	-0.9487520
C	7.0632190	-2.7497200	0.3067430
H	5.3704320	-4.0786490	0.2610810
C	6.6341330	-0.5032260	-0.5062030
N	4.4476910	0.0653810	-1.4058030
C	-5.6470880	-0.9612570	-0.6284920
H	-3.8945850	-0.0902140	-1.2647260
C	7.4932680	-1.4489080	0.0327060
H	7.7437230	-3.4822470	0.7257970
H	7.0054480	0.4949960	-0.7087000
C	4.6794090	1.4981010	-1.3855400
H	3.4809340	-0.2272980	-1.4864950
C	-6.2819200	0.4061710	-0.7428260
O	-6.2534310	-1.9343720	-0.2079680
H	8.5201840	-1.1642830	0.2424640
H	5.6651650	1.7174740	-1.8075150
H	3.9439770	1.9514980	-2.0588090
H	-5.5452900	1.2089910	-0.6679960
H	-7.0430830	0.5051000	0.0319210
H	-6.7723230	0.4831610	-1.7189090
N	-0.2701170	4.9275090	-1.1420890
C	-1.5458270	5.4416860	-1.2249890
H	-1.7145130	6.5099840	-1.1798050
N	-2.4690130	4.5272810	-1.3577350
C	-1.7639180	3.3414540	-1.3651920
C	-2.2088860	1.9879280	-1.4448870
O	-3.3655720	1.5799430	-1.5919750
N	-1.1446560	1.0866370	-1.3303580
H	-1.4139380	0.0911990	-1.2833460
C	0.1781990	1.4276780	-1.1725730
N	1.0725740	0.4148480	-1.0565820
H	1.8794030	0.6715620	-0.4782220
H	0.6926400	-0.5240310	-0.9030440

N	0.6033150	2.6771050	-1.1575980
C	-0.4017890	3.5730330	-1.2276300
C	4.5413250	2.1194090	0.0076760
H	4.9218580	3.1541970	-0.0079190
H	5.1562270	1.5567130	0.7217680
N	3.1497470	2.0295220	0.4239080
H	2.5704440	2.6125780	-0.1865910
C	2.8795010	2.4277770	1.8082020
H	3.1981360	3.4611000	2.0199750
H	3.4545820	1.7738040	2.4743140
C	0.9800220	5.6532420	-1.0226980
H	1.5958420	5.1880860	-0.2500600
H	1.5234890	5.6401990	-1.9702540
H	0.7623070	6.6840890	-0.7419140
C	0.9622360	-3.2725640	-0.8935810
C	1.3912910	2.2977900	2.0312500
C	0.5926800	3.4412600	2.0313020
C	0.7819370	1.0275590	2.0583610
C	-0.7941060	3.3612860	1.9862020
H	1.0731530	4.4172630	2.0292640
C	-0.6374460	0.9366980	2.0243330
C	1.5452510	-0.1990410	2.0722220
C	-1.4292630	2.1162210	1.9524260
H	-1.3950780	4.2667520	1.9451960
C	-1.2775140	-0.3426300	2.0299580
C	0.9360040	-1.4096090	2.1030350
H	2.6288200	-0.1444460	2.0359980
C	-2.8605500	1.9929570	1.8385580
C	-2.6954410	-0.4337230	1.9714320
C	-0.4982670	-1.5276720	2.1037470
H	1.5273220	-2.3222280	2.1130920
C	-3.4635710	0.7788880	1.8462360
H	-3.4461980	2.9036190	1.7408300
C	-3.3020850	-1.6941480	2.0300450
C	-1.1416400	-2.7693450	2.1572450
H	-4.5455750	0.6970300	1.7685080
C	-2.5308360	-2.8483760	2.1310250
H	-4.3862980	-1.7668040	1.9706230
H	-0.5412590	-3.6752910	2.2048940
H	-3.0174000	-3.8184690	2.1705670
72			
8b			
C	-1.5189500	3.3938570	0.7238710
N	-1.2345650	1.0465010	1.2655750
C	-0.1744840	3.6201250	0.8614410
H	-2.2122520	4.1826390	0.4561520
C	-3.3815700	1.7505540	0.7077100
C	0.0973430	1.2610270	1.3895010
C	0.6769800	2.5437520	1.1922050
H	0.2481210	4.6095740	0.7076690
C	-4.5012510	1.3401520	0.4805640
N	0.8414640	0.1714450	1.6968840
C	2.0850920	2.6524870	1.3089430
C	-5.6796420	0.5934000	0.1930210
C	2.1468320	0.3112640	1.7754800
C	2.8358950	1.5489650	1.5955780
H	2.5593960	3.6172390	1.1504740
C	-6.9085290	1.1888520	-0.1106220
C	-5.5387350	-0.8246360	0.1744730

N	2.8192600	-0.8834380	2.0235940
H	3.9122290	1.5819620	1.6723320
C	-8.0081960	0.4117410	-0.4457920
H	-6.9809160	2.2718160	-0.0868200
C	-6.6583680	-1.5920900	-0.1889890
N	-4.3409430	-1.3937690	0.5258010
C	4.1680250	-1.1090720	2.1906630
H	2.2056190	-1.6896560	1.9796390
C	-7.8674800	-0.9775430	-0.4879360
H	-8.9589130	0.8780210	-0.6790080
H	-6.5770250	-2.6730290	-0.2279660
C	-3.9538410	-2.7255210	0.1097670
H	-3.5682140	-0.7387900	0.5937730
C	4.5190350	-2.5706190	2.3556160
O	5.0003350	-0.2215600	2.2489420
H	-8.7173760	-1.5964820	-0.7601650
H	-4.5999550	-3.4748590	0.5819420
H	-4.0615760	-2.8464780	-0.9800970
H	4.3294670	-2.8732170	3.3907200
H	5.5787990	-2.7005750	2.1372290
H	3.9229280	-3.2081390	1.6973340
C	-2.5048370	-2.9988060	0.5423660
H	-2.2174290	-3.9724450	0.1236230
H	-2.4707030	-3.0895940	1.6326820
N	-1.5093940	-2.0123000	0.1580120
H	-1.4951600	-1.1859620	0.7568820
C	-1.5189140	-1.6229290	-1.2462130
H	-2.4785790	-1.1875790	-1.5750590
H	-1.3683490	-2.5312090	-1.8484970
C	-2.0012520	2.0735260	0.9268100
C	-0.4260510	-0.6144330	-1.5164050
C	-0.7700280	0.6889270	-1.8759940
C	0.9321360	-0.9499460	-1.3597330
C	0.1928520	1.6732870	-2.0600650
H	-1.8226480	0.9407450	-1.9863050
C	1.9255420	0.0516980	-1.5432390
C	1.3622130	-2.2866290	-1.0230820
C	1.5487930	1.3792890	-1.8851180
H	-0.1029650	2.6858290	-2.3223290
C	3.3093630	-0.2657130	-1.3696660
C	2.6768340	-2.5944510	-0.8954000
H	0.6055210	-3.0468890	-0.8644560
C	2.5723170	2.3815120	-2.0347150
C	4.2990580	0.7443700	-1.5199000
C	3.7019280	-1.5952080	-1.0552210
H	2.9826490	-3.6124900	-0.6641380
C	3.8819470	2.0814440	-1.8569510
H	2.2651000	3.3924820	-2.2914920
C	5.6474680	0.4107310	-1.3410340
C	5.0611750	-1.8890740	-0.8955080
H	4.6464420	2.8456620	-1.9699310
C	6.0229960	-0.8924400	-1.0327420
H	6.4018780	1.1852080	-1.4508690
H	5.3574230	-2.9079840	-0.6578420
H	7.0728690	-1.1335040	-0.8981770
91			
8c complex			
C	1.3895990	-4.3412090	-0.3367830
N	0.5124220	-2.1552540	-0.8728500

C	0.1355960	-4.8907200	-0.4065330
H	2.2661100	-4.9335570	-0.1027290
C	2.8422510	-2.3616910	-0.5457420
C	-0.7311760	-2.6840630	-0.9306840
C	-0.9684000	-4.0645170	-0.7078110
H	-0.0224670	-5.9513270	-0.2307490
C	3.9764470	-1.9291450	-0.5788920
N	-1.7299560	-1.8083730	-1.2094560
C	-2.3070380	-4.5237780	-0.8129690
C	5.3202350	-1.4653950	-0.7236450
C	-2.9688570	-2.2613060	-1.2552490
C	-3.3097290	-3.6416100	-1.0833660
H	-2.5197330	-5.5801690	-0.6734420
C	6.2458910	-2.2824550	-1.3893430
C	5.7032430	-0.1763160	-0.2669450
N	-3.9266220	-1.2981080	-1.5223890
H	-4.3425440	-3.9466040	-1.1581350
C	7.5357360	-1.8447790	-1.6444590
H	5.9190960	-3.2635500	-1.7198080
C	7.0067550	0.2623090	-0.5646920
N	4.8330280	0.5854620	0.4706610
C	-5.2782050	-1.3648200	-1.2550570
H	-3.5484330	-0.3606290	-1.7158470
C	7.9000700	-0.5601890	-1.2359290
H	8.2403050	-2.4831870	-2.1655240
H	7.3232720	1.2531810	-0.2609930
C	4.9913300	2.0177920	0.6360030
H	3.8698190	0.2679600	0.5136440
C	-6.0232270	-0.1015790	-1.6187040
O	-5.8323010	-2.3483230	-0.7903820
H	8.8996170	-0.1889850	-1.4426800
H	5.9837730	2.2365280	1.0422930
H	4.9035910	2.5473150	-0.3261100
H	-5.4228300	0.7892580	-1.4202210
H	-6.9566650	-0.0714100	-1.0557600
H	-6.2587460	-0.1255350	-2.6880770
N	-0.4371810	5.0094470	-1.0213400
C	-1.7448600	5.4125230	-1.1805500
H	-2.0165020	6.4566080	-1.0908210
N	-2.5642590	4.4296150	-1.4429330
C	-1.7533650	3.3130960	-1.4571610
C	-2.0657780	1.9282730	-1.6257970
O	-3.1641510	1.4164640	-1.8565000
N	-0.9272920	1.1263310	-1.4853620
H	-1.1079240	0.1109590	-1.4743740
C	0.3455870	1.5772250	-1.2318120
N	1.3131520	0.6384650	-1.1550000
H	1.0166850	-0.3368780	-1.0370630
H	2.1052200	0.9193310	-0.5854180
N	0.6506770	2.8564130	-1.0996280
C	-0.4324940	3.6564530	-1.1951220
C	3.9537740	2.5257180	1.6271560
H	4.0807500	3.6104530	1.7655470
H	4.1422860	2.0468220	2.5952850
N	2.6077920	2.1502350	1.2027710
H	2.3219570	2.7216000	0.4037020
C	1.6108850	2.3512630	2.2603230
H	1.3874440	3.4179750	2.4154970
H	2.0504770	1.9855550	3.1970460

C	0.7191940	5.8234410	-0.6978550
H	1.1564050	5.4894270	0.2464750
H	1.4677070	5.7430510	-1.4884850
H	0.3996590	6.8612450	-0.6027330
C	1.5310430	-2.9499620	-0.5837600
C	0.3191980	1.6088170	2.0161780
C	-0.8312620	2.2935800	1.7874500
C	0.2894200	0.1576130	2.1111840
C	-2.1051190	1.6413850	1.6366940
H	-0.8074200	3.3811390	1.7260760
C	-0.9641670	-0.5106180	2.0139840
C	1.4417780	-0.6063650	2.3433280
C	-3.2816920	2.3558780	1.3850130
C	-2.1615780	0.2292300	1.7659810
C	-1.0366420	-1.9199770	2.1921600
H	2.4097940	-0.1168610	2.3941390
C	1.3614290	-1.9859060	2.5156620
C	-4.4995240	1.6929230	1.2698880
H	-3.2301680	3.4346320	1.2606010
C	-3.4113780	-0.4387740	1.6693050
C	0.1364560	-2.6391290	2.4479910
C	-2.3185000	-2.5714330	2.0913900
H	2.2686830	-2.5553200	2.6963430
C	-4.5674110	0.3112850	1.4196500
H	-5.4038050	2.2574870	1.0635890
C	-3.4491580	-1.8690450	1.8358040
H	0.0797650	-3.7169250	2.5790790
H	-2.3538900	-3.6515990	2.2117210
H	-5.5226160	-0.2039870	1.3409100
H	-4.4075420	-2.3728760	1.7330690
72			
8c			
C	-1.1689690	3.2195910	1.4061270
N	-0.9700600	0.8020060	1.4309330
C	0.1840450	3.3625980	1.5657070
H	-1.8334660	4.0716730	1.3231510
C	-3.0823090	1.6654940	1.0277640
C	0.3685410	0.9387470	1.5847880
C	0.9987550	2.2104210	1.6368400
H	0.6433310	4.3464240	1.6145670
C	-4.1935450	1.2929810	0.7125270
N	1.0656870	-0.2189550	1.6528730
C	2.4124990	2.2348890	1.7333040
C	-5.3703970	0.6055710	0.3028790
C	2.3769030	-0.1533470	1.7281240
C	3.1183560	1.0651900	1.7723890
H	2.9274840	3.1916850	1.7617830
C	-6.5837880	1.2557980	0.0534220
C	-5.2501910	-0.8030320	0.1142430
N	2.9865930	-1.4062970	1.7726000
H	4.1962250	1.0354310	1.8236850
C	-7.6917170	0.5467710	-0.3873180
H	-6.6368280	2.3292880	0.2069730
C	-6.3806120	-1.4992230	-0.3499360
N	-4.0700580	-1.4350390	0.4046110
C	4.3236160	-1.7273310	1.7423030
H	2.3146220	-2.1628570	1.7089810
C	-7.5740560	-0.8303850	-0.5890410
H	-8.6299490	1.0554830	-0.5782160

H	-6.3206980	-2.5683170	-0.5205380
C	-3.7710070	-2.7820380	-0.0305540
H	-3.2669940	-0.8294660	0.5447260
C	4.6031270	-3.2119810	1.8154050
O	5.2188110	-0.9000320	1.7072740
H	-8.4300260	-1.3979130	-0.9426890
H	-4.4952890	-3.4831310	0.4009260
H	-3.8516340	-2.8719210	-1.1256760
H	4.8426460	-3.4689310	2.8521210
H	5.4754240	-3.4336820	1.1988970
H	3.7584190	-3.8210490	1.4885840
C	-2.3708510	-3.2005920	0.4432140
H	-2.1759670	-4.1973090	0.0263540
H	-2.3799040	-3.2991690	1.5334310
N	-1.2646760	-2.3233040	0.0941790
H	-1.2022860	-1.4989870	0.6937920
C	-1.2128750	-1.9164060	-1.3056810
H	-2.1439100	-1.4396630	-1.6556610
H	-1.0692400	-2.8143640	-1.9228570
C	-1.6976340	1.9035050	1.3150260
C	-0.0866800	-0.9311230	-1.4912460
C	-0.3801600	0.3864090	-1.6280520
C	1.2993760	-1.3611200	-1.4266530
C	0.6349050	1.4039660	-1.6666970
H	-1.4215210	0.7046840	-1.6586100
C	2.3274190	-0.3776360	-1.4872460
C	1.6648130	-2.7071350	-1.3029960
C	0.3190720	2.7636530	-1.7543810
C	1.9953210	1.0092660	-1.5792450
C	3.6932080	-0.7667360	-1.4255790
H	0.8923120	-3.4635330	-1.2111880
C	3.0069590	-3.0841120	-1.2832510
C	1.3252620	3.7255680	-1.7437710
H	-0.7248610	3.0615020	-1.8127590
C	3.0185180	1.9942870	-1.5856260
C	4.0138330	-2.1275400	-1.3458540
C	4.7111220	0.2532980	-1.4256520
H	3.2666100	-4.1362550	-1.2077580
C	2.6613050	3.3469740	-1.6577270
H	1.0657260	4.7783720	-1.8012070
C	4.3906940	1.5682280	-1.4994530
H	5.0593670	-2.4251950	-1.3154180
H	5.7485720	-0.0620330	-1.3543100
H	3.4445970	4.1008290	-1.6520830
H	5.1671870	2.3289860	-1.4921910
89			
9a complex			
C	1.0911310	-4.0346170	-1.2641220
N	0.1762380	-1.7995900	-1.1059740
C	-0.1627140	-4.5745510	-1.3574660
H	1.9856920	-4.6455120	-1.2836290
C	2.5374810	-2.0910280	-0.9741390
C	-1.0705840	-2.3271270	-1.1780330
C	-1.2867860	-3.7236710	-1.3026770
H	-0.3072740	-5.6469030	-1.4584390
C	3.7128600	-1.8261900	-0.8131090
N	-2.0960530	-1.4411490	-1.1039910
C	-2.6269740	-4.1795150	-1.3489660
C	5.1104080	-1.6206370	-0.6098070

C	-3.3350350	-1.9034760	-1.1112050
C	-3.6559110	-3.2903960	-1.2501840
H	-2.8227470	-5.2436090	-1.4509590
C	5.9559930	-2.7411400	-0.5893580
C	5.6437420	-0.3217040	-0.3976000
N	-4.3097340	-0.9331670	-0.9586840
H	-4.6907140	-3.5963710	-1.2657720
C	7.3149440	-2.6105020	-0.3524780
H	5.5148090	-3.7191900	-0.7557480
C	7.0229520	-0.2114560	-0.1402220
N	4.8336680	0.7809400	-0.4702220
C	-5.6743940	-1.0901650	-0.8373680
H	-3.9544670	0.0231010	-0.8160400
C	7.8366500	-1.3351750	-0.1236380
H	7.9566930	-3.4841640	-0.3385420
H	7.4583140	0.7644670	0.0416280
C	5.2184140	2.0493990	0.1148090
H	3.8325800	0.6107100	-0.4388410
C	-6.3882530	0.2086960	-0.5399350
O	-6.2568910	-2.1565720	-0.9437690
H	8.8974820	-1.2116260	0.0735960
H	5.4615510	1.9351630	1.1834150
H	6.1160550	2.4377630	-0.3779180
H	-6.0630830	0.5951870	0.4311690
H	-7.4619450	0.0267380	-0.5276740
H	-6.1373970	0.9676060	-1.2852590
N	-0.8687210	5.4078780	-0.6333750
C	-2.1595840	5.7977240	-0.3511040
H	-2.3900510	6.8345810	-0.1419620
N	-3.0172820	4.8131080	-0.3689490
C	-2.2508940	3.7094920	-0.6841950
C	-2.5944280	2.3267660	-0.7865120
O	-3.7031960	1.8061370	-0.6256420
N	-1.4807890	1.5395490	-1.0913990
H	-1.6435080	0.5199720	-1.0911040
C	-0.1917010	1.9937370	-1.2247150
N	0.7515240	1.0701910	-1.5062360
H	0.5255920	0.0881210	-1.3142590
H	1.6873920	1.3598430	-1.2248430
N	0.1401220	3.2712680	-1.1263860
C	-0.9169350	4.0612850	-0.8471980
C	4.0916000	3.0639310	-0.0792440
H	4.0654340	3.3763590	-1.1275870
H	4.3190580	3.9497790	0.5353050
N	2.7923790	2.4775220	0.2269060
H	2.0497440	3.1094120	-0.0812760
C	2.5964010	2.1526010	1.6435780
H	2.8106870	3.0196030	2.2914500
H	3.3026630	1.3600800	1.9184350
C	0.3270560	6.2283260	-0.6780100
H	1.0411110	5.8907000	0.0775240
H	0.7897470	6.1605040	-1.6644940
H	0.0484020	7.2627280	-0.4764600
C	1.2125260	-2.6239270	-1.1270090
C	1.1821150	1.6743150	1.8681550
C	0.1446110	2.6169490	2.0228060
C	0.8731020	0.3269850	1.8481250
C	-1.1637460	2.2015580	2.1234100
H	0.3843410	3.6786110	2.0394170

C	-0.4553670	-0.1344240	1.9863370
H	1.6826300	-0.3842850	1.7047980
C	-1.4907920	0.8276300	2.0916790
H	-1.9667460	2.9290240	2.2169840
C	-0.7988550	-1.5494240	2.0248980
C	-2.8633410	0.4035500	2.1453340
C	-2.1645500	-1.9245630	2.0809600
C	0.1741450	-2.5727100	2.0057350
C	-3.1848430	-0.9121400	2.1275140
H	-3.6353240	1.1673330	2.1842630
C	-2.5142820	-3.2925490	2.0856350
C	-0.1876050	-3.9038080	2.0204940
H	1.2289990	-2.3191200	1.9742930
H	-4.2242760	-1.2316570	2.1537220
H	-3.5678850	-3.5598060	2.1128460
C	-1.5449140	-4.2708880	2.0543580
H	0.5811470	-4.6704610	1.9980400
H	-1.8253350	-5.3200190	2.0541630
70			
9a			
C	-0.7189170	2.6160790	1.8491480
N	-0.8388120	0.2171910	1.5008820
C	0.6433230	2.5585460	1.9857780
H	-1.2664740	3.5491590	1.9124220
C	-2.8232770	1.4145640	1.3049040
C	0.5067250	0.1551630	1.6445380
C	1.2975450	1.3134900	1.8648970
H	1.2296320	3.4571500	2.1588910
C	-3.9815650	1.2916180	0.9647670
N	1.0520310	-1.0803620	1.5226530
C	2.7056590	1.1501210	1.9093720
C	-5.2410640	0.8852110	0.4414370
C	2.3603940	-1.1862320	1.5527070
C	3.2548340	-0.0884070	1.7468520
H	3.3375320	2.0225900	2.0551890
C	-6.3476810	1.7376550	0.3644060
C	-5.3110110	-0.4439230	-0.0689310
N	2.8144540	-2.4956980	1.3895330
H	4.3211720	-0.2566990	1.7439130
C	-7.5311390	1.3110920	-0.2202680
H	-6.2559900	2.7428000	0.7642330
C	-6.5115240	-0.8467680	-0.6799600
N	-4.2356970	-1.2842010	0.0667560
C	4.0781080	-2.9403050	1.0697480
H	2.0489370	-3.1519860	1.2760340
C	-7.5960980	0.0182880	-0.7453430
H	-8.3867400	1.9746320	-0.2769040
H	-6.5939140	-1.8428060	-1.1004760
C	-4.0633990	-2.4749010	-0.7374590
H	-3.3710190	-0.8364160	0.3552060
C	4.1312210	-4.4224290	0.7712040
O	5.0607460	-2.2205180	1.0344490
H	-8.5113250	-0.3252000	-1.2188990
H	-4.9052440	-3.1584810	-0.5779320
H	-4.0442190	-2.2294800	-1.8117620
H	3.4849570	-4.6641700	-0.0786120
H	3.7832460	-4.9987450	1.6333050
H	5.1587430	-4.6973510	0.5377210
C	-2.7787460	-3.2103460	-0.3328220

H	-2.6806460	-4.0732300	-1.0046980
H	-2.8993480	-3.6004760	0.6828120
N	-1.5358540	-2.4557070	-0.3663030
H	-1.3958380	-1.8612190	0.4511580
C	-1.2976310	-1.6882380	-1.5821200
H	-1.9509210	-0.8035830	-1.6819930
H	-1.5212740	-2.3447280	-2.4347090
C	-1.4166790	1.4091410	1.5799270
C	0.1488660	-1.2571090	-1.6413420
C	1.1562630	-2.2405920	-1.7429150
C	0.5098330	0.0700390	-1.5405420
C	2.4819580	-1.8799640	-1.7319340
H	0.8666470	-3.2857810	-1.8178270
C	1.8648660	0.4723570	-1.4976740
H	-0.2806970	0.8093870	-1.4474440
C	2.8645090	-0.5267720	-1.5893530
H	3.2625870	-2.6333300	-1.8195900
C	2.2692480	1.8617780	-1.3354670
C	4.2529980	-0.1658710	-1.5108310
C	3.6502570	2.1730460	-1.2456840
C	1.3401060	2.9204790	-1.2341840
C	4.6286270	1.1253410	-1.3428240
H	4.9940680	-0.9586920	-1.5656510
C	4.0537400	3.5123120	-1.0463220
C	1.7546820	4.2212800	-1.0381500
H	0.2763370	2.7171640	-1.2959620
H	5.6794320	1.3938320	-1.2715280
H	5.1166800	3.7293970	-0.9762640
C	3.1251350	4.5240260	-0.9392750
H	1.0173800	5.0141210	-0.9556600
H	3.4464770	5.5491070	-0.7829120
89			
9b complex			
C	1.3600060	-4.1984010	-0.6544370
N	0.4720620	-1.9793620	-1.0369870
C	0.1023140	-4.7388500	-0.6821750
H	2.2451790	-4.8026930	-0.4960290
C	2.8284330	-2.2593940	-0.7571420
C	-0.7787190	-2.5012860	-1.0400100
C	-1.0082650	-3.8909950	-0.8686010
H	-0.0543960	-5.8056560	-0.5476380
C	4.0094220	-2.0100840	-0.6134670
N	-1.7949830	-1.6118020	-1.1838960
C	-2.3528820	-4.3388000	-0.8517240
C	5.4088370	-1.8121140	-0.4156720
C	-3.0391510	-2.0590340	-1.1312410
C	-3.3717380	-3.4430860	-0.9739730
H	-2.5583930	-5.3980810	-0.7231400
C	6.2547510	-2.9323830	-0.4219320
C	5.9389270	-0.5193830	-0.1624380
N	-4.0114050	-1.0811830	-1.2264440
H	-4.4097640	-3.7366610	-0.9485000
C	7.6121090	-2.8063550	-0.1735760
H	5.8157240	-3.9061350	-0.6170290
C	7.3153510	-0.4150180	0.1102120
N	5.1241050	0.5812710	-0.2100240
C	-5.3832100	-1.2269360	-1.2175410
H	-3.6568470	-0.1152210	-1.2396930
C	8.1302660	-1.5379050	0.0982520

H	8.2551450	-3.6791720	-0.1805460
H	7.7472500	0.5556050	0.3259150
C	5.4701510	1.8232110	0.4510380
H	4.1244580	0.4000230	-0.2122240
C	-6.1291490	0.0817670	-1.3415840
O	-5.9626380	-2.2991850	-1.1597980
H	9.1893820	-1.4197150	0.3076380
H	5.6417160	1.6655650	1.5278500
H	6.3974430	2.2299460	0.0350860
H	-5.5523720	0.9249170	-0.9588720
H	-7.0773810	-0.0093180	-0.8096600
H	-6.3450000	0.2593200	-2.4006620
N	-0.4605990	5.1992290	-0.7534140
C	-1.7675040	5.6076110	-0.6007400
H	-2.0013120	6.6441890	-0.3942690
N	-2.6345880	4.6395910	-0.7286630
C	-1.8571890	3.5276130	-0.9819190
C	-2.2111590	2.1572160	-1.1729010
O	-3.3416930	1.6610690	-1.1803430
N	-1.0842780	1.3513130	-1.3595230
H	-1.2679240	0.3360560	-1.3883280
C	0.2191090	1.7837150	-1.3411760
N	1.1730420	0.8482190	-1.5314710
H	2.0787130	1.1223290	-1.1518760
H	0.9104850	-0.1303420	-1.3689460
N	0.5578120	3.0539670	-1.1874850
C	-0.5082020	3.8580580	-0.9987970
C	4.3562310	2.8455980	0.2197740
H	4.4094750	3.2045500	-0.8124490
H	4.5302250	3.7034200	0.8891840
N	3.0395940	2.2449440	0.3959620
H	2.3243970	2.8710710	0.0197650
C	2.7088790	1.9049690	1.7826880
H	2.8186670	2.7759770	2.4512430
H	3.4129650	1.1398200	2.1311060
C	0.7446590	6.0027580	-0.6711250
H	1.4167090	5.5879300	0.0839110
H	1.2553280	6.0179480	-1.6362450
H	0.4677740	7.0188880	-0.3900330
C	1.4974550	-2.7944520	-0.8331040
C	1.2999590	1.3671900	1.8626600
C	1.0445460	0.0110420	1.8691010
C	0.2051840	2.2564030	1.8892810
C	-0.2744060	-0.4927740	1.9173860
H	1.8726600	-0.6966880	1.8497170
C	-1.0923670	1.7904900	1.8977760
H	0.3903300	3.3291180	1.9004230
C	-1.3709210	0.4045220	1.8999010
C	-0.5109480	-1.9074930	2.0233570
H	-1.9045910	2.5097520	1.9202840
C	-2.7266000	-0.1300290	1.9145980
C	-1.7699010	-2.4002060	2.1048570
H	0.3496800	-2.5733100	2.0405720
C	-2.9125870	-1.5292770	2.0442110
C	-3.8726910	0.6886930	1.8065300
H	-1.9432570	-3.4700270	2.1943230
C	-4.2194800	-2.0626930	2.0787330
C	-5.1415550	0.1480030	1.8525190
H	-3.7641690	1.7579290	1.6606320

C	-5.3214210	-1.2401430	1.9930240
H	-4.3396030	-3.1399070	2.1658230
H	-6.0062490	0.7996710	1.7690730
H	-6.3223960	-1.6600980	2.0146160
70			
9b			
C	-0.7718580	0.2287980	1.8110190
N	0.2600670	-1.7238270	0.7954370
C	0.4485870	0.7453630	2.1464700
H	-1.7018180	0.7514950	2.0100030
C	-2.0945780	-1.5074000	0.7036960
C	1.4730750	-1.2051000	1.1118880
C	1.6173520	0.0341930	1.7897400
H	0.5372150	1.7004460	2.6576410
C	-3.2011440	-1.8436110	0.3340150
N	2.5471930	-1.9310000	0.7076640
C	2.9316100	0.5011890	2.0384970
C	-4.5359270	-2.0935450	-0.1024280
C	3.7477660	-1.4472580	0.9342210
C	4.0095430	-0.2232950	1.6173980
H	3.0698470	1.4514520	2.5481010
C	-4.8974820	-3.2950440	-0.7233310
C	-5.4953020	-1.0552460	0.0632300
N	4.7748410	-2.2512990	0.4295470
H	5.0264540	0.1085780	1.7618090
C	-6.1875220	-3.4909630	-1.1966370
H	-4.1425130	-4.0669240	-0.8366670
C	-6.7904370	-1.2645480	-0.4396170
N	-5.1394530	0.0958070	0.7162800
C	6.1212710	-1.9867590	0.3254570
H	4.4246700	-3.0909710	-0.0179960
C	-7.1238760	-2.4644050	-1.0546700
H	-6.4592530	-4.4238120	-1.6780820
H	-7.5359940	-0.4831590	-0.3363120
C	-5.8374470	1.3489030	0.5204070
H	-4.1402180	0.2359550	0.8512750
C	6.8846520	-3.0408800	-0.4460460
O	6.6555140	-0.9928980	0.7862910
H	-8.1337220	-2.5997140	-1.4309630
H	-5.9707600	1.5675210	-0.5512550
H	-6.8385250	1.3150170	0.9656880
H	7.9505940	-2.8979500	-0.2734650
H	6.6780470	-2.9286650	-1.5155060
H	6.5927810	-4.0507530	-0.1470110
C	-5.0352550	2.4591060	1.2089620
H	-5.1620420	2.3695340	2.2917250
H	-5.4433250	3.4331990	0.8961060
N	-3.6081820	2.3175330	0.9272760
H	-3.0769700	2.9056860	1.5658690
C	-3.2433210	2.6539130	-0.4521870
H	-3.5278690	3.6880930	-0.7106220
H	-3.7994830	1.9869670	-1.1203740
C	-0.8091000	-1.0163080	1.1185750
C	-1.7644350	2.4467570	-0.6625090
C	-1.2820240	1.3111660	-1.2789590
C	-0.8382370	3.3898660	-0.1710830
C	0.1030090	1.0761990	-1.4174430
H	-1.9775430	0.5624780	-1.6544780
C	0.5195370	3.1824330	-0.2921850

H	-1.2021870	4.2979310	0.3054070
C	1.0310260	2.0232150	-0.9172030
C	0.5745820	-0.1292160	-2.0421510
H	1.1970120	3.9331060	0.1002310
C	2.4572830	1.7570280	-1.0477920
C	1.9002090	-0.3802180	-2.1574840
H	-0.1617090	-0.8444610	-2.3993900
C	2.8771460	0.5506210	-1.6626400
C	3.4505450	2.6425310	-0.5718690
H	2.2542430	-1.3027740	-2.6100240
C	4.2559670	0.2655890	-1.7744560
C	4.7917600	2.3419940	-0.6868540
H	3.1646530	3.5771290	-0.1010830
C	5.2036680	1.1394400	-1.2892150
H	4.5566010	-0.6678160	-2.2457650
H	5.5331240	3.0379230	-0.3063890
H	6.2594540	0.9001260	-1.3631440
89			
9c complex			
C	0.3635770	-4.7073390	-0.4750640
N	-0.2243620	-2.3907170	-0.8549370
C	-0.9570150	-5.0713670	-0.4752180
H	1.1597750	-5.4281140	-0.3332890
C	2.0646180	-2.9419960	-0.6404780
C	-1.5331300	-2.7379780	-0.8352420
C	-1.9483430	-4.0821690	-0.6519530
H	-1.2528070	-6.1071000	-0.3317920
C	3.2491490	-2.6869770	-0.5579020
N	-2.4138160	-1.7174870	-0.9747800
C	-3.3420350	-4.3398390	-0.6336560
C	4.6389520	-2.3994360	-0.4195290
C	-3.7059630	-1.9865200	-0.9092770
C	-4.2278320	-3.3100610	-0.7557470
H	-3.6944300	-5.3603410	-0.5110680
C	5.4769220	-3.3363150	0.2052450
C	5.1618990	-1.1593240	-0.8728380
N	-4.5239610	-0.8762320	-1.0010210
H	-5.2966530	-3.4582860	-0.7318500
C	6.8191440	-3.0662660	0.4149260
H	5.0430120	-4.2756010	0.5342660
C	6.5243560	-0.8972780	-0.6327820
N	4.3615840	-0.2775280	-1.5570290
C	-5.8814190	-0.7865050	-0.7790930
H	-4.0179110	0.0179820	-1.0790210
C	7.3297450	-1.8349040	-0.0040730
H	7.4573590	-3.7938830	0.9034850
H	6.9551250	0.0451540	-0.9520490
C	4.6544790	1.1447170	-1.6137970
H	3.3793900	-0.5238570	-1.5927310
C	-6.3828810	0.6393430	-0.7959660
O	-6.6099210	-1.7427790	-0.5720920
H	8.3773230	-1.6003340	0.1601370
H	5.6371400	1.3002290	-2.0700170
H	3.9216160	1.5958850	-2.2910830
H	-5.9705910	1.1819230	0.0607250
H	-7.4705390	0.6325970	-0.7411040
H	-6.0487150	1.1601980	-1.6965950
N	-0.1365180	4.8846350	-1.0917810
C	-1.3843700	5.4596320	-0.9895430

H	-1.4927390	6.5333490	-0.9035080
N	-2.3613550	4.5929660	-1.0132030
C	-1.7237400	3.3764660	-1.1408530
C	-2.2386600	2.0455400	-1.1409980
O	-3.4218120	1.6946410	-1.0815100
N	-1.2151200	1.0923810	-1.2032120
H	-1.5269580	0.1121550	-1.1176890
C	0.1312910	1.3696060	-1.2038250
N	0.9869910	0.3139580	-1.1863100
H	1.8415290	0.5353910	-0.6647610
H	0.5734290	-0.5977930	-0.9683110
N	0.6149080	2.5960450	-1.2388380
C	-0.3456040	3.5407660	-1.1791580
C	4.5845720	1.8367260	-0.2503200
H	5.0097090	2.8512170	-0.3268530
H	5.1986360	1.2827100	0.4710110
N	3.2073050	1.8367560	0.2230540
H	2.6405470	2.4460530	-0.3726900
C	3.0483190	2.3011420	1.6038530
H	3.5191460	3.2838250	1.7690020
H	3.5565650	1.5914190	2.2679650
C	1.1544520	5.5458130	-1.0926830
H	1.0324420	6.5560920	-0.7007830
H	1.8404120	4.9886990	-0.4505190
H	1.5646510	5.5928120	-2.1040260
C	0.6851410	-3.3364170	-0.6702560
C	1.5719450	2.4003810	1.9085050
C	0.7683700	1.2281410	1.9795770
C	0.9758900	3.6423480	1.9996120
C	-0.6431480	1.3472300	2.0665950
C	1.3631540	-0.0852730	1.9633240
C	-0.4178150	3.7656710	2.1202320
H	1.5952920	4.5355790	1.9655330
C	-1.4646010	0.1410770	2.1008540
C	-1.2114560	2.6399110	2.1282000
C	0.6028030	-1.2008140	2.0717010
H	2.4390500	-0.1767120	1.8532880
H	-0.8727820	4.7500150	2.1797680
C	-0.8293650	-1.1234810	2.1510020
C	-2.8778500	0.1750070	2.0985970
H	-2.2869850	2.7601920	2.1969940
H	1.0668590	-2.1844720	2.0751170
C	-1.6059700	-2.2974390	2.2601660
C	-3.6198470	-0.9839720	2.2026760
H	-3.3997760	1.1210940	2.0060670
C	-2.9815890	-2.2339250	2.2999080
H	-1.0938840	-3.2569480	2.3032230
H	-4.7052780	-0.9312380	2.1988600
H	-3.5715660	-3.1417640	2.3811850
70			
9c			
C	0.6475550	2.6565800	1.8946460
N	0.6673990	0.2383180	1.6993350
C	-0.7205740	2.6714890	1.9577300
H	1.2361180	3.5661740	1.9309090
C	2.7060480	1.3225290	1.4712490
C	-0.6841710	0.2508080	1.7298020
C	-1.4293460	1.4542680	1.8495360
H	-1.2704440	3.6047160	2.0482390

C	3.8365110	1.1008400	1.0867800
N	-1.2861910	-0.9619650	1.6035280
C	-2.8432740	1.3594960	1.8228870
C	5.0337220	0.5675660	0.5307640
C	-2.5991600	-1.0025090	1.5532250
C	-3.4442840	0.1436880	1.6692460
H	-3.4383580	2.2651830	1.9055810
C	6.2484190	1.2600940	0.5021270
C	4.9331100	-0.7431680	-0.0298040
N	-3.1156630	-2.2891340	1.3973510
H	-4.5164000	0.0260290	1.6240890
C	7.3795840	0.6903480	-0.0649480
H	6.2878390	2.2548070	0.9358960
C	6.0908750	-1.2973150	-0.6099100
N	3.7506220	-1.4137940	0.0287680
C	-4.3865020	-2.6692290	1.0241450
H	-2.3890860	-2.9957320	1.3565670
C	7.2848100	-0.5897020	-0.6182890
H	8.3187110	1.2319230	-0.0811700
H	6.0442640	-2.2833540	-1.0595100
C	3.4921080	-2.7001040	-0.5735960
H	2.9095180	-0.8964990	0.2742400
C	-4.5064110	-4.1486420	0.7357470
O	-5.3225770	-1.8963550	0.9241360
H	8.1598590	-1.0453800	-1.0730490
H	3.5014660	-2.6457020	-1.6743090
H	4.2617290	-3.4218330	-0.2744890
H	-5.5521270	-4.3870120	0.5471040
H	-4.1368100	-4.7433060	1.5757300
H	-3.9113230	-4.4031770	-0.1477590
C	2.1296420	-3.1798960	-0.0677200
H	2.1962980	-3.2926880	1.0190470
H	1.9135870	-4.1716310	-0.4985360
N	1.0948320	-2.2031640	-0.3606290
H	0.3941040	-2.1436950	0.3753240
C	0.4652350	-2.3591450	-1.6666130
H	0.2815800	-3.4203120	-1.9071150
H	1.1445340	-1.9786280	-2.4429820
C	1.2968520	1.4031770	1.7330540
C	-0.8544700	-1.6251590	-1.7148710
C	-0.9138640	-0.2072630	-1.6019920
C	-2.0244860	-2.3487400	-1.8320700
C	-2.1739760	0.4444340	-1.5809610
C	0.2897080	0.5780430	-1.5062640
C	-3.2737480	-1.7065310	-1.8297410
H	-1.9739970	-3.4310120	-1.9270500
C	-2.2265930	1.8940590	-1.4392220
C	-3.3460090	-0.3390320	-1.6904400
C	0.2380460	1.9291630	-1.4179910
H	1.2447580	0.0636860	-1.4699400
H	-4.1867890	-2.2888210	-1.9195620
C	-1.0159940	2.6259520	-1.3752640
C	-3.4412650	2.6094510	-1.3333020
H	-4.3225910	0.1311300	-1.6711660
H	1.1538800	2.5111910	-1.3436170
C	-1.0502720	4.0295790	-1.2213780
C	-3.4543460	3.9796280	-1.1749610
H	-4.3882690	2.0820070	-1.3607410
C	-2.2476630	4.7019380	-1.1211540

H	-0.1073310	4.5685310	-1.1685900
H	-4.4023240	4.5019310	-1.0900580
H	-2.2636700	5.7803170	-0.9973260
89			
9d complex			
C	1.7310410	-4.3984830	-0.3187730
N	0.5398340	-2.3518580	-0.8181630
C	0.5584830	-5.1030080	-0.2671530
H	2.6937100	-4.8666080	-0.1522930
C	2.9148870	-2.2848870	-0.6094390
C	-0.6280710	-3.0367990	-0.7500390
C	-0.6630840	-4.4281330	-0.4758420
H	0.5526070	-6.1688150	-0.0559550
C	4.0469270	-1.8473180	-0.5420600
N	-1.7573270	-2.3051690	-0.9251200
C	-1.9331100	-5.0519410	-0.4023200
C	5.4051640	-1.4250210	-0.4221870
C	-2.9275970	-2.9077150	-0.7979510
C	-3.0669580	-4.3107240	-0.5539760
H	-1.9912050	-6.1195770	-0.2088630
C	6.4071780	-2.4040520	-0.3258610
C	5.7437170	-0.0489820	-0.3405730
N	-4.0228010	-2.0712970	-0.9105510
H	-4.0540540	-4.7410280	-0.4849700
C	7.7339420	-2.0539590	-0.1355870
H	6.1142190	-3.4474560	-0.3920070
C	7.0924750	0.2852150	-0.1223360
N	4.7780950	0.9142070	-0.4941330
C	-5.3517620	-2.3578190	-0.6740250
H	-3.7969050	-1.0708200	-1.0143900
C	8.0637110	-0.7007280	-0.0273280
H	8.4985830	-2.8188720	-0.0594010
H	7.3781180	1.3276390	-0.0383080
C	4.9249820	2.2324190	0.0951070
H	3.8180930	0.5819990	-0.4735370
C	-6.2366390	-1.1346320	-0.7491030
O	-5.7828580	-3.4714830	-0.4256500
H	9.0965800	-0.4072400	0.1356730
H	5.1399860	2.1597190	1.1732730
H	5.7625420	2.7657850	-0.3655960
H	-6.1266820	-0.6422370	-1.7189140
H	-5.9373680	-0.4084610	0.0122360
H	-7.2710090	-1.4384330	-0.5949730
N	-1.4127060	4.6301700	-1.4258100
C	-2.7595960	4.8766630	-1.2842970
H	-3.1329560	5.8918030	-1.2375120
N	-3.4857610	3.7924080	-1.2246800
C	-2.5653330	2.7713360	-1.3278650
C	-2.7220380	1.3560540	-1.2294720
O	-3.7643190	0.7182930	-1.0434230
N	-1.5003920	0.6904440	-1.3597260
H	-1.5365000	-0.3342720	-1.2405190
C	-0.2733460	1.2899130	-1.5089810
N	0.7902820	0.4683370	-1.6513890
H	1.6652730	0.9089270	-1.3709240
H	0.6787180	-0.5023940	-1.3388940
N	-0.1097590	2.6009450	-1.5551860
C	-1.2754710	3.2739300	-1.4459150
C	3.6512200	3.0428970	-0.1461160

H	3.6114350	3.3539880	-1.1944570
H	3.7002200	3.9498810	0.4786140
N	2.4618290	2.2413210	0.1092260
H	1.6326880	2.7352220	-0.2263680
C	2.2890260	1.8362850	1.5071470
H	2.4537890	2.6780660	2.2017040
H	3.0474120	1.0807970	1.7459590
C	-0.3247200	5.5866620	-1.4562200
H	0.3589870	5.3901510	-0.6254620
H	0.2218110	5.5093730	-2.3982420
H	-0.7389090	6.5902990	-1.3560370
C	1.6714700	-3.0040980	-0.5965330
C	0.9206150	1.2338810	1.7193560
C	0.7746880	-0.1108430	1.8381710
C	-0.2503180	2.0891720	1.7743240
C	-0.5087440	-0.7320600	2.0121140
H	1.6521690	-0.7550840	1.8017600
C	-1.5420900	1.5127480	1.9027930
C	-0.1327260	3.4973720	1.7131040
C	-0.6106850	-2.1268060	2.2068170
C	-1.6793020	0.0637910	1.9956800
C	-2.6597720	2.3736090	1.9709070
H	0.8509870	3.9482240	1.6130100
C	-1.2421820	4.3129820	1.7838700
C	-1.8393330	-2.7311500	2.3570850
H	0.3023640	-2.7192160	2.2259270
C	-2.9290490	-0.5865060	2.1029380
C	-2.5187990	3.7440300	1.9157970
H	-3.6562510	1.9574750	2.0659730
H	-1.1275940	5.3924830	1.7370760
C	-3.0082700	-1.9522590	2.2845720
H	-1.9089930	-3.8048100	2.5047190
H	-3.8481250	-0.0138980	2.0477440
H	-3.3971600	4.3795660	1.9613440
H	-3.9813990	-2.4294010	2.3649170
70			
9d			
C	1.0187000	3.2781100	-1.2906070
N	0.7740270	0.8654930	-1.3539870
C	-0.3335520	3.4486900	-1.4276260
H	1.7003380	4.1160200	-1.2028870
C	2.9095150	1.6782670	-0.9822710
C	-0.5638340	1.0291370	-1.4829380
C	-1.1705400	2.3130480	-1.5069760
H	-0.7751010	4.4414800	-1.4527740
C	4.0165830	1.2641330	-0.7069340
N	-1.2828410	-0.1147040	-1.5554730
C	-2.5839840	2.3648530	-1.5892840
C	5.1802290	0.5267090	-0.3500710
C	-2.5935560	-0.0244760	-1.6113980
C	-3.3114630	1.2087530	-1.6353760
H	-3.0814170	3.3311120	-1.6007600
C	6.4170620	1.1308500	-0.0995920
C	5.0205500	-0.8839410	-0.2132100
N	-3.2276620	-1.2656420	-1.6523430
H	-4.3901710	1.2012440	-1.6801560
C	7.5107010	0.3729250	0.2926880
H	6.4998040	2.2074730	-0.2131160
C	6.1376760	-1.6304980	0.2027800

N	3.8164290	-1.4698370	-0.5045850
C	-4.5704480	-1.5588270	-1.6077660
H	-2.5704870	-2.0354070	-1.5911760
C	7.3548760	-1.0068380	0.4445990
H	8.4673470	0.8460040	0.4839780
H	6.0485220	-2.7032530	0.3333980
C	3.4775370	-2.8133400	-0.0860430
H	3.0313420	-0.8339330	-0.6094820
C	-4.8841030	-3.0365590	-1.6762830
O	-5.4472250	-0.7123980	-1.5641160
H	8.1994330	-1.6124730	0.7601970
H	4.1641770	-3.5330340	-0.5474550
H	3.5815150	-2.9255990	1.0051360
H	-4.0426610	-3.6659920	-1.3817770
H	-5.1660000	-3.2827650	-2.7048450
H	-5.7394440	-3.2414420	-1.0306990
C	2.0511210	-3.1710130	-0.5300460
H	1.8303590	-4.1669060	-0.1235360
H	2.0283100	-3.2525740	-1.6214670
N	0.9878060	-2.2593130	-0.1387260
H	0.9307370	-1.4302400	-0.7324690
C	0.9966660	-1.8631950	1.2645780
H	1.9431440	-1.3915050	1.5787840
H	0.8800350	-2.7676860	1.8784160
C	1.5242600	1.9510570	-1.2327100
C	-0.1187350	-0.8793900	1.5153070
C	0.1835320	0.4296190	1.6987120
C	-1.5069420	-1.2961280	1.4848900
C	-0.8255430	1.4451240	1.7966740
H	1.2260310	0.7448620	1.7132070
C	-2.5384130	-0.3319170	1.6321090
C	-1.8560440	-2.6555510	1.3232970
C	-0.4627270	2.8042480	1.9031190
C	-2.1921550	1.0807660	1.7433650
C	-3.8786740	-0.7748310	1.6493630
H	-1.0690510	-3.3851790	1.1648190
C	-3.1743750	-3.0620530	1.3527990
C	-1.4242100	3.7904960	1.9382430
H	0.5938090	3.0595320	1.9363180
C	-3.1568010	2.1101560	1.7845840
C	-4.1949970	-2.1123430	1.5267220
H	-4.6840070	-0.0586400	1.7684310
H	-3.4222550	-4.1138890	1.2426360
C	-2.7831410	3.4359650	1.8741750
H	-1.1365360	4.8350430	2.0090820
H	-4.2129090	1.8708330	1.7235940
H	-5.2343460	-2.4267300	1.5545700
H	-3.5456660	4.2088150	1.8955060
97			
10a complex			
C	1.4387980	-2.7989830	-0.8838280
C	1.2185320	-4.1998150	-0.7747650
N	0.4647150	-1.9194810	-1.0650430
C	-0.0647330	-4.6674880	-0.8659960
H	2.0636760	-4.8611700	-0.6251560
C	2.7977420	-2.3454020	-0.7727620
C	-0.8096420	-2.3718020	-1.1483560
C	-1.1209140	-3.7531130	-1.0605450
H	-0.2819310	-5.7297190	-0.7930940

C	3.9955330	-2.1692600	-0.6588600
N	-1.7687690	-1.4255560	-1.3263520
C	-2.4827250	-4.1303900	-1.1792730
C	5.4143580	-2.1013170	-0.5087360
C	-3.0292310	-1.8104290	-1.4295910
C	-3.4405340	-3.1805260	-1.3679350
H	-2.7501440	-5.1817940	-1.1150940
C	6.1179810	-3.3054020	-0.3445870
C	6.1144480	-0.8654350	-0.5128820
N	-3.9399430	-0.7799500	-1.5811630
H	-4.4894720	-3.4194900	-1.4574840
C	7.4937720	-3.3189990	-0.1796050
H	5.5524520	-4.2322900	-0.3466010
C	7.5105410	-0.8992500	-0.3358800
N	5.4458780	0.3141720	-0.7082010
C	-5.2774150	-0.8578300	-1.9061490
H	-3.5523380	0.1628140	-1.4390000
C	8.1807880	-2.1033200	-0.1759030
H	8.0223360	-4.2571460	-0.0535390
H	8.0712030	0.0283770	-0.3295190
C	6.0478760	1.5898640	-0.3748850
H	4.4401410	0.2942010	-0.5662600
C	-5.9422060	0.4920740	-2.0549870
O	-5.8750240	-1.9016450	-2.1119630
H	9.2586640	-2.0906370	-0.0437380
H	6.4629800	1.5752840	0.6452840
H	6.8810320	1.8076130	-1.0527280
H	-5.9497430	0.7564120	-3.1178580
H	-5.4220720	1.2765080	-1.5033760
H	-6.9760280	0.4081960	-1.7168190
N	-0.1001210	5.3255810	-0.7578290
C	-1.3919080	5.8028080	-0.7034310
H	-1.5847710	6.8571130	-0.5512850
N	-2.2969540	4.8727830	-0.8493110
C	-1.5633090	3.7159440	-1.0164400
C	-1.9778130	2.3561190	-1.1510710
O	-3.1305680	1.9134910	-1.1881670
N	-0.8848260	1.4895210	-1.2227680
H	-1.1203260	0.4858850	-1.2643760
C	0.4396450	1.8593110	-1.1545370
N	1.3463590	0.8729380	-1.2393250
H	1.0377230	-0.0983880	-1.1290790
H	2.2839150	1.1173540	-0.9226750
N	0.8357640	3.1179530	-1.0383320
C	-0.1995230	3.9787530	-0.9554180
C	5.0065130	2.7019360	-0.5179590
H	4.8295660	2.8970450	-1.5797950
H	5.4173470	3.6190150	-0.0679850
N	3.7306270	2.2961340	0.0598970
H	2.9915720	2.9476460	-0.2155410
C	3.7249060	2.1488970	1.5217990
H	3.8569290	3.1132310	2.0366370
H	4.5614900	1.5025460	1.8084400
C	1.1365400	6.0742150	-0.6386960
H	1.7544700	5.6453600	0.1536970
H	1.6897900	6.0447100	-1.5798530
H	0.8960170	7.1082010	-0.3908960
C	2.4175520	1.4981310	1.8949950
C	1.2704870	2.2686980	1.9795140

C	2.3196920	0.1004150	1.9686240
C	-0.0002880	1.6708120	2.0271570
H	1.3397470	3.3544060	1.9328510
C	1.0839580	-0.5322180	2.0611240
H	3.2240610	-0.5049880	1.9260430
C	-0.1020010	0.2569890	2.0282040
C	-1.2031620	2.4436990	2.0024620
C	0.9606590	-1.9711600	2.1557650
C	-1.3853770	-0.3669390	1.9646240
C	-2.4195550	1.8439260	1.8969570
H	-1.1269410	3.5282480	2.0295120
C	-0.2496160	-2.5704980	2.1414610
H	1.8735520	-2.5593140	2.2140580
C	-2.5496250	0.4180080	1.8397900
C	-1.4700130	-1.8025150	2.0078750
H	-3.3046690	2.4669010	1.8431920
H	-0.3344130	-3.6533830	2.1925720
C	-3.8207150	-0.2314920	1.6618190
C	-2.6998730	-2.4094510	1.8934010
C	-3.8825360	-1.6541570	1.6972710
C	-5.0209060	0.4845700	1.4138980
H	-2.7697510	-3.4952600	1.9185520
C	-5.1283070	-2.3054830	1.4900330
H	-5.0014720	1.5663390	1.3459190
C	-6.2125010	-0.1713110	1.2201180
C	-6.2703560	-1.5842990	1.2561870
H	-5.1517310	-3.3923280	1.5066510
H	-7.1153890	0.3986690	1.0223940
H	-7.2150680	-2.0909030	1.0859460
78			
10a			
C	-1.1246430	-0.4876220	1.4967810
C	-1.2454430	0.8939410	1.8190300
N	0.0251430	-1.1342610	1.3968460
C	-0.1007090	1.6111310	2.0322150
H	-2.2311990	1.3466540	1.8521630
C	-2.3420190	-1.1976240	1.2142500
C	1.1621110	-0.4235720	1.6020420
C	1.1477770	0.9597340	1.9265530
H	-0.1328010	2.6728280	2.2647310
C	-3.4133370	-1.6803290	0.9087720
N	2.3234100	-1.1159440	1.4700410
C	2.3934690	1.6073180	2.1191750
C	-4.7103120	-2.1098950	0.4991660
C	3.4564710	-0.4743150	1.6452240
C	3.5583640	0.9085920	1.9830240
H	2.4077270	2.6665210	2.3630890
C	-4.9770740	-3.4478520	0.1840320
C	-5.7325620	-1.1256070	0.3724910
N	4.5861610	-1.2725610	1.4494770
H	4.5305920	1.3606520	2.1104490
C	-6.2318720	-3.8386210	-0.2624310
H	-4.1766260	-4.1734450	0.2913780
C	-6.9910150	-1.5383200	-0.0986040
N	-5.4731080	0.1713470	0.7306730
C	5.9111600	-0.9857170	1.6740400
H	4.3525070	-2.1979770	1.1095610
C	-7.2297630	-2.8720960	-0.4040930
H	-6.4300870	-4.8771210	-0.5033430

H	-7.7831330	-0.8073500	-0.2199250
C	-6.2873650	1.2844850	0.2930120
H	-4.4918100	0.4259050	0.8220480
C	6.8468260	-2.1419700	1.3966410
O	6.3131780	0.0838630	2.1010820
H	-8.2138030	-3.1611640	-0.7617490
H	-6.3812530	1.3062140	-0.8052210
H	-7.3026250	1.2037850	0.6974580
H	6.4341420	-2.8592910	0.6847070
H	7.0545610	-2.6578010	2.3394590
H	7.7858070	-1.7427210	1.0106680
C	-5.6593890	2.5807690	0.8172830
H	-5.8073620	2.6265700	1.9000200
H	-6.1822550	3.4386500	0.3673880
N	-4.2190260	2.5847410	0.5759560
H	-3.7576660	3.2256140	1.2156860
C	-3.8217600	2.8994740	-0.8004730
H	-3.8060580	3.9822260	-0.9928580
H	-4.5683570	2.4639320	-1.4732890
C	-2.4743120	2.2821080	-1.0892010
C	-1.3012540	3.0068740	-0.9624450
C	-2.4079570	0.9158030	-1.4003260
C	-0.0453050	2.3857900	-1.1109690
H	-1.3399600	4.0681580	-0.7229190
C	-1.1920440	0.2682370	-1.5804640
H	-3.3314800	0.3432620	-1.4857340
C	0.0176540	1.0019970	-1.4116400
C	1.1827460	3.0967220	-0.9352920
C	-1.1217590	-1.1412610	-1.8986450
C	1.2825180	0.3478780	-1.5342360
C	2.3845280	2.4646770	-1.0342070
H	1.1409300	4.1593580	-0.7097240
C	0.0674100	-1.7646330	-2.0320670
H	-2.0560800	-1.6851250	-2.0112030
C	2.4789520	1.0650090	-1.3286410
C	1.3158520	-1.0546310	-1.8551730
H	3.2903450	3.0416430	-0.8847740
H	0.1164450	-2.8247730	-2.2660200
C	3.7412830	0.3783530	-1.4312150
C	2.5293370	-1.6891390	-1.9846860
C	3.7509120	-1.0031000	-1.7819950
C	4.9883070	1.0080850	-1.1785790
H	2.5583820	-2.7467060	-2.2386800
C	4.9908230	-1.6856130	-1.9121610
H	5.0187470	2.0481670	-0.8738120
C	6.1728440	0.3217340	-1.2998090
C	6.1788830	-1.0391300	-1.6850300
H	4.9756950	-2.7353750	-2.1952260
H	7.1114920	0.8264930	-1.0930020
H	7.1216940	-1.5678910	-1.7890210
97			
10b complex			
C	1.1858320	-2.7150790	-1.4190130
C	0.9761070	-4.1132340	-1.5878310
N	0.2026570	-1.8283850	-1.4040150
C	-0.3095120	-4.5721280	-1.6800380
H	1.8304490	-4.7790450	-1.6149950
C	2.5331770	-2.2641050	-1.2088690
C	-1.0740760	-2.2748520	-1.4817520

C	-1.3795310	-3.6543100	-1.6001030
H	-0.5213240	-5.6326670	-1.7861850
C	3.7033660	-2.0530240	-0.9556850
N	-2.0397460	-1.3231640	-1.3921780
C	-2.7461040	-4.0264300	-1.6103270
C	5.0920530	-1.9418570	-0.6458610
C	-3.3015200	-1.7111040	-1.3482620
C	-3.7112350	-3.0728250	-1.4739360
H	-3.0117450	-5.0752160	-1.7118330
C	5.8600610	-3.1177870	-0.6321130
C	5.6955760	-0.6941260	-0.3311230
N	-4.2306810	-0.6892290	-1.2056050
H	-4.7629760	-3.3157980	-1.4512720
C	7.2071120	-3.0955590	-0.3103580
H	5.3658600	-4.0526620	-0.8785650
C	7.0620030	-0.6956350	0.0114620
N	4.9727830	0.4662650	-0.3928960
C	-5.4851170	-0.7978450	-0.6491510
H	-3.8677380	0.2657100	-1.3400720
C	7.7965040	-1.8722960	0.0153900
H	7.7872270	-4.0113780	-0.3048180
H	7.5490400	0.2338360	0.2812470
C	5.4859480	1.7331070	0.0838640
H	3.9609930	0.3919930	-0.3943530
C	-6.2420220	0.5095900	-0.5911580
O	-5.9625080	-1.8480150	-0.2458300
H	8.8481710	-1.8324570	0.2837110
H	5.6622960	1.7151240	1.1712220
H	6.4493810	1.9417600	-0.3933790
H	-6.8846270	0.5771880	-1.4752410
H	-5.5762860	1.3746420	-0.5807910
H	-6.8812920	0.5029250	0.2929240
N	-0.5110380	5.4336590	-0.8760790
C	-1.8072840	5.8947530	-0.7948370
H	-2.0101940	6.9414710	-0.6076680
N	-2.7039060	4.9604410	-0.9635320
C	-1.9592540	3.8166270	-1.1691800
C	-2.3587180	2.4609430	-1.3678060
O	-3.5057580	2.0143160	-1.4784540
N	-1.2572240	1.6029990	-1.4303750
H	-1.4761850	0.5945880	-1.4580930
C	0.0615620	1.9854200	-1.3505700
N	0.9865630	1.0098580	-1.4502890
H	0.6896200	0.0348540	-1.3333920
H	1.8894820	1.2608330	-1.0508520
N	0.4424460	3.2448590	-1.2256380
C	-0.5986480	4.0937690	-1.1132390
C	4.5221510	2.8527470	-0.2955820
H	4.5065510	2.9443840	-1.3859560
H	4.9054030	3.7983960	0.1197800
N	3.1612860	2.5583990	0.1388510
H	2.4982900	3.1496270	-0.3677800
C	2.9313150	2.7659800	1.5753030
H	3.2392240	3.7749760	1.8938710
H	3.5441100	2.0546440	2.1409670
C	0.7169090	6.1976650	-0.7665470
H	1.4261490	5.6487240	-0.1434720
H	1.1583260	6.3614650	-1.7522800
H	0.4937410	7.1586290	-0.3021060

C	1.4611770	2.5748860	1.8498240
C	0.8807870	1.2844580	1.7975560
C	0.6419990	3.6827490	2.0078890
C	-0.5314870	1.1485550	1.8468310
C	1.6650510	0.0920890	1.6707400
C	-0.7485720	3.5606520	2.0399640
H	1.0935020	4.6704320	2.0695210
C	-1.1352190	-0.1497080	1.7898920
C	-1.3517890	2.3112020	1.9326640
C	1.0860600	-1.1383710	1.6535760
H	2.7453150	0.1694660	1.5885430
H	-1.3725530	4.4487660	2.1114240
C	-0.3335120	-1.3057700	1.7259840
C	-2.5701050	-0.2622500	1.8109930
C	-2.7903170	2.1651080	1.8921340
H	1.7274190	-2.0076410	1.5633720
C	-0.9534050	-2.6050430	1.7213600
C	-3.1538390	-1.5093790	1.8016510
C	-3.3662040	0.9451100	1.8300430
H	-3.3948310	3.0684880	1.8975110
C	-2.3752120	-2.6920260	1.7661960
C	-0.2117800	-3.8142410	1.6741850
H	-4.2388280	-1.5997620	1.8035300
H	-4.4487650	0.8415790	1.8034890
C	-2.9990870	-3.9681880	1.7673780
H	0.8715720	-3.7868540	1.6283950
C	-0.8416010	-5.0353800	1.6799530
C	-2.2523370	-5.1174960	1.7272900
H	-4.0854120	-4.0098370	1.7872730
H	-0.2503220	-5.9453840	1.6419280
H	-2.7384940	-6.0882970	1.7282730
78			
10b			
C	-1.7526170	-1.5563260	1.4990420
C	-1.1414870	-2.7945550	1.8247830
N	-1.0986070	-0.4048630	1.4149950
C	0.2082160	-2.8070440	2.0662970
H	-1.7435020	-3.6947500	1.8674340
C	-3.1548390	-1.4698940	1.2096900
C	0.2342220	-0.4121820	1.6492850
C	0.9357570	-1.6005780	1.9850320
H	0.7268150	-3.7295520	2.3134430
C	-4.3139430	-1.2549350	0.9191210
N	0.8535850	0.7897200	1.5201480
C	2.3342120	-1.4980270	2.2156230
C	-5.5772720	-0.7438700	0.5038410
C	2.1469040	0.8397990	1.7179800
C	2.9459610	-0.2873430	2.0963910
H	2.9008820	-2.3876780	2.4766360
C	-6.7298370	-1.5319960	0.4164010
C	-5.6172150	0.6349060	0.1419690
N	2.8232760	2.0386730	1.5228180
H	4.0136240	-0.1684040	2.2527690
C	-7.9274230	-0.9905860	-0.0292380
H	-6.6657890	-2.5781380	0.6996230
C	-6.8368610	1.1612440	-0.3170110
N	-4.4896520	1.4031180	0.2681410
C	2.3705240	3.2722030	1.0698400
H	3.8356080	1.9689000	1.4753970

C	-7.9663560	0.3566260	-0.3962340
H	-8.8176070	-1.6063220	-0.0933020
H	-6.8942540	2.2059610	-0.6035010
C	-4.3202550	2.6682840	-0.4141120
H	-3.6326280	0.8776430	0.4107330
C	0.9058720	3.6021800	1.1491070
O	3.2026020	4.0655450	0.6572150
H	-8.8960110	0.7909530	-0.7523950
H	-4.6133860	2.5845160	-1.4721900
H	-4.9631510	3.4363280	0.0332290
H	0.8059010	4.6732550	0.9687700
H	0.4988650	3.3340030	2.1264110
H	0.3365260	3.0342960	0.4055640
C	-2.8558040	3.1271420	-0.2934440
H	-2.6650660	3.4555550	0.7335400
H	-2.7301460	4.0014950	-0.9443170
N	-1.8454820	2.1337620	-0.6192020
H	-1.6654770	1.4805120	0.1455960
C	-2.0330110	1.4204460	-1.8826780
H	-1.7190840	2.0751110	-2.7089620
H	-3.0847070	1.1563090	-2.0726710
C	-1.2365140	0.1401370	-1.8537470
C	0.1705870	0.1701800	-1.7012750
C	-1.8951740	-1.0796610	-1.8519830
C	0.8772770	-1.0396510	-1.4797660
C	0.9182100	1.3897750	-1.7501160
C	-1.2022180	-2.2786610	-1.6706560
H	-2.9770740	-1.0984200	-1.9585510
C	2.2854430	-1.0120400	-1.2255180
C	0.1726280	-2.2783380	-1.4596640
C	2.2619580	1.4070590	-1.5361940
H	0.3911610	2.3177100	-1.9449290
H	-1.7432220	-3.2216140	-1.6556370
C	2.9853290	0.2112690	-1.2232370
C	2.9742400	-2.2450830	-0.9481870
C	0.9012820	-3.5005280	-1.2047890
H	2.7857370	2.3556690	-1.5856650
C	4.3782860	0.2298700	-0.8606700
C	4.3179570	-2.2187160	-0.6479410
C	2.2293360	-3.4849900	-0.9623060
H	0.3453510	-4.4346830	-1.2015140
C	5.0370500	-1.0020530	-0.5773140
C	5.1225810	1.4334140	-0.7214000
H	4.8396190	-3.1492240	-0.4338440
H	2.7705150	-4.4057830	-0.7607520
C	6.4065800	-0.9923210	-0.1952500
H	4.6446220	2.3935530	-0.8884240
C	6.4406640	1.4123800	-0.3317030
C	7.0962680	0.1857230	-0.0723060
H	6.8923230	-1.9431830	0.0082710
H	6.9826010	2.3464160	-0.2212390
H	8.1391700	0.1827680	0.2284610
97			
10c complex			
C	1.3011460	-2.2025400	-1.5726880
C	1.1488730	-3.6003950	-1.7788070
N	0.2806520	-1.3594140	-1.5194390
C	-0.1176470	-4.1101650	-1.8879790
H	2.0289950	-4.2313540	-1.8179990

C	2.6283710	-1.6913990	-1.3733120
C	-0.9752120	-1.8530300	-1.6165350
C	-1.2231720	-3.2387930	-1.7921550
H	-0.2858320	-5.1756480	-2.0193490
C	3.7937270	-1.4080950	-1.1763510
N	-1.9789630	-0.9425240	-1.5024040
C	-2.5747610	-3.6648050	-1.8208780
C	5.1849250	-1.1772180	-0.9528450
C	-3.2238920	-1.3802400	-1.4912660
C	-3.5775560	-2.7559280	-1.6565220
H	-2.7969890	-4.7195720	-1.9574740
C	6.0850410	-2.2247340	-1.2031590
C	5.6605110	0.0675670	-0.4588480
N	-4.1952940	-0.4024610	-1.3394300
H	-4.6188150	-3.0407430	-1.6524410
C	7.4432920	-2.0761380	-0.9715260
H	5.6881220	-3.1620580	-1.5808940
C	7.0404650	0.1928210	-0.2140930
N	4.7934230	1.1113890	-0.2576440
C	-5.4424590	-0.5763100	-0.7758970
H	-3.8582150	0.5688320	-1.3945570
C	7.9090440	-0.8584910	-0.4712340
H	8.1277430	-2.8932640	-1.1700180
H	7.4332470	1.1240300	0.1772640
C	5.1489780	2.2478050	0.5694140
H	3.8071220	0.8729180	-0.2148220
C	-6.2203240	0.7111740	-0.6307220
O	-5.8890670	-1.6589650	-0.4325790
H	8.9684890	-0.7239420	-0.2738490
H	5.4440240	1.9253970	1.5807420
H	6.0107730	2.7692930	0.1398740
H	-6.6681260	0.9696030	-1.5961170
H	-5.5734570	1.5401490	-0.3339060
H	-7.0160200	0.5591490	0.0983840
N	-0.6722720	5.8060480	-0.4228470
C	-1.9787630	6.2425810	-0.3922500
H	-2.2117310	7.2702100	-0.1441180
N	-2.8457370	5.3119040	-0.6887860
C	-2.0692580	4.1977200	-0.9341460
C	-2.4320590	2.8416140	-1.1991460
O	-3.5647040	2.3646990	-1.3271410
N	-1.3086820	2.0176330	-1.2941710
H	-1.4996400	1.0098150	-1.4061350
C	-0.0022140	2.4198920	-1.1571500
N	0.9413380	1.4792260	-1.3392190
H	0.6638040	0.4911720	-1.3450150
H	1.8318700	1.6966300	-0.8927870
N	0.3465080	3.6694470	-0.8877200
C	-0.7196720	4.4874550	-0.7696180
C	3.9808550	3.2373820	0.6290820
H	3.9305610	3.7914060	-0.3132810
H	4.1825200	3.9594520	1.4359410
N	2.7062940	2.5453710	0.7741230
H	1.9420410	3.1884760	0.5602980
C	2.4957380	1.8887040	2.0675330
H	2.3128280	2.6110720	2.8786600
H	3.4152170	1.3542340	2.3265950
C	0.5321210	6.5587810	-0.1268680
H	1.0621890	6.0993840	0.7111840

H	1.1878740	6.5761940	-0.9995660
H	0.2501120	7.5780910	0.1373630
C	1.3805620	0.8724670	1.9777660
C	-0.0150840	1.2955760	1.9625200
C	1.6818870	-0.4426460	1.8683870
C	-1.0398730	0.3065930	1.8421500
C	-0.3876860	2.6352080	2.0689230
C	0.6721880	-1.4680200	1.7570190
H	2.7226560	-0.7631250	1.8692240
C	-0.7109240	-1.0819980	1.7478660
C	-2.4033990	0.7042170	1.8373090
C	-1.7336460	3.0188520	2.0506930
H	0.3731480	3.4050510	2.1643870
C	1.0091350	-2.7982670	1.6479860
C	-1.7250610	-2.0582710	1.6476820
C	-3.4120680	-0.3057960	1.7517000
C	-2.7311990	2.0685160	1.9365010
H	-1.9920350	4.0719300	2.1190160
C	0.0198760	-3.8014780	1.5182570
H	2.0579640	-3.0891230	1.6374440
C	-1.3598030	-3.4447440	1.5220060
C	-3.0908990	-1.6241760	1.6595530
H	-4.4552920	0.0022450	1.7683390
H	-3.7766710	2.3652540	1.9180140
C	0.3915250	-5.1639470	1.3587220
C	-2.3163350	-4.4832840	1.3671760
H	-3.8928700	-2.3490130	1.5738400
C	-0.5572790	-6.1392800	1.1972110
H	1.4498440	-5.4127180	1.3546320
H	-3.3749050	-4.2483880	1.3594980
C	-1.9291070	-5.7904270	1.2017300
H	-0.2633380	-7.1762630	1.0675710
H	-2.6813630	-6.5628380	1.0754320
78			
10c			
C	0.5678620	-0.8147790	-1.4309960
C	0.5030740	0.5153050	-1.9358000
N	-0.4895620	-1.5623290	-1.1597320
C	-0.7282560	1.0591130	-2.1757410
H	1.4257820	1.0633880	-2.0943100
C	1.8762260	-1.3508750	-1.1768720
C	-1.7124390	-1.0142780	-1.3701900
C	-1.8820110	0.2939400	-1.8975740
H	-0.8359300	2.0710280	-2.5585230
C	3.0161000	-1.6966380	-0.9444000
N	-2.7747730	-1.7892770	-1.0280970
C	-3.2046380	0.7592950	-2.1028010
C	4.3763120	-1.9656420	-0.6093930
C	-3.9836160	-1.3064870	-1.2082000
C	-4.2688570	-0.0302890	-1.7777700
H	-3.3589640	1.7548160	-2.5115440
C	4.7764290	-3.2202980	-0.1372330
C	5.3120620	-0.8949260	-0.6806130
N	-4.9956140	-2.1683950	-0.7738260
H	-5.2921760	0.2900560	-1.9007450
C	6.0841770	-3.4441730	0.2734850
H	4.0358570	-4.0126280	-0.0838540
C	6.6250390	-1.1352840	-0.2442330
N	4.9116010	0.3195870	-1.1812750

C	-6.3517490	-1.9537410	-0.6843890
H	-4.6298990	-3.0333020	-0.3916150
C	6.9986070	-2.3912950	0.2200380
H	6.3856870	-4.4197420	0.6386210
H	7.3546500	-0.3329500	-0.2740470
C	5.6366380	1.5438630	-0.9174440
H	3.9052720	0.4807290	-1.1682680
C	-7.0944550	-3.0762410	0.0069760
O	-6.9100820	-0.9510190	-1.0949260
H	8.0220430	-2.5471670	0.5489490
H	5.8040610	1.6946810	0.1634710
H	6.6255970	1.5190200	-1.3888930
H	-6.7611870	-4.0565980	-0.3423410
H	-8.1608630	-2.9593530	-0.1812430
H	-6.9139810	-3.0190960	1.0855500
C	4.8381640	2.7085890	-1.5135520
H	4.8900990	2.6375100	-2.6036630
H	5.3035050	3.6594780	-1.2142450
N	3.4301720	2.6102770	-1.1370460
H	2.8461130	3.0383850	-1.8491510
C	3.0723810	3.1746170	0.1702480
H	2.8870210	4.2565400	0.1149420
H	3.9194660	3.0391010	0.8494980
C	1.8399710	2.4709050	0.6861540
C	1.9539100	1.1476380	1.2936760
C	0.6176900	3.0141220	0.4826420
C	0.7620680	0.4226480	1.5951010
C	3.1832710	0.5682720	1.6042900
C	-0.6080240	2.3177620	0.7983420
H	0.5323510	4.0020760	0.0324940
C	-0.5272580	0.9878730	1.3359580
C	0.8557620	-0.8785150	2.1546520
C	3.2660170	-0.7007200	2.1868500
H	4.1044530	1.1017210	1.3982890
C	-1.8411680	2.8754330	0.5455040
C	-1.7018810	0.2584520	1.6122370
C	-0.3501180	-1.6029450	2.4109920
C	2.1185990	-1.4241120	2.4458350
H	4.2420540	-1.1239780	2.4062900
C	-3.0408630	2.1701140	0.8061800
H	-1.9035400	3.8787100	0.1282350
C	-2.9863300	0.8514420	1.3425520
C	-1.5695110	-1.0636520	2.1483990
H	-0.2712300	-2.6056190	2.8227080
H	2.1773330	-2.4205530	2.8758180
C	-4.3028550	2.7569390	0.5177830
C	-4.2141510	0.1803230	1.5851330
H	-2.4559310	-1.6530730	2.3508430
C	-5.4685350	2.0744860	0.7510330
H	-4.3225550	3.7619500	0.1035320
H	-4.2125540	-0.8251980	1.9917140
C	-5.4207150	0.7702700	1.2949800
H	-6.4273240	2.5295100	0.5224580
H	-6.3448690	0.2305980	1.4772360
97			
10d complex			
C	1.6279710	-2.4226970	-1.1764860
C	1.6042560	-3.8400580	-1.1498580
N	0.5389380	-1.6777840	-1.3054740

C	0.3925430	-4.4719410	-1.2647800
H	2.5311770	-4.3873230	-1.0280120
C	2.8890580	-1.7370160	-1.0945860
C	-0.6607870	-2.2910070	-1.4131390
C	-0.7826320	-3.7033690	-1.4009380
H	0.3228770	-5.5562370	-1.2457130
C	3.9804260	-1.2051190	-1.0914890
N	-1.7334970	-1.4674790	-1.5342210
C	-2.0866760	-4.2478400	-1.5405700
C	5.2729040	-0.6019540	-1.1774040
C	-2.9348330	-2.0053990	-1.6211810
C	-3.1631950	-3.4194510	-1.6499560
H	-2.2137170	-5.3268620	-1.5589770
C	6.2498110	-1.2018250	-1.9853350
C	5.5521760	0.6152680	-0.5022170
N	-3.9691280	-1.0908320	-1.7279150
H	-4.1719490	-3.7915370	-1.7461780
C	7.4917240	-0.6126010	-2.1653510
H	6.0026700	-2.1342250	-2.4835650
C	6.8077720	1.2117890	-0.7206530
N	4.6325500	1.1603060	0.3601010
C	-5.3045150	-1.3004240	-1.4575910
H	-3.6658670	-0.1090010	-1.7863020
C	7.7544700	0.6037410	-1.5329260
H	8.2369180	-1.0826720	-2.7972630
H	7.0453840	2.1561000	-0.2451950
C	4.6788030	2.5542620	0.7616330
H	3.6958290	0.7684780	0.3386440
C	-6.1528390	-0.0637620	-1.6431960
O	-5.7711760	-2.3789630	-1.1260050
H	8.7150630	1.0903450	-1.6739630
H	5.6475290	2.7759400	1.2204090
H	4.5617740	3.2265790	-0.1035780
H	-6.4550420	-0.0017880	-2.6942660
H	-5.6034060	0.8447030	-1.3867860
H	-7.0499630	-0.1570390	-1.0299190
N	-0.8821940	5.3227770	-0.4507750
C	-2.2231730	5.6381280	-0.4690740
H	-2.5607810	6.6313410	-0.2019680
N	-2.9875150	4.6420000	-0.8301440
C	-2.1028500	3.6088570	-1.0617480
C	-2.3282280	2.2441090	-1.4236600
O	-3.3982020	1.6910540	-1.6884760
N	-1.1325020	1.5178330	-1.4485550
H	-1.2446150	0.4994480	-1.5695410
C	0.1204990	2.0286980	-1.2131580
N	1.1522760	1.1678560	-1.3421150
H	0.9351970	0.1647460	-1.3107600
H	1.9830120	1.4447510	-0.8323730
N	0.3455930	3.2976580	-0.9188230
C	-0.7946740	4.0148900	-0.8288870
C	3.5937510	2.8167430	1.7962060
H	3.6322460	3.8736530	2.1035800
H	3.8110100	2.2096740	2.6833570
N	2.2898080	2.4064610	1.2863690
H	1.9831320	3.0476470	0.5511030
C	1.2569980	2.4075760	2.3265750
H	0.9411280	3.4291360	2.5897240
H	1.7072070	1.9783340	3.2315580

C	0.2341950	6.1726540	-0.0814490
H	0.8115300	5.6963960	0.7147940
H	0.8828680	6.3434500	-0.9430820
H	-0.1561930	7.1257930	0.2752670
C	0.0326720	1.5921470	1.9840730
C	0.1367000	0.1377460	1.8909550
C	-1.1798680	2.1869600	1.8892040
C	-1.0691760	-0.6440620	1.7686080
C	1.3477130	-0.5168560	1.9732360
C	-2.4015630	1.4392820	1.6994500
H	-1.2611840	3.2698490	1.9793830
C	-1.0170820	-2.0545160	1.7860910
C	-2.3316850	0.0192830	1.6543470
C	1.4318720	-1.9304610	2.0108610
H	2.2711450	0.0524170	2.0335520
C	-3.6374850	2.0715430	1.5861410
C	0.2496620	-2.7190960	1.9459770
C	-2.2395320	-2.7854880	1.6248300
C	-3.5271810	-0.7309090	1.5192370
C	2.6949640	-2.5715650	2.1237920
C	-4.8105760	1.3246720	1.4389970
H	-3.6796440	3.1578910	1.5953610
C	0.3791180	-4.1288820	2.0576030
C	-3.4384760	-2.1570150	1.4906370
H	-2.2119490	-3.8683220	1.5795910
C	-4.7590040	-0.0581970	1.4124980
C	2.7870760	-3.9370280	2.2120700
H	3.5877660	-1.9510840	2.1384510
H	-5.7650480	1.8337190	1.3446830
H	-0.5043070	-4.7576800	2.0438290
C	1.6108660	-4.7217930	2.1934480
H	-4.3497030	-2.7301220	1.3362930
H	-5.6687750	-0.6449330	1.3037910
H	3.7567080	-4.4162310	2.3054640
H	1.6828920	-5.8017230	2.2803160
78			
10d			
C	-2.4314010	1.9598730	1.1416360
C	-2.1252430	3.3469890	1.1050640
N	-1.5391070	1.0087610	1.3785970
C	-0.8195340	3.7253100	1.2759600
H	-2.9149890	4.0666230	0.9239090
C	-3.7530260	1.4775940	0.8620910
C	-0.2461360	1.3775680	1.5433890
C	0.1663690	2.7353040	1.4823290
H	-0.5271900	4.7712340	1.2344060
C	-4.7920070	0.9213200	0.5717820
N	0.6275750	0.3633070	1.7437920
C	1.5519100	3.0038950	1.6137440
C	-5.8476990	0.0371990	0.2103910
C	1.9065390	0.6527230	1.8451390
C	2.4366260	1.9773110	1.7863980
H	1.9020050	4.0314180	1.5608010
C	-7.1338860	0.4793010	-0.1177210
C	-5.5212350	-1.3494160	0.1496090
N	2.7125200	-0.4669590	2.0399720
H	3.5016330	2.1333780	1.8681180
C	-8.1126990	-0.4194390	-0.5165510
H	-7.3464170	1.5424640	-0.0609720

C	-6.5219940	-2.2404180	-0.2759420
N	-4.2721720	-1.7741640	0.5216130
C	4.0864240	-0.5574700	2.1115250
H	2.1793760	-1.3295800	2.0713000
C	-7.7908370	-1.7762460	-0.5973900
H	-9.1076530	-0.0714050	-0.7705600
H	-6.3016830	-3.2996140	-0.3500230
C	-3.7494580	-3.0770790	0.1696580
H	-3.5757500	-1.0415310	0.6184760
C	4.5784930	-1.9515760	2.4210160
O	4.8335070	0.3958280	1.9757250
H	-8.5431040	-2.4898570	-0.9209610
H	-4.3580900	-3.8630540	0.6322590
H	-3.7882860	-3.2389920	-0.9195260
H	4.1037140	-2.6946980	1.7733760
H	4.3411590	-2.1978720	3.4611720
H	5.6575530	-1.9819330	2.2771250
C	-2.3101050	-3.2260060	0.6848710
H	-1.9365310	-4.1939320	0.3260900
H	-2.3268290	-3.2675130	1.7786060
N	-1.3647540	-2.1897530	0.3025260
H	-1.4508750	-1.3385290	0.8599620
C	-1.3488100	-1.8545090	-1.1165240
H	-2.3316420	-1.5330060	-1.5011000
H	-1.0718450	-2.7570300	-1.6797410
C	-0.3664390	-0.7363700	-1.3574580
C	1.0670600	-0.9623760	-1.2076410
C	-0.8285000	0.5017270	-1.6412900
C	1.9693400	0.1570800	-1.3243800
C	1.5859150	-2.2130620	-0.9605370
C	0.0416400	1.6475470	-1.7504090
H	-1.9001850	0.6682280	-1.7412290
C	3.3605960	-0.0200830	-1.1713080
C	1.4407690	1.4646160	-1.5666310
C	2.9825700	-2.4373420	-0.8658410
H	0.9188350	-3.0600150	-0.8296700
C	-0.4591560	2.9244110	-1.9881380
C	3.8900360	-1.3449850	-0.9706530
C	4.2062570	1.1367930	-1.2174850
C	2.3036140	2.5878630	-1.6314390
C	3.4883950	-3.7526720	-0.6777100
C	0.3958370	4.0305200	-2.0334790
H	-1.5300980	3.0568360	-2.1198640
C	5.2796320	-1.6205640	-0.8753790
C	3.7040420	2.3817880	-1.4376970
H	5.2721700	1.0246100	-1.0585050
C	1.7584930	3.8669940	-1.8547310
C	4.8385000	-3.9858220	-0.6029170
H	2.7787240	-4.5726280	-0.6024000
H	-0.0143450	5.0206750	-2.2075710
H	5.9994200	-0.8135530	-0.9494940
C	5.7420690	-2.9036500	-0.7029660
H	4.3655310	3.2437180	-1.4623960
H	2.4256680	4.7242820	-1.8895240
H	5.2151990	-4.9947320	-0.4668990
H	6.8102790	-3.0868060	-0.6407750
97			
10e complex			
C	1.3715340	-2.4705970	-1.3011480

C	1.4298860	-3.8856600	-1.1563090
N	0.2349570	-1.7977770	-1.3909960
C	0.2545150	-4.5860460	-1.1073630
H	2.3958190	-4.3710560	-1.0811810
C	2.6115150	-1.7476370	-1.3355730
C	-0.9345680	-2.4786560	-1.3245240
C	-0.9714240	-3.8896430	-1.1883550
H	0.2493220	-5.6670640	-0.9964060
C	3.7323050	-1.2794480	-1.3151080
N	-2.0607500	-1.7252980	-1.3829410
C	-2.2437450	-4.5056230	-1.1075110
C	5.0932960	-0.8485810	-1.2617430
C	-3.2333660	-2.3281070	-1.2768810
C	-3.3759830	-3.7447630	-1.1421870
H	-2.3072270	-5.5859290	-1.0092240
C	6.0987890	-1.8012690	-1.4824570
C	5.4404230	0.4871870	-0.9258690
N	-4.3236420	-1.4786680	-1.3286890
H	-4.3635130	-4.1738350	-1.0700060
C	7.4408310	-1.4680330	-1.3771790
H	5.7989290	-2.8151650	-1.7294980
C	6.8052310	0.8007660	-0.8052310
N	4.4586620	1.4340010	-0.7452180
C	-5.6344920	-1.7562120	-1.0015000
H	-4.0918500	-0.4828180	-1.4497070
C	7.7824070	-0.1597710	-1.0326010
H	8.2074180	-2.2150120	-1.5504910
H	7.1022530	1.8067160	-0.5322940
C	4.7305310	2.6729670	-0.0424820
H	3.5385900	1.0631180	-0.5216390
C	-6.5446540	-0.5567000	-1.1260590
O	-6.0384150	-2.8575980	-0.6652540
H	8.8271990	0.1194950	-0.9329620
H	5.1420700	2.4825720	0.9640730
H	5.4845550	3.2542290	-0.5830810
H	-7.4692080	-0.7612360	-0.5864330
H	-6.7772900	-0.3920850	-2.1835460
H	-6.0638470	0.3482130	-0.7470980
N	-1.6329250	5.1619930	-0.6387030
C	-2.9888810	5.4010420	-0.5794930
H	-3.3661090	6.3887520	-0.3470900
N	-3.7153750	4.3439380	-0.8261380
C	-2.7881700	3.3503940	-1.0650990
C	-2.9544610	1.9563910	-1.3278980
O	-4.0092330	1.3289240	-1.4614060
N	-1.7237310	1.2994210	-1.4252680
H	-1.7763120	0.2729180	-1.5117850
C	-0.4879280	1.8894430	-1.3082620
N	0.5820120	1.0929130	-1.4777470
H	1.4453080	1.4621130	-1.0836880
H	0.4479800	0.0763220	-1.4329170
N	-0.3232200	3.1847790	-1.0823790
C	-1.4933050	3.8415810	-0.9509080
C	3.4510770	3.5108800	0.0394470
H	3.2328460	3.9199480	-0.9519060
H	3.6296280	4.3559290	0.7222190
N	2.3087790	2.6886090	0.4169610
H	1.4404590	3.1437020	0.1290130
C	2.2301970	2.2987870	1.8308980

H	1.7464180	3.0677150	2.4457830
H	3.2432410	2.2178570	2.2256610
C	-0.5474340	6.1022170	-0.4310200
H	0.1592630	5.6930290	0.2945580
H	-0.0253820	6.2942840	-1.3708940
H	-0.9612510	7.0345690	-0.0465950
C	1.5017820	0.9742190	1.9434980
C	2.2423500	-0.2516780	1.9419430
C	0.1126200	0.9471900	1.9299480
C	1.5568820	-1.5041960	1.9498220
C	3.6686510	-0.2729460	1.9383160
C	-0.5920140	-0.3117140	1.9241830
C	-0.6827000	2.1620750	1.9127690
C	0.1187830	-1.5276640	1.9461570
C	2.3231240	-2.7009330	1.9528350
C	4.3766380	-1.4469990	1.9393940
H	4.2275510	0.6546440	1.9310120
C	-2.0262510	-0.3239330	1.9051140
C	-2.0331590	2.1380910	1.8854000
H	-0.1798140	3.1229160	1.9133590
C	-0.6230820	-2.7553740	1.9644260
H	1.8219750	-3.6615450	1.9534070
C	3.6947290	-2.6807030	1.9447100
H	5.4622880	-1.4223080	1.9236730
C	-2.7327240	-1.5545010	1.9258290
C	-2.7624830	0.8930150	1.8717310
H	-2.6009480	3.0654920	1.8698490
C	-1.9824500	-2.7703960	1.9558590
H	-0.0972240	-3.7025580	1.9841220
H	4.2526420	-3.6119750	1.9417230
C	-4.1393760	-1.5515980	1.9115020
C	-4.1555240	0.8593380	1.8392050
H	-2.5221700	-3.7136640	1.9705720
H	-4.6697150	-2.5009160	1.9090730
C	-4.8406740	-0.3584170	1.8666820
H	-4.7047180	1.7963290	1.7917080
H	-5.9268440	-0.3683780	1.8483050
78			
10e			
C	-1.9064300	1.6423660	1.6402830
C	-1.3997170	2.9600130	1.7889340
N	-1.1567780	0.5483710	1.6689370
C	-0.0439150	3.1219040	1.8986330
H	-2.0819340	3.8019820	1.7734820
C	-3.2891360	1.4171640	1.3373310
C	0.1835270	0.7027680	1.7968470
C	0.7904270	1.9832800	1.8849020
H	0.4014900	4.1104070	1.9742990
C	-4.3968380	1.1043530	0.9512430
N	0.9088290	-0.4435660	1.8055870
C	2.2071060	2.0368920	1.9350880
C	-5.5495630	0.4738300	0.4055230
C	2.2189540	-0.3511430	1.8487010
C	2.9363140	0.8841330	1.9084860
H	2.7010330	3.0042630	1.9811630
C	-6.7774310	1.1232630	0.2406580
C	-5.3806260	-0.8778100	-0.0192570
N	2.8645720	-1.5879840	1.8728610
H	4.0157050	0.8789410	1.9185590

C	-7.8531080	0.4692110	-0.3424650
H	-6.8683830	2.1518240	0.5761840
C	-6.4780740	-1.5154550	-0.6267600
N	-4.1872120	-1.5080170	0.1869950
C	4.2058900	-1.8713380	1.7490530
H	2.2135640	-2.3656590	1.8719710
C	-7.6863880	-0.8483060	-0.7768640
H	-8.8036170	0.9756080	-0.4670540
H	-6.3780060	-2.5341750	-0.9843470
C	-3.8473870	-2.8069210	-0.3435480
H	-3.4135660	-0.9302740	0.4982010
C	4.5431410	-3.3346190	1.9242920
O	5.0617560	-1.0210740	1.5698300
H	-8.5152290	-1.3682200	-1.2485620
H	-4.6224100	-3.5341750	-0.0728620
H	-3.7914500	-2.7892900	-1.4438150
H	3.7294980	-3.9939080	1.6152760
H	4.7593410	-3.5151830	2.9823560
H	5.4375950	-3.5599500	1.3430570
C	-2.5183370	-3.2865640	0.2564460
H	-2.2845160	-4.2544430	-0.2080200
H	-2.6592720	-3.4638930	1.3275330
N	-1.3675970	-2.4139320	0.1044750
H	-1.3451160	-1.6333850	0.7620680
C	-1.1094670	-1.9526060	-1.2533610
H	-1.9004430	-1.3074530	-1.6577110
H	-1.0965290	-2.8339440	-1.9080980
C	0.2367420	-1.2632390	-1.3154260
C	1.4121940	-2.0782930	-1.2473480
C	0.3555150	0.1171010	-1.3942510
C	2.7063430	-1.4903910	-1.3203850
C	1.3190150	-3.4943500	-1.1151300
C	1.6640530	0.7324030	-1.3785040
C	-0.7969280	0.9994990	-1.4335720
C	2.8288080	-0.0583150	-1.3336350
C	3.8426660	-2.3431050	-1.3521730
C	2.4371040	-4.2890960	-1.1245910
H	0.3444990	-3.9483340	-0.9817320
C	1.7800350	2.1609070	-1.3814370
C	-0.6735230	2.3431250	-1.4562740
H	-1.7936470	0.5738110	-1.4032050
C	4.1050340	0.5905530	-1.2562360
H	4.8347040	-1.9185550	-1.4523710
C	3.7157100	-3.7070180	-1.2704710
H	2.3394090	-5.3660010	-1.0259580
C	3.0572800	2.7781060	-1.3107930
C	0.6193820	2.9826440	-1.4218710
H	-1.5593330	2.9735030	-1.4648920
C	4.2159180	1.9451480	-1.2455470
H	5.0040440	-0.0059590	-1.1632160
H	4.5997060	-4.3368040	-1.3004590
C	3.1516230	4.1823680	-1.2775720
C	0.7501040	4.3683790	-1.3873460
H	5.1925980	2.4157750	-1.1700570
H	4.1352390	4.6406030	-1.2171860
C	2.0120480	4.9666860	-1.3136450
H	-0.1457390	4.9835330	-1.4092310
H	2.0956330	6.0486730	-1.2837490

10f complex

C	1.1458100	-3.6366130	-0.5238250
C	0.7571360	-4.9849210	-0.3105070
N	0.2854970	-2.6628560	-0.7894380
C	-0.5767340	-5.2953250	-0.3862980
H	1.5113930	-5.7332640	-0.0988500
C	2.5345440	-3.2788080	-0.4474890
C	-1.0313950	-2.9584580	-0.8619830
C	-1.5125490	-4.2778470	-0.6670480
H	-0.9239970	-6.3132450	-0.2314440
C	3.7143640	-3.0034190	-0.3641090
N	-1.8557050	-1.9098590	-1.1136490
C	-2.9156690	-4.4794040	-0.7506300
C	5.0839200	-2.6214160	-0.2406000
C	-3.1566410	-2.1297980	-1.1755390
C	-3.7428640	-3.4265090	-1.0031420
H	-3.3204490	-5.4775310	-0.6072030
C	6.0015330	-3.4660330	0.4020420
C	5.4965310	-1.3469590	-0.7177940
N	-3.9173760	-0.9997890	-1.4061560
H	-4.8153750	-3.5309500	-1.0672480
C	7.3099840	-3.0630450	0.6154040
H	5.6570830	-4.4361670	0.7465990
C	6.8206770	-0.9459820	-0.4660980
N	4.6191060	-0.5552140	-1.4182460
C	-5.2820820	-0.8937360	-1.5698000
H	-3.3769750	-0.1246330	-1.4638080
C	7.7050640	-1.7921810	0.1869280
H	8.0112210	-3.7196380	1.1181500
H	7.1556470	0.0272980	-0.8100170
C	4.6540940	0.8987870	-1.3551180
H	3.6758880	-0.9237610	-1.4897050
C	-5.7413210	0.5232350	-1.8289990
O	-6.0532900	-1.8391370	-1.5515450
H	8.7239420	-1.4574420	0.3579980
H	5.5388340	1.2854680	-1.8731940
H	3.7748880	1.2430140	-1.9044100
H	-5.7407400	0.7003310	-2.9098850
H	-5.0827850	1.2590550	-1.3622740
H	-6.7623820	0.6305250	-1.4611040
N	0.7601090	4.5656010	-1.6294410
C	-0.4517390	5.1965230	-1.7906160
H	-0.5069360	6.2739670	-1.8816840
N	-1.4683240	4.3754820	-1.8247840
C	-0.8945970	3.1296830	-1.6742020
C	-1.4794990	1.8269390	-1.6206140
O	-2.6688990	1.5168440	-1.7387970
N	-0.5100860	0.8434610	-1.3975050
H	-0.8791190	-0.1117030	-1.2786230
C	0.8368750	1.0645420	-1.2308750
N	1.6113210	-0.0233410	-0.9774370
H	2.3485110	0.1841940	-0.2802610
H	1.1020940	-0.8939380	-0.8018950
N	1.3922250	2.2565100	-1.3234210
C	0.4861190	3.2326620	-1.5372260
C	4.6014540	1.4713470	0.0737200
H	4.1843360	2.4823030	0.0136460
H	5.6100770	1.5543750	0.5072150
N	3.7249790	0.6732730	0.9368090

H	4.2177240	-0.1839040	1.1860390
C	3.3566400	1.3786720	2.1755110
H	4.1881650	1.9985800	2.5427780
H	3.1591510	0.6282550	2.9464670
C	2.0768400	5.1662220	-1.5418150
H	2.6265490	4.6930250	-0.7253700
H	2.6251710	5.0295230	-2.4769670
H	1.9648980	6.2317450	-1.3368700
C	2.1416780	2.2546530	1.9728280
C	0.8301000	1.6793140	1.8726960
C	2.2903230	3.6160920	1.8779470
C	-0.2977000	2.5277000	1.6544310
C	0.6241580	0.2830590	2.0028210
C	1.1772650	4.4584260	1.6558910
H	3.2817770	4.0529720	1.9761680
C	-1.6159510	1.9536680	1.5697300
C	-0.0804980	3.9271370	1.5415930
C	-0.6364940	-0.2752110	1.9691440
H	1.4769120	-0.3770390	2.1367100
H	1.3224560	5.5319390	1.5739250
C	-1.7803520	0.5654960	1.7494980
C	-2.7846580	2.7448570	1.3105950
H	-0.9149770	4.5952400	1.3615950
C	-0.8402420	-1.6925740	2.1756170
C	-3.0837100	-0.0211780	1.7242900
C	-4.0259810	2.1906750	1.2710150
H	-2.6850920	3.8066080	1.1188910
C	-2.0784810	-2.2329530	2.1762830
H	0.0376910	-2.3143410	2.3357060
C	-4.2229860	0.7911360	1.4905600
C	-3.2504860	-1.4168870	1.9485130
H	-4.8950870	2.8101830	1.0645060
H	-2.2199180	-3.2994930	2.3349720
C	-5.5004940	0.2017260	1.4765780
C	-4.5320870	-1.9638620	1.9225080
H	-6.3687790	0.8300180	1.2936570
C	-5.6504240	-1.1591210	1.6866310
H	-4.6540540	-3.0321900	2.0820200
H	-6.6393220	-1.6057970	1.6586770
78			
10f			
C	0.3657780	-0.8751450	-1.5359900
C	0.4637710	0.4921420	-1.9252650
N	-0.7749730	-1.5182200	-1.3535160
C	-0.6946060	1.2017730	-2.0897120
H	1.4435410	0.9446810	-2.0381580
C	1.5696560	-1.6042110	-1.2500430
C	-1.9247240	-0.8180340	-1.5112800
C	-1.9350870	0.5556010	-1.8746320
H	-0.6779630	2.2544600	-2.3612320
C	2.5548090	-2.2125780	-0.8846050
N	-3.0671660	-1.5093740	-1.2715480
C	-3.1935070	1.1959520	-1.9838880
C	3.7360110	-2.8461270	-0.4010630
C	-4.2104560	-0.8682080	-1.3517730
C	-4.3415440	0.5017350	-1.7227000
H	-3.2331980	2.2447990	-2.2661460
C	3.7368040	-4.1984110	-0.0364240
C	4.9136870	-2.0610770	-0.2493840

N	-5.3221410	-1.6690270	-1.0680620
H	-5.3197350	0.9553780	-1.7798090
C	4.8775700	-4.7975500	0.4782840
H	2.8199620	-4.7662510	-0.1627210
C	6.0549240	-2.6809120	0.2916250
N	4.9037350	-0.7575890	-0.6502400
C	-6.5941250	-1.2772360	-0.7205950
H	-5.0698380	-2.6378350	-0.9055780
C	6.0293840	-4.0245350	0.6411500
H	4.8702080	-5.8454620	0.7567550
H	6.9612580	-2.1040730	0.4400260
C	5.9617620	0.1879760	-0.3890920
H	4.0040470	-0.3257530	-0.8427970
C	-7.4890250	-2.4266660	-0.3119620
O	-6.9694820	-0.1169620	-0.7306920
H	6.9273870	-4.4747050	1.0544960
H	6.0658130	0.4004250	0.6870890
H	6.9226810	-0.2103410	-0.7337260
H	-7.1525360	-2.8401650	0.6440160
H	-7.4619940	-3.2279640	-1.0550950
H	-8.5076470	-2.0569840	-0.2038630
C	5.6564130	1.4614330	-1.1756900
H	5.7413860	1.2343300	-2.2424700
H	6.4082110	2.2277920	-0.9279630
N	4.2887090	1.9138060	-0.9276010
H	4.0002390	2.5290300	-1.6849820
C	4.1439030	2.6494080	0.3320710
H	4.8985000	3.4477970	0.4233130
H	4.3171610	1.9582860	1.1645030
C	2.7697180	3.2662950	0.4099950
C	1.6126700	2.4821220	0.7281590
C	2.6267250	4.5980220	0.1026140
C	0.3242740	3.0976760	0.7074000
C	1.7200100	1.1129640	1.0805140
C	1.3554150	5.2111010	0.0888640
H	3.5088160	5.1871400	-0.1353660
C	-0.8427060	2.3092270	1.0070090
C	0.2349470	4.4769760	0.3791910
C	0.6142220	0.3605030	1.4171430
H	2.6947760	0.6310530	1.0794770
H	1.2679890	6.2654410	-0.1535780
C	-0.6935880	0.9511170	1.3514650
C	-2.1698790	2.8511390	0.9484950
H	-0.7289930	4.9712300	0.3616270
C	0.7345650	-1.0282520	1.8049740
C	-1.8414120	0.1422700	1.6236640
C	-3.2651590	2.0840700	1.1964380
H	-2.3176990	3.8926370	0.6889520
C	-0.3557270	-1.7817690	2.0634420
H	1.7325820	-1.4547800	1.8624610
C	-3.1423690	0.7005510	1.5356000
C	-1.6884830	-1.2298780	1.9693780
H	-4.2613230	2.5136540	1.1263200
H	-0.2534060	-2.8274970	2.3409900
C	-4.2648530	-0.1106360	1.7822390
C	-2.8239930	-2.0004160	2.2112220
H	-5.2587250	0.3213990	1.6906110
C	-4.1032650	-1.4445450	2.1176620
H	-2.7043270	-3.0479140	2.4751550

H	-4.9735380	-2.0644840	2.3129910
97			
10g complex			
C	1.4217170	-3.0413100	-0.4261240
C	0.8362770	-4.3179840	-0.2184680
N	0.7270780	-1.9708830	-0.7884850
C	-0.5066010	-4.4626870	-0.4570310
H	1.4581450	-5.1468930	0.0973780
C	2.8459770	-2.8910200	-0.3074430
C	-0.6024880	-2.0996090	-1.0070010
C	-1.2609700	-3.3490720	-0.8803200
H	-0.9959560	-5.4248550	-0.3323530
C	4.0582980	-2.8217410	-0.3337220
N	-1.2553170	-0.9665590	-1.3673960
C	-2.6465340	-3.3910190	-1.1804530
C	5.4781590	-2.7310890	-0.4476470
C	-2.5524090	-1.0367480	-1.6151860
C	-3.3001630	-2.2548790	-1.5535590
H	-3.1810830	-4.3332010	-1.0943430
C	6.2166070	-3.8514400	-0.8527710
C	6.1276120	-1.4859030	-0.2259460
N	-3.1440140	0.1757500	-1.9194520
H	-4.3557560	-2.2385310	-1.7787500
C	7.5826780	-3.7641330	-1.0743580
H	5.6901540	-4.7886320	-1.0048930
C	7.5056330	-1.4077130	-0.4949870
N	5.3930080	-0.4135750	0.2095630
C	-4.4254950	0.4153840	-2.3665030
H	-2.5421690	0.9951060	-1.7606880
C	8.2126640	-2.5295140	-0.9062440
H	8.1452800	-4.6354960	-1.3899950
H	8.0227310	-0.4609870	-0.3905780
C	5.9693200	0.8238300	0.7106590
H	4.4823370	-0.6146160	0.6164290
C	-4.7172850	1.8777490	-2.6183470
O	-5.2513480	-0.4554200	-2.5854440
H	9.2772630	-2.4351500	-1.0992830
H	7.0052640	0.6707370	1.0303190
H	5.9733870	1.5925390	-0.0742940
H	-4.7213940	2.0464770	-3.6998630
H	-3.9845480	2.5403930	-2.1544080
H	-5.7180290	2.0968270	-2.2400430
N	2.0780530	5.0581320	-0.5502160
C	0.9518570	5.8508740	-0.5907390
H	1.0181190	6.9145990	-0.4015280
N	-0.1392660	5.1912320	-0.8746190
C	0.2903320	3.8897610	-1.0346340
C	-0.4395510	2.6841850	-1.2704260
O	-1.6581200	2.5546280	-1.4242170
N	0.4002710	1.5680160	-1.2996050
H	-0.0848660	0.6603700	-1.3858150
C	1.7607290	1.5860460	-1.1052610
N	2.3983030	0.4064460	-1.2305220
H	3.3530970	0.3830200	-0.8898000
H	1.8480270	-0.4510950	-1.1129150
N	2.4452440	2.6917130	-0.8607310
C	1.6602220	3.7905850	-0.8310210
C	5.1518210	1.2949810	1.9117950
H	5.4952790	2.2951850	2.2223270

H	5.3322440	0.6113040	2.7505640
N	3.7346090	1.2317810	1.5891530
H	3.5077190	1.9308620	0.8770670
C	2.8684690	1.4327400	2.7458920
H	3.0121500	2.4216850	3.2141490
H	3.1401590	0.6814290	3.4970410
C	3.4400140	5.4492360	-0.2380570
H	3.7833100	4.9236170	0.6566380
H	4.0995390	5.2056830	-1.0731370
H	3.4616290	6.5240230	-0.0576050
C	1.4181860	1.2637600	2.3630510
C	0.6233360	2.3974010	2.0676870
C	0.8430700	0.0169010	2.2897660
C	-0.7001830	2.2689610	1.7243130
H	1.0722640	3.3875960	2.1230310
C	-0.5323370	-0.1483330	1.9803400
H	1.4356170	-0.8686290	2.5141060
C	-1.3228940	0.9960630	1.6690670
H	-1.2680020	3.1649140	1.4987490
C	-1.1392720	-1.4279490	2.0406550
C	-2.7152590	0.8220590	1.3513710
C	-2.4858940	-1.5983870	1.8081480
H	-0.5244010	-2.2893830	2.2979420
C	-3.2887620	-0.4628200	1.4360620
C	-3.5524150	1.9187280	0.9608150
C	-3.1222530	-2.8924010	1.9353670
C	-4.6732960	-0.6566320	1.1366100
C	-4.8701060	1.7400040	0.6761150
H	-3.1240620	2.9081230	0.8572980
C	-4.4353920	-3.0598740	1.6688000
H	-2.5053180	-3.7328200	2.2447890
C	-5.4767090	0.4456410	0.7459450
C	-5.2584680	-1.9524880	1.2338590
H	-5.4840630	2.5858820	0.3773410
H	-4.9010290	-4.0374730	1.7640750
C	-6.8318810	0.2371130	0.4319340
C	-6.6045020	-2.1174590	0.9140270
H	-7.4377530	1.0859960	0.1258020
C	-7.3846880	-1.0294780	0.5089420
H	-7.0478550	-3.1070700	0.9877180
H	-8.4305170	-1.1814930	0.2611430
78			
10g			
C	-1.3560060	-0.7915280	1.3512650
C	-1.4423370	0.5432910	1.8416010
N	-0.2242500	-1.4542920	1.1811960
C	-0.2810670	1.1953330	2.1474650
H	-2.4156720	1.0161760	1.9209220
C	-2.5915250	-1.4225040	0.9744900
C	0.9309060	-0.8088930	1.4859480
C	0.9503310	0.5254280	1.9719960
H	-0.2859610	2.2229020	2.5031740
C	-3.6761220	-1.8328730	0.6154560
N	2.0740370	-1.5148150	1.2873020
C	2.2099440	1.1131440	2.2426590
C	-4.9815850	-2.1758600	0.1548100
C	3.2226890	-0.9283100	1.5435090
C	3.3574770	0.4040290	2.0344340
H	2.2515130	2.1385350	2.6016600

C	-5.2904490	-3.4715180	-0.2760260
C	-5.9644200	-1.1461940	0.0969300
N	4.3333930	-1.7314390	1.2744400
H	4.3387930	0.8173550	2.2110520
C	-6.5485780	-3.7760700	-0.7760940
H	-4.5186260	-4.2328290	-0.2155810
C	-7.2245350	-1.4691260	-0.4353230
N	-5.6676290	0.1021720	0.5797460
C	5.6666690	-1.4928450	1.5129060
H	4.0793130	-2.6137170	0.8453500
C	-7.5054650	-2.7622960	-0.8571570
H	-6.7792530	-4.7827560	-1.1064660
H	-7.9865530	-0.7012200	-0.5132330
C	-6.4126460	1.2885140	0.2162900
H	-4.6810440	0.3026110	0.7291500
C	6.5700750	-2.6457490	1.1334490
O	6.0942310	-0.4714520	2.0236730
H	-8.4907200	-2.9802160	-1.2592870
H	-6.4137060	1.4450870	-0.8753340
H	-7.4589470	1.1978020	0.5280740
H	6.6489600	-3.3292810	1.9850610
H	7.5620090	-2.2508250	0.9118690
H	6.1942720	-3.2017480	0.2718080
C	-5.7947030	2.4878400	0.9418160
H	-6.0033350	2.3888360	2.0109180
H	-6.2767040	3.4113750	0.5869620
N	-4.3430080	2.4929660	0.7786970
H	-3.9044440	2.9833440	1.5527040
C	-3.8568660	3.0522590	-0.4876650
H	-3.7527140	4.1459290	-0.4480280
H	-4.6001260	2.8269980	-1.2609530
C	-2.5464390	2.3994130	-0.8532290
C	-2.5706230	1.0696240	-1.3457360
C	-1.3339510	3.0035020	-0.6398360
C	-1.4115790	0.3864830	-1.6024490
H	-3.5317830	0.5839010	-1.5049800
C	-0.1102960	2.3153120	-0.8769240
H	-1.2896000	4.0222030	-0.2578300
C	-0.1417620	0.9763200	-1.3610010
H	-1.4802160	-0.6339550	-1.9619430
C	1.1319110	2.9289810	-0.5902040
C	1.0952330	0.2728800	-1.5665710
C	2.3248210	2.2595130	-0.7618810
H	1.1386460	3.9497810	-0.2128470
C	2.3142110	0.9093850	-1.2546050
C	1.1379710	-1.0719360	-2.0627270
C	3.5933270	2.8718610	-0.4331760
C	3.5550900	0.2194370	-1.4309660
C	2.3146060	-1.7284150	-2.2418860
H	0.2142060	-1.5853880	-2.3006510
C	4.7578910	2.2035960	-0.5816780
H	3.5822110	3.8901360	-0.0528260
C	3.5658190	-1.1072220	-1.9332690
C	4.7857160	0.8515020	-1.0939020
H	2.3208320	-2.7468660	-2.6211180
H	5.7040220	2.6720650	-0.3233780
C	4.7937750	-1.7705710	-2.1089670
C	5.9819110	0.1585600	-1.2739990
H	4.7941880	-2.7839230	-2.5026650

C	5.9857640	-1.1417170	-1.7868670
H	6.9184920	0.6424240	-1.0097710
H	6.9292110	-1.6607410	-1.9281890
97			
10h complex			
C	1.1638140	-2.8720440	-1.0617070
C	0.7916880	-4.2442470	-1.0383790
N	0.3008340	-1.8840230	-1.2460350
C	-0.5281380	-4.5647800	-1.2123760
H	1.5535730	-4.9990940	-0.8852500
C	2.5528900	-2.5741160	-0.8471240
C	-1.0126920	-2.1899350	-1.3887310
C	-1.4720140	-3.5322700	-1.3895130
H	-0.8608460	-5.5993310	-1.2041310
C	3.7481740	-2.5352470	-0.6289300
N	-1.8609190	-1.1365570	-1.5015890
C	-2.8650960	-3.7511960	-1.5288060
C	5.1482110	-2.6130590	-0.3614290
C	-3.1607930	-1.3754840	-1.5803370
C	-3.7169140	-2.6919400	-1.6226380
H	-3.2450280	-4.7692520	-1.5388050
C	5.7207740	-3.8815430	-0.1768890
C	5.9548760	-1.4482110	-0.2682330
N	-3.9558090	-0.2443820	-1.6228410
H	-4.7860690	-2.8117320	-1.7018960
C	7.0701180	-4.0266870	0.1033660
H	5.0756410	-4.7514720	-0.2547670
C	7.3198900	-1.6149900	0.0310890
N	5.4132690	-0.2103890	-0.4937730
C	-5.3308750	-0.1616690	-1.5349290
H	-3.4484130	0.6489040	-1.5521970
C	7.8609370	-2.8804180	0.2079080
H	7.4998520	-5.0122160	0.2431900
H	7.9589620	-0.7440270	0.1205640
C	6.0950030	1.0040170	-0.0958720
H	4.4011580	-0.1404050	-0.4440870
C	-5.8479130	1.2581320	-1.5678930
O	-6.0763740	-1.1254480	-1.4685840
H	8.9191990	-2.9718050	0.4343670
H	6.3525770	0.9838530	0.9754540
H	7.0346120	1.1083610	-0.6492540
H	-5.9025310	1.5913870	-2.6099330
H	-5.1888630	1.9413250	-1.0293890
H	-6.8517290	1.2720040	-1.1426400
N	0.5316660	5.3531410	-0.7029090
C	-0.6946000	5.9615040	-0.5452180
H	-0.7620670	7.0163340	-0.3112080
N	-1.7038320	5.1483720	-0.7075960
C	-1.1115340	3.9335360	-0.9883750
C	-1.6801440	2.6445170	-1.2235790
O	-2.8759040	2.3433570	-1.2931100
N	-0.6932140	1.6663450	-1.3755850
H	-1.0367480	0.6951840	-1.4457130
C	0.6646430	1.8859940	-1.3402510
N	1.4614280	0.8139060	-1.5280630
H	1.0503390	-0.1178380	-1.4089320
H	2.4055890	0.9438700	-1.1650770
N	1.1998260	3.0837580	-1.1771600
C	0.2730330	4.0440580	-0.9845260

C	5.2116910	2.2084590	-0.4145880
H	5.1730000	2.3503310	-1.4989280
H	5.6752170	3.1026440	0.0318650
N	3.8450790	1.9904070	0.0448890
H	3.2270320	2.7167650	-0.3247200
C	3.7012460	1.9365610	1.5058950
H	4.2161880	2.7781680	1.9983680
H	4.1628170	1.0102330	1.8688410
C	1.8475200	5.9550110	-0.6090240
H	2.4892550	5.3224980	0.0077840
H	2.2943270	6.0604520	-1.6001610
H	1.7519870	6.9372890	-0.1457620
C	2.2299390	1.9554180	1.8324220
C	1.4884700	0.7983800	1.7680270
C	1.5771030	3.1962870	2.0388480
C	0.0722980	0.8170780	1.8542840
H	2.0082350	-0.1376210	1.5779370
C	0.2099330	3.2604050	2.0795250
H	2.1734020	4.1023690	2.1228440
C	-0.5749160	2.0831240	1.9498350
C	-0.7316760	-0.3765810	1.8147400
H	-0.2999750	4.2162040	2.1804640
C	-1.9861100	2.1611750	1.8784390
C	-2.1350890	-0.2623150	1.7486380
C	-0.1585400	-1.6895800	1.8804490
C	-2.7623200	1.0320600	1.7435180
H	-2.4573720	3.1420720	1.8967050
C	-2.9543520	-1.4340630	1.7029950
C	-0.9344210	-2.8072320	1.8752220
H	0.9183140	-1.7995960	1.9550710
C	-4.2014410	1.1116290	1.6173390
C	-2.3594210	-2.7200410	1.7730230
C	-4.3694800	-1.3206070	1.5866360
H	-0.4773750	-3.7917490	1.9372540
C	-4.9630610	-0.0010160	1.5375290
H	-4.6526140	2.1000210	1.5861260
C	-3.1799840	-3.8630610	1.7388550
C	-5.1451120	-2.4766510	1.5289310
H	-6.0432630	0.0694010	1.4328600
H	-2.7161230	-4.8447010	1.7996620
C	-4.5530950	-3.7405730	1.6145330
H	-6.2219460	-2.3835080	1.4174500
H	-5.1755060	-4.6294020	1.5780420
78			
10h			
C	-1.3608590	-0.5480970	1.5071430
C	-1.4064940	0.8018370	1.9639780
N	-0.2504750	-1.2515550	1.3683190
C	-0.2239560	1.4264500	2.2502140
H	-2.3646130	1.3069750	2.0284370
C	-2.5905420	-1.1917180	1.1323700
C	0.9249580	-0.6332800	1.6438140
C	0.9885820	0.7161030	2.0832370
H	-0.1977430	2.4623640	2.5788600
C	-3.6197930	-1.7284080	0.7766210
N	2.0391280	-1.3797920	1.4458330
C	2.2712110	1.2732580	2.3056070
C	-4.8657260	-2.2444530	0.3102210
C	3.2116300	-0.8173770	1.6434550

C	3.3943470	0.5246010	2.0892350
H	2.3517680	2.3057100	2.6360660
C	-5.0162620	-3.5910410	-0.0439270
C	-5.9459570	-1.3358300	0.1455390
N	4.2849790	-1.6713990	1.3786530
H	4.3906550	0.9168380	2.2248090
C	-6.2100560	-4.0548340	-0.5782760
H	-4.1737730	-4.2616860	0.0946560
C	-7.1372310	-1.8175910	-0.4210660
N	-5.8042390	-0.0323760	0.5538840
C	5.6346620	-1.4145240	1.4124140
H	3.9831880	-2.5755330	1.0339360
C	-7.2615780	-3.1556240	-0.7713710
H	-6.3190320	-5.0985070	-0.8516580
H	-7.9690200	-1.1366800	-0.5702660
C	-6.4998560	1.0533870	-0.1089890
H	-4.8547650	0.2375510	0.8043390
C	6.4992060	-2.6126290	1.0868440
O	6.1142400	-0.3362000	1.7214520
H	-8.1969740	-3.5035800	-1.1999290
H	-6.4330290	0.9551670	-1.2043950
H	-7.5647380	1.0590210	0.1490680
H	7.3730470	-2.2711040	0.5299000
H	5.9720850	-3.3750520	0.5104850
H	6.8445580	-3.0561210	2.0261110
C	-5.8770500	2.3732080	0.3534670
H	-6.1888240	2.5759550	1.3823690
H	-6.2600390	3.1831940	-0.2877120
N	-4.4181570	2.2876430	0.3504070
H	-4.0365390	3.0993830	0.8303740
C	-3.8358070	2.1968760	-0.9922210
H	-4.2912790	2.9330500	-1.6786670
H	-4.0485310	1.1999110	-1.3970540
C	-2.3440210	2.4128990	-0.9318910
C	-1.4504670	1.4079230	-1.2207920
C	-1.8562960	3.6846690	-0.5320990
C	-0.0456770	1.6010410	-1.1214680
H	-1.8454490	0.4400210	-1.5138130
C	-0.5115070	3.9094590	-0.4220080
H	-2.5609030	4.4876450	-0.3253860
C	0.4261470	2.8819090	-0.7134940
C	0.9133350	0.5621820	-1.3920840
H	-0.1359580	4.8835790	-0.1195240
C	1.8135970	3.1259290	-0.5958130
C	2.2912920	0.8394330	-1.2647720
C	0.5216270	-0.7642440	-1.7721340
C	2.7417430	2.1458680	-0.8681120
H	2.1481770	4.1126700	-0.2823470
C	3.2626850	-0.1766410	-1.5326060
C	1.4397560	-1.7359240	-2.0179980
H	-0.5313890	-1.0106070	-1.8472670
C	4.1601000	2.3890510	-0.7307350
C	2.8432080	-1.4779410	-1.9094970
C	4.6531540	0.1030440	-1.4069670
H	1.1167800	-2.7355600	-2.2956610
C	5.0671200	1.4205950	-0.9805100
H	4.4765880	3.3776810	-0.4087630
C	3.8090390	-2.4700820	-2.1603110
C	5.5806280	-0.8999570	-1.6825350

H	6.1306890	1.6073750	-0.8601510
H	3.4797450	-3.4653090	-2.4468530
C	5.1600030	-2.1801600	-2.0557420
H	6.6413090	-0.6781380	-1.5921070
H	5.8980690	-2.9504250	-2.2595880
97			
10i complex			
C	1.7647840	-1.8285730	-1.5768220
C	2.0508580	-3.2087150	-1.7635470
N	0.5347470	-1.3448210	-1.4935700
C	1.0043680	-4.0892890	-1.8171070
H	3.0820900	-3.5344830	-1.8268010
C	2.8746560	-0.9300250	-1.4247040
C	-0.5079060	-2.2067440	-1.5442840
C	-0.3156080	-3.6037590	-1.6906500
H	1.1739310	-5.1560460	-1.9349130
C	3.9087090	-0.3143050	-1.2548910
N	-1.7427710	-1.6514710	-1.4211940
C	-1.4670910	-4.4287880	-1.6702490
C	5.1737150	0.3144400	-1.0485460
C	-2.7930080	-2.4514170	-1.3835090
C	-2.7020680	-3.8730820	-1.5064520
H	-1.3533890	-5.5038120	-1.7823640
C	6.3394000	-0.4347960	-1.2725720
C	5.2676830	1.6558470	-0.5899630
N	-4.0165590	-1.8123800	-1.2505030
H	-3.6020220	-4.4677160	-1.4759450
C	7.5953020	0.1069200	-1.0493380
H	6.2322340	-1.4570760	-1.6224640
C	6.5509030	2.1824420	-0.3539950
N	4.1353160	2.4082630	-0.4106460
C	-5.1725490	-2.3500820	-0.7237330
H	-3.9833500	-0.7847660	-1.2967060
C	7.6873710	1.4207060	-0.5848420
H	8.4877390	-0.4821200	-1.2287890
H	6.6540670	3.1983290	0.0095310
C	4.1410270	3.6064600	0.4053010
H	3.2587630	1.8968950	-0.3650240
C	-6.2947970	-1.3460460	-0.5937200
O	-5.2950420	-3.5210870	-0.4026820
H	8.6620550	1.8613100	-0.3966970
H	4.5396330	3.3978670	1.4110170
H	4.7920720	4.3655900	-0.0412570
H	-6.7451140	-1.1804070	-1.5779610
H	-5.9276880	-0.3820270	-0.2335270
H	-7.0498900	-1.7508850	0.0796600
N	-2.5286340	5.2150020	-0.5167530
C	-3.9037190	5.2307970	-0.4293770
H	-4.4319770	6.1449810	-0.1906980
N	-4.4533760	4.0689830	-0.6621480
C	-3.3823930	3.2393340	-0.9236080
C	-3.3221630	1.8281530	-1.1364410
O	-4.2574510	1.0231620	-1.1959350
N	-2.0048370	1.3845760	-1.2668400
H	-1.8816680	0.3640510	-1.3535180
C	-0.8801660	2.1714040	-1.2018350
N	0.2971470	1.5554550	-1.4082720
H	0.3357870	0.5301500	-1.3672990
H	1.0975520	2.0508600	-1.0192090

N	-0.9206860	3.4766390	-0.9786370
C	-2.1817940	3.9340920	-0.8326520
C	2.7239360	4.1838620	0.4890070
H	2.4868400	4.6976200	-0.4475930
H	2.7030810	4.9290780	1.2996130
N	1.7327750	3.1268850	0.6495620
H	0.8009470	3.5005220	0.4602600
C	1.7700930	2.4362630	1.9421270
H	1.4547340	3.0890770	2.7721420
H	2.8095330	2.1564690	2.1426860
C	-1.6036910	6.3110090	-0.2985950
H	-0.8958640	6.0464090	0.4907860
H	-1.0528570	6.5287810	-1.2158440
H	-2.1710530	7.1915300	0.0031320
C	0.9435380	1.1706920	1.9031240
C	1.5655680	-0.0369180	1.7784200
C	-0.4960590	1.2320130	1.9530660
C	0.8519900	-1.2771390	1.7194500
H	2.6502790	-0.0475800	1.7291390
C	-1.2332580	0.0183750	1.8786030
C	-1.1996590	2.4469010	2.0710190
C	1.5217580	-2.5462200	1.5980160
C	-0.5548040	-1.2364950	1.7756480
C	-2.6586950	0.0546280	1.9206270
H	-0.6549370	3.3848050	2.1337420
C	-2.5843770	2.4688780	2.0965620
C	0.7405650	-3.7370920	1.5536000
C	2.9329510	-2.6721050	1.4954570
C	-1.3228420	-2.4530720	1.7341580
C	-3.3122130	1.2798330	2.0198150
C	-3.3975810	-1.1874860	1.8687450
H	-3.1089140	3.4179100	2.1666350
C	-0.6709210	-3.6606210	1.6318840
C	1.3854030	-4.9947000	1.4096630
H	3.5604350	-1.7880960	1.5148870
C	3.5306660	-3.9017170	1.3548480
C	-2.7658110	-2.3771530	1.7877920
H	-4.3988170	1.3035950	2.0287080
H	-4.4837620	-1.1368480	1.9039250
H	-1.2493560	-4.5816540	1.5953600
C	2.7502500	-5.0800540	1.3102750
H	0.7692070	-5.8899480	1.3773680
H	4.6114310	-3.9682430	1.2746660
H	-3.3308240	-3.3048720	1.7331440
H	3.2332580	-6.0457080	1.1975030
78			
10i			
C	-1.6554710	1.2517340	1.7002810
C	-1.1624860	2.5473760	2.0157380
N	-0.8986190	0.1666080	1.6269950
C	0.1876160	2.7004400	2.1859550
H	-1.8488240	3.3840020	2.0707060
C	-3.0318700	1.0231180	1.3671770
C	0.4370700	0.3120750	1.7967690
C	1.0334000	1.5748390	2.0549830
H	0.6209170	3.6757420	2.3914330
C	-4.1248560	0.6564550	0.9869320
N	1.1644370	-0.8206080	1.6629490
C	2.4470210	1.6220590	2.1392730

C	-5.2777940	-0.0053670	0.4789980
C	2.4747940	-0.7315160	1.7311940
C	3.1844790	0.4828410	1.9708090
H	2.9369120	2.5747860	2.3225950
C	-6.5084550	0.6379510	0.3068620
C	-5.1178120	-1.3737050	0.1106480
N	3.1151290	-1.9571960	1.5507480
H	4.2634460	0.4772250	2.0012820
C	-7.5942750	-0.0378370	-0.2304910
H	-6.5924040	1.6802620	0.5989720
C	-6.2267140	-2.0346370	-0.4476460
N	-3.9220140	-2.0075280	0.3243690
C	4.4586380	-2.2354130	1.4643090
H	2.4607090	-2.7069180	1.3564520
C	-7.4373180	-1.3733150	-0.6081120
H	-8.5458240	0.4650840	-0.3614240
H	-6.1361100	-3.0705570	-0.7546280
C	-3.5963480	-3.2851620	-0.2727150
H	-3.1331140	-1.4066170	0.5439750
C	4.7763380	-3.7025250	1.2775090
O	5.3336370	-1.3929160	1.5730780
H	-8.2749500	-1.9127680	-1.0408500
H	-4.2981520	-4.0507100	0.0793440
H	-3.6903640	-3.2442230	-1.3696580
H	5.0644640	-4.1199230	2.2474700
H	5.6294880	-3.7913800	0.6030080
H	3.9355230	-4.2765670	0.8837250
C	-2.1798480	-3.7232930	0.1283450
H	-1.9684870	-4.6565250	-0.4097920
H	-2.1681130	-3.9543080	1.1982300
N	-1.1014640	-2.7806100	-0.1257320
H	-1.0471440	-2.0413730	0.5772030
C	-1.0963840	-2.1926980	-1.4612890
H	-2.0541800	-1.7165120	-1.7303330
H	-0.9299950	-2.9942690	-2.1939080
C	-0.0182790	-1.1410100	-1.5313580
C	-0.3800020	0.1691400	-1.4545150
C	1.3770130	-1.5001040	-1.5630340
C	0.5708380	1.2323320	-1.3506000
H	-1.4405500	0.3976980	-1.4035130
C	2.3468600	-0.4649150	-1.4838290
C	1.8115570	-2.8350910	-1.6618430
C	0.1677550	2.6039130	-1.1960320
C	1.9392380	0.8998250	-1.3417380
C	3.7333870	-0.7925770	-1.5056960
H	1.0779730	-3.6342040	-1.6833890
C	3.1632410	-3.1373650	-1.7246360
C	1.1681880	3.5953560	-0.9819640
C	-1.1903990	3.0174350	-1.2226960
C	2.9342030	1.9247090	-1.1801090
C	4.1209610	-2.1229560	-1.6511490
C	4.7087500	0.2638570	-1.3483430
H	3.4813990	-4.1714810	-1.8206850
C	2.5358950	3.2297390	-0.9867010
C	0.7780140	4.9448800	-0.7632200
H	-1.9767090	2.2905540	-1.3947210
C	-1.5383840	4.3303120	-1.0185640
C	4.3301540	1.5504080	-1.1890840
H	5.1805440	-2.3651990	-1.6840200

H	5.7601570	-0.0106310	-1.3468570
H	3.2858580	4.0037480	-0.8372160
C	-0.5441080	5.3071210	-0.7750580
H	1.5540290	5.6865410	-0.5919690
H	-2.5845120	4.6200880	-1.0386310
H	5.0697100	2.3358530	-1.0578320
H	-0.8307090	6.3406540	-0.6070540
97			
10j complex			
C	0.5539690	-3.0812120	-1.2732940
C	-0.0300940	-4.3765480	-1.3055910
N	-0.1503990	-1.9618180	-1.3486550
C	-1.3926540	-4.4737460	-1.4170890
H	0.6065510	-5.2510640	-1.2437610
C	1.9759470	-2.9684670	-1.1126010
C	-1.4985940	-2.0487640	-1.4340040
C	-2.1689480	-3.2974430	-1.4823610
H	-1.8849990	-5.4421810	-1.4467980
C	3.1718700	-2.9549670	-0.9018740
N	-2.1637870	-0.8671690	-1.4381840
C	-3.5851180	-3.2776000	-1.5520100
C	4.5655880	-2.9589750	-0.5997360
C	-3.4856040	-0.8866750	-1.4558160
C	-4.2535680	-2.0891580	-1.5375160
H	-4.1292220	-4.2171790	-1.5970820
C	5.1560080	-4.1308750	-0.1021680
C	5.3381000	-1.7763450	-0.7539290
N	-4.0715620	0.3650090	-1.3854270
H	-5.3308460	-2.0285150	-1.5605440
C	6.4900980	-4.1585970	0.2694900
H	4.5350930	-5.0163120	-0.0048600
C	6.6862620	-1.8197200	-0.3487760
N	4.7823670	-0.6574150	-1.3196570
C	-5.4033410	0.6917360	-1.2523740
H	-3.4052330	1.1504200	-1.4099450
C	7.2438980	-2.9886560	0.1476660
H	6.9345400	-5.0683420	0.6570480
H	7.3025030	-0.9315580	-0.4305020
C	5.3476430	0.6685060	-1.1507480
H	3.7830780	-0.6963670	-1.4822240
C	-5.6420740	2.1846920	-1.2017390
O	-6.3116830	-0.1207870	-1.1946300
H	8.2886130	-2.9851220	0.4444250
H	6.3909540	0.6692640	-1.4813070
H	4.8058380	1.3372660	-1.8282640
H	-5.6594870	2.5771450	-2.2238720
H	-4.8460580	2.7052460	-0.6645880
H	-6.6101480	2.3699400	-0.7367360
N	1.2933620	5.1479080	-0.8078960
C	0.1777630	5.9551060	-0.8552940
H	0.2636160	7.0246850	-0.7120000
N	-0.9297400	5.3010460	-1.0829620
C	-0.5232840	3.9869410	-1.1944410
C	-1.2716330	2.7870380	-1.3932530
O	-2.4889170	2.6770800	-1.5690540
N	-0.4506870	1.6536740	-1.3595500
H	-0.9486240	0.7500270	-1.4025940
C	0.9094580	1.6581310	-1.1537070
N	1.5367320	0.4568610	-1.1112950

H	2.3553750	0.4654370	-0.4942140
H	0.9411350	-0.3744420	-1.0504410
N	1.6148480	2.7661670	-1.0219680
C	0.8499450	3.8765650	-1.0221830
C	5.2394120	1.2022960	0.2809400
H	5.8458400	2.1176120	0.3820690
H	5.6491130	0.4616210	0.9795450
N	3.8349690	1.4088000	0.6017050
H	3.4525740	2.1591430	0.0197040
C	3.5547490	1.7442780	2.0000590
H	4.0569400	2.6710660	2.3207290
H	3.9445050	0.9379590	2.6324770
C	2.6729540	5.5390430	-0.5895790
H	2.6929440	6.5627680	-0.2150750
H	3.1238420	4.8728780	0.1492520
H	3.2411740	5.4792760	-1.5205840
C	2.0582910	1.8974840	2.1461620
C	1.5003060	3.1806470	2.2285220
C	1.2156560	0.7817380	2.0400020
C	0.1347790	3.3805070	2.1443860
H	2.1649190	4.0365000	2.3250390
C	-0.1958930	0.9711980	1.9681610
C	1.7340320	-0.5697710	1.9508930
C	-0.7323970	2.2856800	1.9885330
H	-0.2792450	4.3857550	2.1680480
C	-1.0785540	-0.1512520	1.8475560
C	0.9087400	-1.6345600	1.8608120
H	2.8089950	-0.7186180	1.9341750
C	-2.1441870	2.4545980	1.8308340
C	-2.4733890	0.0394650	1.7518080
C	-0.5269920	-1.4790190	1.8330170
H	1.3129870	-2.6415080	1.7912920
C	-2.9734880	1.3826430	1.7143880
H	-2.5438400	3.4650050	1.7973460
C	-3.3447450	-1.1062660	1.7033200
C	-1.3686430	-2.5667960	1.7747450
H	-4.0376560	1.5557850	1.5984410
C	-2.7747630	-2.4123950	1.7288310
C	-4.7585480	-1.0003720	1.6290420
H	-0.9490980	-3.5713120	1.7558540
C	-3.6259420	-3.5499240	1.7006220
H	-5.2303840	-0.0245480	1.5933520
C	-5.5580730	-2.1174330	1.5956740
C	-4.9883690	-3.4101230	1.6402350
H	-3.1685570	-4.5364000	1.7235930
H	-6.6354300	-2.0031230	1.5280670
H	-5.6296510	-4.2858030	1.6179540
78			
10j			
C	-0.7134580	-1.0847990	-1.4137750
C	-0.8246620	0.2766760	-1.8189170
N	0.4328970	-1.7280650	-1.2677740
C	0.3246730	0.9775910	-2.0609150
H	-1.8075180	0.7344040	-1.8825390
C	-1.9272780	-1.7780170	-1.0803930
C	1.5752720	-1.0301930	-1.4873850
C	1.5707120	0.3325830	-1.8908920
H	0.2974760	2.0262980	-2.3477800
C	-2.9743110	-2.2658020	-0.7070210

N	2.7306370	-1.7129770	-1.2817870
C	2.8219480	0.9747630	-2.0650050
C	-4.2350710	-2.7181610	-0.2185790
C	3.8687310	-1.0742080	-1.4311070
C	3.9812310	0.2905340	-1.8350570
H	2.8446230	2.0185610	-2.3671760
C	-4.4212680	-4.0379340	0.2101580
C	-5.2994640	-1.7761990	-0.1276720
N	4.9897120	-1.8674280	-1.1753570
H	4.9560760	0.7421180	-1.9413530
C	-5.6367350	-4.4527800	0.7357000
H	-3.5883450	-4.7295060	0.1277240
C	-6.5165270	-2.2105930	0.4273030
N	-5.1192570	-0.5054570	-0.6029180
C	6.3016620	-1.4883680	-1.0087120
H	4.7376950	-2.8108320	-0.9019540
C	-6.6754470	-3.5259380	0.8436460
H	-5.7721050	-5.4768790	1.0652010
H	-7.3389010	-1.5117680	0.5327790
C	-6.0174780	0.5928090	-0.3239870
H	-4.1609430	-0.2078320	-0.7663440
C	7.1938640	-2.6118780	-0.5300710
O	6.7132800	-0.3583980	-1.2077570
H	-7.6289940	-3.8311430	1.2650110
H	-7.0392400	0.3293990	-0.6179990
H	-6.0421290	0.8382760	0.7505100
H	7.0338810	-3.5242740	-1.1104560
H	6.9679550	-2.8334530	0.5185190
H	8.2332110	-2.2970130	-0.6132030
C	-5.5730990	1.7975510	-1.1523990
H	-6.2252930	2.6552020	-0.9251380
H	-5.6995050	1.5487690	-2.2101220
N	-4.1582720	2.0912080	-0.9271670
H	-3.7740960	2.5559800	-1.7465970
C	-3.9161290	2.9506390	0.2366400
H	-4.3292520	2.4552220	1.1224280
H	-4.4371230	3.9172600	0.1463420
C	-2.4342900	3.1897360	0.3935150
C	-1.8930710	4.4173450	-0.0083830
C	-1.5824470	2.1726480	0.8504550
C	-0.5288780	4.6477700	0.0199650
H	-2.5647370	5.1977030	-0.3575640
C	-0.1739170	2.3919820	0.8723960
C	-2.0872090	0.8839630	1.2722160
C	0.3513270	3.6393380	0.4439840
H	-0.1252680	5.6035010	-0.3032510
C	0.7218980	1.3435960	1.2613170
C	-1.2516680	-0.1016680	1.6647060
H	-3.1567370	0.7012040	1.2439490
C	1.7718080	3.8183370	0.4280990
C	2.1188820	1.5355410	1.2123120
C	0.1809270	0.0720000	1.6530910
H	-1.6445470	-1.0700690	1.9632970
C	2.6135890	2.8148470	0.7910340
H	2.1682800	4.7771900	0.1046370
C	2.9983800	0.4485380	1.5498920
C	1.0327600	-0.9615190	1.9756180
H	3.6823340	2.9906000	0.7499920
C	2.4362940	-0.8040350	1.9318260

C	4.4155460	0.5556760	1.5072400
H	0.6208350	-1.9283930	2.2564980
C	3.2951390	-1.8896640	2.2578020
H	4.8827630	1.4860080	1.2047190
C	5.2216590	-0.5045350	1.8417360
C	4.6570720	-1.7456160	2.2226730
H	2.8437410	-2.8367500	2.5416050
H	6.3012590	-0.3910960	1.7985340
H	5.3025390	-2.5778100	2.4885000